

FINAL REPORT OF TIC

VOLUME 2

**THEORETICAL
INVESTIGATIONS OF
THE PHYSICAL
PROPERTIES OF
WVER-TYPE
URANIUM-WATER
LATTICES**

AKADÉMIAI KIADÓ, BUDAPEST

TEMPORARY INTERNATIONAL COLLECTIVE (TIC)
FOR JOINT RESEARCH INTO
THE PHYSICS OF WWER-TYPE REACTORS

THEORY OF THE PROPERTIES
OF THE WWER-TYPE
REACTOR WATER LATTICES

AKADEMIA

TEMPORARY INTERNATIONAL COLLECTIVE (TIC)
FOR JOINT RESEARCH INTO
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OF WWER-TYPE
URANIUM-WATER LATTICES

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REPORTS

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1. Р.Беккер. Результаты анализа расчетов по модельной задаче YANKEE.
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KFKI-ZR6-538/1984.
3. Я.Гадо. Расчет выгорания асимптотической ячейки.
KFKI-ZR6-539/1984.
4. Я.Гадо, А.Керестури. Многогрупповые кинетические расчеты для ячейки бесконечных топливных решеток.
KFKI-ZR6-544/1986.
5. В.Лелек. Численный метод подгонки линейных уравнений реактора на основе измерений.
KFKI-ZR6-545/1986.
6. В.Лелек. Сеточная программа BRETISLAV для расчета реактора в гексагональной геометрии.
KFKI-ZR6-547/1986.
7. А.Мюллер, Г.Агте, Р.Беккер, Г.Хайнрих, В.Мюллер, З.Томас. Комплекс программы ГДР для расчета стационарных нейтронно-физических характеристик ядерных реакторов типа ВВЭР.
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8. Г.Агте. Параметризация зависимости макроскопических малогрупповых констант от параметров состояния.
KFKI-ZR6-549/1987.
9. Т.Апостолов, М.Манолова, З.Вознишки. Факторизационные методы решения.
KFKI-ZR6-550/1987.
10. В.Крысл, М.Леман, Я.Махачек. Теоретические основы модульной микрокодовой системы MOBY-DICK.
KFKI-ZR6-551/1987.
11. В.Ллек, М.Пецка. Использование измерений на критической сборке для уточнения групповых констант ячеек с топливом и другими материалами.
KFKI-ZR6-553/1988.
12. Р.Беккер. Обсчет критических измерений для невозмущенных решеток по спектральным диффузионным и кинетическим программам.

- KFKI-ZR6-554/1988.
13. Р.Беккер. Описание метода расчета для ячеек типа Вигнера-Зейтца по программе NESSEL-4.
KFKI-ZR6-555/1988.
 14. Г.Агте, Р.Беккер. Физические основы программы FLEX.
KFKI-ZR6-556/1989.
 15. Г.Агте, Р.Беккер. Параметризация зависимости макроскопических малогрупповых констант от спектра.
KFKI-ZR6-557/1989.
 16. Г.Агте, Х.Вокенфус. Физические основы трехмерной крупносеточной программы POLEX.
KFKI-ZR6-559/1988.
 17. Т.Куликовска, Б.Садовска. Расчеты выгорания в программе WIMSD-4.
KFKI-ZR6-559/1988.
 18. Т.Апостолов, В.Лелек. Проблемы составления и проверки диффузионных программ.
KFKI-ZR6-560/1988.
 19. Т.Апостолов, М.Манолова, К.Иванов. HEXAB - семейство малогрупповых диффузионных программ для гексагональной геометрии.
KFKI-ZR6-561/1988.
 20. Л.Майоров, Ю.Ване. использование прецизионных расчетов для анализа экспериментов на сборке ZR-6.
KFKI-ZR6-563/1989.
 21. М.Юдкевич. Константное обеспечение прецизионных реакторных программ.
KFKI-ZR6-564/1989.
 22. Р.Беккер. Использование коррекции малогрупповых параметров по методу спектрального индекса в тонкосеточных диффузионных программах.
KFKI-ZR6-565/1989.
 23. Р.Беккер, Х.Хайнрих. Обеспечение малогрупповых констант в программе NESSEL-4.
KFKI-ZR6-566/1989.
 24. П.Вертеш. Система обеспечения расчетов многогрупповыми константами - программная система ФЭДГРУП.
KFKI-ZR6-606/1985.

FOREWORD
TO VOLUME 2 OF THE FINAL REPORT OF TIC

The Temporary International Collective (TIC) for Studying Physics of WWERS was established by an international agreement of the governments of Bulgaria, Czechoslovakia, Hungary, Poland, Romania and the Union of Soviet Socialist Republics. Later, further countries and organizations joined the cooperation: Cuba, the State Institute for Nuclear Research of Vietnam and the Technical Center of Finland.

The activity of the TIC was based on the experimental program carried out on the critical assembly ZR-6 operated by the Central Research Institute for Physics of the Hungarian Academy of Sciences, Budapest. In volumes 1 and 3 of the Final Report of TIC, the experiments are assessed and evaluated. These volumes were published earlier in English and Russian.

Along with the experiments, in the laboratories taking part in the TIC also a calculational-theoretical development took place. Within this activity, not only the calculational models were verified, validated and improved but also the actual problems of WWER operation were solved.

It was decided in 1980 to publish the most outstanding results of the calculational-theoretical activity of the TIC. Collection of contributions to volume 2 helped understand and model better the physics of WWERS. Notwithstanding, the preparation was underway when the activity of TIC was abandoned. Still TIC decided to publish later on a volume assessing results of theoretical investigations. Volume 2 of the Final Report of TIC was finalized in 1993.

It is worth mentioning that the present volume does not reflect all the theoretical investigations, efforts and achievements of TIC experts. Because of the extraordinary circumstances of the preparatory work, the thematic of the volume has been selected to some extent subjectively, reflecting in a restricted extent the potential and sphere of interest of the authors, who agreed to go on working on volume 2 after the TIC ceased to exist. Hence, this volume does not include results of practical operational calculation of WWERS.

The authors are convinced that the material published in the present volume is useful, gives a correct impression of a considerable part of the joint research done in the TIC and may be of interest for a fairly large circle of reactor physics experts.

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1. INTRODUCTION

The theoretical results presented in Volume 2 of the Final Report of the TIC are based on investigations carried out between 1972 and 1990. The investigations themselves were carried out by specialists of TIC member countries and institutes. The authors of individual investigations published their results in internal reports of the TIC, in Proceedings of the Annual TIC Symposia (from the first in 1972 until the nineteenth in 1990) and in other materials. Many results were not published being only presented as working materials at meetings of the so called thematical groups.

This volume reflects only one part of the TIC theoretical activities connected with nuclear data and code validation based on utilizing the ZR-6 assembly experimental data. The ZR-6 critical facility was operated in the Central Research Institute for Physics (Budapest, Hungary). The objective of the measurements was to investigate WWER type uranium fuelled water moderated lattices.

The experiments were carried out to validate both nuclear data libraries and the design codes applied to calculations the performance of WWER-440 and WWER-1000 type power reactors.

In the experiments both regular and perturbed lattices were investigated. The influence of the main lattice parameters (fuel enrichment, lattice pitch, boric acid concentration in the moderator, temperature) on the neutron physics characteristics was mainly studied for the regular lattices. In addition the characteristic perturbations of WWER (absorber rods, water holes) were studied modelling them as irregularities introduced into the basic regular lattice.

A review of the experimental results is published in Volumes 1 and 3 of the Final Report of the TIC ((TIC, 1985), (TIC, 1991)).

The ZR-6 experiments form a very important part of the WWER global investigation program including the following tasks:

- creation of evaluated nuclear data libraries,
- development of the theory and numerical methods for the description of the strongly non-uniform hexagonal WWER lattices,
- computer code development, verification and validation, increasing the code accuracy in elaborating new generation codes,
- experimental study of fuel lattice characteristics,
- collection and generalization of measured data obtained at reactor

INTRODUCTION

start-up and during operation,
- fuel pattern optimization, etc.

All these items formed part of the TIC activities. The results of the first three items of the program are partly discussed in Volume 2. The data evaluation problems, constant preparation and fine mesh codes used for design purposes are considered taking into account comparisons with ZR-6 experimental results.

Chapter 2 describes the data bases elaborated, being evaluated or adapted, and validated in the TIC institutes. Some of them are original data files. One of the goals of the evaluation was to elaborate a data base comparable in accuracy with ENDF/B-5 data when applied to WWER type reactors. It seems that this goal was achieved. Another important target was elaborating the design data libraries utilizing both the original evaluations and the commonly used ones. The data validation was carried out utilizing both the ZR-6 experimental results and the international benchmarks. Many criticality calculations being necessary for the data validation were carried out by Monte Carlo methods.

A lot of TIC efforts was devoted to elaborate new approaches permitting one to calculate the WWERs strongly non-uniform lattices with high accuracy. Principally new methods were created. As a rule, they are based on disregarding the homogenization concept and replacing it by synthesis type methods which differ from the nodal type methods usually used to solve the homogenized equations. From various points of view these methods are discussed in Chapters 3 to 7.

Chapter 3 contains a brief description of the TIC Monte Carlo codes. Its basic part concerns their application to both the design code and verification and validation of the new methods. Thus the new ingenious approaches are briefly described as well. Different methods for calculating the diffusion coefficients are discussed. The Monte Carlo and the ZR-6 results are compared.

Chapter 4 is devoted to the methods and codes to calculate the few group constants by solving the transport equation. It contains verification and validation results based particularly on the ZR-6 experimental results.

The fine mesh calculation methods and codes, their verification and validation are described in Chapter 5.

Chapters 6 and 7 describe the new design approaches to solve the transport equation. They mainly concern the fine mesh calculation problems. These methods are also extensively used now in coarse mesh calculations. In

particular some new generation three-dimensional WWER codes utilize these approaches instead of nodal ones based on the homogenization theory.

A mixed referencing system is used throughout this book: TIC reports are referred by their numbers, while other papers, articles or books are referred to by author(s) and year of appearance.

This Volume, similarly to Volumes 1 and 3, is published both in Russian and English.

2. NUCLEAR DATA FOR REACTOR CODES

M.S. Yudkevich

2.1 INTRODUCTION

By this time a lot of experimental information on parameters of neutron interaction with nuclei for the whole reactor spectrum has been collected through all the world. Theoretical models able to predict these parameters have been created should the experimental information be inadequate.

Certain techniques have been developed for dealing with nuclear data applied to reactor calculations. Physicists, usually nuclear physics experts, evaluate all known information about each specific isotope. As a result, they generate the most trustworthy data available at the time of the evaluation. This information forms the base for computer nuclear data files. Libraries of such files have been developed in several countries : ENDF/B in the USA, BROND in Russia, JENDL in Japan, etc. The most of those libraries have been written in ENDF/B format and have been transferred to IAEA for the international access.

Existing libraries are not able to satisfy all the user requirements. Nevertheless, one may set and in many cases successfully solve a problem of reactor parameters calculation on the basis of the cross sections and other nuclear data only.

Creating the computer codes for calculating the WWER type reactor parameters with sufficient accuracy was one of the TIC targets. Those codes had to be based on primary nuclear data. In general the tasks have been performed as can be seen from comparing the calculated and measured parameters of many critical assemblies including the ZR-6. Created codes use the evaluated nuclear data libraries (mostly ENDF/B-4) or original author evaluations.

Most codes adopt cross sections and other nuclear data not directly from total files of nuclear data. Each code has its own data library formed on the basis of files or other sources of evaluated neutron data. Various algorithms were utilized during this process. Main approximations are connected with neutron energy spectrum. For example, NESSEL-4 and some other codes use the equivalence theorem to treat resonance effects; the

SAPFIR code uses the subgroup approach. Consequently, the *NESSEL-4* library contains a dependence on resonance self-shielding factors versus dilution cross section and the *SAPFIR* library includes subgroup parameters of resonance cross sections. Algorithms of engineering codes are described in Chapter 4 in detail.

In Section 2 of this chapter brief information is given on codes for preparing libraries from evaluated nuclear data. In Section 3 the work libraries are described for reactor codes created by the TIC country members. Section 4 presents the calculation results of the critical assemblies. These calculations have been performed by Monte Carlo method on the basis of evaluated nuclear data.

2.2. NUCLEAR DATA PROCESSING CODES

2.2.1 Codes created by TIC

FEDGROUP

The *FEDGROUP* code (Vertes, 1981) calculates group constants in the energy region of slowing down neutrons using data files in ENDF/B, KEDAK or UKNDL format. This code has been long used by TIC member countries to generate libraries for engineering codes. The *FEDGROUP* code consists of 6 units. Each unit can operate independently or all units can be called consecutively.

Units carry out:

1. Reconstruction of pointwise data from the resonance parameters. Calculation of the cross sections in any energy point are executed taking into account Doppler broadening. The choice of points ensures assigned precision when linear interpolation is carried out.
2. Calculation of the group cross sections on the basis of the pointwise ones. Energy boundary and a weighting flux should be assigned by the user.
3. Calculation of the Grueling-Goertzel type slowing down parameters on the basis of information on the elastic scattered neutron angular distribution.
4. Calculation of the inelastic cross section and cross section for transfer between groups (transfer matrix) from the information on excitation function of discrete levels and continuum of levels.
5. Calculation of the angular moments of the scattering cross section.

6. Calculation of self-shielded cross sections versus dilution cross section and temperature. Initial data are the resonances parameters in the energy region of fully resolved resonances and the average ones in the unresolved resonance region. It is used the narrow resonance approximation.

FEDGROUP-R

This code (Golubarge, 1985) is a modified and extended version of the *FEDGROUP* code. It is intended for processing of data in ENDF/B format and it is used to obtain the group constants *ABBN* (*BNAB*) and *WIMS* type.

CND

The *CND* code (Becker, 1989) was written with the same goal as *FEDGROUP*. It processes files in ENDF/B-4 and ENDF/B-5 format. Specifically it allows the user to obtain higher momentums of the elastic cross section.

The code has been used to create a group constant library for the *LIB-4* code (see 2.3.2).

CROS

That code (Abagyan et al, 1984) generates the cross sections in an energy point of a resolved resonance region on the basis of the nuclear levels parameters. The (ψ, χ) approach is used to take into account Doppler broadening of the resonance levels. A relatively short run time gives an opportunity to use *CROS* as the module in Monte Carlo codes which cancel any doubt about cross section interpolation accuracy.

SAPFIR

SAPFIR code package utilizes generalized subgroup method in order to calculate resonance absorption (Tebin, Yudkevich, 1985; Tebin, 1989). One code of *SAPFIR* prepares the subgroup parameters of cross sections. The number of subgroups is chosen so as to provide an assigned precision of resonance absorption of neutrons in fuel rods. The momentum method is used to calculate part and cross sections of the subgroups.

TERMAC

The codes of this package (Gomin, Maiorov, 1982) are designed so as enable a library to be generated in the thermal neutrons energy region. The chemical bond effects and thermal motion of the nuclei are important in this region. The number of groups, their boundaries and their inner group spectrum should be assigned by user.

NEWRAS (Liman and Maiorov, 1981) and more advanced *STEN* (Gomin et al, 1990) codes have been written for calculating scattering law and double differential scattering cross section $\sigma(E_0 \rightarrow E, \mu)$ in incoherent Gauss

approximation. The *ELCOHR* code (Liman, 1982) is used for elastic coherent cross section calculations. Listed codes use the phonon spectrum of the moderator as an input data. The differential scattering cross section may also be calculated in gas approximation.

TERMAC codes have been used to generate multigroup library *TEPCON*, *KORT* and *LIPAR* libraries (see 2.3.4.), *CROS*, *NEWRAS* (or *STEN*) and *ELCOHR* codes are used jointly with *TERMAC* codes to calculate the cross sections in an energy point.

2.2.2. Adopted codes

Several codes of wide usage in many countries for processing neutron data have been adopted by TIC country members. Let us enumerate them here. *NJOY* (MacFarlane, Muir, 1987), *GRUCON* (Sinitisa et al, 1979)

These codes are similar *FEDGROUP*. Unlike the latter *NJOY* can prepare cross sections and scattering transfer matrices for thermal neutrons and *GRUCON* can generate subgroup parameters in energy regions of resolved and unresolved resonances.

LINEAR, *RECENT*, *SIGMA1* (Cullen, 1979)

These codes are intended to work with cross sections in the resonance energy region. Total the combination of the 3 codes gives an opportunity for reconstructing pointwise cross sections with Doppler broadening on the basis of the resonance parameters of the nucleus. Input information must be written in ENDF/B format, output data are written in this format too.

THERMOS (Stam'ler, 1963)

This complex is intended for calculating the cross sections as well as the spectrum of thermal neutrons. The *GAKE* subroutine of *THERMOS* is similar to *NEWRAS* code of *TERMAC* package.

2.3. NEUTRON DATA LIBRARIES OF TIC *

2.3.1 Data library of KFKI (Budapest)

The library is based on the ENDF/B-4 files and is used in *BETTY* (Gado, Zsoldos, 1978), *CERES* (Kereszturi, 1981), *PEANICO* (Kereszturi, 1981) and

* Author of 2.1.3 is A.Kereszturi, 2.3.2 - R.Becker and H.Heinrich,
2.3.3 - K.Zalesky.

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THERMOS codes, in MASI and CERES modules of the KARATE system (Gado, Kereszturi et al, 1990).

The library consists of four parts.

a) **Pointwise cross sections** of certain resonance isotopes. They are utilized by PEANICO code.

PEANICO has been obtained from the PEACO code (Ishiguro, Takano, 1971) after generalizing the latter. It allows one to calculate neutron spectrum in reactor cells by the first collision probability method. Non-isotropic hydrogen scattering and the detailed description of the resonance cross section are taken into account. Tables of energy dependent absorption, fission and scattering cross sections have been calculated by using LINEAR, RECENT and SIGMA1 codes for ^{235}U , ^{238}U , and ^{239}Pu isotopes. The energy region from 4 KeV to 0,625 eV was divided into 3000 groups. The width of the groups is determined by the resonance structure of the ^{238}U isotope. Cross sections are tabulated for temperatures 300, 900 and 2100 K.

b) **Data for CERES code.**

CERES obtains the self-shielded cross sections by means of equivalence theorem approach. The following data are used for this purpose:

- The group cross sections and resonance integrals $I(\sigma_{\text{ex}})$ for ^{235}U , ^{238}U and ^{239}Pu isotopes versus the dilution cross section σ_{ex} for temperatures 300, 900 and 2100 K. Resonance integrals were calculated using the PEANICO code in the energy region of fully resolved resonances for homogeneous material with hydrogen as the moderator. The FEDGROUP code have been used in unresolved resonance energy region. The values of the dilution cross section σ_{ex} are listed below.

U-235	U-238	Pu-239
10.000	7.0	10.000
31.623	10.0	31.623
100.000	32.4	100.000
316.230	67.6	316.230
1000.000	115.6	1000.000
3162.300	176.4	3162.300
10000.000	250.0	10000.000
31623.000		31623.000
100000.000		100000.000

- Bell factors of the each group versus dilution cross section (for ^{235}U , ^{238}U and ^{239}Pu isotopes). These data were obtained when calculation results of infinite uniform media were compared with ones of isolated fuel rods.
- Goldstein factors were calculated accordance with Forti approach by the *FEDGROUP* code.

All the mentioned data related to 21 groups from 41 Kev to 1.84 ev energy region.

c) Data in the energy region of slowing down neutrons for the *BETTY* code and the *MASI* module, namely:

- Absorption, fission and elastic scattering cross sections from 10 MeV to 0.625 eV (35 energy groups). These values were obtained by the *FEDGROUP* code.
- Parameters from Greuling-Goertzel approach calculated by the *FEDGROUP* code.
- Inelastic scattering cross sections and inelastic transfer matrices calculated by the *FEDGROUP* code.

d) Data for the thermal energy region. These data are used by *BETTY* and *THERMOS* codes and *MASI* module. The upper boundary of the region is 1.84 eV, thus it permits one to describe correctly the ^{240}Pu isotope principal resonance.

That part of the library contains:

- Absorption, fission and scattering cross sections at the 35 energy points. These data were obtained by means of interpolation by *RECENT* code. The numbers of fission neutrons do not depend on energy.
- First two angular moments of the double differential scattering cross section of hydrogen. Those were generated by the *GAKER* code of *THERMOS* in Nelkin approximation. Scattering matrices of other isotopes are calculated in the gas approximation and only the first angular moments are taken into account.
- G and H functions for the differential equation of thermalization in Cadilhac approximation (Cadilhac et al, 1962).

All the data mentioned describe 53 isotopes. Absorption and scattering cross section are available only for 145 fission products.

2.3.2. Group library LIB-4 (KKAB, Berlin)

This library is used by the *NESSEL-4* code (Heinrich, 1981).

LIB-4 (Becker, 1989) contains 34-group constants, information about

fission products, prompt and delay fission neutrons, the radioactive parameters of ^{135}Xe and ^{241}Pu isotopes.

LIB-4 is similar to *ABBN* in the 24 upper groups, but there are some peculiarities. They are as follows.

- inelastic transfer matrices have been updated;
- hydrogen scattering cross section above 0.465 eV have been corrected to take into account chemical bond effect and thermal movement of atoms;
- resonances self-shielding is considered through 13th to 24th groups (4.65 Kev - 0.465 eV).

The energy region below 0.465 eV includes 10 groups; transfer cross sections between those have been calculated on the basis of the Koppel-Young model.

Library content has been increased considerably in comparison with *ABBN* by means of processing ENDF/B files using the *CND* code.

2.3.3. Library of *MICROBE* code (NRI, Res)

The *MICROBE* code is described in (Zalesky, 1984).

Group library *ABBN* type is used to perform calculations in the slowing down energy region. Self-shielding factors are input into the library to provide resonance absorption calculations in the equivalence theorem approach.

Multigroup *THSIG* code is used in the thermal neutron energy region.

All data were generated on the basis of ENDF/B-4 files by the *FEDGROUP-R* code. The library contains data for all isotopes of a reactor core as well as for fission products.

2.3.4. Neutron data bank (IAE, Moscow)

Direct application of evaluated neutron data files in reactor *codrsis* extremely complicated because of the large volume of data. However, it is not necessary in practice to use them totally. In each reactor type one may pick out the most important parts of the neutron spectrum. Each item of data should be presented in all details there and in the less important energy intervals they could be described more roughly. As it is known, in thermal reactors the most significant regions are those of the thermal neutrons and low placed resonances.

To support thermal reactor calculations on the basis of evaluated neutron data several libraries have been created in the I.V.Kurchatov IAE. Each of those libraries describes the cross sections and other neutron data with sufficient accuracy in their own energy region. These are libraries of group constants, resonance parameters, thermal neutron data. The libraries were prepared as a result of the original authors' evaluations and critical analyses of certain data files.

All libraries are included in the "IAE Bank of neutron data" (Yudkevich, 1984). Apart from libraries, the Bank contains some codes for data search and retrieving, editing and so on.

The IAE Bank was formed long ago. For the last several years it has been developed within the *MCU* project (Gomin et al., 1990). The project aimed at providing precise reactor calculations by the Monte Carlo method. The *MCU* Monte Carlo code created in the framework of the project is described in Chapter 3.

The *MCU* code uses libraries of the Bank directly. The libraries of *UNIRASOS-2*, *TVS*, *RAFORIN*, *SAPFIR* codes (see below) are based on the Bank too. This means that the Bank gives opportunity to perform reactor parameter calculations on the general data base by different methods. Thus it is possible to obtain a methodical bias of simplified codes by comparing their results with results of the more precise Monte Carlo code.

The data libraries of the IAE Bank are described below.

Library *BNAB/MCU* of group constants

Neutron data of *ABBN* (*BNAB*) system (Abagyan et al., 1964; Abagyan et al., 1981); Bondarenko et al., 1964) have been used for a long time. Being applied to thermal reactors they can be used to calculate spectra of slowing down neutrons in the range from 10.5 MeV to a thermal region.

The philosophy of *ABBN* system and the algorithms for obtaining the reactor macro constants were described in detail by its authors. Here we should like to point out that there are two ways of describing cross section resonance structure in *ABBN* system:

- the Bondarenko resonance self-shielding factors (*f*-factors). In agreement with reactor cell calculations those factors may be used together with the equivalence theorem;
- subgroup parameters of cross sections which can be used in different calculation methods, for example the first collisions probability method.

Bondarenko's *f*-factors and subgroup parameters are obtained in narrow

resonance approach. This assumption fails for low placed strong resonances. So for application to thermal reactors the *ABBN* system must be used with care.

The basic sources of information in the current version of the Bank are the *ABBN* libraries (Abagyan *et al*, 1980; Abagyan *et al*, 1981). To these were added the constants of isotopes, which either were obtained as the result of an independent evaluation or were generated from different evaluated nuclear data files. The data of some isotopes have been reevaluated and in some cases have been renewed. Currently the *BNAB/MCU* library contains information on 92 isotopes and elements.

Library of *LIPAR* resonance parameters

This library (Abagyan *et al*, 1984) is used to describe the cross sections energy dependence in the fully resolved resonances region. Currently *LIPAR* contains information for 87 isotopes.

The library has been created as the result of evaluations which were performed on the basis of the reference book (Mughabghab, Garber, 1973; Mughabghab, 1984), papers and available evaluated data files. During the evaluation process the resolved resonances boundary were found for each isotope. In a slow neutron energy region the cross sections obtained by means of *LIPAR* agree with those of the *KORT* library (see below).

LIPAR data are utilized by the *CROS* code calculating the cross sections in the desired energy points.

Libraries *KORT*, *BFS*, *TEPCON* of thermal constants

These libraries provide calculations in a region of thermal neutrons, where it is necessary to take into consideration thermal movement and the chemical bonds of atoms.

The basic library is the *KORT* library (Abagyan and Yudkevich, 1981; Abagyan *et al*. 1990). It can support calculations for energies below 5 eV. The *KOPT* has been created on the basis of the experimental information, evaluated data files and on the basis of the different publications.

The following information is recorded in the *KORT* for each isotope: - absorption, fission and scattering cross sections at the thermal point ($E=0.0253$ eV);

- the number of fission neutrons;
- recommendation on the method to generate cross sections: they either

follow the $1/v$ law or can be calculated on the basis of the resonance parameters (*LIPAR* library);

- the energy dependence of absorption and fission cross sections for other than $1/v$ isotopes.

Besides for each isotope the library contains additional comment information. It includes resonance integrals, g-factors, precision of cross sections at the thermal point and so on. These data are not used directly in calculations, but are useful for reference purposes.

The *BFS* library contains generalized phonon spectra for important moderators mainly from (Koppel and Huston, 1979; (Egelstaff and Pool, 1969). It allows one to calculate the scattering law with accounting for thermal movement and chemical bonds of atoms.

The library of thermal constants *TEPCON* is formed for a assigned isotopes list on the basis of *KORT*, *LIPAR* and *BFS* by means of the *TERMAC* code. Energy groups boundaries are prescribed by the user. 40 group library with the upper energy 1 eV and with linear scale on velocity are now widely employed. Another library option has the upper energy equal to 2.15 eV. This option is used in calculations of large plutonium content reactors.

TEPCON contains the following information for each isotope:

- absorption, fission and scattering cross sections at the thermal point, the numbers of fission neutrons;
- group cross sections if these do not follow the $1/v$ law;
- cross section for transfer between groups (first two angular momenta) for hydrogen in different compounds, deuterium, beryllium and carbon (other isotopes are considered in free gas approach);
- averaged cosine of scattering angle.

2.3.5. Libraries of *MCU*, *UNIRASOS-2*, *RAFORIN*, *SAPFIR* codes (IAE, Moscow)

Each of these codes uses the same data base - the IAE Neutron data bank.

MCU

The *MCU* codes (Gomin et al, 1990) perform calculations by the Monte Carlo method and use the information from the Bank directly. We should like to point out that *MCU* results were taken into account while evaluating the data.

The *BNAB/MCU* library with the subgroup description of the cross sections is used in an energy region of slowing down neutrons. For the thermalization region the *TEPCON* library is used. The boundary between these regions is to be assigned by the user. Usually it is equal to 1 eV.

Cross sections in simulation of collision are calculated by the *LIPAR* library in a region of strong resonances of uranium, plutonium, gadolinium and other resonance absorbers. The highest energy for calculating the cross sections with precise description are to be assigned by the user too. Usually one accepts: 100 eV for ^{235}U , 465 eV for ^{238}U , 215 eV for ^{239}Pu , 100 eV for ^{240}Pu .

UNIRASOS-2

UNIRASOS-2 code (Pshenin *et al.*, 1989) uses three libraries:

- 14-group constant library for the epi-thermal energy region ($E > 0.625\text{ eV}$);
- the table of effective resonance integrals depending upon the dilution cross section for important uranium and plutonium isotopes and resonance absorbers;
- the cross sections in the thermal energy region ($E \leq 0.625\text{ eV}$).

In the energy region of fission spectrum and unresolved resonances the group library is based on the *BNAB/MCU* library. So that applies to nonresonance isotopes in whole energy region above 1 eV. Effective resonance integrals for single rods have been calculated on the basis of the *LIPAR* library. The Goldstein factors secure equality calculated resonance absorption by *UNIRASOS-2* and by the Monte Carlo code *MCU*.

A thermal neutron spectrum is calculated by means of Laletin differential model (Laletin, 1974). The absorption and fission cross sections are taken from *KOPT* and *LIPAR* libraries.

RAFORIN (Pshenin *et al.*, 1989), TVS (Pshenin *et al.*, 1989)

The same data as in *UNIRASOS-2* code were used to provide calculations in the energy region of slowing down neutrons.

The *TEPCON* multigroup library is used to calculate thermal neutron spectrum ($E \leq 0.625\text{ eV}$). It was formed by means of the *TERMAC* code.

SAPFIR (Tebin, 1989)

In the epi-thermal energy region the *BNAB/TR* group library is used. It was been created on the basis of *BNAB/MCU* from the IAE Bank. In comparison

with the latter *BNAB/TR* contains the parameters of generalized subgroup approach.

One employs an additional correction values if the algorithm of an engineering reactor program is based on *ABBN* or other libraries with *f*-factors. So the accuracy of resonance absorption calculations is improved. As another possibility a generalized subgroup approach has been developed with reference to thermal reactor cells. The generalized subgroup parameters are an expanded set of original *ABBN* ones. These parameters are following:

- a^i - part of subgroup i ($\sum a^i = 1$);
- σ_x^i - averaged subgroup total and partial cross sections;
- $\omega_{(i,j)}^x$ - transfer matrix between subgroups i and j ;
- $\alpha_{(i,k)}^{(1,j)}$ - correlation coefficient between subgroups i isotope l and subgroups j isotope k .

All these parameters depend on temperature.

Generalized subgroup parameters have been obtained for a resolved resonances energy region. The *LIPAR* library was used as initial data. The number of subgroups was chosen to ensure a lower 3% bias of resonance absorption calculation results for each group.

For sufficiently high neutron energy the narrow resonance approximation has enough accuracy. It is therefore possible to use subgroup parameters a^i and σ_x^i from the original *ABBN* system.

For the thermal energy region is used 40 group *TEPCON* library retrieved from the IAE Bank is used.

2.4. VERIFICATION OF THE NEUTRON DATA BANK

Approximately 250 critical assemblies have been studied to verify the IAE Neutron data bank and to judge on prediction accuracy of the multiplication coefficient and other reactor parameters. They are assemblies of thermal and fast reactors with different fission and fertile materials and with different moderators. The descriptions and the calculated neutron spectra, multiplication factors, reaction rates and some important integral parameters of assemblies are gathered in the computer library *CLAD* (Alekseev *et al*, 1991) created in the framework of *MCU* project (Gomin *et al*, 1990).

This chapter contains results for assemblies connected with WWER type reactors (Gomin *et al*, 1987), (Alekseev *et al.*, 1991). The calculations

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were carried out using the Monte Carlo *MCU* code, versions mainly *MCU-1* and *MCU-2*.

The geometry and composition of assemblies have been modelled in full accordance with the experimentator's description without any simplifications. That is why only well described assemblies have been considered.

The *MCU* code gives an opportunity for simulating neutron and nuclei collision with different level of detail. The results presented here were obtained using the physical model corresponding to the data libraries *BNAB/MCU*, *LIPAR* and *TEPCON* (see 2.3.4). This model enable to obtain a reasonable compromise between accuracy of results and run time.

Fulfilled verification confirms that the accuracy on the reactor parameter calculation is comparable with existing experimental data precision. The reliability of the reactor criticality prediction satisfies all the practical requirements.

Notations used during the description of the critical assemblies

- R - spherical core radius, cm.
- D, H - diameter and height of cylindrical core, cm.
- d - fuel rod diameter in a heterogeneous assembly core, cm.
- h - lattice pitch in a heterogeneous assembly core, cm.
- V_M/V_F - moderator (water) to fuel volume ratio in unit cell of a heterogeneous assembly.
- B_R^2, B_Z^2, B^2 - radial, axial and total buckling, M^{-2}
- $H/U5, H/Pu$ - ratio of H to $^{235}U, Pu$ nuclear density.
- $B10/U5$ - ratio of ^{10}B to ^{235}U nuclear density.
- ^{235}W - enrichment in ^{235}U of uranium, weight per cent.
- PuW - content of PuO_2 in PuO_2-UO_2 fuel, weight per cent.
- $^{240}W, ^{241}W$ - content $^{240}Pu, ^{241}Pu$ in plutonium isotopes mixture, weight percent.

Notation used during the description of the calculation results.

- K_{eff} - multiplication factor.
- K_{∞} - the same one for the infinite array of cells.
- M_f^2 - square length of neutron's migration from birth to fission $(1/6\langle R_f^2 \rangle)$, cm^2 .
- P - probability of neutron leakage.

- ρ^{28}, ρ^{40} - ratio of epi-cadmium to sub-cadmium neutron capture rates in $^{238}\text{U}, ^{240}\text{Pu}$.
- δ^{25}, δ^{49} - ratio of epi-cadmium to sub-cadmium neutron fission rates in $^{235}\text{U}, ^{249}\text{Pu}$;

The cadmium cut-off energy E_c value for assemblies, where measuring of ρ^{28} and ρ^{25} have been done, corresponds to the cadmium cover thickness used (Beckurts, 1964). Otherwise $E_c = 0.625$ eV is assumed.

- δ^{28} - ratio of fission rate in ^{238}U to fission rate in ^{235}U .
- δ^{25}_{49} - ratio of fission rate in ^{235}U to fission rate in ^{249}Pu .
- ξ_{25} - ratio of ^{235}U fission rate in fuel to ^{235}U fission rate in moderator.

Presentation of the results.

All results of calculations are given together with their statistical probability errors. For example, 5.02(6) means 5.02 ± 0.06 where 0.06 is a probability error (one standard deviation).

2.4.1. Homogeneous critical assemblies with highly enriched uranium

The core in these assemblies is an aqueous solution of an uranium acid. Enrichment in ^{235}U is equal approximately 93%.

In the process of evaluation 23 assemblies without reflector and 10 assemblies with a reflector were investigated from several tens of the described assemblies. These selected assemblies embrace the scope of all values of the measured uranium concentrations. The "infinite medium" was added to them. In this case the critical concentration of uranium has been determined by extrapolating buckling to zero.

The main characteristics of assemblies are given in Table 2.1. Information was retrieved from (Thermal Benchmark, 1974) for ORNL assemblies, from (Gwin, Magnusen, 1962) for assemblies with $\text{UO}_2(\text{NO}_3)_2$ and from (ANL-5800, 1963) for assemblies with UO_3F_2 . Results of calculations are presented in Table 2.2. Assemblies are arranged in increasing order of their H/U5 ratio. For the best visualization the calculated values of K_{eff} upon H/U5 are shown in Fig.2.1.

First of all one should point out the strong scattering of results

especially for reflected assemblies even between these with similar parameters. It appears that precision of determination of the critical parameters does not allow one to check the accuracy of K_{eff} calculation better 0.2% for high $H/U5$ and 0.5% for low ones.

For unreflecting assemblies with low uranium concentration, including benchmark assemblies, the calculations predict the criticality almost exactly. For assemblies with a high neutron leakage the calculations give rather too high values of K_{eff} . This could indicate evidence of too soft fission neutron spectrum.

No conclusions can be made for reflected assemblies because of the too wide scattering of calculated K_{eff} .

Table 2.1. Main Characteristics of Homogeneous Critical Assemblies with Highly Enriched Uranium

Solution UO_2F_2						
<u>Bare cylinder</u>			<u>Reflected cylinder</u>			
H/U5	D	H	H/U5	D	H	
27	25.4	38.9	26	16.5	44.5	
44	25.4	35.1	43	25.4	12.5	
50	25.4	34.8	59	15.2	71.8	
61	25.4	34.1	79	20.3	19.4	
73	25.4	33.7	127	25.4	14.4	
83	25.4	34.4	192	20.3	28.1	
169	25.4	41.2	329	25.4	22.4	
331	30.5	32.8	499	38.1	16.9	
331	38.1	22.9	755	38.1	27.1	
755	38.1	43.6	999	38.1	44.3	

Solution $\text{UO}_2(\text{NO}_3)_2$						
<u>Bare cylinder</u>			<u>Bare sphere</u>			
H/U5	D	H	H/U5	B10/U5	R	
1021	154.8	74.2	ORNL-4	972	0.0037	34.6
1604	154.8	46.5	ORNL-3	1033	0.0032	34.6
1634	154.8	48.8	ORNL-2	1177	0.018	34.6
1905	154.8	106.8	ORNL-1	1378	0.0	34.6
1955	273.6	90.9	ORNL-5	1835	0.0	61.0
1981	154.8	205.0				
2004	273.6	119.4				
2052	273.6	241.0				
2110±20	infinite					

Table 2.2. Integral Parameters of Homogeneous Critical Assemblies with Highly Enriched Uranium

Bare core				Reflected core		
H/U5	K_{eff}	P	δ^{25}	H/U5	K_{eff}	δ^{25}
27	1.006(3)	0.444	0.777	26	0.992(2)	0.193
44	1.012(3)	0.456	0.447	43	0.981(3)	0.150
50	1.010(3)	0.451	0.395	59	1.003(3)	0.196
61	1.008(3)	0.459	0.321	79	0.999(3)	0.181
73	1.005(3)	0.462	0.266	127	0.999(3)	0.142
83	1.012(3)	0.459	0.233	192	1.017(3)	0.082
169	1.010(4)	0.452	0.117	329	1.012(3)	
331	1.008(3)	0.423	0.064	499	1.006(3)	
331	1.011(3)	0.420	0.064	755	1.015(3)	
755	0.993(2)	0.331	0.032	999	1.006(2)	
972 [*])	0.997(2)	0.168	0.029			
1021	1.005(2)	0.069	0.018			
1033 [*])	0.999(2)	0.168	0.029			
1177 [*])	0.999(2)	0.170	0.024			
1378 [*])	0.997(2)	0.176	0.021			
1604	1.004(2)	0.122	0.019			
1634	0.998(2)	0.115	0.018			
1835 [*])	0.999(2)	0.067	0.017			
1905	1.003(2)	0.051	0.017			
1955	0.995(2)	0.043	0.016			
1981	1.000(2)	0.035	0.016			
2004	0.994(2)	0.031	0.016			
2052	1.005(2)	0.012	0.016			
2110	0.999(2)	0.000	0.016			

* benchmark

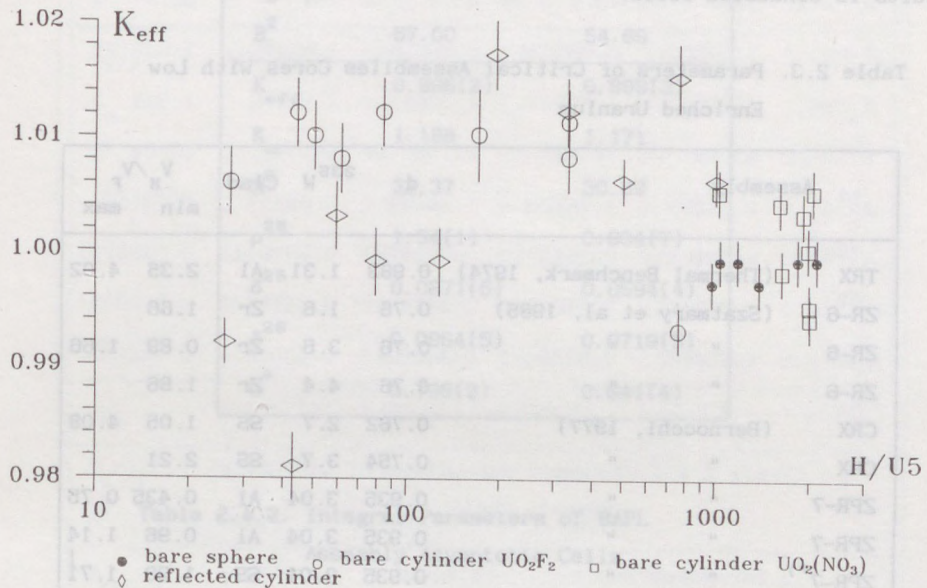


Fig.2.1. Calculated K_{eff} values for homogeneous critical assemblies with highly enriched uranium. Calculation probability errors are indicated.

2.4.2. Asymptotic cells of critical assemblies with low enriched uranium

Most of the asymptotic cells described in the literature have been investigated in the following calculations. There are 43 asymptotic cells whose buckling has been measured at the critical assemblies of various laboratories. One or another integral parameters have been measured in the majority of the assemblies.

The cells of any assembly differ from those of another only by the lattice pitch, that is moderator to fuel volume ratio V_M/V_F . Table 2.3

gives a general idea about calculated cells. The used information sources are pointed out too. The cells of TRX and BAPL are recommended as benchmarks (Thermal Benchmark, 1974). Calculated K_{eff} and important spectral parameters are presented in Table 2.4. A brief discussion of results is conducted below.

Table 2.3. Parameters of Critical Assemblies Cores with Low Enriched Uranium

Assembly		d	^{235}W	Clad	V_M/V_F	
					min	max
TRX	(Thermal Benchmark, 1974)	0.983	1.31	Al	2.35	4.02
ZR-6	(Szatmary et al, 1985)	0.76	1.6	Zr	1.66	
ZR-6	" "	0.76	3.6	Zr	0.89	1.66
ZR-6	" "	0.76	4.4	Zr	1.66	
CRX	(Bernocchi, 1977)	0.762	2.7	SS	1.05	4.08
CRX	" "	0.754	3.7	SS	2.21	
ZPR-7	" "	0.935	3.04	Al	0.435	0.75
ZPR-7	" "	0.935	3.04	Al	0.96	1.14
ZPR-7*)	" "	0.935	3.04	SS	1.28	1.71
BAPL	(Thermal Benchmark, 1974)	0.973	1.31	Al	1.43	2.40
BAY	(Bernocchi, 1977)	1.03	2.50	Al	1.37	
TCA	" "	1.25	2.60	Al	1.50	3.00
NORA	" "	1.27	3.41	SS	1.66	4.51
ZPR	" "	1.524	2.07	Al	1.01	4.02
DIMPLE	(Broun, 1967)	2.024	3.00	SS	0.78	3.16

*) polycell 4x4, loaded 16, 14 or 12 fuel rods

Table 2.4.1. Integral Parameters of TRX
Assembly Asymptotic Cells

Parameter	Value	
V_M/V_F	2.35	4.02
B^2	57.00	54.69
K_{eff}	0.996(2)	0.999(2)
K_∞	1.188	1.171
M^2	32.37	30.89
ρ^{28}	1.34(1)	0.834(7)
δ^{25}	0.0971(5)	0.0594(4)
δ^{28}	0.0964(5)	0.0719(5)
C^*	0.796(3)	0.641(4)

Table 2.4.2. Integral Parameters of BAPL
Assembly Asymptotic Cells

Parameter	Value		
V_M/V_F	1.43	1.78	2.40
B^2	32.59	35.47	34.22
K_{eff}	0.997(4)	1.009(4)	1.002(4)
K_∞	1.146	1.152	1.142
M^2	43.75	41.41	38.9
ρ^{28}	1.41(1)	1.15(1)	0.901(8)
δ^{25}	0.0833(5)	0.0666(4)	0.0512(3)
δ^{28}	0.0770(5)	0.0662(2)	0.0550(4)
C^*	0.813(5)	0.733(4)	0.656(4)
ξ_{25}	1.13(1)	1.14(1)	1.15(1)

Table 2.4.3. Integral Parameters of ZPR Assembly Asymptotic Cells

Parameter	Value				
V_H/V_F	1.012	1.515	2.017	3.011	4.016
B^2	57.6	79.8	83.2	74.8	60.6
K_{eff}	1.008(4)	0.985(3)	0.996(3)	1.004(3)	1.003(3)
K_∞	1.272	1.307	1.306	1.273	1.211
M^2	42.93	38.99	37.02	35.14	32.24
ρ^{28}	2.44(2)	1.70(2)	1.36(1)	0.95(1)	0.75(1)
δ^{25}	0.159(1)	0.106(7)	0.0824(6)	0.0579(4)	0.0462(3)
δ^{28}	0.0931(7)	0.0741(5)	0.0614(4)	0.0478(3)	0.0408(3)
C^*	0.708(5)	0.564(4)	0.495(3)	0.423(3)	0.384(3)

Table 2.4.4. Integral Parameters of DIMPLe Assembly Cells

Parameter	Value		
V_H/V_F	0.779	1.001	1.001 ^{*)}
B^2	50.96	66.00	62.58
K_{ef}	0.998(4)	1.002(4)	1.003(4)
K_∞	1.224	1.268	1.264
M^2	40.99	30.08	39.87
ρ^{28}	5.06(4)	3.96(3)	4.03(3)
δ^{25}	0.310(2)	0.237(2)	0.241(2)
δ^{28}	0.106(9)	0.0901(6)	0.0921(6)
C^*	0.752(4)	0.646(4)	0.653(4)
ξ_{25}	1.222(9)	1.239(8)	1.241(9)

*) T=583 K

Table 2.4.5 Integral Parameters of CRX Assembly Asymptotic Cells

Parameter		Value				
V_M/V_F		1.048	1.2	1.405	1.853	2.166
B^2		40.7	47.5	53.2	63.3	68.8
K_{eff}		1.008(3)	1.005(4)	1.012(3)	1.010(3)	1.008(4)
K_∞		1.174	1.195	1.218	1.243	1.247
M^2		39.48	38.16	37.16	34.72	34.07
ρ^{28}	*)	3.80(3)	3.44(3)	2.89(2)	2.25(2)	2.00(2)
δ^{25}	*)	0.220(1)	0.201(1)	0.163(1)	0.124(1)	0.107(1)
δ^{28}		0.0848(1)	0.0789(5)	0.0703(4)	0.0581(4)	0.0521(4)
C^*		0.702(4)	0.653(4)	0.591(4)	0.508(3)	0.470(3)
ξ_{25}		1.175(7)	1.18(3)	1.20(1)	1.21(2)	1.207(1)
V_M/V_F		3.372	4.078	2.212	**)	
B^2		59.5	54.4	95.1		
K_{eff}		1.033(3)	1.036(3)	1.008(4)		
K_∞		1.236	1.257	1.349		
M^2		32.68	31.97	33.72		
ρ^{28}	*)	1.36(1)	1.12(1)	2.59(2)		
δ^{25}	*)	0.0706(5)	0.0929(6)	0.136(1)		
δ^{28}		0.0376(2)	0.0329(2)	0.0508(3)		
C^*		0.384(3)	0.348(2)	0.399(3)		
ξ_{25}		1.24(1)	1.26(1)	1.26(1)		

*) $E_c = 0.55$ eV**) $d = 0.754$ cm $^{235}\text{W} = 3.7$.

Table 2.4.6. Integral Parameters of TCA Assembly
Asymptotic Cells

Parameter	Value			
V_M/V_F	1.501	1.833	2.482	2.999
B^2	83.3	93.2	98.3	95.2
K_{ef}	1.013(4)	0.997(4)	1.000(4)	1.006(4)
K_∞	1.364	1.386	1.372	1.352
M^2	39.6	38.14	35.39	34.62
ρ^{28}	2.14(2)	1.81(2)	1.40(1)	1.19(1)
δ^{25}	0.129(1)	0.109(1)	0.082(1)	0.0697(5)
δ^{28}	0.0700(5)	0.0627(4)	0.0510(4)	0.0450(3)
C^*	0.512(3)	0.464(3)	0.405(3)	0.373(3)
ξ_{25}	1.31(1)	1.32(2)	1.37(2)	1.38(2)

Table 2.4.7 Integral Parameters of BAY Assembly
Asymptotic Cell

Parameter	Value
V_M/V_F	1.377
B^2	70.1
K_{ef}	1.009(4)
K_∞	1.328
M^2	42.44
$\rho^{28} *$	2.34(2)
$\delta^{25} *$	0.137(9)
δ^{28}	0.0726(5)
C^*	0.571(4)

*) $E_c = 0.55$ eV

Table 2.4.8. Integral Parameters of ZR-6 Assembly
Asymptotic Cells

Parameter	Value			
^{235}W	1.6	3.6	3.6	4.0
V_M/V_F	1.66	1.66	0.888	1.66
B^2	50.57	98.58	67.13	112.58
K_{eff}	0.989(3)	1.008(3)	0.995(4)	1.001(3)
K_{∞}	1.196	1.421	1.309	1.455
M^2	40.47	38.74	45.37	37.91
ρ^{28}	1.47	2.91	5.12	3.46
δ^{25}	0.0794	0.155	0.292	0.189
δ^{28}	0.0610	0.0539	0.0837	0.0529
C^*	0.686	0.523	0.0837	0.411

Table 2.4.9. Integral Parameters of NORA Assembly
Asymptotic Cells

Parameter	Value		
V_M/V_F	1.66	3.03	4.51
B^2	91.89	98.8	86.4
K_{eff}	1.010(4)	1.015(4)	1.011(4)
K_{∞}	1.351	1.355	1.296
M^2	34.66	32.30	31.31
ρ^{28}	2.63(2)	1.53(2)	1.10(1)
δ^{25}	0.158(10)	0.0887(6)	0.0623(5)
δ^{28}	0.0649(4)	0.0439(3)	0.0344(2)
C^*	0.438(3)	0.322(3)	0.272(2)
ξ_{25}	1.41(1)	1.53(1)	1.60(1)

Table 2.4.10. Integral Parameters of ZPR-7 Assembly Asymptotic Cells

Parameter	Value			
V_M/V_F	0.435	0.7544	0.9596	1.371
B^2	24.36	55.38	70.76	91.82
K_{eff}	0.989(3)	0.987(3)	0.986(3)	0.982(3)
K_∞	1.139(3)	1.265(3)	1.329(3)	1.380(3)
M^2	58.7	48.6	45.15	40.8
ρ^{28}	8.85(5)	5.04(4)	3.95(3)	2.86(2)
δ^{25}	0.561(3)	0.301(2)	0.230(1)	0.160(1)
δ^{28}	0.1412(7)	0.0999(6)	0.085(5)	0.066(4)
C^*	1.034(5)	0.743(4)	0.637(5)	0.523(3)

Table 2.4.11. Integral Parameters of ZPR-7 Assembly Asymptotic Polycells

Parameter	Value		
V_M/V_F *)	1.708	1.281	0.962
B^2	74.27	61.99	47.47
K_{eff}	1.000(3)	1.002(3)	1.006(3)
K_∞	1.278(3)	1.255(8)	1.201(3)
M^2	36.03	38.24	39.4
ρ^{28}	2.51(2)	3.22(2)	2.86(2)
δ^{25}	0.141(1)	0.187(1)	0.253(1)
δ^{28}	0.063(4)	0.075(4)	0.066(4)
C^*	0.483(3)	0.561(3)	0.523(3)

*) Averaged over the polycell

The K_{eff} values from Tables 2.4 are shown in Fig 2.2. The $B^2 M_f^2$ value is taken as a parameter determining neutron leakage from a cell.

The calculated K_{eff} of most assemblies lies between 0.99 and 1.01. Evidently the scattering is connected with a methodological error in B^2 determinations or in the fact that some assemblies are not asymptotic.

K_{eff} of benchmark assemblies TRX and BAPL coincides with 1 if one takes into account statistical probability errors.

K_{eff} of CRX assembly exceeds 1 by more than 1% and in two of the assemblies more 3%. The experimental results on ρ^{28} and δ^{28} deviates from other authors data too (see Tables 2.6 and 2.7 below).

K_{eff} averaged over all cells except CRX is equal to 1.002.

The measured and calculated values of integral parameters C^* , ρ^{28} , δ^{28} and δ^{25} are compared in Tables 2.5 - 2.8.

In general, the picture looks mixed and contradictory. One can clearly recognize it from Figs. 2.3, 2.4 and 2.5. In a number of cases various cells, which have nearly equal parameters but have been investigated in various assemblies, display very different results. In some cases the results of calculations of K_{eff} and integral parameters contradict one another. No doubt it is connected not with the data in the libraries used but with the experimental results.

At the same time it is important to point out that the calculated results practically coincide with all experimental data for benchmark assemblies TRX and BAPL.

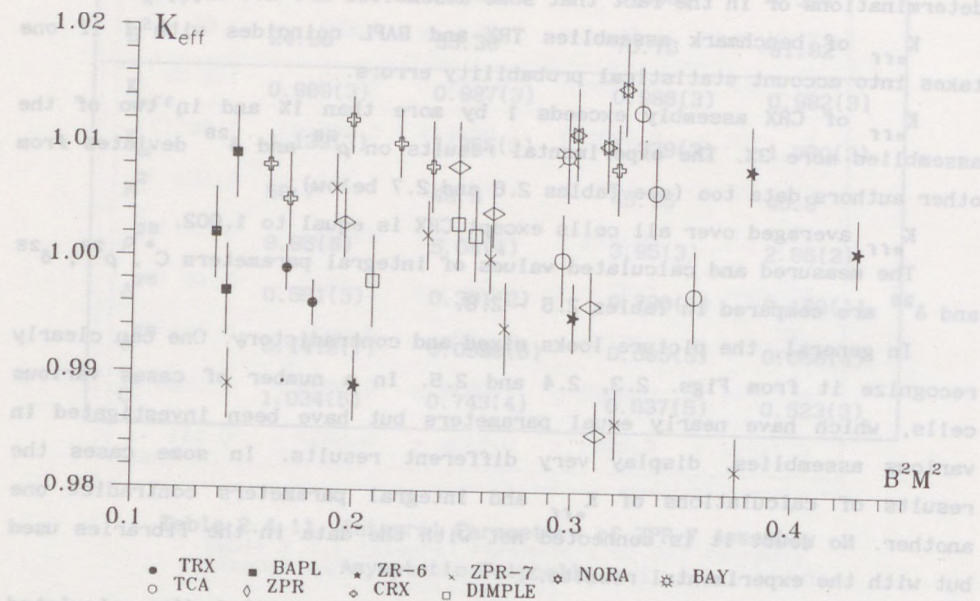


Fig.2.2. Calculated K_{eff} values for asymptotic cells with low enriched uranium. Calculation probability errors are indicated.

K_{eff}	1.006(3)	1.006(3)	1.006(3)
B^2M^2	0.38	0.38	0.38
σ	2.51(2)	3.23(2)	2.56(2)
σ	0.141(1)	0.187(1)	0.253(1)
σ	0.083(4)	0.075(4)	0.086(4)
σ	0.483(3)	0.561(3)	0.523(3)

Table 2.5. Integral Parameter C^* in the Asymptotic Cells

Assembly	V_H/V_F	C^*		(c/e-1)%
		exp.	calc.	
TRX	2.35	0.797±0.008	0.796(3)	0
	4.02	0.647±0.006	0.641(4)	-1
DIMPLE	0.779	0.725±0.018	0.752(4)	+3
	1.001	0.628±0.012	0.646(4)	+3
	1.001 ^{*)}	0.645±0.016	0.653(4)	-1
ZPR-7	0.962	0.679±0.009	0.679(5)	+10

*) T=583 K

Table 2.6 Integral Parameter ρ^{28} in the Asymptotic Cells

Assembly	V_H/V_F	ρ^{28}		(c/e-1)%
		exp.	calc.	
TRX	2.35	1.320±0.021	1.341	+1.5
	4.02	0.837±0.016	0.834	+1.3
BAPL	1.43	1.39±0.01	1.41(1)	0
	1.78	1.12±0.01	1.150(9)	+3
	2.40	0.906±0.010	0.901(8)	+0.3
NORA	3.03	1.524±0.016	1.53(2)	+0.4
	4.51	1.065±0.013	1.10(1)	+3
BAY	1.38	2.28±0.01	2.36(3)	+5
CRX	1.05	2.77±0.08	3.80(3)	+35
	1.20	2.78±0.16	3.44(3)	+25
	1.405	2.22±0.5	2.89(2)	+30
	1.85	1.83±0.10	2.25(2)	+25
	2.17	1.72±0.07	2.00(2)	+15
	3.37	1.22±0.10	1.36(1)	+10
	4.08	1.06±0.06	1.12(1)	+5
	2.12	1.96±0.08	2.59(2)	+30

Table 2.7. Integral Parameter δ^{28} in the Asymptotic Cells

Assembly	V_M/V_F	δ^{28}		
		exp.	calc.	(c/e-1)%
TRX	2.35	0.0946±0.0041	0.0964(5)	+2
	4.02	0.0693±0.0035	0.0719(5)	+4
BAPL	1.43	0.078±0.004	0.0770(5)	-1
	1.78	0.070±0.004	0.0662(5)	-5
	2.40	0.057±0.003	0.0550(4)	-4
DIMPLE	0.78	0.1113±0.0018	0.106(9)	-5
	1.00	0.0928±0.0009	0.0901(6)	-5
ZPR	1.52	0.067±0.001	0.0741(5)	+10
	3.01	0.046±0.001	0.0478(3)	+4
CRX	1.20	0.097±0.007	0.0789(5)	-20
	1.41	0.076±0.002	0.0703(4)	-8
	1.85	0.060±0.005	0.0581(4)	-3
	2.12	0.054±0.002	0.0508(4)	-6
	2.17	0.066±0.002	0.0521(4)	-21
	3.37	0.037±0.001	0.0376(2)	+2
	4.08	0.037±0.001	0.0348(2)	-6
NORA	1.66	0.062±0.003	0.0649(4)	+5

Table 2.8. Integral Parameter δ^{25} in the Asymptotic Cells

Assembly	V_M/V_F	H/U5	δ^{25}		
			exp.	calc.	(c/e-1)
TRX	2.35	250	0.0987±0.0010	0.0971(5)	-1.5
	4.02	430	0.0614±0.0008	0.0594(4)	-3
BAPL	1.43	305	0.084±0.002	0.0833(5)	-1
	1.78	385	0.068±0.001	0.0666(4)	-2
	2.40	510	0.052±0.001	0.0512(3)	-1.5
BAY	1.38	155	0.151±0.001	0.137(9)	-9
NORA	1.66	135	0.126±0.002	0.158(10)	+25

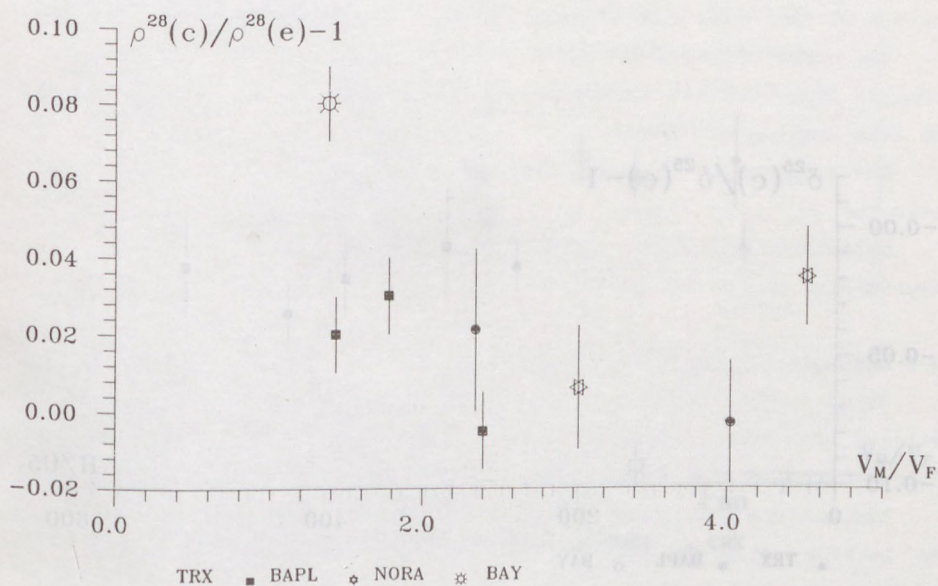


Fig.2.3. Comparison of measured (e) and calculated (c) ρ^{28} values.
Experimental probability errors are indicated.

Table 2.7. Integral Parameter δ^{25} in the Asymptotic Cells

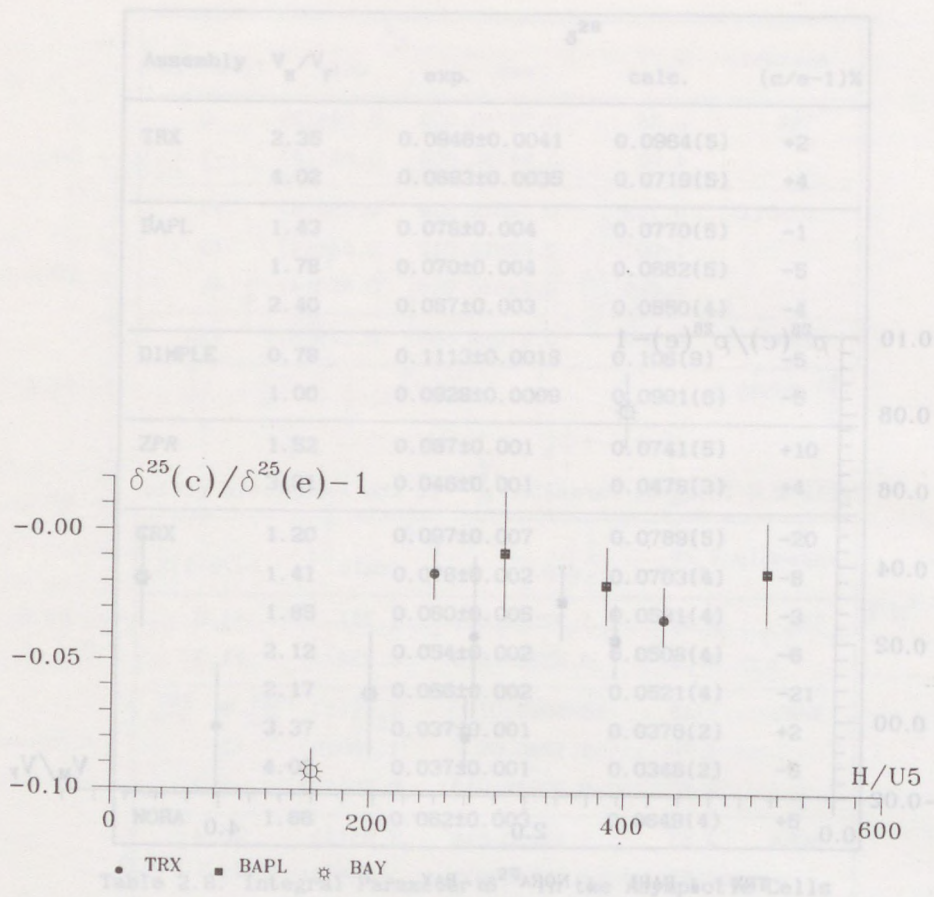


Fig.2.4. Comparison of measured (e) and calculated (c) δ^{25} values. Experimental probability errors are indicated.

Assembly	V_s/V_r	$H/U5$	exp. δ^{25}	calc. δ^{25}	(c/e-1)
TRX	2.35	250	0.087 ± 0.0010	$0.0971(5)$	-1.5
	4.02	430	0.0814 ± 0.0008	$0.0563(4)$	-3
	2.40	510	0.052 ± 0.001	$0.0512(3)$	-1.5
BAY	1.38	165	0.151 ± 0.001	$0.137(9)$	-9
NORA	1.60	135	0.128 ± 0.002	$0.128(10)$	+25

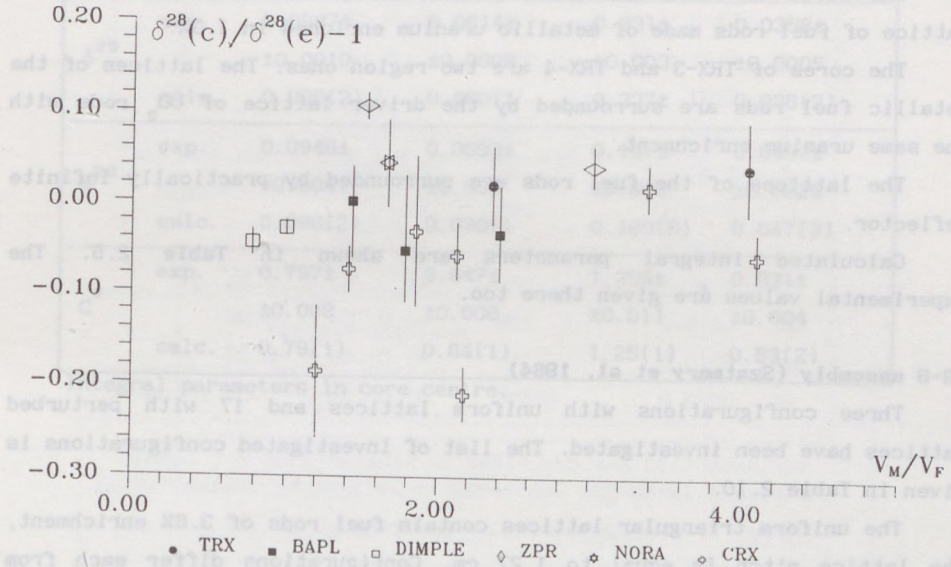


Fig.2.5. Comparison of measured (e) and calculated (c) δ^{28} values.
Experimental probability errors are indicated.

2.4.3. Full-scale heterogeneous assemblies

Calculations of these assemblies were performed without any simplifications in the plane perpendicular to the Z-axis. Leakage in Z-direction was considered in asymptotic approximation with experimental values of B_Z^2 .

TRX assembly (Thermal Benchmark, 1974)

The cores of TRX-1 and TRX-2 consist of water moderated triangular lattice of fuel rods made of metallic uranium enriched in 1.3%.

The cores of TRX-3 and TRX-4 are two-region ones. The lattices of the metallic fuel rods are surrounded by the driver lattice of UO_2 rods with the same uranium enrichment.

The lattices of the fuel rods are surrounded by practically infinite reflector.

Calculated integral parameters are shown in Table 2.5. The experimental values are given there too.

ZR-6 assembly (Szatmary et al, 1984)

Three configurations with uniform lattices and 17 with perturbed lattices have been investigated. The list of investigated configurations is given in Table 2.10.

The uniform triangular lattices contain fuel rods of 3.6% enrichment, the lattice pitch is equal to 1.27 cm. Configurations differ each from other in the number of fuel rods, water level and boron concentration in water.

In regularly perturbed lattices of X7 type every 7th fuel rod of the uniform lattice is replaced by an absorbing rod (B, Eu, Gd) or by water.

Configurations of K331 type imitate the core of WWER-1000 type reactors.

Calculated integral parameters of ZR-6 assembly are presented in Table 2.11.

The value of K_{eff} averaged over all cases is equal to 1.0035. The average variance is about 0.005.

Table 2.9. Integral Parameters of TRX Assembly

Parameter		Value			
		TRX-1	TRX-2	TRX-3	TRX-4
K_{eff}	exp.	1.0	1.0	1.0	1.0
	calc.	0.993(3)	0.996(1)	0.999(2)	0.998(3)
ρ^{28}	exp.	1.320 $\pm$ 0.021	0.837 $\pm$ 0.016	3.03 $\pm$ 0.05	0.481 $\pm$ 0.011
	calc.	1.33(2)	0.84(2)	3.1(1)	0.50(3)
δ^{25}	exp.	0.0987 $\pm$	0.0614 $\pm$	0.231 $\pm$	0.0358 $\pm$
		$\pm$ 0.0010	$\pm$ 0.0008	$\pm$ 0.003	$\pm$ 0.0005
	calc.	0.096(2)	0.060(1)	0.237 $\pm$	0.036(2)
δ^{28}	exp.	0.0946 $\pm$	0.0693 $\pm$	0.167 $\pm$	0.0482 $\pm$
		$\pm$ 0.0041	$\pm$ 0.035	$\pm$ 0.008	$\pm$ 0.0020
	calc.	0.096(2)	0.070(1)	0.180(6)	0.047(2)
C^*	exp.	0.797 $\pm$	0.647 $\pm$	1.255 $\pm$	0.531 $\pm$
		$\pm$ 0.008	$\pm$ 0.006	$\pm$ 0.011	$\pm$ 0.004
	calc.	0.79(1)	0.64(1)	1.25(1)	0.53(2)

Integral parameters in core centre.

Table 2.10. List of investigated configurations of ZR-6 assembly^{a)}

	Lattice	N ^{b)}	Perturbation
1	12.7/3.6/0.0	175	no
2	12.7/3.6/0.0	11	no
3	12.7/3.6/0.0	154	no
4	D7/0.0	57	B ₄ C
5	E7/0.0	58	H ₂ O
6	F7/0.0	141	Eu ₂ O ₃ +Al
7	F7/1.8 ^{c)}	146	Eu ₂ O ₃ +Al
8	K331	88	Al, H ₂ O
9	K331	90	B, H ₂ O
10	K331	145	Eu, H ₂ O
11	I7/0.0	298	Al ₂ O ₃
12	J7/0.0	312	Al ₂ O ₃ , Gd ₂ O ₃ , 2%
13	K7/0.0	303	Al ₂ O ₃ , Gd ₂ O ₃ 1.0%
14	L7/0.0	296	Al ₂ O ₃ , Gd ₂ O ₃ 2.0%
15	M7/0.0	307	Al ₂ O ₃ , Gd ₂ O ₃ 5.0%
16	N7/0.0	310	Al ₂ O ₃ , Gd ₂ O ₃ 7.5%

a) Variants 1-10 are described in (Szatmary et al, 1985), variants 11-16 are described in (Vidovszky, Gazso, 1990).

b) Number of configurations in reference.

c) With boron in water.

B&U assembly (BAU-1810, 1984)

The core of this assembly comprises square lattices of the fuel rods in water ($V_H/V_F=1.34$). The rods are made of 2.46% enriched UO_2 . The first lattice is uniform. In the second lattice 20 rods are replaced by rods with gadolinium addition (1 nucleus Gd for 3 nuclei ^{235}U). Some amount of boron is added in water.

The calculated integral parameters are given in Table 2.12.

Table 2.11.1. Integral Parameters of ZR-6 Assembly
Uniformly Lattices

Parameter	Value		
N^*	175	11	154
B_z^2	17.87	21.70	18.29
K_{eff}	1.007(2)	1.003(3)	1.005(4)
ρ^{28}	2.426	2.504	2.496
δ^{25}	0.129	0.132	0.132
δ^{28}	0.0488	0.0490	0.0493
C^*	0.404	0.412	0.411

Integral parameters are averaged over the core.

*) Number of configurations.

Table 2.11.2. Integral Parameters of ZR-6 Assembly
X7 Type Lattices

Parameter	Value			
Lattice	D7	E7	F7	F7 ^{*)}
Perturbation	B ₄ C	H ₂ O	Eu ₂ O ₃ +Al	Eu ₂ O ₃ +Al
B_z^2	19.89	50.22	27.31	13.02
K_{eff}	1.007(2)	1.001(3)	1.000(1)	1.002(3)
ρ^{28}	2.671	2.491	2.670	2.818
δ^{25}	0.143	0.132	0.141	0.150
δ^{28}	0.0521	0.0494	0.0516	0.0538
C^*	0.428	0.411	0.429	0.443

Integral parameters are averaged over the core.

*) With boron in water.

Table 2.11.3. Integral parameters of ZR-6 Assembly
X7 Type Lattices, Gadolinium Absorbers

Parameter	Value					
Lattice	I7	J7	K7	L7	M7	N7
W Gd %	0.0	0.2	1.0	2.0	5.0	7.5
B_z^2	48.2	43.0	39.5	37.8	36.0	35.4
K_{eff}	1.000(4)	1.008(1)	1.005(2)	1.007(2)	1.007(3)	1.003(2)
ρ^{28}	2.552	2.562	2.5802	2.6039	2.619	2.633
δ^{25}	0.1355	0.1367	0.1380	0.1388	0.1396	0.1393
δ^{28}	0.0499	0.0501	0.0505	0.0509	0.507	0.0509
C^*	0.4164	0.4173	0.4194	0.4217	0.4229	0.4251
$A_{155}^{*})$		0.0014	0.0029	0.0035	0.0042	0.0046
$\rho^{155}^{**})$		0.012	0.29	0.051	0.106	0.135
$A_{157}^{*})$		0.0062	0.013	0.015	0.018	0.019
$\rho^{157}^{**})$		0.0011	0.0029	0.0043	0.0107	0.135

Integral parameters are averaged over the core..

*) A_{155} , A_{157} - neutron capture rate for ^{155}Gd , ^{157}Gd .

**) ρ^{155} , ρ^{157} - as ρ^{28} for ^{155}Gd , ^{157}Gd .

Table 2.11.4. Integral Parameters of ZR-6 Assembly
K331 Type Lattices

Parameter	Value		
Absorber	no	B_4C	Eu_2O_3
B_z^2	50.7	14.9	44.7
K_{eff}	1.005(2)	1.004(2)	1.006(2)
ρ^{28}	2.34(1)	2.34(1)	2.39(1)
δ^{25}			
δ^{28}	0.1297(6)	0.1262(6)	0.1243(6)
δ	0.0472(5)	0.0486(5)	0.0457(5)
C^*	0.395(2)	0.401(2)	0.374(2)

Integral parameters are averaged over the core.

Table 2.12. Integral Parameters
of B&U Assembly

Parameter	Value	
	without Gd	with Gd
K_{eff}	0.997(2)	1.001(2)
ρ_{28}	2.056	2.028
δ_{25}	0.0800	0.116
δ_{28}	0.0627	0.0601
C^*	2.780	2.618

Integral Parameters are averaged over the core.

2.4.4. Infinite heterogeneous lattices

The cell calculations are often used for comparing results of the different WWER design codes.

Here the results from the *MCU* code are compared with those obtained by *SAM-SE* (Lichtenstein et al, 1979) and *MCNP* (Biesmeister, 1986). Those Monte Carlo codes use the ENDF/B-V data. The *SAM-SE* and *MCNP* results are retrieved from the literature, e.g. (Williams, 1985).

As one can see from Table 2.13 the *MCU* code using the IAE neutron data bank produces practically the same results as the other Monte Carlo codes using ENDF/B-V data.

Table 2.13. Different Monte Carlo Codes Results

Code	Parameter, Value				
	K_{∞}	ρ^{28}	δ^{25}	δ^{28}	c^*
<u>TRX-1</u>					
MCU	1.188(4)	1.283(6)	0.0935(6)	0.0883(6)	0.779(5)
MCNP	1.180(1)	1.318(5)	0.0966(3)	0.0912(4)	0.788(2)
SAME-CE	1.185(1)	1.300(7)	0.0947(4)	0.0913(4)	0.782(2)
<u>TRX-2</u>					
MCU	1.169(3)	0.808(7)	0.0577(4)	0.0641	0.633(4)
MCNP	1.168(1)	0.824(4)	0.0594(2)	0.0656(3)	0.637(2)
SAME-CE	1.170(1)	0.815(5)	0.0583(3)	0.0661(3)	0.633(2)
<u>BAPL-1</u>					
MCU	1.149(4)	1.34(1)	0.0799(5)	0.0705(4)	0.793(5)
MCNP	1.146(2)	1.385(6)	0.0826(3)	0.0717(3)	0.804(2)
SAME-CE	1.142(1)	1.370(15)	0.0797(4)	0.0719(3)	0.799(3)
<u>NB-4</u>					
MCU	1.338(4)	2.63(2)	0.156(1)	0.0615(4)	0.547(3)
SAME-CE	1.345(2)	2.66(3)	0.159(1)	0.0613(5)	0.551(3)
<u>NB-5</u>					
MCU	1.137(4)	8.52(2)	0.541(4)	0.130(1)	1.009(6)
SAME-CE	1.145		0.556(4)	0.133(6)	1.007(4)

2.4.5. Critical assemblies with plutonium

The situation for systems with plutonium fuel in *MCU-1* code calculations was not as acceptable as for systems with uranium. Accuracy of calculations was far from satisfying the practical requirements.

However, the state of affairs is considerably improved in the new *MCU-2* code. It was achieved by reevaluation of all plutonium isotopes data and by developing advanced algorithms. The results of this activity have been summarized in (Abagyan et al, 1991).

In this section the results of the *MCU-2* code for the PNL assemblies recommended as benchmark (Thermal Benchmark, 1974) are presented. The values of K_{eff} obtained by *MCU-1* code are given for comparison too.

The cores of homogeneous PNL assemblies are the spherical or cylindrical vessels filled with an aqueous solution of plutonium nitrate $\text{Pu}(\text{NO}_3)_4$. Some cores are surrounded by a thick water reflector. The assemblies differ one from another with regard to geometry, plutonium concentration and isotopic composition of plutonium. The general parameters of the assemblies are given in Table 2.14.

The minimum critical concentration value of ^{239}Pu in water are taken from (Testing Report, 1981).

The K_{eff} calculated by MCU codes are presented in Table 2.15. The same values obtained by MCNP code based on ENDF/B-V data (Testing Report, 1981) are cited for comparison. MCU-2 code predicts the criticality with a precision of about 0,5%. It seems that the fission neutron spectrum should be defined more accurately to increase the calculation accuracy.

The heterogeneous PNL assemblies are the square lattices of the fuel rods dipped into water which acts as moderator and reflector. The rods are manufactured of UO_2 -2wt% PuO_2 mixture. The fraction of ^{240}Pu in the plutonium isotopic composition equals 8%. Critical configurations were determined for three lattice spacings, with borated and unborated moderator water. The main assembly parameters are given in Table 2.16.

The calculated values of K_{eff} are presented in Table 2.17.

As one can see, the calculated values of K_{eff} practically coincide with 1, except those of PNL-34 (The last fact can be explained by some ambiguity of the PNL-34 top reflector description in reference (Thermal Benchmark, 1974)).

Some interesting integral parameters of homogeneous and heterogeneous assemblies are given in Tables 2.18 and 2.19

PNL-30	1.778	1.18	184	0.000
PNL-31	1.778	1.18	184	0.013
PNL-32	2.200	2.02	280	0.000
PNL-33	2.208	2.08	280	0.000
PNL-34	2.514	2.08	280	0.000
PNL-35	2.514	2.08	280	0.001

Table 2.14. Homogeneous Critical Assemblies with Plutonium,
Main Characteristics

Assembly	H/Pu	^{240}W	Geometry
PNL-1	668	4.58	Sphere R=19.5 cm.
PNL-2	125	4.55	Sphere R=19.5 cm.
PNL-3	1154	4.18	Sphere R=22.7 cm.
PNL-4	873	4.18	Sphere R=22.7 cm.
PNL-5	554	4.15	Sphere R=20.1 cm.
PNL-6	125	4.55	Sphere R=19.3 cm, vessel h=0.12 cm.
PNL-7	980	0.54	Sphere R=17.8 cm, vessel h=0.12 cm. reflector 30 cm.
PNL-8	758	4.65	Sphere R=19.3 cm, vessel h=0.78 cm.
PNL-9	910	13.8	Cylinder R=45.4 cm, H=36.4 cm, vessel h=0.16 cm.
PNL-10	210	8.36	Cylinder R=61.0 cm, H=15.4 cm, vessel h=0.9 cm, side and down reflector 20 cm, pipe r=2.5 cm.
PNL-11	623	42.9	Similar PNL-10, H=80.9 cm.
PNL-12	1067	4.54	Sphere R=19.3 cm, vessel h=0.12 cm, reflector 20 cm.
	3695	0.0	Endless medium.

Table 2.15. Homogeneous Critical Assemblies with Plutonium,
Calculated K_{eff} Values

Assembly				H/Pu	^{240}W	refl.	K_{eff}		
							MCU-2	MCU-1	MCNP *)
1	PNL-1	668	4.58	no			1.0189(34)		1.0211(21)
2	PNL-2	125	4.55	no			1.0018(34)		
3	PNL-3	1154	4.18	no			1.0033(41)		1.0003(23)
4	PNL-4	873	4.18	no			1.0049(34)		1.0072(23)
5	PNL-5	554	4.15	no			1.0088(34)		1.0110(24)
6	PNL-6	125	4.55	no			1.0075(34)	1.028(4)	1.0118(24)
7	PNL-7	980	0.54	yes			1.0006(34)	1.016(5)	1.0129(22)
8	PNL-8	758	4.55	no			1.0026(34)	1.009(5)	1.0153(23)
9	PNL-9	910	13.8	no			1.0063(34)	1.021(5)	1.0115(23)
10	PNL-10	210	8.35	yes			1.0020(34)	1.025(4)	1.0075(23)
11	PNL-11	623	42.9	yes			1.0128(32)	1.032(4)	1.0098(22)
12	PNL-12	1067	4.54	yes			1.0110(34)	1.023(4)	1.0073(20)
13		3695	0.0				1.0011(15)		0.9999(14)

*) (Testing Report, 1981)

Table 2.16 Heterogeneous Critical Assembly with
Plutonium, Main Characteristics

d=1.43 $\text{UO}_2 + \text{PuO}_2$ $^{235}\text{W}=0.71$ $\text{PuW}=2.0$ $^{240}\text{Pu}=8$				
Assembly	h	V_H/V_F	H/ ^9Pu	B10/ ^9Pu
PNL-30	1.778	1.19	184	0.000
PNL-31	1.778	1.19	184	0.019
PNL-32	2.209	2.52	390	0.000
PNL-33	2.209	2.52	390	0.030
PNL-34	2.514	3.64	562	0.000
PNL-35	2.514	3.64	562	0.021

Table 2.17. Heterogeneous Critical Assemblies with Plutonium, Calculated K_{eff} Values

Assembly	V_M/V_F	boron	K_{eff}	
			MCU-2	MCU-1
PNL-30	1.19	no	0.9979(37)	1.018(3)
PNL-31	1.19	yes	0.9992(32)	1.021(3)
PNL-32	2.52	no	0.9985(33)	1.015(3)
PNL-33	2.52	yes	1.0004(31)	1.015(3)
PNL-34	3.64	no	0.9915(33)	1.018(3)
PNL-35	3.64	yes	0.9988(32)	1.024(3)

Table 2.18. Homogeneous Critical Assemblies with Plutonium Integral parameters

PNL-	P	ν fission ^{a)}		capture ^{a)}			δ^{39}	ρ^{40}	
		^{239}Pu	^{240}Pu	^{239}Pu	^{240}Pu	^{241}Pu		0.625	2.1 ^{b)}
1	0.362	1.019		0.165	0.021	0.000	0.039	9.914	0.07
2	0.389	1.002		0.186	0.049	0.000	0.150	9.947	
3	0.310	1.003		0.157	0.014	0.000	0.025	1.853	0.06
4	0.322	1.005		0.160	0.017	0.000	0.032	2.369	0.06
5	0.366	1.009		0.166	0.021	0.000	0.047	3.496	0.02
6	0.386	1.003	0.004	0.185	0.049	0.000	0.192	10.16	0.03
7	0.006	1.001		0.158	0.002	0.000	0.027	2.306	
8	0.353	0.999	0.004	0.161	0.020	0.0005	0.035	2.659	
9	0.293	1.006		0.159	0.051	0.000	0.029	1.802	0.05
10	0.061	0.990	0.011	0.174	0.055	0.001	0.104	5.122	0.01
11	0.019	0.762	0.248	0.121	0.186	0.031	0.029	1.084	0.03
12	0.020	1.007	0.004	0.158	0.016	0.0005	0.024	1.928	
endless		1.0015		0.150			0.011		

^{a)} Reaction rate

^{b)} Cd cut-off energy

Table 2.19. Heterogeneous Critical Assemblies with Plutonium,
Integral parameters

Parameter		PNL-30	PNL-31	PNL-32	PNL-33	PNL-34	PNL-35
ν fission *	^{239}Pu	0.775	0.773	0.793	0.792	0.790	0.796
	^{241}Pu	0.004	0.004	0.004	0.004	0.004	0.004
	^{235}U	0.145	0.142	0.154	0.149	0.158	0.154
	^{238}U	0.073	0.080	0.046	0.054	0.038	0.044
fission *	^{239}Pu	0.270	0.270	0.277	0.276	0.276	0.278
	^{235}U	0.059	0.058	0.063	0.061	0.065	0.063
	^{238}U	0.026	0.028	0.016	0.019	0.014	0.016
capture *	^{239}Pu	0.135	0.137	0.131	0.134	0.136	0.132
	^{240}Pu	0.035	0.038	0.025	0.030	0.022	0.025
	^{235}U	0.014	0.014	0.013	0.013	0.012	0.013
	^{238}U	0.167	0.182	0.113	0.131	0.097	0.110
δ^{49}		0.131	0.149	0.065	0.086	0.050	0.063
δ^{25}		0.246	0.290	0.110	0.152	0.080	0.105
ρ^{28}		4.087	4.833	1.915	1.205	1.402	1.940

* Reaction rate

REFERENCES

Abagyan L.P. et al (1964). The group constants for the reactor calculations. In Russian.

Абагян Л.П., Базазянц Н.О., Бондаренко И.И., Николаев М.Н. Групповые константы для расчета ядерных реакторов. Москва. Атомиздат. 1964.

Abagyan L.P., Bazazyants N.O., Nikolaev M.N., Tsybulya A.M. (1981). Group Constants for Reactors and Shielding Calculation. In Russian.

Абагян Л.П., Базазянц Н.О., Николаев М.Н., Цибуля А.М. Групповые константы для расчета реакторов и защиты. Справочник. Москва. Энергоиздат. 1981.

Abagyan L.P., Bazazyants N.O., Nikolaev M.N., Tsybulya A.M. (1981). New Group Constants for Fast Reactor Calculation. In Russian.

Абагян Л.П., Базазянц Н.А., Николаев М.Н., Цибуля А.М.: Новая система групповых констант для расчета быстрых реакторов. Атомная энергия, 1980, т.48, вып.2, с.117.

Abagyan L.P., Yudkevich M.S. (1981). Neutron Data Library for Thermal Reactor Calculation. VANT, Series YK, V 1(40), p 39. In Russian.

Абагян Л.П., Юдкевич М.С.: Библиотека нейтронных данных для расчета тепловых реакторов. Вопросы атомной науки и техники. Сер.: "Ядерные константы", вып.1(40), с.39, 1981.

Abagyan L.P., Tebin V.V., Yudkevich M.S. (1984). CROSS - code and constants library for cross sections calculation in resolved resonances region. Kurchatov Institute, IAE-4009/5. In Russian.

Абагян Л.П., Тебин М.С., Юдкевич М.С. CROSS - пакет программ и библиотек для расчета сечений в области разрешенных резонансов. Препринт ИАЭ-4009/5, М., 1984.

Abagyan L.P., Prosvetova M.P. Yudkevich M.S. (1990). Neutron Data Library for Thermal Reactor Calculation. VANT, Series YK, V 4, p 3. In Russian.

Абагян Л.П., Просветова М.П., Юдкевич М.С.: Нейтронные данные для расчета тепловых реакторов. ВАНТ. Сер.: Ядерные константы, вып.4, стр.3, 1990.

Abagian L.P., Gomin E.A. and Yudkevich M.S. (1992). Evaluation of constants of isotopes ^{239}Pu - ^{242}Pu and their Verification Conformably to the Calculations of Thermal Reactors. 1992 Topical Meeting on Advances in Reactor Physics, Charleston, USA.

Alekseev et al (1991). The MCU-1 code verification. In Russian.

Алексеев Н.И., Брызгалов В.И., Владимиров Т.М., Гомин Е.А., Капитонова А.В., Майоров Л.В., Носовский И.В., Юдкевич М.С. Верификация константного обеспечения версии MCU-1 применительно к реакторам с водой в качестве замедлителя. Препринт ИАЭ-5407)5. Москва. 1991.

ANL-5800. (1963). Reactor Physics Constants.

BAW-1810. (1984). Nuclear Model Development and Critical Experiment Nuclear Benchmark, DOE/ET/34212-41, April 1984.

Becker R., Heinrich H. (1989). Multigroup Constants Supply in NESSEL-4 Code. KFKI-ZR-6-566/1989. In Russian.

Р.Беккер, Х.Хайнрих: Обеспечение многогрупповых констант в программе NESSEL-4. KFKI-ZR-6-566/1989.

Beckurs K.H. and Wirtz K. (1964). Neutron Physics, Springer-Verlag, 1964.

Bernocchi E., Martinelli R. editors. (1977). Light Water Lattice Data, NEACRP-U-190, December 1977.

Biesmeister J.F. (1986). MCNP - A General Monte-Carlo Code for Neutron and Photon Transport, LA-7396-M.

Bondarenko I.I. Editor. (1964). Group Constants for Nuclear Reactor Calculations, Consultants bureau, New York, 1964.

Brown W.A.V. et al. (1967). Measurements of Material Buckling and Detailed Reaction rates in a Series of Low Enrichment UO_2 Fueled Cores Moderated by Light Water, A.E.E., Winfrith.

Cadilhak M. et al. (1962). BNL-713 (c32), 1962, vol. 2, p.439.

CHAPTER 2

- Cullen P.E. (1979). Program *LINEAR*, UCRL-5-400, vol. 17, Part A.
- Cullen P.E. (1979). Program *RECENT*, UCRL-5-400, vol. 17, Part C.
- Cullen P.E. (1979). Program *SIGMA1*, UCRL-5-400, vol. 17, Part B.
- Egelstaff P.A., Pool M.J. (1969). Experimental Neutron Thermalization, Pergamon Press.
- Gado J., Zsoldos J. *BETTY* - The Pin-Cell Burnup Code, KFKI- report, KFKI-1978-35.
- Golubarge A. (1985). *FEDGROUP-R* Code (Version in INI Res). UJV 7349 R, 1985. In Russian.
- Голубарж А.: *FEDGROUP-R* (версия программы в ИЯИ Ржеж). UJV 7349 R, 1985.
- Gomin E.A., Kapitonova V.I., Kononov S.L., Maiorov L.V., Marin S.V., Yudkevich M.S. (1987). Experimental Data Analysis for validating nuclear data. In Russian.
- Гомин Е.А., Капитонова А.В., Кононов С.Л., Майоров Л.В., Марин С.В., Юдкевич М.С. Анализ экспериментов на критических сборках с целью проверки константного обеспечения реакторных расчетов. Доклад на XVI Симпозиуме специалистов ВМК по физике ВВЭР. Москва. Сентябрь 1987.
- Gomin E.A., Maiorov L.V. (1982) *TERMAC* - the Program Complex for Calculation of Neutron Group Cross Sections in Thermalization Region. VANT, Series FiTYR, V 5(27), pp 70-73. In Russian.
- Гомин Е.А., Майоров Л.В. Комплекс *TERMAC* для расчета групповых сечений нейтронов в области термализации. ВАНТ. Физика и техника ядерных реакторов. 1982. Вып. 5(27). С. 70-73.
- Gomin E.A., Maiorov L.V., Yudkevich M.S.. (1990). Some Aspects of Monte-Carlo Method Application to Nuclear Reactor Analysis, Prog. in Nucl. Ener, v. 24, p. 211, 1990.
- Gwin R. and Magnuson D. (1962). The Measurement of Eta and other Nuclear Properties of U^{233} and U^{235} in Critical Aqueous Solutions, NSE 12,

p. 364-380.

Heinrich H. (1981). Das Programm NESSEL-4 zur Berechnung des Lokalen Abbrands in H_2O -moderierten Kernreaktoren. Kernenergie 24, p. 465.

Ishiguro V., Takano H. (1971). PEACO - a Code for Calculation of Group Constants of Resonance Energy Region in the Heterogeneous Systems, JAERI 1912 Report, 1971.

Kereszturi A. (1981). Engineering Code CERES for Resonance Capture Calculation. XI TIC Symposium, Erevan, 1981. In Russian.

А. Керестури. Инженерная программа CERES для расчета резонансного поглощения. Материалы XI симпозиума ВМК. Ереван, 1981.

Kereszturi A. (1989). Multigroup Constants Library of KFKI. XVIII TIC Symposium, Prachatice. In Russian.

А. Керестури: Библиотека многогрупповых констант в ЦИФИ ВАН. Материал 18 Симпозиума ВМК, Prachatice, 1989.

Koppel J., Huston D. (1979). Reference Manual for ENDF Thermal Neutron Scattering Data, GA-8874, Revised (ENDF-269).

Laletin N.I. (1974). Simplifying Equation of Neutron Thermalization. In Russian.

Лалетин Н.И.: Приближенные уравнения термализации нейтронов. В кн. Методы расчета полей тепловых нейтронов в решетках реакторов. М. Атомиздат. 1974.

Lichtenstein H. et al. (1979). The SAM-SE Monte Carlo System for Radiation Transport and Criticality Calculations in Complex Configurations, EPY-CCM-8, July 1979.

Liman G.F., Maiorov L.V. (1981). NEWRAS Code for Calculation of Slow Neutrons Cross Sections. VANT, Series FiTYR, V 8(21), pp 32-28. In Russian.

Лиман Г.Ф., Майоров Л.В.: Программа NEWRAS для расчета дифференциальных сечений рассеяния медленных нейтронов. ВАИТ, Сер.: Физика и техника ядерных реакторов. вып. 8(21), с. 32-38, 1981.

Liman G.F. (1982). CALCST and ELCOHR Codes for Calculation of Total and

CHAPTER 2

Coherent Elastic of Slow Neutrons Cross Sections. VANT, Series FiTYR, V 5(27), pp 74-77. In Russian.

Лиман Г.Ф.: Программы *CALCST* и *ELCOHR* для расчета полных и упругих когерентных сечений рассеяния тепловых нейтронов. ВАНТ, Сер.: Физика и техника ядерных реакторов. Вып. 5(27), с.74-77, 1982.

Macfarlane R.E., Muir D.W. (1987). *NJOY 87.0*, ANL Memo t-1-10991.

Mughabghab S.F., Garber D.I. (1973). *Neutron Cross Sections*, BNL-325, v.1.

Mughabghab S.F. (1984). *Neutron Cross Sections*, V.1. Part A, 1981, Part B, Academic Press.

Pshenin V.V. et al. (1989). Calculations Result for Gadolinium in Fuel Rod Lattices, Material of CRP on Safe Core Management with Burnable Absorbers in VVRS, IAEA, Vienna.

Pshenin V.V. et al. (1989). *UNIRASOS-2 code*. In Russian

В.В.Пшенин, В.А.Лазоренко, В.Д.Сидоренко: УНИРАСОС-2: алгоритмы и результаты тестирования. Материалы совещания специалистов ТГ-3 ВМК. Москва, 1989.

Pshenin V.V. et al. (1989). *RAFORIN-code*. In Russian

В.В.Пшенин, А.Л.Лазаренко, Н.В.Султанов, И.И.Сурначева: Программа РАФАРИН - назначение, алгоритмы и предварительные результаты тестирования. Материал 18 симпозиума ВМК, СССР, 1989.

Sinitza V.V. et al (1979). *GRUCON* - Computer Code Package for Processing Evaluated Nuclear Data Files. In Book: Nuclear-physic Research in USSR, Series 27, p.31, CNIIAtominform. In Russian.

Синица В.В. и др.: ГРУКОН. В кн. Ядерно-физические исследования в СССР, вып. 27, с.31, М., ЦНИИАтоминформ, 1979.

Stam'ler R.J.J. (1963). *K-7 THERMOS*, Kjeller report, KR-47.

Szatmary Z. Editor. (1985). *Final Report of TIC, Volume 1, Experimental Investigations of the Physical Properties of WWER-type Uranium-Water*

lattices. Akademiai Kiado, Budapest, 1985.

Tebin V.V., Yudkevich M.S. (1985). Generalized Subgroup Approach for Resonance Capture Calculation. Atomic Energy, v,59(2), p.96-101. In Russian.

Тебин В.В., Юдкевич М.С.: Обобщенный подгрупповой подход к расчету резонансного поглощения нейтронов. Атомная энергия, т.59, вып.2, с.96-101, 1985

Tebin V.V. (1989). Advanced PWRs (APWRs) and Related Safety Considerations. Nuclear Data for the Calculation of Thermal Reactor Reactivity Coefficients, IAEA-TECDOC-491, 1989.

Testing Report ENDF/B-V Data. (1981).

Thermal Benchmark Compilation. (1974). CHEW Data Testing Subcommittee. June 1974.

Vertes P. (1981). FEDGROUP-3. A Program System for Processing Evaluated Nuclear Data in ENDF/B, KEDAK or UKNDL Format to Constants to be Used in Reactor Physics Calculation, KFKI-1981-34, 1981.

Vidovszky I., Gazso J. (1990). Results of the Experiments Carried out on VVER Type Lattices Containing Gd Absorber Rods, IAEA-TECDOC-567, p.245.

Williams M.Z. et al. (1985). Analysis of Thermal Reactor Benchmarks with Design Codes Based on ENDF/B-V Data, Nuclear Technology, 71(7), 386.

Yudkevich M.S. (1984). Kurchatov IAE Neutron Data Bank. VANT, Series YK, V 5, p 3. In Russian.

М.С.Юдкевич: Банк нейтронно-физических констант Института атомной энергии им. И.В.Курчатова. ВАНТ Сер.: Ядерные константы, вып.5, с.3, 1984.

Zalesky K. (1984). MICROBE-02 Code for Burnup Calculation. UJU 6880-R, A, 1984. In Russian.

К.Залески : Программа MICROBE-02 для расчета локального выгорания. UJU 6880-R, A, 1984.

3. THE MONTE CARLO CODES AND THEIR APPLICATIONS

L. MAIOROV

3.1 INTRODUCTION

The target of high precision neutronic computations is to solve the transport equation with an accuracy limited only by used evaluated nuclear data. The Monte Carlo method is the most convenient tool for this purpose.

The geometrical complexity of investigated assemblies or their detailed cross-section description are not serious obstacles to applying the Monte Carlo method, which is why the Monte Carlo codes are used widely as a source of mathematical reactor benchmarks. On the other hand the crude enough approximations are used in the WWER transport design codes. The transport equation is solved on the basis of simplified reactor models mostly utilizing the homogenization approach (cf. Chapter 5). The diffusion equation coefficients are also calculated approximately (See Chapter 4). Therefore it is necessary to use the benchmark results for verification and validation of the design codes. Comparison of the benchmark and of the engineering calculations permits one to be sure of the reliability of the engineering code predictions. Analysis both of the different design approximations and of their influence on the calculation accuracy are a very important part of the verification task carried out on the basis of the Monte Carlo codes.

In the first stage of the TIC activities the design code verification and validation were carried out mostly using the ZR-6 experimental results. However, mathematical benchmarks are more informative and more reliable means often excluding the nuclear data evaluation of course.

Throughout the long period of TIC activities the Monte Carlo methods were used intensively for interpretation of the experiment results (TIC-1, 1985) and for the design code verification. Parallely, the Monte Carlo codes themselves were developing intensively.

Now the Monte Carlo benchmarks play a not less important role in the verification and validation process than experimental ones.

The Monte Carlo code place was different throughout the different TIC activity periods. Initially Monte Carlo methods were applied to solve the most important but only the separate problems of the design code verification and validation. They were applied to solve many problems which were important as a means of understanding the role of the various

approximations used in the design codes, to interpret experimental results and to improve nuclear data base (Seifert, 1976,1977), (Maiorov, 1977), Kurka et al,1981), (Maiorov and Yudkevich, 1988).

Some of these problems are as follows:

- analysis of the design calculation accuracy for the resonance and thermal regions of energy (see Chapter 4),
- analysis of accuracy of the different homogenization theory approaches,
- estimation of different experimental corrections, in particular effects of dry lattice, of detector finite size, the perturbations, caused by detectors (see (TIC, volume 1)).

Section 3.2 describes briefly Monte Carlo codes applied for these tasks.

The second generation Monte Carlo code development permitted one to utilize these codes as a main tool of design code verification. This generation code *MCU* is described in Sect. 3.3. Its applications for nuclear data validation were discussed in Chapter 2. Chapter 4 contains many examples of *MCU* application for verifying and validating the design codes used in calculating the cell parameters. Therefore below we shall restrict ourself to considering some special problems concerning the advanced design methods.

Throughout the period of TIC activities the theory of Monte Carlo methods was also developed in the TIC institutes (cf. (Zolotukhin and Maiorov, 1983), (Lux and Koblinger, 1991)). The main targets of these activities were as follows:

- investigations of efficiency of various simple and combined estimators for calculating the flux functionals,
- development of theory concerning the K_{eff} calculations by Monte Carlo methods (in particular, the well known problem of biasing the estimators utilized),
- investigating the possibilities for diminishing the calculational cost.

In particular, the equations were derived for the variances of scores both depending on events at two neighbouring collision points and various combined estimators (cf. collision + track estimators, collision + absorption estimators, etc (Maiorov and Frank-Kamenetsky, 1969). The original approaches were developed by Lux for treating the estimators using two neighbouring collision points and for evaluating the calculational cost (Lux, 1978, 1978 b).

The problem of biasing the K_{eff} estimators was considered from the point of view of the cost optimization in (Zolotukhin and Maiorov, 1983).

CHAPTER 3

In (Ogibin, 1967) was derived the general equation for the calculation cost of algorithms utilizing the roulette and splitting methods:

$$C = (D_0 + \frac{D_1}{n_1} + \frac{D_2}{n_1 n_2} + \dots + \frac{D_k}{n_1 n_2 \dots n_k}) (T_0 + n_1 T_1 + n_1 n_2 T_2 + n_1 n_2 \dots n_k T_k)$$

where $C=DT$ is the cost of calculation defined as the product of the estimator variance D and the average calculation time T per one primary particle, T_1 are the average modelling time spend to model the history part between two splitting surfaces, n_1 are the number of particles that the particle is splitted into when intersects the i surface, D_1 are the problem parameters.

The cost optimization is achieved by special choice of the n_i values.

The cost of modelling the fission process is also described by the similar equation (Zolotukhin and Maiorov, 1984). The traditional methods for calculating the K_{eff} are optimal ones from the point of view of the cost value. However, this optimization is paid by bias of Monte Carlo eigenvalue calculations (Lieberoth, 1968), (Gelbard and Prael, 1974), (Zolotukhin and Maiorov, 1984), (Brissenden and Garlick, 1985). One may hope that approach for calculating both unbiased and inexpensive eigenvalues will be elaborated in future. The reviews of problems concerning both the estimator efficiencies and the K_{eff} bias problem are given in (Gelbard, 1991), (Zolotukhin and Maiorov, 1984), (Lux and Koblinger, 1991)). These reviews include partly the results of TIC's authors. Therefore theoretical problems of Monte Carlo method are beyond the scope of present Report.

3.2 THE FIRST GENERATION TIC MONTE CARLO CODES

Below we describe the TIC first generation Monte Carlo codes briefly.

MMKFK

The three dimensional code (VANT, 1981) for special geometry assemblies. The code uses as a basis the 21 and 26-group data (one thermal group).

PIT

The three dimensional code (VANT, 1981) for thermalization calculations, when the effects of thermal motion and chemical bonds were taken into account.

MONRI

The MMKFK option (Sboev, 1981) allowing the evaluation of the resonance effects and utilizing the CROSS code (Tebin et al, 1978) to calculate the resonance cross sections at the every energy point when it was necessary.

OMK78, MKPRT

The combined options (VANT, 1981) of all the three codes mentioned above. They allowed one to model the 3-dimensional system taking into account both the resonance effects and the thermalization ones.

The description of these codes and their application for reactor calculations were published in special issue of VANT journal (VANT, 1981) devoted to memory of A.D.Frank-Kamenetsky who was author of the MMKFK code.

OMEGA

This code (Seifert, 1978) allows for a rather general three-dimensional geometric arrangement of circular cylinders, rectangular and hexagonal prisms. The code can consider a great variety of practically important geometric arrangements which often appear inside and outside a reactor. The 26-group ABBN subgroup library and the THERMOS library are used for the basic microscopic cross-sections in the epithermal and in the thermal range, respectively. The epithermal data can be used in two different ways. First, spectrum averaged macroscopic group cross-sections can be generated. Secondly, the subgroup parameters can be used directly according to the so called subgroup method or the probability tables method. The thermal range can be divided into a number of groups and the corresponding cross sections are generated as in the THERMOS code. Although group cross sections are used the neutrons are described by continuous energy variables. The epithermal elastic slowing down is calculated according to the laws of the elastic slowing down and the library elastic slowing down data are not used by the code. OMEGA solves the homogeneous transport equation with K_{eff} as an eigenvalue. Some global parameters are evaluated, for example K_{eff} . Furthermore, the fluxes and the reaction rates can be calculated for the special sub zones and for any desired energy group structure. The OMEGA application for design codes verification is described in Sect. 4.2,4.3.

3.3 MCU CODE

3.3.1 General description

The MCU project has been developed in Kurchatov IAE over the long period of time (Maiorov and Yudkevich, 1988), (Gomin et al, 1991). The project goal is to provide high precision of the reactor parameter calculation.

The project includes:

- development of the nuclear data base,
- creation of Monte-Carlo codes, their verification and validation,
- creation of CLAD library containing the critical experiment description in MCU language,
- development of the approaches permitting one to utilize Monte-Carlo codes for design code verification and validation,
- the design code verification and validation.

Main features of the MCU code are as follows.

The code architecture, based on the modular principle, allows one to compute the transport equation functionals on the basis of a wide set of different algorithms and mutually-changeable program modules, utilizing the different data libraries in particular.

The MCU code utilizes the original data libraries based on the recommended neutron data.

Throughout one code run the point wise and the group cross section descriptions are allowed.

The code permits one to use a detailed description of cross section energy dependence in the resolved fully resonance region. The resonance cross sections need not obligatory be tabulated in advance. Throughout the modelling they may be calculated in every energetic point on the basis of the resonance parameter library (see Chapter 2). It cancel any doubt about cross section calculation accuracy and allows the user to model the systems having various temperature having independence on the cross section library state. It is important for analyzing temperature effects.

Collision modelling in the thermal region is performed taking into account the chemical bonds, nuclei thermal moving and the coherent effects. The user is permitted to update the scattering law library utilizing the phonon spectrum library. Parallel with the resonance region modelling algorithm it allows one to calculate the temperature effects.

It is possible to model a wide class of three dimensional systems.

MCU allows one to take into account effects of double heterogeneity. For this purpose the special algorithm was developed (Bryzgalov et al, 1989). In particular, the HTGR type system were modelled having the sphere elements which contained to 10^4 micro elements of fuel.

Some standard sets of the most important functionals and those needed for the advanced design code verification are calculated (see Sect.3.4).

The latest portable MCU-3 version is written in FORTRAN-77. Now MCU is exploited in computers having SVM, OS (IBM), UNIX, VMS operating systems and in various PC.

The previous MCU-1 and MCU-2 versions were exploited for a long time. They were validated using about 200 benchmarks and were verified by solving thousands of practical problems. The CLAD library contains about 250 experiment descriptions.

The data base used for MCU is described in detail in Sects.2.3.4, 2.3.5. Its main parts are as follows.

ABBN/TR 26-group library, allowing one to use, in particular the subgroup approach describing the unresolved resonance self shielding.

LIPAR library (see Sect. 2.3.4) contains the nuclear resonance parameters for the fully resolved resonance region. In the modern LIPAR version format ENDF/B-6 is used. The LIPAR data are directly utilized in the process of modelling for calculating every energy point cross-section taking into account Doppler broadening.

TEPCON thermal neutron data multi group library contains the cross-sections for energies less than 5 eV and for the different temperatures. It includes itself the zero and the first angular moments of the scattering cross sections. The most important moderator scattering cross-sections are calculated in the Gauss incoherent approximation, the elastic coherent cross section are used if it is necessary. The different library options differ by the group structure.

VESTA - the scattering law library for the thermal energy region. This library is used for point wise modelling in the thermalization region.

The special scattering law $S(\alpha, \beta)$ calculation algorithm and code are used to update the VESTA library. They are based on using the recurrent relationship

$$S(\alpha + \Delta\alpha, \beta) = \int_{-\infty}^{\infty} S(\alpha, \beta - \beta') S(\Delta\alpha, \beta') d\beta'$$

where for the small $\Delta\alpha$ the scattering law $S(\Delta\alpha, \beta')$ is expressed through the

phonon spectrum.

NEDAM library (Markovsky and Borisov, 1989) compiled on the basis of the ENDF/B-4 and the ENDL-83 files describes neutron-nuclei interaction for the point wise modelling in the energy region 0.1-15.2 MeV.

The **MCU** architecture. The Monte-Carlo methods allow one to apply a wide spectrum of algorithms for the particle history modelling. They are based on using the different probability density functions and the different tallies of values of interest. The code structure permits one to simulate random walk of several types of particles. From the code architecture point of view the particle random walk is a random sequence of many abstract events: the particle birth from the external source, collision, the flight between two collision points, the death, the birth of the different type secondary particles, weight changing, etc.

Concretization of physical meaning and the event interpretation algorithms are realized by modules contained in the code library. The **MCU** module is a set of segments, where each has its functional destination and interfaces strictly determined by the code architecture. With regard to their destination **MCU** module types are classified, as follows:

C - control (governing), P - physical, G- geometric,

T - tallies, S - sources.

As a rule every type of module has alternative versions corresponding to its different modelling algorithms.

The executable program variant (EP) is assembled according to the equation:

$$EP = C + P + G + T + S$$

where C, P, G, T, S are the alternative concretized names of the corresponding types of modules.

Physical modules. The **MCU** library contains the physical submodule set. Every submodule uses the different data libraries and the different particle-nuclei interaction models for different energy regions.

The physical module operating variant (OP) is assembled according to the equation:

$$OP = P_1 + P_2 + P_3 + P_4$$

where P_i - are the alternative concretized names of the corresponding types of submodules: three ones for neutron collision modelling and one for photon collision modelling.

For neutrons the whole energetic region is divided into three unintersected subregions serviced by P_1, P_2, P_3 submodules (conditionally the

fast, the resonance and the thermal ones) having the boundaries (E_1, E_{1-1}). Most submodules perform continuous energy modelling but the group approach may also be used utilizing both the point wise and the group cross sections.

Nuclei concentrations and temperatures allow to be depended continuously on the spatial coordinates.

Cross section resonance structure may be taken into account by using any of three methods: Bondarenko's self-shielding f-factors, the subgroups, resonance cross section calculation in every energy point in limits of resolved resonances region. The elastic scattering anisotropy is taken into account by the set of equiprobable bins of scattering angle cosines in cms, scattering is sampled by kinematic formulas.

In the thermalization region the inelastic scattering is modelling in ideal gas approximation or in incoherent Gauss approximation. The correlation between energy change and scattering angle cosine is taken into account. Coherent elastic cross sections are used when it is necessary.

Geometric modules. The MCU code permits one to model arbitrary complex three dimensional systems. The geometric module library contains 11 specialized geometric modules and two universal ones. Specialized modules are designed to model the special class systems (the WWER, RBMK, TOPAZ reactors, etc).

The universal type modules are based on the combinatorial method, which allows one to construct different geometric systems using Boolean operations under the definite primitives, contained in the special primitive library. They allow one to use hierarchical principle for describing complex systems with one time description of repeating elements. The regular lattices may be described fixing only their basic elements and translation vectors.

Control modules. These modules provide the possibility to solve transport equation using the different alternative algorithms solving the transport equation (in particular, analog and non-analog approaches).

All the control modules use the common banker segment. The banker allows one to place particles into the external memory and to get them from the external memory with differing particles by types, queue numbers and by priority in queues.

The banker is a main tool for realizing nonanalogue methods, e.g.: the Russian roulette, splitting, weight window methods, etc.

Criticality problems are solved by using the method of the forced regulation of the number of particles in generation.

Besides traditional criticality problems, the *MCU* allows one to solve the asymptotic system problems, when the leakage is given by buckling vector (see Sect 3.4.2).

The different types of boundary conditions may be considered, in particular the different conditions of symmetry, fixed by the symmetry planes.

The source modules permit one to define the different space, angle and energy distribution functions.

Tally modules. The *MCU* calculates the standard set of functionals: the fluxes and the reactions rates in the spatial and energetic regions defined by the user, fraction - linear functionals, migration lengths, neutron lifetime, sets of the cell few group diffusion constants, β_{eff} , etc. In particular it is possible to calculate the diffusion coefficients corresponding to the different definitions.

The *MCU* tally module architecture permits to the user himself to widen calculated values set and supplies him by the necessary service.

3.3.2 *MCU* verification

MCU has been verified with the help of special tests by comparing calculation results with those obtained by other codes and with experimental data. Assemblies with different fuel and different moderators in particular (ENDF-202), (BAW-1810, 1984), (TIC-1, 1985) and many other assemblies have been examined.

The CLAD library has been compiled (Alekseev et al, 1992). CLAD contains assembly descriptions on *MCU* input language. There are ~250 assignments of different experimental assemblies. They include data about reactors of practically all types which differ in fissile nuclei, moderators and neutron spectrum. Critical assemblies sufficiently simple in geometry are used to verify nuclear data. Geometry and materials of assemblies are described as precisely as the various authors' documents permit. A review of calculation results comparison with experimental data is given in (Maiorov and Yudkevich, 1988), (Alekseev et al, 1992), (Yudkevich, 1993).

Briefly *MCU* verification results may be summed up as follows: criticality of thermal reactors with U^{235} - fuel with moderators H_2O , D_2O or C is predicted with precision ~0.5% (experimental errors ~0.5%); computed K_{eff} of assemblies with Pu-fuel do not exceed of the experimental errors.

Criticality of fast reactors is predicted better than 1% and discrepancies are unsystematic.

MCU is widely used now in Russia for the calculating parameters of Russia reactors of practically all types, in-pool storage and shipping casks, etc.

Large series of calculations of vapour effect had been done when the causes of the Chernobyl accident were analyzed. The first calculation results carried out in May 1986 permit one not only to conclude that RBMK reactors have the large positive vapour coefficient but calculate also all the function showing dependence K_{eff} on water density.

3.3.3 ZR-6 assembly modelling

The ZR-6 experimental results were intensively used to validate both the MCU data libraries and the MCU code as a whole. Chapter 2 contains the data validation results obtained on the criticality analysis basis. The examples comparing the MCU and experimental flux distribution and reaction rates in ZR-6 macrocells are given in Chapter 4.

Many calculations were performed to supplement experimental data describing the flux and reaction rate distributions over all the ZR-6 assembly, for every core cell.

As example we illustrate some MCU results of modelling configuration 154 of the ZR-6 assembly (TIC-1, 1985): the uniform lattice of 12.0/3.6/0 type, 10^6 histories (Maiorov *et al*, 1993).

The third energy group absorption cross section map is given in fig. 3.1. The results for the thermal neutron group and for every cell are shown in fig. 3.2 -3.6, as follows: the source power, the cell absorption and neutron generation cross sections, the flux, the ratio of the edge flux to the flux averaged over the volume of the cell.

Similar data so as the transfer cross sections were calculated for the every energy group. In addition the reaction rate for every nuclei types was calculated. The diffusion coefficients corresponding to their different definitions may be calculated as well (see Sect. 3.4.3). For this goal the fluxes, one side currents and levels (see Sect. 3.4.3) are estimated for the cell sides (see also Sect. 3.4).

Examples of energy release maps (for every cell) calculated by MCU code (Maiorov *et al*, 1993) are given in fig. 3.7-3.12. Analogous experimental maps were given in (TIC, 1985) but only for the certain cells. Fig. 3.7-3.12 permits also one to compare the experimental and MCU results.

$\nu \Sigma_f = 10^3$

									215
								207	226
							207	210	
					197	208	221		
				196	200	207	224		
			202	203	199	213			
		196	200	202	205	225			
	196	197	199	198	212				
	201	198	199	202	204	224			
	196	199	199	200	199	210			
	196	199	198	199	200	202	215		
	203	196	200	198	197	200	209	228	
	197	199	199	198	198	201	202	217	
	196	198	201	199	202	199	204	207	226
197	195	201	200	197	201	199	196	214	

Fig.3.3 The secondary neutron generation cross sections.

Group 4. Assembly ZR-6-154/154

							125		
						121	131		
					118	121			
				116	120	127			
			114	114	120	131			
		117	114	114	122				
	112	116	117	118	128				
	117	115	114	116	124				
	117	115	116	118	118	128			
	113	116	115	117	115	122			
	114	115	115	115	118	117	125		
	118	114	115	115	113	116	121	134	
	114	117	116	115	115	115	117	125	
	116	116	118	114	117	116	117	119	132
116	113	116	113	115	119	118	114	122	

Fig. 3.4 The thermal neutron absorption cross sections.

Assembly ZR-6-154/154.

0 (4.3) 156
 1 143 (-4.0)
 2 (-3.0) 146 146 (-1.5)
 3 143 144 (0.6)
 4 (-5.0) 140 142 134 (-2.3)
 5 141 144 139 (1.7)
 6 (4.0) 145 142 142 137 (0.1)
 7 137 138 136 133 (-3.5)
 8 (-2.0) 132 132 134 134 129 (-1.5)
 9 131 132 131 127 127 (4.0)
 10 (2.0) 130 127 127 124 122 126 (7.0)
 11 122 122 120 120 118 113 (0.4)
 12 (2.5) 121 118 117 115 116 111 107 (-0.6)
 13 110 113 109 113 108 107 102 (-0.6)
 14 (-4.0) 105 108 112 103 101 98 99 93 (-2.5)
 15 102 98 100 96 96 93 93 87 (-1.5)
 16 (-1.5) 96 97 92 94 89 90 86 85 78 (-4.3)
 17 89 93 88 90 87 83 81 76 79 (7.0)
 18 (0.5) 84 84 87 83 83 79 77 72 72 68 (2.0)
 19 81 78 77 75 75 72 68 67 64 59 (-2.3)
 20 (-2.3) 70 72 71 69 72 67 65 63 58 57 55 (-0.4)
 21 63 65 65 67 62 63 60 56 58 54 55 (-1.8)
 22 (0.4) 61 62 60 58 62 58 59 55 58 61 63 74 (7.0)
 23 57 61 57 59 60 61 56 66 66 72
 24 (2.0) 59 61 64 68 67 70 71 75
 25 71 69 73
 26

0 1 2 3 4 5 6 7 8 9 0 1 2 3 4 5 6 7 8 9 0 1 2

Fig.3.9 Energy release distribution. Assembly ZR-6 12.7/3.6/5.8.
 Configuration 161 (T=300 K) Statistical error - 3.0%
 Deviations from experiment are given in parentheses (%)

0	(5.0)	156 (5.0)
1		145 (-3.7)
2	(1.0)	146 145 (0.6)
3		145 142 (0.0)
4	(-2.7)	142 140 141 (1.6)
5		141 139 135 (-1.1)
6	(-2.1)	137 140 139 136 (-0.8)
7		134 137 132 137 (2.5)
8	(-2.0)	131 133 133 128 129 (0.3)
9		132 128 130 126 120 (-0.5)
10	(-2.0)	123 127 126 124 121 118 (0.4)
11		120 120 118 119 114 116 (3.6)
12	(1.0)	119 116 114 114 110 112 109 (1.6)
13		110 109 111 108 103 102 100 (-0.8)
14	(-4.5)	105 105 103 103 103 97 98 95 (0.0)
15		98 101 99 99 94 94 90 88 (0.1)
16	(-2.5)	95 94 94 93 90 88 87 84 80 (-2.5)
17		88 87 88 85 86 83 80 73 71 (-4.0)
18	(-4.0)	81 82 81 80 80 78 75 72 71 67 (-0.5)
19		76 76 76 74 73 72 70 67 65 62 (2.5)
20	(-2.8)	70 73 71 69 68 66 67 64 60 59 57 (-0.2)
21		65 65 66 63 63 61 60 61 56 57 56 (-5.0)
22	(-2.4)	61 60 61 61 60 60 59 56 59 58 63 74 (3.0)
23		59 58 58 58 60 61 60 63 67 73
24	(-2.4)	58 60 62 64 68 70 71 73
25		69 71 77

Fig.3.10 Energy release distribution. Assembly ZR-6 12.7/3.6/4.0.
Configuration 161(T=350 K) Statistical error - 2.0%
Deviations from experiment are given in parentheses (%)

0	(7.0)	156 (7.0)
1		146 (1.4)
2	(-1.2)	145 146 (4.0)
3		140 140 (-0.8)
4	(-3.5)	140 142 143 (4.0)
5		139 139 138 (0.1)
6	(-3.6)	134 136 135 134 (-1.0)
7		134 133 132 132 (-2.4)
8	(0.0)	133 130 129 128 129 (0.0)
9		126 128 127 124 119 (2.0)
10	(0.0)	126 124 121 125 119 117 (0.6)
11		120 121 118 118 116 113 (1.9)
12	(0.9)	115 115 114 115 111 109 108 (2.5)
13		110 112 109 110 107 102 102 (2.5)
14	(-1.0)	108 105 108 103 101 100 98 95 (-1.2)
15		102 103 100 98 96 93 92 90 (2.4)
16	(1.0)	96 96 96 90 91 89 87 86 80 (-1.8)
17		91 91 88 87 85 84 82 77 74 (0.0)
18	(-0.6)	84 82 82 82 82 80 75 73 73 70 (1.4)
19		78 78 77 77 74 72 69 66 64 62 (-0.3)
20	(-5.0)	69 72 72 71 70 70 66 65 61 61 58 (0.7)
21		68 65 66 65 64 63 62 60 60 60 60 (-0.7)
22	(-0.2)	63 64 64 62 61 60 60 61 60 60 66 75 (-0.5)
23		61 60 61 65 62 62 64 65 70 80
24	(-1.3)	61 61 63 67 74 74 74 79
25		72 74 79
26		

Fig.3.11 Energy release distribution. Assembly ZR-6 12.7/3.6/4.0.
Configuration 161 (T=400 K). Statistical error - 2.0%
Deviations from experiment are given in parentheses (%)

0	(-3.4)	145	(-3.4)
1		149	(2.0)
2	(-1.2)	145	145 (1.0)
3		145	144 (0.5)
4	(-4.0)	141	145 141 (-1.0)
5		139	140 142 (-1.2)
6	(-0.5)	139	138 141 138 (1.0)
7		135	135 134 132 (1.0)
8	(1.0)	135	133 132 131 129 (0.5)
9		132	130 128 127 124 (-0.7)
10	(2.6)	129	127 126 124 124 120 (-0.8)
11		123	121 121 117 118 115 (1.4)
12	(0.7)	118	116 117 115 112 111 107 (-2.0)
13		112	112 111 107 107 108 100 (-1.3)
14	(-1.0)	106	105 106 105 103 102 99 97 (3.0)
15		101	104 99 96 97 93 90 88 (0.2)
16	(-0.2)	97	95 94 95 92 91 87 85 82 (1.3)
17		90	90 89 86 86 82 79 77 72 (-1.1)
18	(-0.7)	83	82 82 82 79 77 75 73 69 66 (1.1)
19		76	76 75 74 73 70 68 65 63 60 (-0.9)
20	(-0.7)	71	70 69 70 68 65 61 61 61 57 55 (1.7)
21		65	64 63 63 61 58 57 57 54 64 54 (1.1)
22	(1.1)	60	60 59 60 58 57 56 55 53 53 59 66 (1.4)
23		55	56 56 57 57 56 56 59 62 67
24	(3.0)	56	56 56 61 64 65 64 70
25		64	64 69

0 1 2 3 4 5 6 7 8 9 0 1 2 3 4 5 6 7 8 9 0 1 2

Fig.3.12 Energy release distribution. Assembly ZR-6 12.7/3.6/5.8.
Configuration 161(T=300 K) Statistical error - 1.0%
Deviations from experiment are given in parentheses (%)

3.4 THE APPLICATION OF THE MONTE CARLO METHODS FOR VERIFICATION AND VALIDATION OF THE DESIGN CODES

3.4.1 The general remarks

The design codes have a limited accuracy because they use very approximate reactor mathematical models. These models are based on a definite set of a priori hypotheses, which are not accurate enough as a rule. Besides the approximate nature of the design models, their parameters are usually calculated approximately as well. Additionally it is often difficult to interpret the quality of the design code result because the nuclear data used in the various codes are usually different.

The important targets in applying Monte Carlo method are as follows.

- Verification and accuracy evaluation of the different design methods.
- Quality analysis of the hypotheses used as the basis of the design methods.
- Analysis of the real advantages of the new approaches and of the new design methods proposed regularly (cf. Chapters 5-7).
- Clarifying the reasons influencing on the design code accuracy and the elaboration of the recommendations allowing their accuracy to be increased.

The mentioned problems were considered in (Maiorov et al, 1978, 1988, 1993). Their main target was to verify the WWER fine mesh design codes (cf. Chapter 5) and to analyze the possibility improving their accuracy.

The investigations were based on the following principles.

1. A set of mathematical benchmark problems is calculated by the Monte Carlo methods.
2. A special theoretical analysis is carried out to elaborate Monte Carlo algorithms of calculating the design equation parameters.
3. The design equation coefficients are calculated by Monte Carlo codes with the same accuracy as the test benchmark problems. Identical nuclear data and geometry models are used (both for solving the benchmarks and for calculating the design equation coefficients).
4. The Monte Carlo and the design code solutions of the transport equation are compared in application to a full assembly. The reasons for discrepancies are investigated and cleared up.

A similar approach permits one to avoid the influence of data discrepancies and of the approximate design parameter determination on the

results. Initially the investigations were based on the surface flux method (SFM) (Maierov et al, 1970). Later the approach developed for this method was used to investigate the other new ones.

One should note that in the SFM or in the other response matrix type methods, every cell flux is synthesized as the sum of a prescribed number of trial functions. Every trial function is the transport equation solution corresponding to some boundary condition. Then the reactor equations are constructed by way of linking the different moments of these linear combinations in the neighbouring cells taking into account the continuity conditions of different moments of flux. The goal of (Maierov et al, 1970) was to verify synthesis type methods in their application to WWER calculation problems.

The WWER lattices are nonuniform and contain many singularities, e.g. the absorbers, the water holes, the water gaps between the assemblies, etc. These singularities significantly influence the neutron spectrum inside the cells. In the design calculations, it is important to take into account both the spectrum change and the possible non-diffusion effects near the singularities.

Traditionally, the few group homogenization methods were used in the WWER design codes (cf. Chapters 4,5). These methods are based on replacement of the real heterogeneous cell by an equivalent homogenized one. Then the hypothesis is used that the flux in the model reactor consisting of similar equivalent cells may be described by the diffusion equation with good enough accuracy. An irreversible loss of information has already taken place during the first homogenization step of constructing the design models. It limits the accuracy of the design codes in principle. Additional losses take place when the diffusion equations are solved by the approximate finite difference methods.

Earlier it was generally supposed that the diffusion equation coefficients did not depend on the cell position in the assembly. The approximate character of this hypothesis is obvious for the few group WWER design model. One of the means of improving the typical design code accuracy is to increase the energy group number (in the thermal region in particular). It permits one to take into account the cell diffusion parameter dependence on the surroundings. It does not however eliminate the other information losses connected with using the homogenization procedure (e.g., transport effects and effects of significant flux variation on the cell boundaries).

TIC specialists have expended a great deal of effort on improving the

accuracy of the traditional design methods. These efforts seem to be successful. As a result it became possible, using only one thermal group to predict the reaction rates with 5-10 times higher accuracy than before (for the cells adjacent to singularities).

The new approaches were developed where authors disregarded homogenization methods using different approximate methods of solution of the transport equation instead (see below and the Chapters 5-7). The equations of new approaches are formally similar to the traditional ones thereby allowing one to solve them using the traditional codes.

Another way was chosen by authors who improved the traditional diffusion equation accuracy taking into account changing the cell energy spectra in dependence on the cell surroundings (the spectral index and Bonalumi methods, see below and Chapter 5).

In (Laletin et al, 1977), diffusion type equations based on the synthesis principle were derived. These equations were formally similar the simplest finite difference ones usually being derived on the basis of homogenized diffusion theory. It was shown that the homogenization step is not necessary to obtain the equations analogous to those usually used in the fine-mesh design codes. The new equations have better accuracy and may be solved using the traditional codes.

The synthesis approaches are very popular now. They are discussed below and in Chapters 6 and 7. Even so it is worth noting that the use of synthesis methods does not automatically improve the codes quality. It should be taken into account that the definite freedom exist both in choosing the trial functions and in constructing the balance equations. In principle, it is possible to derive even worse equations than the traditional ones if this freedom would be used not the right way (cf. Maiorov et al, 1970). So the analysis of real quality of the proposed equations is always necessary.

The Monte Carlo codes were used to verify new methods and to evaluate their real advantages in comparison with traditional ones. In Sect.3.4.3 we consider an example of similar analysis for the simplest synthesis balance equations of diffusion type. The Monte Carlo code *MCU* was used for this analysis based on numerical benchmark modelling of the WWER (and the ZR-6) type assemblies.

More complex synthesis methods are considered in Chapters 6 and 7. In Sect.3.4.4 the possibilities of their analysis using *MCU* code are discussed.

As a rule the solution of the set of model problems is necessary to

calculate the parameters of the synthesis type equations. These solutions are used as trial functions.

The asymptotic lattice problem plays an important role for this purpose and similarly for the homogenization procedure. This is the reason we consider this problem first.

3.4.2 Asymptotic lattice problem

Problem description. The aim of transport calculations is to determine the different neutron distribution parameters. These parameters may be expressed through the linear functional R of the transport equation solution $\Psi(r, v)$:

$$R = \int \varphi(r, v) \Psi(r, v) dr dv, \quad (3.4.1)$$

Here the φ function defines the functional.

The transport equation may be written as follows:

$$\begin{aligned} & \frac{v}{v} \nabla \Psi(r, v) + \Sigma_t(r, v) \Psi(r, v) - \\ & - \int \Sigma_s(r, v, v') \Psi(r, v') dv' - \frac{1}{K_{eff}} \int \Sigma_f(r, v, v') \Psi(r, v') dv' \quad (3.4.2) \\ & = S(r, v) \end{aligned}$$

Here $\Sigma_t(r, v)$ is a total cross section of the neutron having velocity v and placed at point r . Functions Σ_s and Σ_f describe the changes of particle number and their energies in scattering and fission reactions respectively. S is the density of the external sources.

The equation in the form (3.4.2) may be used to describe the source (inhomogeneous) or criticality (homogeneous) problems. In the latter case $S=0$ and it is necessary to calculate the maximal eigenvalue K_{eff} and functionals of the corresponding eigenfunction (for the source problem $K_{eff}=1$).

The mathematical models of the real assemblies are defined by assignment of the boundary conditions for Eq. (3.4.2) and by assignment of the functions $\Sigma_t(r, v)$, $\Sigma_s(r, v, v')$, $\Sigma_f(r, v, v')$. The latter depend on the geometry and materials of the reactor to be investigated.

An important practical problem is the determination of the so called asymptotic solution (cf. Benoist, 1964) of the transport equation. That solution is defined for the uniform infinite lattices having translation

symmetry under the condition that leakage from the lattice is described by a buckling vector B (cf. Deniz, 1986).

The asymptotic problems are important for analysing the criticality experiments and for calculating the design equation coefficients.

By definition an asymptotic solution of the transport equation may be expressed in the form

$$\Psi(r, v) = \psi_B(r, v) \exp(iBr) \quad (3.4.3)$$

where $\psi_B(r, v)$ is some periodical function with the period to be equal to the lattice period.

Asymptotic criticality problems and the source ones may be considered equally.

For the inhomogeneous problem the source distribution function is usually presented in the form:

$$S(r, v) = s_B(r, v) \exp(iBr)$$

where $s_B(r, v)$ is some periodical real or complex value function.

For a criticality problem the main eigenvalue should be determined.

It seems that the generally conventional formulation of the asymptotic problem does not exist. Usually the following positions may be opened.

With which value of B should the asymptotic problem be solved for?

Which problem should be solved: the criticality problem or that corresponding to the fixed source?

What function $s_B(r, v)$ should be chosen if the source problem should be solved, for example complex value or real value function?

It should be noted that these questions are not too important from the practical point of view because:

- Asymptotic problem solutions are used mainly for calculating the coefficients of the crude enough homogenized equations.
- Asymptotic problems used to be solved approximately utilizing the design codes.

However it is useful to have in view all the mentioned ambiguity when comparing the results of different authors. In the opposite case one may compare the solutions of the different problems attempting to understand the reasons for their discrepancies.

As the formulation of the asymptotic problem has been fixed both the solution methods and the usage of results may be discussed.

Experiment analysis. As a rule, the asymptotic method is used in the experiment analysis, when the assembly configuration is not described

accurately enough, for example:

- in the XY-geometry plane the lattice has a finite size and it is described accurately but the leakage along the Z-axis is fixed by assignment of the buckling component B_z (as a rule, on a measurement basis),
- all the lattice is described as an asymptotic one with the measured leakage vector B .

Many benchmark-experiments, for the ZR-6 assembly in particular, are described as two dimensional ones or as the zero dimensional models with the measured buckling.

The Monte Carlo method makes it possible to analyze the similar experiments without additional approximations.

Design calculations. In the design calculations the asymptotic solutions are used traditionally in the homogenization step. As a rule these solutions are determined approximately. The especially considerable approximations are used in the resonance and in the thermalization energy regions. The Monte Carlo codes give the opportunity to estimate discrepancies appearing at the step of the diffusion equation parameter calculations.

As asymptotic problem has been formulated and solved, its results may be applied in many variants for calculating the homogenization parameters. This multivariancy, for example, is discussed in (Deniz, 1986). In the cited work the homogenization problem is formulated in a general enough form.

Suppose, following (Deniz, 1986) that two arbitrary functions $W(r,v)$ and $N(r,v)$ are chosen for the lattice cell homogenization procedure and we know the solution of the asymptotic problem with a priori fixed B .

Then, using Eq.(3.4.2) we may write the balance correlation for every energy group having the number $g^{1)}$:

¹⁾ We included the fission term of (3.4.2) in the external source term, noted as S .

$$\frac{\langle (\nabla \nabla \Psi(r, v) + \sum_t (r, v) \Psi(r, v)), W(r, v) \rangle_g}{\langle \Psi, N \rangle_g} \quad (3.4.4)$$

$$\frac{\langle W, \int \sum_s (r, v, v') \Psi(r, v') dv' \rangle_g}{\langle \Psi, N \rangle_g} = \langle W, S \rangle_g$$

Here the symbol $\langle \dots \rangle$ denotes the scalar product, and Ψ is the solution of the asymptotic problem.

On the other hand the asymptotic problem may be described by the diffusion homogenized equation. Its asymptotic solution must satisfy the equation:

$$(DB^2 + \sum_t) \phi_g - \sum_s \Sigma_s^{g \rightarrow g'} \phi_{g'} = S_g \quad (3.4.4a)$$

Therefore the equivalent homogenized cell parameters are calculated from the condition that the coefficients in Eq. (3.4.4) should be equal to the analogous ones of Eq. (3.4.4a). In this procedure the variable ϕ is interpreted as $\langle \Psi, N \rangle_g$.

In particular from Eq. (3.4.4) the equation for the diffusion coefficient of homogenized lattice comes out in the form:

$$D_g = \frac{\langle (\nabla \nabla \Psi(r, v), W(r, v)) \rangle_g}{B^2 \langle \Psi, N \rangle_g} \quad (3.4.5)$$

where B is the buckling component for the direction of interest.

This algorithm of the homogenized cell parameter calculation gives a solely the obvious guarantee: namely, that the reaction rates both of the real lattice and of the homogenized one would be equal for the chosen asymptotic model problem only. From the principle of continuity one may hope that the homogenized diffusion equation solutions will also be close to the real solution for the case of the real nonuniform lattice. But not more than that! Nevertheless all the traditional design codes are based on the principle mentioned above.

One may recall that the freedom of choosing the model asymptotic problem and the weighting functions W and N still remains. This is used widely in the design calculations. For example, in (Deniz, 1986) about ten different definitions of diffusion coefficients are given on basis of Eq. (3.4.5). They differ one from the other mainly by the choice of the W and N functions and parameters B . Some of them should be mentioned: corrected and uncorrected Benoist coefficients, coefficients of Bonalumi, Deniz, Gelbard, Larsen etc. The definitions of (Laletin, 1958) and (Shevelev, 1958) may be

added to this set. All these definitions are based on different forms of the equivalence principle.

Two popular diffusion parameter normalization procedures tend to be: averaging the flux over the whole cell volume and its normalization on the cell edge. For this purpose two options of N functions (3.4.4) are used respectively: $N=1$ or N to be equal to the δ -function which differs from zero at the edge of the cell only (we have in mind the space variable dependence).

The latter option often allows one to achieve more accurate results because the flux-current continuity conditions should be realized on the cell edge. The development of modern design methods (cf. below and Chapters 6 and 7) confirmed the good quality of the edge normalization procedure recommended in (Bonalmi, 1973).

From arbitrariness of the above mentioned N and W functions, it follows that parameters calculated using the different normalization rules differ by factors which are equal to the ratio of the cell edge fluxes to the fluxes averaged over the volume. For WWER cells these factors may be large enough. So it may be dangerous to use the diffusion coefficients normalized on the cell edge and the cross sections averaged over its volume in one calculation scheme. They should be renormalised before.

In general, one should always have in mind that all the coefficients of the homogenized diffusion equation should be calculated in accordance with each other: on the basis of the same pair of functions W and N . One of the typical errors is an attempt to use the averaged cross sections and diffusion coefficients without taking into account this rule.

Modelling of the asymptotic lattice by MC methods. In the *MCU* code it is possible to determine the different functionals of neutron flux in the asymptotic lattices with pre assigned buckling.

As a rule the asymptotic problem is solved by the *MCU* in the approximation that fission neutron distribution does not depend on B inside the cell. However it takes into account the complex value neutron slowing down distribution.

The *MCU* method is based on a very simple transformation of Eq. (3.4.3).

Let r_s be the arbitrary point on the cell edge and $r_s + l(r_s)$ be the point on the opposite cell edge. Of course the vector $l(r_s)$ may be defined uniquely.

From Eq. (3.4.3) it is obvious that the asymptotic solution may be calculated if we solve the transport equation for a single cell with the boundary condition on its sides:

$$\Psi^*(\mathbf{r}_s + \mathbf{l}(\mathbf{r}_s), \mathbf{v}) = \Psi^-(\mathbf{r}_s, \mathbf{v}) \exp(i \mathbf{B} \mathbf{l}(\mathbf{r}_s)) \quad (3.4.6)$$

where

$\Psi^*(\mathbf{r}_s, \mathbf{v})$ is the flux of neutron flying into the cell;

$\Psi^-(\mathbf{r}_s, \mathbf{v})$ is the flux of neutron flying out of the cell;

$\mathbf{B}$ is the buckling vector.

The functionals of neutron flux for the transport equation with boundary conditions (3.4.6) may be calculated by Monte Carlo method as follows (Gelbard and Pego, 1979), (Maierov et al, 1984).

The trajectories are modelled inside the single cell with the boundary condition of translation (Eq. (3.4.6) where $\mathbf{B} = 0$).

After the particle leaves the cell at point $\mathbf{r}_s$ it returns into the same cell at the opposite point $\mathbf{r}_s + \mathbf{l}(\mathbf{r}_s)$ not changing the direction of its movement. The particle weight is multiplied by the factor $\exp(i \mathbf{B} \mathbf{l}(\mathbf{r}_s))$, that imitates the boundary condition (3.4.6). Then the particle weights are traditionally used for the different tally calculations.

The described procedure is used for calculating every group functionals which are evaluated by taking into account the complex value of particle weights. For example the group source S is equal to the expected value of $\text{Re}(W_g^{(\text{enter})})$ and the removal rate A_g equal to the expected value of $\text{Re}(W_g^{(\text{exit})})$. Here $W_g^{(\text{enter})}$ and $W_g^{(\text{exit})}$ are the particle weights on the moments when the neutrons enter into the group and leaves it respectively.

Cell leakage L_g is estimated for every energy group as the difference of the expected values:

$$L_g = \text{Re}(W_g^{(\text{enter})}) - \text{Re}(W_g^{(\text{exit})}).$$

The migration lengths and the diffusion coefficients are estimated as:

$$M_g^2 = \frac{L_g}{B^2 A_g}$$

$$D_g = M_g^2 \sum_{\text{rem}}^{(g)}$$

where all the quantities (including removal cross-sections $\sum_{\text{rem}}^{(g)}$) are calculated for every group.

For example in the rhomboid lattice the removal rate may be estimated as the expectation value of the complex value tally:

$$A = A_0 \text{Re} \left[\exp \left(i \sum_{k=1}^3 (\Delta \eta_k B \mathbf{l}_k) \right) \right]$$

where

A_0 is a removal rate on condition $B=0$,

Δn_k is the algebraic number of the intersections of the cell sides in the directions of the translation vectors l_k to be calculated beginning when the neutron enters into the group till its exit from this group (this may be the result of absorption).

It is obvious, that for small B

$$L \approx 0.5 \sum_k \overline{(\Delta n_k)^2} (B l_k)^2$$

Thus in a general case the neutron leakage from the heterogeneous lattice can not be expressed through the migration area, but depends on the average value of $\overline{(\Delta n_k)^2} (B l_k)^2$ every direction.

If the lattice is uniform in the Z direction the value l_z^2 may be chosen as small as desired. So in this special case the leakage is expressed through the migration area.

3.4.3 Application of the Monte Carlo method for verifying the simplest design codes

Verification of the WWER design fine-mesh codes was carried out using the *MCU* code (Maigorov et al, 1984). Below we shall describe some verification results.

The verified methods coming from specific practical and theoretical reasons were chosen. Thus only four group approaches used in the WWER design calculations were verified. Moreover, only those methods were considered that were based on the following premises:

- the space distribution of the neutron sources over every cell does not depend on the cell position inside the reactor,
- the flux on the cell surface does not strongly depend on azimuth angle.

In the framework of these limitations it is possible to compare the efficiency of new approaches developed for WWER design calculations in the TIC institutes.

It is necessary to begin with a formal and extended introduction in order to make the subject of investigations more clear.

As a matter of fact the verification work required to carry out the analysis of both the traditional and of the new proposed design methods. In this analysis we tried to conserve as possibly the generally accepted formalism of the design fine mesh equations. However the goal was not to conserve the homogenization approach as obligatory condition.

Diffusion homogenized equations for every energy group have the form:

$$-D \nabla^2 \Phi + \Sigma \Phi = q \quad (3.4.7)$$

where

q is a source power,

Σ is a removal cross section,

D is a diffusion coefficient.

As a rule one Φ is taken to mean a flux, averaged over the volume of the cell.

Variable Φ is generally some arbitrary functional of the cell flux $\Psi(r, \Omega, E)$ defined by choice of the weight function $N(r, \Omega, E)$, depending on the space, the energy and the angle variables (see Eq. (3.4.4)):

$$\Phi = \iiint N(r, \Omega, E) \Psi(r, \Omega, E) \, dr d\Omega dE$$

Here the integration is performed over all the cell volume, over the energy group interval and over the full solid angle.

The specific choice of the weighting function N determines the values of the diffusion equation coefficients and the physical meaning of Φ .

We shall use notation $\bar{\Phi}$ if Φ is a flux averaged over the whole cell volume ("The folk" method: $N=1$). If N is a δ -function depending on the position vector (normalization on the cell edge) then Φ means the "flux" averaged over the cell surface. In this case we shall use notation $\tilde{\Phi}$. The analogous notation will be used for the corresponding parameters of Eq. (3.4.7), for example $\bar{\Sigma}$ and $\tilde{\Sigma}$.

Usually the three different options of angle dependence on the weighting functions N are considered. They are reduced to utilizing the different angular moments Φ in the diffusion equation:

- 1) the scalar flux Φ or the zero angle moment of Ψ (The folk and the Bonalumi methods);
- 2) the 'albedo flux' used in (Malorov, 1977) is:

$$\Phi_A = 2 \left(I_n^+ + I_n^- \right) \quad (3.4.8)$$

where $I_n^+ + I_n^-$ are the inward and the outward currents,

- 3) The level Φ_L , or the second angle moment of Ψ (Laletin et al, 1985) is:

$$\Phi_L = 3 \int (\Omega p)^2 \Psi(r, \Omega, E) \, dr d\Omega dE = 3 \mu_n^2 \cdot (\text{scalar flux})_n \quad (3.4.9)$$

where μ^2 is the notation for $(\Omega, p)^2$, p is the normal to surface of the cell.

The values of the diffusion equation coefficients depend on the choice of angular moments in the equivalent Eq. (3.4.4). The two last moments Φ_A

and Φ_L may be used if edge cell normalization ($\Phi = \tilde{\Phi}$) is considered.

In most cases the diffusion equation for the scalar flux $\Phi = \bar{\Phi}$ is considered in the design codes. However possible advantages in using other moments were discussed (cf. (Maierov, 1977), (Laletin et al, 1977)). Therefore similar options will be illustrated below.

As a rule the coefficients of the diffusion equation are determined by solving the asymptotic problem (see. Sect.3.4.2 and Chapter 4).

Then

$\Sigma = \Sigma_{as}$ is the removal cross section calculated for the infinite asymptotic lattice with fixed B.

$D = D_{as}$ is the diffusion coefficient of the same lattice.

The simple connection between the similar type parameters is obvious for the different choices of the space and the angular moments Φ used in the diffusion equation.

For example the removal cross sections and the diffusion coefficients calculated on the basis of $\bar{\Phi}$ and $\tilde{\Phi}$ are connected by the relations:

$$\tilde{\Phi}_{as} \tilde{\Sigma}_{as} = \bar{\Sigma}_{as} \bar{\Phi}_{as}$$

$$\tilde{\Phi}_{as} \tilde{D}_{as} = \bar{D}_{as} \bar{\Phi}_{as}$$

These relations reflect the fact that the reaction rates and the leakage in the asymptotic lattice do not depend on the formalism of their description.

As was mentioned earlier the use of the asymptotic problem solutions to describe the flux behavior in the real reactor is based on the simple hypothesis: parameters D and Σ of similar cells do not depend on the cell position inside the reactor. This proposition is not always true for WWER reactors.

The simplest algorithm taking into account the dependence of D and Σ on surroundings was proposed in (Bonalmi, 1973, 1974).

He approximated the cell flux in the limits of the one energy group as superposition of two or more trial functions: for example, the asymptotic spectrum $\Phi_{as} = q\varphi_{as}$ and some transient spectrum φ_t (it is possible to consider the φ_{as} normalization on the unit source for every group).

$$\Phi = q\varphi_{as} + \varphi_t = \Phi_{as} + \varphi_t \quad (3.4.10)$$

Evidently for every spectrum the average cross sections are different. We shall denote the removal cross sections of the transient spectrum and the asymptotic spectra by Σ_t and by Σ_{as} respectively.

From Eq. (3.4.10) it follows, that the removal rate may be expressed by the correlation

$$\Sigma\Phi = q + \Sigma_t(\Phi - q/\Sigma_{as}) \quad (3.4.11)$$

Equation (3.4.11) will be referenced as the Bonalumi transformation below.

In addition Bonalumi proposed the analogous approximate correlations for Fick's law, connecting the flux gradient with the current I and for the cell leakage L :

$$I = -D_t \nabla(\Phi - \Phi_{as}) - D_{as} \nabla \Phi_{as} \quad (3.4.12)$$

$$L = -D_t \nabla^2 \Phi - (D_{as} - D_t) \nabla^2 \Phi_{as} \quad (3.4.13)$$

Substituting Eq. (3.4.11) and Eq. (3.4.13) into Eq. (3.4.7) one finds:

$$-D_t \nabla^2 \Phi + ((D_t - D_{as})/\Sigma_{as}) \nabla^2 q + \Sigma_t \Phi - q\Sigma_t/\Sigma_{as} = 0 \quad (3.4.14)$$

As it follows from Eq. (3.4.10), the x-type reaction rates are expressed by equation

$$R^{(x)} = r_{as}^{(x)} \Phi_{as} V + r_t^{(x)} (\Phi - \Phi_{as}) V \quad (3.4.15)$$

where

$$r_{as}^{(x)} = \frac{\Sigma_{as}^{(x)}}{\Sigma_{as}} \quad \text{and} \quad r_t^{(x)} = \frac{\Sigma_t^{(x)}}{\Sigma_t}$$

Bonalumi proposed to use the two simple problems as models for calculating the transient spectrum parameters: the cylindrised cell surrounded by the infinite layer of moderator with the sources removed to infinity. In the first problem the sources do not depend on the azimuth angle φ , in the second one they depend on φ as $\cos(\varphi)$. Then using a simple procedure parameters D_t and Σ_t are determined from solutions of these model problems (Bonalumi, 1973, 1974).

The cell parameter dependence on the surroundings is described by Eq. (3.4.14) in a very simple way. However the considered scheme retains definite deficiencies. One of them is the additional uncertainty of the discretization step of the calculation scheme. Another deficiency is connected with the uncertainties of the homogenization procedure by itself. The difficulties of the Monte Carlo verification are due to these uncertainties. The above deficiencies may be removed by disregarding the

homogenization procedure as a whole.

Finite difference homogenized equations. In practice diffusion homogenized equations are solved by using the simplest finite difference approach.

For every cell (with the fixed number 0) of two dimensional lattice the finite difference equations may be written in the form (see Chap.5):

$$\frac{2S}{hNV} \sum_{n=1}^N (D_n^{-1} + D_0^{-1})^{-1} (\Phi_n - \Phi_0) + \Sigma_0 \Phi_0 = q_0 \quad (3.4.16)$$

with summation over all the neighbouring cells having numbers n (we suppose that every cell has N edges).

Here S, V are the cell surface area and volume respectively, h is the pitch of the lattice.

To analyze the accuracy of Eq. (3.4.16) using Monte Carlo codes it is convenient to consider them as the source equations of the reactor mathematical model. It means that one should not take into account their origin: the previous steps of the homogenization and of the diffusion equation discretization. For this purpose we need to be able to interpret all the members of Eq. (3.4.16) as physically measurable quantities. It will be then much more convenient to investigate the model accuracy as whole using the mathematical benchmark results. The possibility of diminishing the discretization uncertainties is another advantage of the chosen way.

Having in mind the above remark one may interpret Eq. (3.4.16) as the simple balance correlation for neutrons inside the cell:

$$\text{LEAKAGE} + \text{ABSORPTION} = \text{SOURCE}$$

In this equation Σ, Φ, q are the physically measurable quantities.

The connection of D with the physically measurable quantities should be analyzed specially.

Now we shall carry out a similar analysis for two of the most important flux moment options which may be used in the finite difference equations: $\bar{\Phi}$ and $\tilde{\Phi}$. These moments are averaged over the cell volume and over the cell surface respectively. The equations for these moments were used in the works of TIC (see Chapters 5-7).

Equation for the volume flux (model (V)). Let us define formally parameter D_{0n}^* for every side (number n) of every cell, having the conditional number 0:

$$I_n = D_{0n}^* (\bar{\Phi}_n - \bar{\Phi}_0) / h \quad (3.4.17)$$

Here

$\bar{\Phi}_n$ is the flux averaged over the whole cell volume,

I_n is the net current through the cell edge (the inward normal direction is considered as positive).

It is obvious, that parameters $\bar{D}_{0n}^*$ are the physically measurable ones.

It follows from Eq. (3.4.17), that the net current J averaged over the full surface of the cell equals

$$J = \frac{1}{hN} \sum_{n=1}^N \bar{D}_{0n}^* (\bar{\Phi}_n - \bar{\Phi}_0) \quad (3.4.18)$$

Here

$$J = \frac{1}{N} \sum_{n=1}^N I_n$$

Taking into account that leakage L from the cell equals $-JS$, we may write the balance equation:

$$-JS + \sum \bar{\Phi} V = qV \quad (3.4.19)$$

or

$$-\frac{S}{hNV} \sum_{n=1}^N \bar{D}_{0n}^* (\bar{\Phi}_n - \bar{\Phi}_0) + \sum \bar{\Phi}_0 = q \quad (3.4.20)$$

Equation (3.4.16) is identical to the finite difference homogenized Eq. (3.4.14) when the neighbouring cells have the same diffusion coefficients ($\bar{D}_0 = \bar{D}_n$).

The opposite case may be considered when these coefficients are the different ones.

Let us define formally the new cell parameters $\bar{D}_{0(n)}$ (for every cell side) which are the physically measurable ones:

$$I_n = 2\bar{D}_{0(n)} (\bar{\Phi}_n - \bar{\Phi}_0)/h \quad (3.4.21)$$

where $\bar{\Phi}_n$ is the flux averaged over the edge having the number n of the cell numbered 0.

From the flux-current continuity conditions on the cell edges and from Eq. (3.4.18) it follows that:

$$\bar{D}_{0n}^* = 2 (\bar{D}_{0,(n)}^{-1} + \bar{D}_{n,(0)}^{-1})^{-1} \quad (3.4.22)$$

Substituting the right part of Eq. (3.4.22) into Eq. (3.4.20) instead of $\bar{D}_{0n}^*$ one finds the equation similar to the source mathematical model Eq. (3.4.16):

$$-\frac{2S}{hNV} \sum_{n=1}^N (\bar{D}_{0,(n)}^{-1} + \bar{D}_{n,(0)}^{-1})^{-1} (\bar{\Phi}_n - \bar{\Phi}_0) + \sum \bar{\Phi}_0 = q \quad (3.4.23)$$

In this equation parameters $\bar{D}_{0,(n)}$ are the physically measurable ones and the equation itself is absolutely accurate. It may be seen that Eq. (3.4.16) may be derived from the accurate Eq. (3.4.23) in approximation when the diffusion coefficients $\bar{D}_{k,(n)}$ do not depend on the edge number (for every cell having the number k):

$$\bar{D}_{k,(n)} \approx \bar{D}_k \quad (3.4.24)$$

So one may now interpret the few group design equations as ones being derived from the exact balance equations neglecting the approximation (3.4.24). Therefore one may investigate the inaccuracy of approximation (3.4.23), dependence D_k on the cell place inside the reactor by calculating D_k on the basis of the Monte Carlo results (using Eqs. (3.4.17), (3.4.21), (3.4.23)) and considering all the parameters to be "measured".

These possibilities are illustrated below.

The verification of the V model. The different approximative methods for calculating the average cross sections and diffusion coefficients are considered in Chapters 5-7. They permit one to take into account the surroundings influence on the design equation coefficients.

The Bonalumi approximation is the simplest recipe for taking into account the neutron spectrum dependence on the cell position. Using Eq. (3.4.11) one may transform Eq. (3.4.20) to:

$$-\frac{2}{hN} \frac{S}{V} \sum_{n=1}^N (\bar{D}_0^{-1} + \bar{D}_n^{-1})^{-1} (\bar{\Phi}_n - \bar{\Phi}_0) + \bar{\Sigma}_t \bar{\Phi}_0 = \frac{\bar{\Sigma}_t}{\bar{\Sigma}_{as}} q \quad (3.4.25)$$

Equation (3.4.25) may be solved using the traditional design codes on the condition that the coefficients of Eq. (3.4.16) should be changed compared with traditional ones as follows:

$$\Sigma \leftarrow \bar{\Sigma}_t \quad q \leftarrow \frac{\bar{\Sigma}_t R_{mod}}{\bar{\Sigma}_{as} V}$$

Here R_{mod} is the slowing down rate.

In this way it is possible to improve the traditional code accuracy if one consider the equation coefficients do not depending on the cell position.

The above algorithm permits one to understand Lelek's numerical results (see Sect. 5.8), for example. Lelek calculated the coefficients in Eq. (3.4.16) using the fitting procedure and the ZR-6 experimental data. He proposed that the Eq. (3.4.16) coefficients do not depend on the cell position and determined the set of good constants which describes the

experimental results accurately enough. On the other hand the four group real cell cross sections depend obviously on the position in the ZR-6 assembly (cf. Sect.3.3.3, fig.3.1-3.4). The seeming contradiction is removed if Lelek's good fitting results are interpreted as implicit determination of coefficients of Bonalumi type Eq. (3.4.25).

Another simple recipe for taking into account the spectrum change effect inside the cell (Spectral index method) is described in Chapter 5.

We shall now consider the diffusion coefficient calculation problem.

For nonuniform lattices the diffusion coefficients may be calculated using Monte Carlo code results and Eqs. (3.4.17, 18, 21, 23). The Monte Carlo results also permit one to verify the hypothesis $D_n \approx D$.

It follows from the diffusion coefficient definition (3.4.17), that:

$$D_{on}^* = hI / (\bar{\Phi}_n - \bar{\Phi}_0);$$

where n and 0 are the neighbouring cell numbers and I is the current through the common surface of two cells.

In the simplest case the approximation may be used that D does not depend on the cell position. Then on condition that the diffusion coefficients D of all the neighbouring cells are equal, it follows from Eq. (3.4.18) that:

$$D^* = \bar{D} = Jh / (\bar{\Phi}_{AV} - \bar{\Phi}_0) \quad (3.4.26)$$

where J is the average current per unit of all the cell surface and

$$\bar{\Phi}_{AV} = \frac{1}{N} \sum_{n=1}^N \bar{\Phi}_n \quad (3.4.27)$$

In the design codes the diffusion coefficients are determined usually on the basis of the asymptotic problem approximate solutions with prescribed buckling (mostly in the zero limit, (see Sect.3.4.2). Eq. (3.4.26)¹⁾ may be used for this case also. It is enough to substitute into it the flux to be proportional $\exp(iB_1 r_n)$. The asymptotic diffusion coefficient calculations based on Eq. (3.4.26) are more preferred in the framework of (V) model than those which are calculated for the diffusion equation. It is explained that one avoids of the information losses

¹⁾ According to Eq. (3.4.3) the leakage from the cell equals $u \exp(iBr_n)$ and the absorption equals $a \exp(iBr_n)$, where u and a do not depend on the cell position. D^* does not depend on the cell position either.

connected with the discretization step.

Equations for the surface flux (model S). We shall now consider the alternate option of the diffusion equation for the flux normalized on the edge of the cell. This case corresponds to the choice of the δ -function to be the N function in Eq. (3.4.3). To contrast to the V-model we shall derive the equations for the surface flux without using differential analog. We shall follow the approach described in (Maierov, 1978), although the different methods were applied ((Laletin et al 1977), (Novikov, 1980), etc) for this goal.

It may be seen that the basic (V) model Eq. (3.4.23) follows from the current-flux continuity conditions, from the balance Eq. (3.4.19) and from the diffusion coefficient definition by Eq. (3.4.21).

We may rewrite Eq. (3.4.19) and Eq. (3.4.21) in the equivalent form using where possible the surface flux ϕ_n instead of the flux $\bar{\phi}$ averaged over the volume.

Then one finds three equations, viz:

$$\tilde{\Sigma}\tilde{\phi}V = JS + qV \quad (3.4.28)$$

$$(I_n - J) = 2D(\phi_n - \tilde{\phi})/h \quad (3.4.29)$$

$$J = 2D(\tilde{\phi} - \bar{\phi}_0)/h \quad (3.4.30)$$

where $\tilde{\Sigma}\tilde{\phi}V$ is the removal rate normalized on the cell edge and:

$$J = \frac{1}{N} \sum_{n=1}^N I_n \quad \text{and} \quad \tilde{\phi} = \frac{1}{N} \sum_{n=1}^N \phi_n$$

Now analogously to the V-model consideration we shall consider Eq. (3.4.28) and Eq. (3.4.29) as the definitions of the parameters $\tilde{\Sigma}$ and D respectively.

More precisely we shall define the new $\tilde{D}_{(n)}$ parameters for every cell side by the relation:

$$\tilde{D}_{(n)} = 0.5h(I_n - J)/(\phi_n - \tilde{\phi}) \quad (3.4.31)$$

where n is a number of the side.

It is evident that $\tilde{\Sigma}$ and $\tilde{D}_{(n)}$ are the measurable parameters and may be calculated (using their definition) by the Monte Carlo codes.

Therefore we may consider parameters $\tilde{\Sigma}$ and $\tilde{D}_{(n)}$ as the fixed ones. Then for every reactor cell the following equations are true:

$$\tilde{\Sigma}\tilde{\Phi}V = JS + qV \quad (3.4.32)$$

$$I_n - J = 2\tilde{D}_{(n)}(\Phi_n - \tilde{\Phi})/h$$

The balance Eqs.(3.4.29) added by the flux-current continuity equations for the cell sides are the full set of reactor equations (one should naturally take into account the external boundary conditions). It is important to note that the Eq. (3.4.30) is not included in the considered set. In the V-model this equation is used to calculate the reaction rates ($\tilde{\Phi}$ in particular) and its analog will be necessary for the S-model (see below). But for the S-model it is preferable to disregard Eq.(3.4.30) because the parameter connection given by this equation seems too unreal.

Equation set (3.4.32) is similar to Eq.(3.4.28), (3.4.29) of the V-model. Again we shall restrict ourselves to the approximation $\tilde{D}_n \approx \tilde{D}$ ($\tilde{D}_n$ does not depend on the cell side number). Then using the flux-current continuity equations and excluding Φ_n from (3.4.29) we have (Maiorov, 1978):

$$J_0 = \frac{1}{N} \sum_{n=1}^N (\tilde{D}_0^{-1} + \tilde{D}_n^{-1})^{-1} (F_n - F_0) \quad (3.4.33)$$

where n are the subscripts of the cells surrounding the cell with subscript 0 and:

$$\tilde{\delta}_n = 2\tilde{D}_n / h \quad (3.4.34)$$

$$F_n = \tilde{\Phi}_n - \tilde{\delta}_n^{-1} J_n \quad (3.4.35)$$

We shall call F_n quantity (Laletin, 1977) by a pseudo flux.

From the balance condition (the first of Eqs.(3.4.32)) it follows that

$$J = \left[F - \frac{q}{\tilde{\Sigma}} \right] \frac{\tilde{\Sigma}V/S}{1 - \tilde{\Sigma}V/(S\tilde{\delta})} \quad (3.4.36)$$

Substituting (3.4.36) into (3.4.33) we have:

$$- \frac{2}{hN} \sum_{n=1}^N (\tilde{D}_0^{-1} + \tilde{D}_n^{-1})^{-1} (F_n - F_0) + \tilde{\Sigma} F_0 = q \quad (3.4.37)$$

where

$$\tilde{\Sigma}^* = \frac{\tilde{\Sigma}}{1 - \tilde{\Sigma}V/(S\tilde{\delta})} \quad q^* = \frac{q}{1 - \tilde{\Sigma}V/(S\tilde{\delta})} \quad (3.4.38)$$

The equation for the pseudo flux F is an alternative one to equation for the flux averaged over the cell volume. One should note that any

angular flux moment may play a role of Φ : scalar flux, albedo flux, level. Their choice is a matter of taste.

Now we should supplement Eq.(3.4.37) by the new equations for every group reaction rates instead of Eq.(3.4.30) of the V-model.

For example, on the basis of Eq.(3.4.36) one may write the equations, describing the flux averaged over the cell volume.

$$qV + JS = \Sigma^* V \left[F - \frac{qV}{\tilde{\Sigma}S} \right]$$

$$\tilde{\Phi} = \Sigma^* \left[F - \frac{qV}{\tilde{\Sigma}S} \right] / \tilde{\Sigma} \quad (3.4.39)$$

$$\bar{\Phi} = \tilde{\Sigma} \tilde{\Phi} / \bar{\Sigma}$$

Analogously other reaction rates may be calculated using the ratio $\tilde{\Sigma}^{(*)} / \tilde{\Sigma}$.

Verification of (S) model with use of Monte Carlo codes. To take into account the cell parameters dependence on the cell surroundings the Bonalumi approximation may be used again.

In this approximation we have

$$\tilde{\Sigma} \tilde{\Phi} - q = \tilde{\Sigma}_t (\tilde{\Phi} - q / \tilde{\Sigma}_{as}) \quad (3.4.40)$$

Then Eq. (3.4.37) is transformed into the standard few group equation whose coefficients do not depend on surroundings:

$$- \frac{2S}{hNV} \sum_{n=1}^N (\tilde{D}_0^{-1} + \tilde{D}_n^{-1})^{-1} (\tilde{F}_n - \tilde{F}_0) + \sum_{t \neq as} \tilde{\Sigma}_t \tilde{\Phi}_0 = \frac{\tilde{\Sigma}_t}{\tilde{\Sigma}} q^* \quad (3.4.41)$$

where $\tilde{\Sigma}_t^*$ differs from $\tilde{\Sigma}_t$ by substituting $\tilde{\Sigma}_t$ instead of $\tilde{\Sigma}$.

The alternative equivalent option of Eq. (3.4.41) is used in the some design codes of the TIC.

For example (Novikov, 1983), the auxiliary variable is introduced for every cell:

$$\epsilon = (\tilde{\Phi} - \tilde{\delta}^{-1} J) / \bar{\Phi}$$

Then a pseudo flux F is replaced by the product $\epsilon \bar{\Phi}$. After substitution of this variable into Eq.(3.4.36) we have (see Sect. 6.1, 6.3):

$$- \frac{2S}{hNV} \sum_{n=1}^N (\tilde{D}_0^{-1} + \tilde{D}_n^{-1})^{-1} (\epsilon_n \bar{\Phi}_n - \epsilon_0 \bar{\Phi}_0) + \bar{\Sigma} \bar{\Phi}_0 = q \quad (3.4.42)$$

where

$$\begin{aligned}\varepsilon &= \varepsilon_{as} (\bar{\Phi}_{as} / \bar{\Phi}) + \varepsilon_t (1 - \bar{\Phi}_{as} / \bar{\Phi}) \\ \bar{\Sigma} &= \bar{\Sigma}_{as} (\bar{\Phi}_{as} / \bar{\Phi}) + \bar{\Sigma}_t (1 - \bar{\Phi}_{as} / \bar{\Phi}) \\ \bar{\Phi}_{as} &= q \bar{\varphi}_{as}\end{aligned}\quad (3.4.43)$$

The WWER design code PERMAC is based on these equations.

The accuracy of Bonalumi approximation in the framework of (V) and (S) models may be verified by comparing approximate cross sections with the ones calculated by Monte Carlo method.

The diffusion coefficients for (S) model may be calculated by the Monte Carlo methods using different approaches:

(a) In the approximation of nearly equal values of δ parameters for the neighbouring cells:

$$\tilde{D} = Jh / (\tilde{\Phi}_{av} - \tilde{\Phi}_0) \quad (3.4.44)$$

where

$$\tilde{\Phi}_{av} = \frac{1}{N} \sum_{n=1}^N \tilde{\Phi}_n; \quad (3.4.45)$$

(b) On the basis of definition (3.4.29):

$$\tilde{D} = 0.5h(I_n - J) / (\tilde{\Phi}_{av} - \tilde{\Phi}_0); \quad (3.4.46)$$

(c) On the basis of Fourier finite sum expansion for the currents

$$\tilde{D} = 0.5h \frac{\sum_{n=1}^N I_n \cos[2\pi(n-1)/N]}{\sum_{n=1}^N \Phi_n \cos[2\pi(n-1)/N]} = \tilde{D}_c \quad (3.4.47)$$

$$\tilde{D} = 0.5h \frac{\sum_{n=1}^N I_n \sin[2\pi(n-1)/N]}{\sum_{n=1}^N \Phi_n \sin[2\pi(n-1)/N]} = \tilde{D}_s \quad (3.4.48)$$

(d) On the basis of the solution of the Eq (3.4.33) using the values of J and $\tilde{\Phi}$ calculated by Monte Carlo method for every cell of assembly.

(e) For every side from the definition

$$\tilde{D} = 0.5h(I_n - I_{n'}) / (\tilde{\Phi}_n - \tilde{\Phi}_{n'}); \quad (3.4.49)$$

This definition follows from Eq. (3.4.29) if one proposes that D coefficients corresponding to the cell opposite edges are equal one to

another. Then Eq. (3.4.49) may be interpreted as Fick's law: the average current $0.5(I_n - I_n')$ on the cell central plane is proportional the flux gradient (I_n and I_n' have the different signs because the edge normals have different directions).

Numerical examples. The following was shown above.

- (a) The simplest traditional design equations for flux may be considered as the balance equations. It is not necessary to use the homogenization step for their derivation. It permits one to verify both the equations and their coefficients using Monte Carlo codes directly.
- (b) The single approximation used in deriving the balance equations is hypothesis about independence of D parameters from the side numbers.
- (c) Simple design formulae exist which permit to describe the equation coefficient dependence on the cell position.

The target of Monte Carlo benchmark calculations was to verify quality of (a), (b) and the design formulae of (c) type in the framework of the four group scheme traditionally used in the WWER design calculations.

The set of different ZR-6 configurations was modelled using MCU code (some of them are described in Chapter 2). All the coefficients of the equations mentioned in this section are calculated by MCU.

We shall consider here, as an example, the calculation results for three WWER type macrocells. The cell distribution of different functionals was calculated, in particular four group cell parameters (The WWER design group boundaries are: 821 KeV, 4.65 KeV, 0.625 eV).

The D type macrocell structure is shown in figs. 3.13 and 3.15. They are the fragments of ZR-6 assemblies (pitch 12.7 mm, enrichment 3.6%, see description in (TIC-1, 1985)). The external part of macrocells is presented by one (for macrocell 1) or two (for macrocell 2) layers of water cells. The macrocells are bounded by symmetry planes. The central macrocell cell is the absorber ($B_4C + H_2O$) in macrocells 1 and 2 or the water hole (macrocell 3 is surrounded by the one water cell layer similar to macrocell 1).

For the thermal group the calculation results are shown in figs. 3.14 and 3.16. These results are obtained:

- by MCU code,
- by using the (V) design model,
- by using the (S) design model.

The group cross-sections, the diffusion coefficients and the source distribution for S and V models were calculated by MCU code simultaneously with benchmark calculations. So the single source of differences between

three calculations are the approximations in V and S model because the same data base and the exact calculation of the equation coefficients are used.

The macrocell 1 parameters needed for the thermal flux calculations with use of the fine mesh equations are shown in fig.3.17.

The other group parameters are given in the Appendix (Fig.3.22 - 3.25).

The S-model diffusion coefficients were calculated by using both the values of the surface currents and flux and using the leakage values. The table 3.1 of Appendix contains the necessary information.

The results of the examples used for illustration hardly differ one from the others. They are not sensitive to the choice of S or V model and very close to Monte Carlo results. It may be concluded that the main effect which should be taken into account is the spectral effect which may be described in the Bonalumi approximation.

Numerical results confirm the conclusions made in Chapter 5 that earlier observed discrepancies between experiment and calculations may be reduced significantly by using the Bonalumi or spectral index methods.

Evidently the more exact approximations may be necessary in more complex cases.

Cell numbers				Material numbers					
			28						2
		6						1	2
		5	27					1	2
		4	11				1	1	2
	3	10	26				1	1	2
2		9	15		1		1	1	2
1	8	14	25		1		1	1	2
7		13	18		1		1	1	2
	12	17	24			1	1	1	2
		16	20				1	1	2
		19	23				1	1	2
		21						1	2
		22							2

1 - ($\text{UO}_2 + \text{H}_2\text{O}$) Cell, 2 - H_2O , 3 - ($\text{B}_4\text{C} + \text{H}_2\text{O}$) Cell

Energy release	$\times 10^4$	
		499
		393
		338 454
		303 367
	260	325 441
	294	361
	260	326 443
	301	366
		335 460
		391
		498

Fig. 3.13 Macrocell 1. Structure and energy release.

three calculations are the approximations in V and S model because the same data base and the exact calculation of the equation coefficients are used.

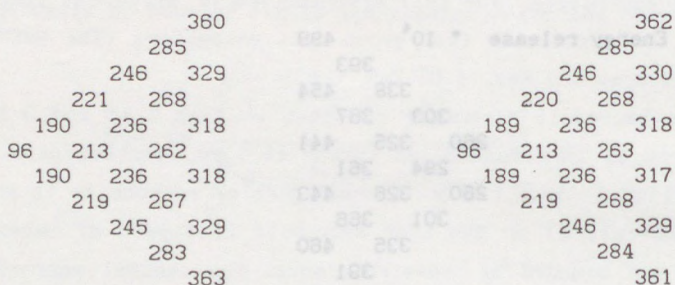
The macrocell 1 parameters needed for the thermal flux calculations with use of the fine mesh equations are shown in Fig. 3.17.

The other group parameters are given in the Appendix (Fig. 3.22 - 3.25).

The S-model diffusion coefficients were calculated by using both the values of the surface currents and flux and the leakage values. The table 3.1 of Appendix contains the results of the calculations. The results of the calculations are very close to Monte Carlo results. The results of the calculations are very close to Monte Carlo results. The results of the calculations are very close to Monte Carlo results.

Numerical results confirm the calculations. The results of the calculations are very close to Monte Carlo results. The results of the calculations are very close to Monte Carlo results.

Evidently the more exact approximation is necessary in more complex systems.



(S) model calculation

(V) model calculation

Fig. 3.14 Thermal flux distribution in Macrocell 1.

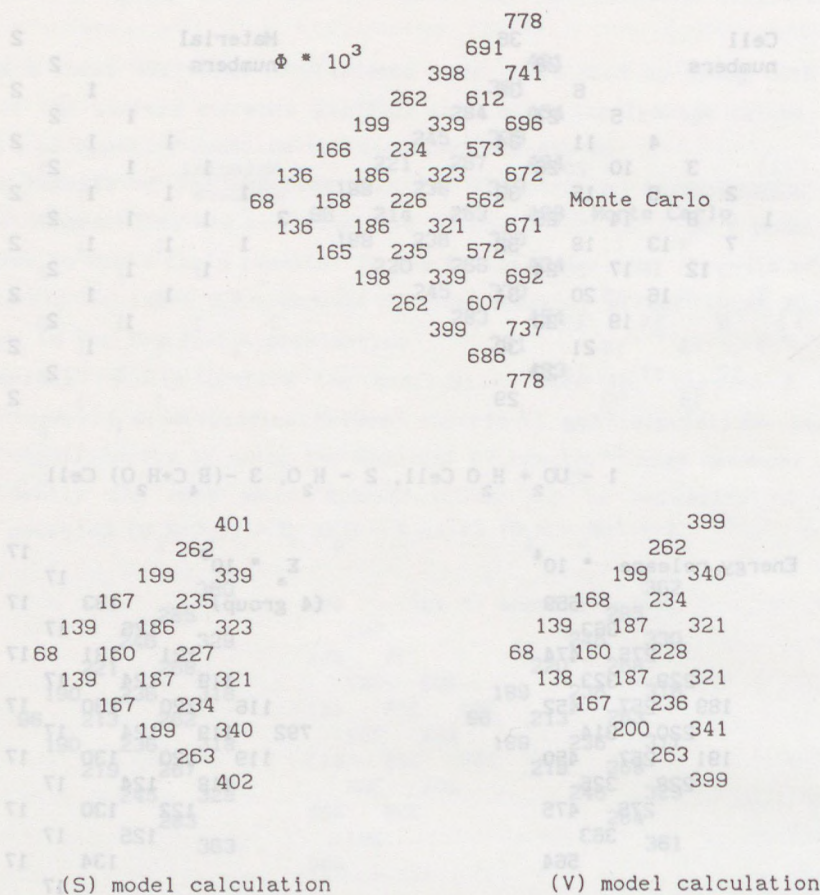


Fig. 3.16 Thermal flux distribution in Macrocell 2.

- Leakage*10 -60
 26
 12 -61
 6 20
 2 9 -60
 -1 4 18
 81 1 8 -60
 -1 4 18
 2 9 -60
 5 20
 12 -61
 26
 -61

Absorption
 rates
 * 10³
 11
 63
 48 10
 40 57
 36 45 10
 30 39 55
 106 35 44 9
 30 39 55
 36 45 10
 40 57
 48 10
 63
 11

($\tilde{\Phi}/\bar{\Phi}$)*100 96
 110
 109 96
 109 110
 108 109 96
 108 109 110
 173 108 109 96
 108 109 109
 109 109 96
 109 110
 109 96
 110
 96

$\bar{\Phi} \cdot 10^3$ 481
 361
 284 454
 245 329
 220 267 434
 188 236 319
 96 214 263 428
 188 236 319
 220 266 434
 245 329
 283 454
 361
 484

$\Sigma_a \cdot 10^3$ 16
 126
 121 16
 118 124
 116 120 16
 116 118 123
 796 116 119 16
 115 118 124
 116 120 16
 118 124
 120 16
 125
 16

$\nu \Sigma_f \cdot 10^3$ 217
 208
 204 214
 200 206
 199 203 213
 201 206
 199 202 214
 200 206
 204 214
 208
 216

Fig 3.17 Macrocell 1 parameters for thermal group

Full number of particles 4000200. $K_{eff} = 1.3772$.

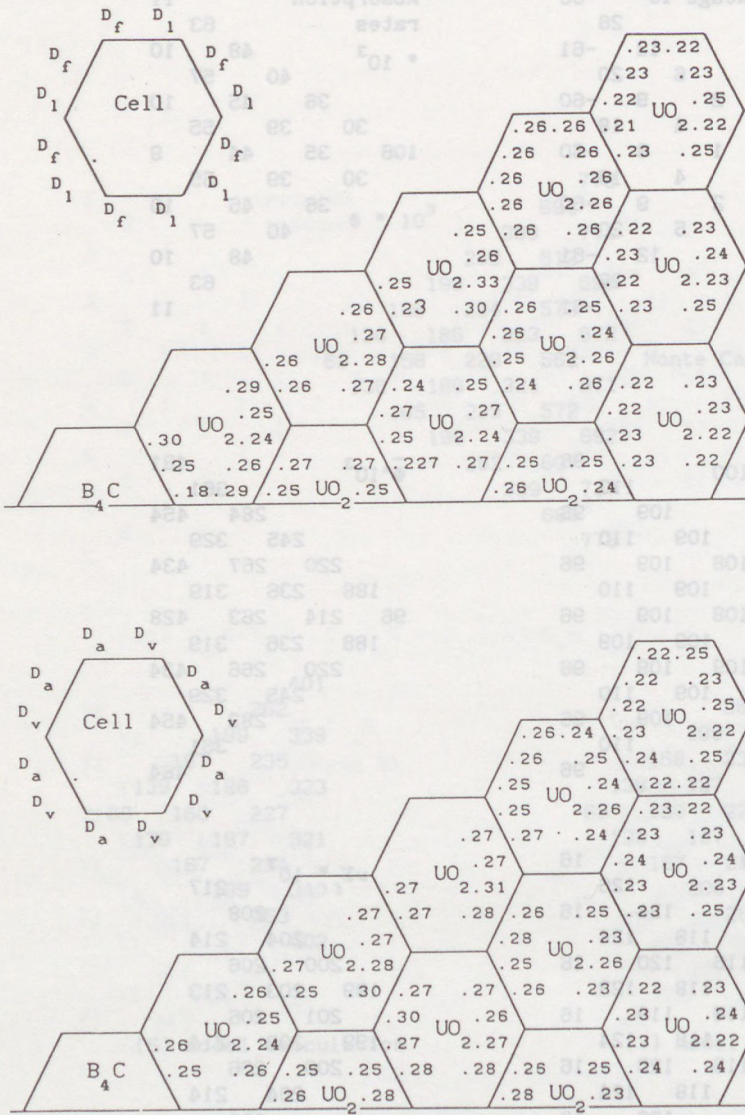


Fig. 3.18 Macrocell 1. The cell diffusion coefficients.

D_f, D_l, D_a are the S-model diffusion coefficients calculated for scalar flux, level and albedo flux formalisms respectively. Eq.(3.4.48) was used. D_v are the V-model diffusion coefficients, calculated by Eq.(3.4.17)

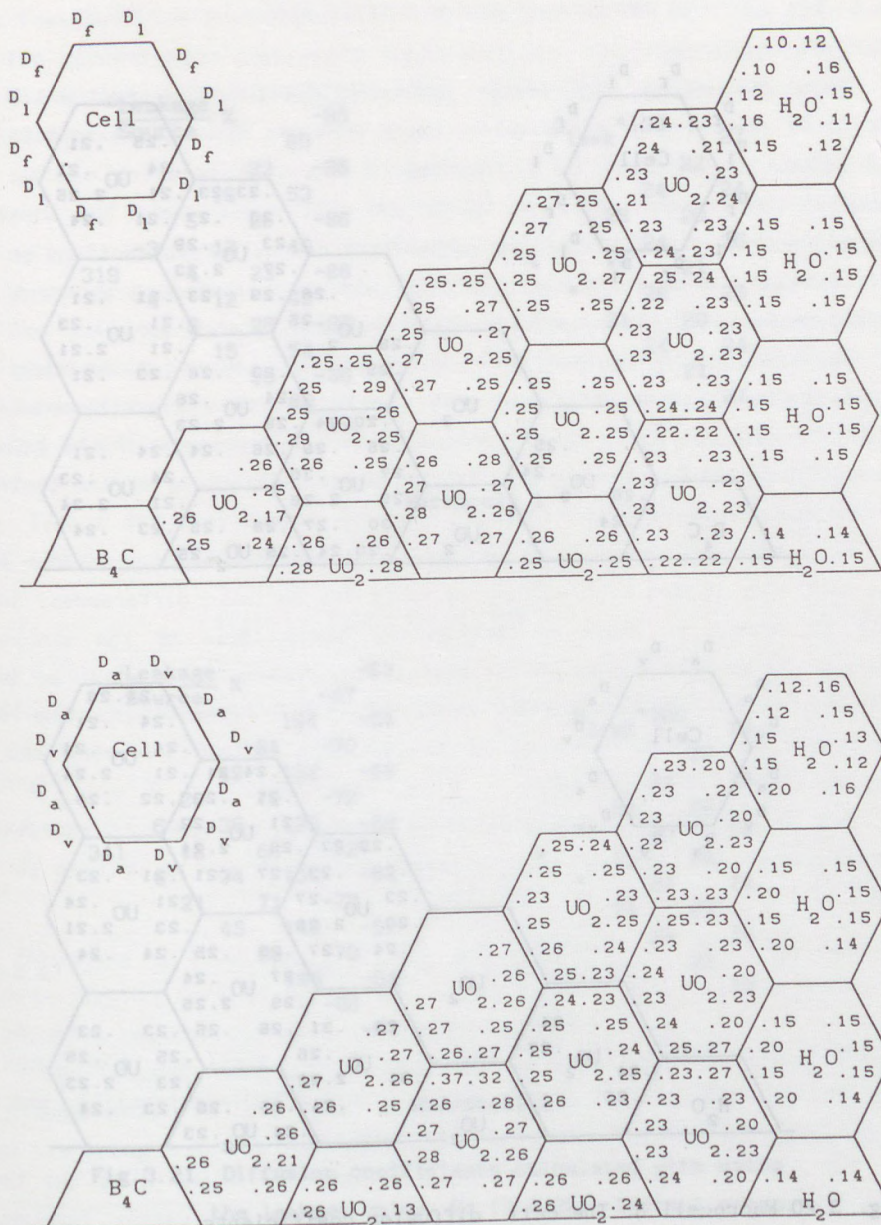


Fig. 3.19 Macrocell 2. The cell diffusion coefficients.

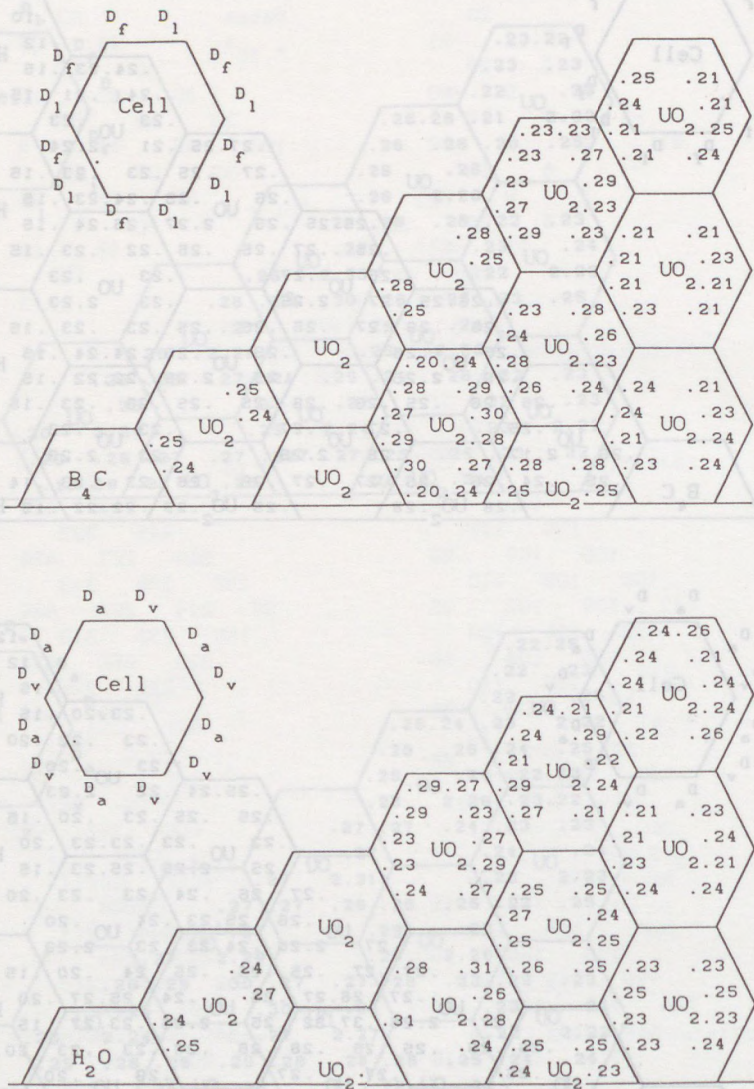


Fig. 3.20 Macrocell 3. The cell diffusion coefficients.

D_s, D_b, D_l are the S-model diffusion coefficients calculated for scalar flux. D_a, D_v are the V-model diffusion coefficients, calculated by Eq. (3.4.17). The cell diffusion coefficients for the S-model and V-model are used, respectively, in the calculation of the macrocell diffusion coefficients.

3.4.4 THE ADVANCED ENGINEERING METHOD VERIFICATION

When discussing the design code verification in Sect.3.4.3 we restricted ourselves by the simplest cases when one may neglect by both the cell source distribution as a function of the cell position and by the diffusion coefficient variation along the cell edges. Only the Bonalumi type approximation describing the dependence of cell cross sections on the position was discussed. Though mentioned was about analogous approach for the diffusion coefficient approximations (see Eqs.(3.4.12,13)).

The advanced approaches were developed as a means of avoiding the mentioned restrictions (cf.Chapters 6 and 7). The new algorithms may be verified using the Monte Carlo codes also in the framework of the general approach described in Sect.3.4.1. This work was carried out on the basis of the MCU code in particular.

As a rule the new methods are based on the synthesis approach. Also they have many common lines naturally there are definite differences. So it would be useful to describe shortly the basic ideas of the synthesis approach. It is most convenient to discuss the common lines mentioned using the well known response matrix formalism. This formalism is the most convenient for the application of Monte Carlo codes to verify and to validate the new methods.

Let us consider the lattices of cells having N edges. In the lowest approximations the response matrix method equations may be written in the form:

$$I(g) = \sum_{g'=1}^G \hat{\Gamma}(g, g') \Phi(g') + Qi(g) \quad (3.4.50)$$

Here the matrix $\hat{\Gamma}(g, g')$ and the vector $i(g)$ are the equation coefficients considered as fixed. Matrix $\hat{\Gamma}$ have $N \cdot N$ dimensionality, and all the vectors in Eq.(3.4.50) are N -dimensional ones.

The variables g, g' are the energy group numbers and G is the total group number; Q is the source integral power. The vector components $I_n(g)$, $\Phi_n(g)$, $i_n(g)$ are to be referred to the cell edges having the subscripts n ($n=1, \dots, N$).

As above (see Sect.3.4.3) $I_n(g)$ and $\Phi_n(g)$ are the edge currents and the "fluxes" respectively. Again the "fluxes" $\Phi_n(g)$ may be considered as any of the angular flux moments: the scalar flux, the albedo flux, the

level (see Eqs. (3.4.8-9)).¹⁾

The current-flux continuity conditions and the expressions allowing one to calculate the x-type reaction rates $R^{(x)}$ should be added to Eq. (3.4.50) as follows:

$$I(g) = I'(g) \quad (3.4.51)$$

$$\Phi(g) = \Phi'(g) \quad (3.4.52)$$

$$R^{(x)} = (r^{(x)}, \Phi) + Qr_0^{(x)} \quad (3.4.53)$$

Here symbol "'" is used to mark the neighbouring cell flux and current.

The response matrix Eqs. (3.4.50-53) added by the external boundary conditions allow one to calculate all the transport equation functional. It should be noted that these equations have many options yet. The most known ones are as follows.

1. For the criticality problems one may consider Q to be equal to zero. Then $\hat{\Gamma}$ matrices depend on K_{eff} parametrically: $\hat{\Gamma} = \hat{\Gamma}(g, g', K_{eff})$, and Eq. (3.4.50) transforms into:

$$I(g) = \sum_{g'=1}^G \hat{\Gamma}(g, g', K_{eff}) \Phi(g') \quad (3.4.54)$$

2. The approximative $\hat{\Gamma}$ matrix parameterization may be utilized. For this goal one may use Eq. (3.4.53) having in mind the neutron generation rate $R^{(\nu)}$ as $R^{(x)}$. Introducing the K_{eff} definition into (3.4.53) and considering Q as the second neutron generating power one has:

$$R^{(\nu)} = \frac{1}{K_{eff}} \left[(r^{(\nu)}, \Phi) + Qr_0^{(\nu)} \right] \quad (3.4.55)$$

Excluding Q from Eqs. (3.4.50) and (3.4.55) one gets the special parameterization form of the $\hat{\Gamma}$ matrix. As a result Eq. (3.4.54) describes the relation between the currents and fluxes again.

3. The response matrix equations may be considered for every energy group separately. In this case, matrix $\hat{\Gamma}$ depends only on the one argument to be the group number g and the global reactor problem is solved as usual

¹⁾ One should notice the small difference of Eq. (3.4.50) from the traditional response matrix equations where the one side currents are mostly used. Though this difference is not a principal one the (3.4.50) type equations for the arbitrary moments were referred to in (Maiorov et al, 1970) as the Surface Flux Method equations to mark the small detail mentioned. Evidently for the "albedo" fluxes both equation forms are equivalent.

in group by group order. It seems that for the few group WWER calculation this approach is the optimal one (taking into account the simple additional recipes, described in Sect.6.1 as being analogous to the Eqs.(3.4.8-9) for Fick's law).

Similar to the traditional design methods all the problem may now be divided into two parts: calculation of the coefficients of Eqs.(3.4.50) and (3.4.54) and the final response matrix equation solution. Initially we shall consider the first problem.

For two-dimensional symmetrical cells it is usually assumed that $\hat{\Gamma}$ -matrices depend on the edge number as follows:

$$\hat{\Gamma}_{nm} = \hat{\Gamma}_{|n-m|} \quad (3.4.56)$$

So in this approximation the $\hat{\Gamma}$ -matrices have only $[N/2]+1$ different components (for the fixed g and g' values). It gives the very pleasant possibility solving only one model problem to determine all the matrix elements corresponding to the neutron flying into the cell through any of its edge and belonging to g' group. Evidently it is supposed that the angular, the energy and the space flux edge distributions are a priori fixed. But this simplification is a tricky one. In (Maierov et al, 1970) it was shown that for WWER type lattices a similar approach to calculating $\hat{\Gamma}$ -matrices leads to about 10% errors in the reaction rates.

However the accuracy problem may be solved and the accuracy may be increased significantly in the framework of Eqs. (3.4.50-53). It requires utilizing the less simplified approach to calculating the $\hat{\Gamma}$ -matrices than mentioned above.

Let us propose that the neutron spectrum in identical cells having different surroundings may be well approximated by a superposition of some arbitrary trial functions. Let their number be equal to $N \cdot G + 1$.

$$\Psi(r, v) = \sum_{n=1}^{NG} C_n \Psi_n(r, v) + Q \Psi_0(r, v) \quad (3.4.57)$$

It is obvious that in this approximation all the identical cell parameters of Eqs.(3.4.50) and (3.4.52) are constant and do not depend on the identical cell positions inside the reactor. These coefficients depend only on the chosen set of functions approximating the flux inside the cells.

But on the other hand Eq.(3.4.57) allows one to approximate the cell

surface flux much more than one a priori distribution, not changing Eqs.(3.4.50) and (3.4.52). This is the principal reason for increasing the response matrix equation accuracy compared to the trivial traditional response matrix method.

Similarly to the diffusion design methods the coefficients for Eqs.(3.4.50-54) may be calculated before the global reactor calculations. For this goal both the Monte Carlo and the engineering codes may be used.

For the matrix determination it is sufficient to solve $M \geq G \cdot N + 1$ model problems every one on condition that Eq.(3.4.57) is considered to be valid for all model problems. Then matrices may be found by minimizing functionals, constructed on the basis of relations (3.4.50),(3.4.52) connecting currents, fluxes and the reaction rates calculated in model problems. For example, in one group case:

$$\min \sum_{m,n} \left[I_n^{(m)} - \sum_{n'} \Gamma_{nn'} \cdot \phi_{n'}^{(m)} - Q^{(m)} i_0 \right]^2$$

where subscript m is the model problem number.

If the model problem number equals $NG+1$ the coefficients may be calculated as the solution of (3.4.50), (3.4.52).

All the matrices describing the identical cells may be obtained as a byproduct of full scale Monte-Carlo reactor or macrocell calculations. In reactor or macrocell calculations different model problems may be defined such as calculating the fluxes and the currents on the surfaces of identical cells placed in different environments on the condition that neutrons flying into the cell have fixed energy distribution (within different energy groups). The most attractive feature of Monte-Carlo methods is the possibility to solve a set of model problems during one code run (Maierov et al, 1970).

The engineering codes should be modified slightly to calculate the matrices Γ . The new approach (Gado et al, 1983) allowing one to perform similar calculations is described in Sect.6.3.

It seems that the response matrix equations might be directly used in engineering calculations. However in practice (see Chapters 6 and 7) many authors prefer to use the traditional diffusion type equations but based on the same synthesis principle. It is explained mainly by the user's desire to utilize the codes written earlier both for calculating the equation

coefficients and for solving the final reactor equations.¹⁾ In principle it may be carried out by modifying the traditional codes.

As a matter of fact the response matrix method may be reformulated to the form usually considered in calculation practice (see Chapters 6 and 7). For this goal it is enough to transform Eqs.(3.4.50) and (3.4.52), utilizing the other set of basis vectors in the N-dimensional linear space.

Let us expand Φ, I vectors by the non-zero basis vectors e_n , which are defined as follows (cf.(Maierov, 1978, 1983), (Laletin and Elshin, 1980), (Gado et al, 1983), (Maierov and Yudkevich, 1988)):

$$e_n^{(m)} = \begin{cases} \cos\left[2\pi n(m-1)/N\right] \\ \sin\left[2\pi n(m-1)/N\right] \end{cases} \quad (3.4.58)$$

where $n = 0, \dots, [N/2]$ and m are a component number of vectors e_n ($m=1, \dots, N$).

It is obvious that on condition (3.4.53) e_n are the $\hat{\Gamma}$ - matrix eigenvectors, i.e.:

$$\hat{\Gamma}(g, g') e_n = \Lambda_n(g, g') e_n \quad (3.4.59)$$

where $\Lambda_n(g, g')$ is the notation used for the corresponding eigenvalues and the variables g, g' are considered as parameters.

It is obvious that:

$$\Lambda_n(g, g') = \frac{(e_n, \hat{\Gamma}(g, g') e_n)}{(e_n, e_n)} \quad (3.4.60)$$

In the new basis the response matrix equations are transformed in the form:

$$j_n(g) = \sum_{n=1}^G \Lambda_n(g, g') f_n(g') + Q i_n(g) \quad (3.4.61)$$

where $j_n(g), f_n(g), i_n(g)$ - are the I, Φ, i new representations:

¹⁾ It seems that it may be less expensive to rewrite the design reactor calculation codes on the basis of the response matrix method than to modify them taking into account the effects discussed above.

$$\begin{aligned}
 j_n(g) &= (I(g), e_n) / (e_n, e_n) \\
 f_n(g) &= (\Phi(g), e_n) / (e_n, e_n) \\
 i_n(g) &= (i(g), e_n) / (e_n, e_n)
 \end{aligned}
 \quad (3.4.62)$$

It is obvious that both representations of the response matrix equations are equivalent (see Sect 6.3). In the reactor codes both representations have equal rights; moreover it is possible to combine them. But if the second representation is used one can utilize the modified traditional design codes to calculate both the Γ matrices and Λ functions.

In Sect 6.3 the new design approach (Gado *et al*, 1983) is described where the $\Lambda_n(g, g')$ parameters are calculated but the response matrix equations are solved (for this goal the authors proposed the original method also described in Sect.6.3). For the similar combined method the Γ -matrices may be calculated utilizing the transformation.

$$\Gamma_{km}(g, g') = \sum_{n=1}^N (e_n^{(m)}, \Lambda(g, g') e_n^{(k)}) \quad (3.4.63)$$

In (Laletin *et al*, 1980) it is recommended that the second representation as a whole be used. It means that not only Eq.(3.4.61) is utilized, but it is recommended that one should also transform the current-flux continuity equations to the new representation. The authors called their approach as the Surface Harmonic Method (See Chapter 7).

In the above framework the design methods based on the modernized Galanin-Feinberg approach should be mentioned. In (Gorodkov, 1988) and (Kochurov, 1982) it is proposed utilizing $\Lambda_0(g, g')$ and $\Lambda_1(g, g')$ matrices in the modified Galanin-Feinberg type equations. Then the finite difference equations are constructed on the basis of the Galanin-Feinberg diffusion type equation and their coefficients are calculated on the basis of the definite equivalence principle utilizing the fixed $\Lambda_0(g, g')$ and $\Lambda_1(g, g')$ matrices. The design code calculating these matrices is described in (Kochurov *et al*, 1982). The reactor codes (Gorodkov, 1988) and (Kochurov, 1982) based on this approach are widely used in practical calculations for graphite and heavy water reactors.

Finally one should consider the connection between the advanced methods reviewed briefly in this Section and the (S) type methods investigated numerically in Sect.3.4.4.

For the two dimensional lattices having symmetrical cells it is possible to consider the case when only two first azimuthal harmonics of I_n and Φ_n are important. Then from (3.4.61) (Maiorov, 1978), (Maiorov and Yudkevich, 1988) the basic (S) model equations (3.4.28-29) follows:

$$J = \tilde{\Sigma} \frac{V}{S} \tilde{\Phi} - q \frac{V}{S} \quad (3.4.64)$$

$$I_n - J = \frac{2\tilde{D}}{h} (\Phi_n - \tilde{\Phi})$$

where $J, \tilde{\Phi}$ are the current and the flux averaged along all the faces of the cell and:

$$\tilde{\Sigma} = \frac{S}{V} \Lambda_0, \quad \tilde{D} = \frac{h}{2} \Lambda_1.$$

From Eq.(3.4.64) the response matrix equation follows in the form:

$$I_n = \frac{2\tilde{D}}{h} \Phi_n + N^{-1} \left(\tilde{\Sigma} \frac{V}{S} - \frac{2\tilde{D}}{h} \right) \sum_n \Phi_n - q \frac{V}{S} \quad (3.4.65)$$

Thus the (S) model equations may be interpreted as the response matrix equations based on the simplified Γ -matrix defined by Eq. (3.4.65).

The MCU code was utilized for calculating the Γ or Λ matrices in the different representations described above (Gorodkov, 1993), (Maierov and Yudkevich, 1988), (Barkov et al, 1992). It should be noted that the special tally modules were written by Gorodkov and by Barkov et al. These modules calculate $\Lambda_0(g, g', K_{eff})$ parameters (for the angular moment pair current-scalar flux with using the approximate K_{eff} parameterization) and $\hat{\Gamma}(g, g', K_{eff})$ (for the the angular moment pair current-"albedo flux" using the direct calculation of the $\hat{\Gamma}(g, g', K_{eff})$ dependence on K_{eff}).

3.5 First collision probability (FCP) calculations

The first collision probability (FCP) method is one of the most popular ones for the design calculations of the cell parameters. It based on considering the transport integral equation which is solved by the different numerical methods as follows.

The cell or the macro cell is divided into zones. For each of these zones it is supposed that the zone flux may be described by the set of the trial functions. It allows one to reduce the flux evaluation problem to the solution of a system of linear algebraic equations.

The equation coefficients are the multidimensional integrals. For the flat flux approximation these integrals may be interpreted as the first collision probabilities. The FCP describes the neutron possibility to collide in the marked zones, under the condition that neutrons are born in the other zones. It is supposed that the birth events are described by an uniform probability density function.

For the complex geometry objects the basic efforts are usually concentrated on the calculation of multi-dimensional integrals, describing FCP. The Monte-Carlo (MC) codes allows one to use the effective tools for calculating these integrals. These tools are the geometrical modules (GM) for solving the problem of calculating the path lengths in the various regions crossed by particles between collisions.

In principle the Monte Carlo codes may be used to calculate FCP but computer time needed is too large. From the other hand FCP may be calculated much faster than by the direct Monte Carlo method not losing the high accuracy. At the same time it is possible to utilize the earlier elaborated Monte Carlo geometry module for faster calculations..

The new approach was proposed (Gomin and Maiorov, 1981) allowing one to realize the above possibility. It is based on using the known Monte Carlo method interpretation as utilizing the simple quadrature formula for evaluating the multidimensional integrals. That formula allows one to calculate the multi-dimensional integrals J by transforming the integration domain into an unit cube (by transforming the integration variables). It may be written in the form:

$$J = N^{-1} \sum_{n=1}^N f(\gamma_n) \quad (3.5.1)$$

where γ_n is the point vector in multi-dimensional unit cube and $f(\gamma)$ is the function integrated over the cube. Equation (3.5.1) is the basic one used in the Monte Carlo method on the condition that γ_n points are the ones distributed randomly.

The new approach is based on applying Eq.(3.5.1) to FCP calculations utilizing the improved integration point nets including the different so-called uniformly distributed sequences (cf. (Holton, 1960, Korobov, 1963, Sobol, 1973, 1979)). On the other hand Eq.(3.5.1) allows one to utilize the Monte Carlo code geometry modules in the FCP codes. Both factors means that one can calculate FCP for the complex system effectively enough. We shall describe now the above approach in more details.

Let us consider the whole system (R) to be divided into a finite number of closed regions R_1 (zones) having volumes V_1 .

For 3-dimensional systems the probability that a neutron born in the zone numbered i will experience the first collision in zone j , is expressed by a 5-dimensional integral:

$$P_j^i = \oint_{R_1} \frac{d\Omega}{4\pi} \int \frac{dr}{V_1} f_j(r, \Omega) \quad (3.5.2)$$

Here $f_j(r, \Omega)$ is the probability that a neutron, born at point r and having flight direction Ω , will experience the first collision in j .

One may consider that $f_j(r, \Omega)$ may be presented in the form:

$$f_j(r, \Omega) = \exp(-\tau_j(r, \Omega)) (1 - \exp(-\Delta\tau_j(r, \Omega)))$$

where τ_j - is the optical distance travelled by the neutron from point r until the first intersection with surface i of zone j . $\Delta\tau_j(r, \Omega)$ - is the optical distance, travelled inside zone j .

Since $1/(4\pi V_1)$ may be considered as the probability density function of a neutron's birth, we may proceed to new variables in Eq. (3.5.2):

$$r = r(\gamma_1, \dots, \gamma_5) = r(\gamma); \quad \Omega = \Omega(\gamma_1, \dots, \gamma_5) = \Omega(\gamma),$$

where $d\gamma = d\gamma_1 \dots d\gamma_5 = (4\pi V_1)^{-1} dr d\Omega$ and all the values γ_i are the point coordinates in a 5-dimensional unit cube, i.e. $0 < \gamma_i < 1$.

In new variables, probability P_j^1 is expressed in the form:

$$P_j^1 = \int d\gamma f_j(r(\gamma), \Omega(\gamma))$$

The integral may be calculated using Eq. (3.5.1):

$$P_j^1 = N^{-1} \sum_{n=1}^N f_j(r_n, \Omega_n) \quad (3.5.3)$$

where $r_n = r(\gamma^{(n)})$; $\Omega_n = \Omega(\gamma^{(n)})$ and $\gamma^{(n)}$ - are the coordinates of points, chosen "at random", in a unit 5-dimensional cube.

At the same time (3.5.3) is a standard formula of the approximate integral calculation after the necessary replacement of variables is made. It is common knowledge (Sobol, 1973) that Monte Carlo integration is just a particular case of applying this quadrature formula, on the condition that a certain net is chosen. It is also known that a such net is not an optimal one (cf. Sobol, 1973, 1979).

The quality of a "random" net is determined by the equation justified for the large N values:

$$|W - n/N| \approx CN^{-0.5},$$

where W is the volume of any considered region of a unit cube and n is the number of those points from the general number N , which are falling into region W .

It is the reason why the application of Eq. (3.5.3) leads to an error of order $N^{-0.5}$.

The nets are known characterized by the knots distributed more uniformly in the unit cube. For similar nets the following equation is satisfied:

$$|W-n/N| \approx C/N.$$

For a wide class of functions the usage of similar nets in Eqs. (3.5.1) and (3.5.2) leads to an error of order $N^{-(1-\varepsilon)}$ (where ε is an infinitely small number).

So, on the one hand the FCP calculation algorithm has good convergency on the condition that "good" nets are employed and on the other hand the Monte Carlo algorithm differs from that only by knot choice from the formal point of view. It permits one to utilize efficiently the Monte Carlo code geometry modules for calculating of FCP.

The *PIJMMK* and *VEPS* code calculating FCP by utilizing approach described were elaborated (Gomin and Maiorov, 1985). The modern *VEPS* version (Gomin, Gurevich, 1992) allows one to utilize the universal type geometry modules that satisfy to the *MCU* standard. *PIJMMK* and *VEPS* use the various quadrature nets and various quadrature schemes describing the FCP integrals. In particularity it is used possibility to introduce the integral dimensionality performing the integration part analytically.

The *WERTER* and *PERST* codes (Gomin, 1985) are also elaborated. They solve the thermalization problems calculating the thermal neutron flux functionals. In practice, it is usually to use the quadrature nets having the number of knots varying from several hundreds to several thousands. For real objects (*WVER* macrocells), divided into many zones, it permits one to achieve an accuracy about 1% for the neutron fluxes.

Now *PERST* is used both as the *MCU* thermal sub module permitting one to perform deterministically part of calculations (Gomin, 1992) and as sub medullae of the set of deterministic codes. The results the *ZR-6* macrocell calculations are contained in (Gomin and Maiorov, 1981).

REFERENCES^{*})

Abagyan L et al (1964) The group constants for the reactor calculations. In Russian.

Абагян Л.П., Базазянц Н.О., Бондаренко И.И., Николаев М.Н. Групповые константы для расчета ядерных реакторов. Москва. Атомиздат. 1964.

Abagyan L.P., Bazazyants N.O., Nikolaev M.N., Tsybulya A.M. (1981) Group Constants for Reactors and Shielding Calculation. Energoizdat. Moscow. In Russian.

Абагян Л.П., Базазянц Н.О., Николаев М.Н., Цибуля А.М. Групповые константы для расчета реакторов и защиты. Справочник. Москва. Энергоиздат. 1981.

Abagyan L.P., Tebin V.V., Yudkevich M.S. (1984) CROSS - code and constants library for cross sections calculation in resolved resonances region. Kurchatov Institute IAE-4009/5. In Russian.

Абагян Л.П., Тебин М.С., Юдкевич М.С. CROSS - пакет программ и библиотек для расчета сечений в области разрешенных резонансов. Препринт ИАЭ-4009/5, М., 1984.

Abagyan L.P., Yudkevich M.S. (1981). Kort library. Voprosy Atomnoy Nauki i Tekhniki (VANT) Series: Yadernye Constanty. V 1(40), p. 39. In Russian.

Abagyan L et al (1989). Neutron data for calculating the thermal reactors.

Абагян Л.П., Просветова М.П., Юдкевич М.С. Нейтронные данные для расчета тепловых реакторов. ВАНТ. Сер. Ядерные константы. 1989. Вып 4, с.3ю

^{*}) VANT: The problems of atomic science and technique journal. In Russian. (Вопросы атомной науки и техники). It is published in the form of special series. The "Physics of nuclear reactors" series is issued by RNC Kurchatov's Institute.

Abagyan L.P., Alekseev N.I., Gomin E.A., Gurevitch M.I., Maiorov L.V. Marin S.V., Rogov A.D., Romanov A.C., Yudkevich M.S. (1991) The MCU 2 code. In Russian.

Л.П.Абагян, Н.И.Алексеев, Е.А.Гомин, М.И.Гуревич, Л.В.Майоров, С.В.Марин, А.Д.Рогов, А.С.Романов, М.С.Юдкевич

Пакет программ MCU-2 для расчета методом Монте-Карло нейтронно-физических характеристик ядерных реакторов.

том 1. Общее описание.

том 2. Константное обеспечение.

том 3 Архитектура пакета

Отчет ИАЭ Инв.36/1-1493-91

Alekseev et al (1991). The MCU-1 code verification. In Russian. Алексеев Н.И., Брызгалов В.И., Владимирова Т.М., Гомин Е.А., Капитонова А.В., Майоров Л.В., Носовский И.В., Юдкевич М.С. Верификация константного обеспечения версии MCU-1 применительно к реакторам с водой в качестве замедлителя.

Препринт ИАЭ-5407)5. Москва. 1991.

Alekseev et al (1991). The CLAD library for validating the MCU code. In Russian. Н.И.Алексеев, В.И.Брызгалов, Т.М.Владимирова, А.В.Капитонова, С.В.Марин, В.А.Чистякова, М.С.Юдкевич

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Содержание библиотеки расчетных заданий CLAD.

Версия CLAD-2. Отчет ИАЭ Инв.36-1/769/92

Allen P.R. (1971). Verbal communication at the EACRP meeting on heterogenous methods. Paris.

BAW-1810, DOE/ET/34212-41. (1984). UC-78 Urania Gadolinia: Nuclear Model Development and Critical Experiment Benchmark.

Becker R., Pshenin V., Lazarenko A., Alekseev N., Vaneev Yu. (1990). Results of Spectral Codes Verification using Numerical and Experimental Benchmarks. Kernenergie, Vol.33, No 8, pp 335-341.

Benoist P. (1964). Theorie du coefficient de diffusion des neutrons dans un reseau comportant des cavites. Report CEA R 2278.

- Berna Ph. (1973) Comparison between Benoist and Selengut diffusion coefficients in one-velocity theory, when absorbing media are present in the cell. Jour. Nucl. Enrg. v.27, p.633.
- Bonalumi R.A. (1971). A unified theory of cell diffusion coefficient. Energia Nucleare. v.18, n.7/8, p.395.
- Bonalumi R.A. (1973). A rigorous diffusion model for cell homogenization. Energia Nucleare. v.20, n.1, p.39.
- Bonalumi R.A. (1974) Diffusion equation and cell homogenization made rigorous. Energia Nucleare. v.21, N4, p.231.
- Brissenden R.J., Garlick A.R. (1986). Biases in the estimation of k_{eff} and its error by Monte-Carlo methods. Ann. Nucl. Energy, Vol. 13, No.2, pp.63-68
- Bryzgalov V.I., Gomin E.A., Gurevich M.I., Kaminsky A.S., Subbotin E.S., Tebin V.V. (1989) Calculation and Experimental Research of Double Heterogeneity Fuel Elements of HTGR. VANT. Series Fizika i Tekhnika Yadernykh Reaktorov (FiTYR), V 2, pp. 44-50. In Russian.
- Deniz V.C. (1986). The theory of neutron leakage in reactor lattices. CRC-handbook of Nuclear Reactors Calculations. V.2, p.409. CRC Press Inc.
- ENDF-202.THERMAL REACTOR BENCHMARK COMPILATION. June 1974
- Gado J., Devenyi A., Kereszturi A., and Makai et al. (1984). A new approach for calculating non-uniform lattices. Ann. nucl. Energy 11, 559.
- Gelbard E.M., Prael R.E., (1974). Report ANL-75-2.(NEACRP-L-118), 202.
- Gelbard E.M., Pego R., (1979). Monte-Carlo Computation of Directional Diffusion Coefficients Proceedings of the Topical Meetings on Computational Methods in Nuclear Engineering. v.2, p.7-9. USA, Virginia. April 23-25.

- E.M.Gelbard (1991) Present Status and Future Prospects of Neutronic Thermalization. Prog. in Nucl. Ener. V 24, N 1-3, p.3.
- E.A.Gomin and L.V. Maiorov (1981). The Thermalization codes. In Russian.
Гомин Е.А., Майоров Л.В. Пакет программ для нейтронно - физических расчетов в области термализации. Материалы 10 симпозиума ВМК. Ереван. Изд. ИАЗ. С.547. 1981.
- E.A.Gomin and L.V. Maiorov (1981). On the Computation of Probabilities of the Collisions in the Systems with Complicated Geometry. Voprosy Atomnoy Nauki i Tekhniki, Series: Fizika i Tekhnika Yadernykh Reaktorov, 8(21), p. 62. In Russian.
- Gomin E.A., Maiorov L.V. (1981b) The codes for calculating thermalization effects. In Russian.
Пакет программ для нейтронно-физических расчетов в области термализации. Материалы 10 симпозиума ВМК. Ереван 1981 г.
- Gomin E.A., Maiorov L.V. (1982) TERMAC - the Program Complex for Calculation of Neutron Group Cross Sections in Thermalization Region. VANT, Series FiTYR, V 5(27), pp 70-73. In Russian.
Гомин Е.А., Майоров Л.В. Комплекс TERMAC для расчета групповых сечений нейтронов в области термализации. ВАНТ. Физика и техника ядерных реакторов. 1982. Вып.5(27). С.70-73.
- Gomin E.A. (1985). PERST Code for Thermal Neutrons Functionals Calculations in Three Dimensional Systems. Kurchatov Institute IAE-4208/5. In Russian.
Гомин Е.А. Программа ПЕРСТ расчета функционалов потока тепловых нейтронов в трехмерных системах. Препринт. ИАЗ-4208/5. М.. 1985.
- Gomin E.A., Maiorov L.V. (1985). VEPS Code for First Collisions Probabilities Calculations in Three Dimensional Systems. Kurchatov Institute IAE-4207/5. In Russian.
Гомин Е.А., Майоров Л.В. Программа ВЕПС для расчета вероятностей первых столкновений в трехмерных системах. Препринт. ИАЗ-4207/5. М.. 1985.

- Gomin E.A., Kapitonova V.I., Kononov S.L., Maiorov L.V. Marin S.V., Yudkevich M.S. (1987). Experimental Data Analysis for validating nuclear data. In Russian. *Вестн. АЭС*, v.27, p.533.
- Гомин Е.А., Капитонова А.В., Кононов С.Л., Майоров Л.В., Марин С.В., Юджевич М.С. Анализ экспериментов на критических сборках с целью проверки константного обеспечения реакторных расчетов. Доклад на XVI Симпозиуме специалистов ВМК по физике ВВЭР. Москва. Сентябрь 1987.
- Gomin E.A., Maiorov L.V. (1988). Monte-Carlo Method Usage for Precision Analysis of Heterogeneous Reactors Calculation Modern Methods. VANT, Series FiTYR, V 2, pp 24-33. In Russian.
- Гомин Е.А., Майоров Л.В. Использование метода Монте-Карло для проверки точности современных методов расчета гетерогенных реакторов. ВАНТ. Сер. Физика и техника ядерных реакторов. 1988. Вып. 2. С. 24.
- Gomin E.A., Maiorov L.V., Yudkevich M.S. (1991). Some Aspects of Monte-Carlo Method Application to Nuclear Reactors Analysis. Prog. in Nucl. Ener. V 24, N 1-3, p. 211.
- Gorodkov S.S. (1984). HEM-3 code. In Russian.
- Городков С.С. Аннотация программы HEM=3. ВАНТ. Сер. Физика и техника ядерных реакторов. 1984, вып.8(45), с.40=41.
- Gorodkov S.S. (1988). Comparison of mesh algorithms for calculating the neutron fields. In Russian.
- Городков С.С. Сравнение сеточных алгоритмов расчета нейтронных полей в больших реакторах. АЭ, 1988, т.65, вып.3, с.184=190.
- Gorodkov S.S. (1989). The Limit Error of Modern Mesh Algorithms for Calculation of Neutron Flux in RBMK. Atomn. Energ. 68, p. 155. In Russian.
- Городков С.С. Предельная погрешность современных сеточных алгоритмов при расчете нейтронных полей в РБМК. АЭ, 1990, т.68, вып.3, с.155.
- Gorodkov S.S. (1990). About discrepancies of the certain 3D-algorithms for calculating the neutron fields. In Russian.
- Городков С.С. Погрешность некоторых сеточных алгоритмов при трехмерном расчете нейтронных полей в РБМК. АЭ. т.69, вып.1, 1990.

- Gurevich M.I. (1990). First Collisions Probabilities Calculations for Compact Systems. Kurchatov Institute IAE-5122/5. In Russian.
- Gurevich M.I., (1990). First Collisions Probabilities Calculations for Poly-cells. Kurchatov Institute IAE-5123/5. In Russian.
- Gurevich M.I. and Gomin E.A. (1991). Application of the geometrical module of Monte Carlo method for the first collisions probabilities method with the expanding in the spherical modes. Proc. of the Int. Top. Meeting Adv. in Math., Comp. and Reac. Phys. April 28- May 2, 1991, Pittsburgh, PA, USA, p. 2.2 3-1.
- Halton J.H. (1960). On the Efficiency of Certain Quasi-Random Sequences of Points in Evaluating Multi-Dimensional Integrals, Numer. Math., 27, N 2 p 84
- Hrennikov N.N., Stchukin A.V. (1988). Analysis of calculations and experiments for the uranium-graphite lattices. In Russian.
- Хренников Н.Н., Шукин А.В. Сравнительный анализ расчета и эксперимента для уран-графитовых решеток на природном и слабообогатенном уране. Препринт ИАЭ-4709/4, М., 1988г.
- Kvartzhely A.Yu., Kochurov B.P. (1985). Method for calculating the cell physical parameters. In Russian.
- Кварцхели А.Ю., Кочуров Б.П. Метод вычисления физических характеристик ячейки гетерогенного реактора. АЭ, 1985, т.58, вып.2, с.83=91.
- Korobov N.M., (1963). Theoretically-Numerical Methods in Approximate Analysis. Fizmatgiz, Moscow. In Russian.
- Kochurov B.P. (1980) Numerical methods of the heterogeneous reactor. In Russian.
- Кочуров Б.П. Численные методы в теории гетерогенного реактора. Атомиздат, М., 1980.
- Kurka R. et al (1981). The two-dimensional non-uniformity investigation. In Russian.
- Р.Курка и др. Исследование двумерных неоднородностей. Материалы 9 симпозиума ВМК. СРР, Ереван, с.350. 1981 г.

- Laletin N.I., Elshin A.V. (1977). Increasing the homogenization method accuracy. In Russian.
- Лалетин Н.И., Ельшин А.В. Уточнение метода гомогенизации гетерогенного реактора. АЭ, 1977, т.43, вып.4, с.247.
- Laletin N.I., Elshin A.V. (1980). The Derivation of Finite-difference Equations for Heterogeneous Reactors. Kurchatov Institute IAE-3280/5. In Russian.
- Лалетин Н.И., Бояринов В.Ф. (1985). The efficient diffusion coefficient. In Russian.
- Лалетин Н.И., Бояринов В.Ф. Эффективный одnogрупповой коэффициент диффузии нейтронов в решетках реакторов. АЭ, 1985. т.59, вып.2, с.91.
- Leman M. (1978). The spectral index method. In Russian.
- Леман М. Расчет влияния неоднородности решетки на диффузионные константы элементарных ячеек методом спектральных индексов. Материалы 7-ого Симпозиума ВМК, 2, 300, Дзержинское, 1978.
- Leslie D.C. (1963) Report AEEW-M-292.
- Lieberoth J. (1968). A Monte Carlo Technique to solve the static eigenvalue problem. Nukleonik 11. Band 5. Heft, 203.
- Liman G.F., Maiorov L.V. (1981) The NEWRAS Program for Computation of the Slow Neutron Scattering Cross Sections. VANT.Series: FiTYR 8(21), pp. 32-38. In Russian.
- Лиман Г.Ф., Майоров Л.В. Программа NEWRAS для расчета дифференциальных сечений рассеяния медленных нейтронов. Вопросы атомной науки и техники. Сер. Физика и техника ядерных реакторов. 1981. Вып.8(21), С. 32-38.
- Liman G.F. (1982) Codes CALCST and ELCOHR for Calculation of Total and Elastic Coherent Scattering Cross Section for Thermal Neutrons. In Russian.
- Лиман Г.Ф. Программа CALCST и ELCOHR для расчета полных и упругих когерентных сечений рассеяния медленных нейтронов. Вопросы атомной науки и техники. 1982. Сер. Физика и техника ядерных реакторов. 1982. Вып.5(27). С.74.

- Liman G.F., Maiorov L.V and Yudkevich M.S.. (1985) The MCU code. In Russian.
- Лиман Г.Ф., Майоров Л.В., Юдкевич М.С. Пакет программ MCU для решения методом Монте-Карло задач переноса излучений в реакторах// Вопросы атомной науки и техники. Сер. Физика и техника ядерных реакторов. 1985. Вып.7. С.27-31.
- Lux I. (1978). Remark on the efficiency of tack-length estimators in reaction rare estimators. Nucl. Sci. Eng. 66, p.258.
- Lux I. (1978). Systematic study of some standard variance reduction techniques. Nucl. Sci. Eng. 67, p.317.
- Lux I. and Koblinger L. (1991). Monte Carlo methods and photon transport calculations. CRC - book.
- Maiorov L.V., Frank-Kamenetsky A.D. (1969) Comparative efficiency of various Monte Carlo estimators. Preprint IAE-1791. Moscow. In Russian.
- Maiorov L.V., Frank-Kamenetsky A.D., Trukhanov G.Ya. (1970) The Application of Monte-Carlo Method to Calculation of Clusters. Kurchatov Institute IAE-4208/5. In Russian.
- Майоров Л.В., Труханов Г.Я., Франк=Каменецкий А.Д. Применение альбедного метода к расчету пучка стержней. Препринт ИАЭ=1987, М., 1970. См. также в сб. Методы расчета полей тепловых нейтронов в решетках реакторов. Атомиздат, М., 1974, с. 216.
- Maiorov L.V. (1976) Using the precision codes to verify and validate experiment interpretation (In Russian).
Report KFKI-ZR-6-408/1976.
- Maiorov L.V. (1977) The neutron field calculations for complex heterogeneous assemblies. In Russian.
- Майоров Л.В. Расчет полей нейтронов в сложных гетерогенных системах, Материалы 6-го симпозиума ВМК, Бухарест, 1977, с.626.

- Maierov L.V. (1978) Some problems of WWER type reactor homogenization. In Russian.
- Майоров Л.В. Некоторые вопросы теории гомогенизации реакторов ВВЭР, Материалы 7-го симпозиума ВМК, Добжиховице, 1978, т.1, с.141.
- Maierov L.V. (1983) Calculation of parameters of the diffusion finite-difference equations. In Russian.
- Майоров Л.В. О расчете констант диффузионных конечно-разностных уравнений для гетерогенных реакторов. Вопросы атомной науки и техники. Серия: Физика и техника ядерных реакторов, выпуск 5(34), с.1 (1983).
- Maierov L.V., Yudkevich M.S. (1988) Neutron Physical Constants in Thermal Reactors Calculations. Energoatomizdat. Moscow. In Russian.
- Майоров Л.В., Юдкевич М.С. Нейтронно-физические константы в расчетах реакторах на тепловых нейтронах. Энергоатомиздат. М., 1988.
- Maierov L.V., Vaneev Yu.E. (1989) Report KFKI-ZR-6-563/89.
- Майоров Л.В., Ванев Ю.Е. Использование прецизионных расчетов для анализа экспериментов на сборке ZR-6. Отчет KFKI-ZR-6-563/89. Будапешт, 1989 г.
- Maierov L.V., Alekseev N.I., Gomin E.A., Gurevitch M.I., Danilin A.A., Romanov A.C., Molitkova N.E. (1993) The ZR-6 assembly calculations by Monte Carlo MCU code. In Russian.
- Майоров Л.В., Н.И.Алексеев, Е.А.Гомин, М.И.Гуревич, Данилин А.А., Молоткова Н.В. А.С.Романов. Двумерные расчеты некоторых конфигураций сборок ZR-6 и модельных задач по программе MCU-3. Отчет РНЦ Курчатовский Институт. ИЯР-36/1-1839-92.
- Markovsky D.V., Borisov A.A. (1989) Physical Module FORTUN-88 for Calculations by Monte-Carlo Method with Micro Constants Based on Evaluated Data Files. Kurchatov Institute IAE-4774/5. In Russian.
- Марковский Д.В., Борисов А.А. Физический модуль FORTUN-88 для расчетов методом Монте-Карло с микроконстантами на основе файлов оцененных данных. Препринт ИАЭ-4774/ 5. 1989.

- Novikov A.N. (1982) About improving accuracy of the fine-mesh calculations. In Russian.
- А.Н.Новиков, Повышение точности мелкосеточных расчетов, Материал ТГ-4 ВМК (София, НРБ, 1982).
- Ogibin V.I. (1967). Application of the splitting and roulette methods in the particle transport problems. In Russian.
- Огибин И.И. О применении эсщепления и рулетки в расчетах переноса частиц методом Монте-Карло. В кн. Метод Монте-Карло в проблеме переноса излучений. С. 72. М. Атомиздат.
- Sboev A. (1981). The MONR code for calculating the resonance absorption. In Russian.
- Сбоев А. ВАНТ. Сер. Физика и техн. ядер. реакторов. Вып. 5(18).
- Seifert E. (1976) Report KFKI-ZR-6-526-1976. In Russian.
- Э.Зайферт Отчет KFKI-ZR-6-526-1976
- Seifert E. (1976) The ZR-6 macrocell calculations by Monte Carlo Method. In Russian.
- Э.Зейферт и др. Расчеты суперячеек сборки ЗР-6 методом Монте-Карло. Материалы 6 симпозиума ВМК. CPP, Бухарест. с.724. 1977.
- Seifert E. (1978) The Monte Carlo criticality Code OMEGA. Zfk Rossendorf Report. Zfk-364.
- Selegnut D.S. (1959) Report HW 60220, p.65.
- Shevelev Ya.V. (1957). Neutron diffusion in a one-dimensional uranium-water lattice. J.Nucl.Energy. II. V.6, p.132.
- Shevelev Ya.V.(1989). Private communication. In Russian.
- Shevelev Ya.V.(1993). Private communication. In Russian.
- Sobol I.M. (1969) Many Dimensional Quadrature Formulas and Haar's Functions. Nauka, Moscow. In Russian.
- Sobol I.M.,(1973) Numerical Monte Carlo Methods. Nauka, Moscow. In Russian.
- Соболь И.М. Численные методы Монте-Карло. М. Наука. 1973.

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Sobol I.M., (1979) On the Systematic Search in a Hypercube, SIAM J. Numer. Anal. Vol. 10, No. 5, (1979), p. 790

TIC Collected Works. (1985). Final Report of TIC Vol. 1, Akademiai Kiado, Budapest.

VANT (1981) The problems of atomic science and technique journal. Special issue devoted to A.D. Frank-Kamenetsky. In Russian.
Вопросы атомной науки и техники. Сер. Физика и техника ядерных реакторов. Вып. 8(21), 9(22).

Yudkevich M.S. (1992). The MCU code verification. In Russian.
М.С. Юдкевич Пакет программ MCU-2 для расчета методом Монте-Карло нейтронно-физических характеристик ядерных реакторов.
Верификация MCU-2. Отчет ИАЭ Инв.36-1/768/92

Zolotukhin V.G., Maiorov L.V. (1983) Criticality parameter biasing for Monte Carlo Calculations. In Russian. Золотухин В.Г., Майоров Л.В. Оценка систематических погрешностей при расчете критичности методом Монте-Карло. АЭ. 1983. Вып. 3, с. 173.

Zolotukhin V.G., Maiorov L.V. (1984) Reactors Criticality Parameters Evaluation by Monte-Carlo Method. Energoatomizdat. Moscow. In Russian.
Золотухин В.Г., Майоров Л.В. Оценка параметров критичности реакторов. М. Атомиздат. 1984.

APPENDIX TO CHAPTER 3

Table 3.1. Currents, fluxes, albedo fluxes and levels on edges of macrocell 1. D_c and D_s - diffusion coefficients (3.4.47), (3.4.48)..

CELL 1			
I - current.	$\tilde{\Phi}$ - flux.	$\tilde{\Phi}_L$ - level.	$\tilde{\Phi}_A$ - albedo flux.
***** ***** ***** ***** *****	***** ***** ***** ***** *****	***** ***** ***** ***** *****	***** ***** ***** ***** *****
.0134 X .0136	.1204 X .1220	.1098 X .1096	.1142 X .1138
CELL 7			
$D_c = .2842$			
I	$\tilde{\Phi}$	$\tilde{\Phi}_L$	$\tilde{\Phi}_A$
.0002 -.0136 .0037 .0002	.1460 X .1590 .1460	.1450 X .1558 .1450	.1450 X .1588 .1450
.0037 X .0047	.1220 X .162	.1096 X .1540	.1138 X .1560
CELL 2			
$D_c = .2728$ $D_s = .2728$			
I	$\tilde{\Phi}$	$\tilde{\Phi}_L$	$\tilde{\Phi}_A$
-.0002 .0041 -.0134 -.0002	.1460 X .160 .1460	.1450 X .1550 .1450	.1450 X .1570 .1450
.0041 X .0045	.1600 X .162	.1556 X .1550	.1570 X .1588
CELL 12			
$D_c = .2686$			
I	$\tilde{\Phi}$	$\tilde{\Phi}_L$	$\tilde{\Phi}_A$
-.0012 -.0047 .0025 -.0012	.1710 X .1810 .1710	.1660 X .1750 .1660	.1680 X .1780 .1680
.0025 X .0038	.1628 X .1828	.1558 X .1770	.1588 X .1794
CELL 8			
$D_c = .2655$ $D_s = .2273$			
I	$\tilde{\Phi}$	$\tilde{\Phi}_L$	$\tilde{\Phi}_A$
.0011 -.0041 -.0037	.1720 X .1780 .1780	.1670 X .1720 .1720	.1690 X .1750 .1750
.0035 X .0035	.1600 X .1590	.1550 X .1540	.1570 X .1560
CELL 3			
$D_c = .2480$ $D_s = .248$			
I	$\tilde{\Phi}$	$\tilde{\Phi}_L$	$\tilde{\Phi}_A$
-.0011 .0025 -.0045 -.0011	.1720 X .1790 .1720	.1670 X .1750 .1670	.1690 X .1770 .1690
.0038 X .0025	.1834 X .1790	.1774 X .1750	.1800 X .1770

Table 3.1. (Continued)

CELL 16	$D_c = .2611$			
I	$\tilde{\Phi}$	$\tilde{\Phi}_L$	$\tilde{\Phi}_A$	
-.0016	.1910	.1850	.1870	
-.0038  .0033	.1828  .2010	.1770  .1960	.1794  .1980	
.0033  .0058	.2010  .2060	.1960  .2000	.1980  .2020	
-.0016	.1910	.1850	.1870	
CELL 13	$D_c = .2697E$			
I	$\tilde{\Phi}$	$\tilde{\Phi}_L$	$\tilde{\Phi}_A$	
-.0001	.1860	.1810	.1830	
-.0035  .0043	.1780  .1960	.1720  .1900	.1750  .1920	
-.0025  .0046	.1810  .1970	.1750  .1920	.1780  .1940	
.0016	.1910	.1850	.1870	
CELL 9	$D_c = .2501$	$D_s = .2502$		
I	$\tilde{\Phi}$	$\tilde{\Phi}_L$	$\tilde{\Phi}_A$	
.0013	.1900	.1850	.1870	
-.0025  .0048	.1790  .1980	.1750  .1920	.1770  .1950	
-.0035  .0042	.1780  .1970	.1720  .1910	.1750  .1930	
.0001	.1860	.1810	.1830	
CELL 4	$D_c = .2653$	$D_s = .2652$		
I	$\tilde{\Phi}$	$\tilde{\Phi}_L$	$\tilde{\Phi}_A$	
-.0013	.1900	.1850	.1870	
.0032  .0057	.2010  .2060	.1950  .2020	.1970  .2040	
-.0038  .0032	.1834  .2010	.1774  .1950	.1800  .1970	
-.0013	.1900	.1850	.1870	
CELL 19	$D_c = .2398$			
I	$\tilde{\Phi}$	$\tilde{\Phi}_L$	$\tilde{\Phi}_A$	
-.0023	.2150	.2090	.2120	
-.0058  .0060	.2060  .2370	.2000  .2300	.2020  .2320	
.0060  .0101	.2370  .2480	.2300  .2420	.2320  .2440	
-.0023	.2150	.2090	.2120	
CELL 17	$D_c = .2555$	$D_s = .2466$		
I	$\tilde{\Phi}$	$\tilde{\Phi}_L$	$\tilde{\Phi}_A$	
-.0007	.2080	.2020	.2040	
-.0046  .0067	.1970  .2260	.1920  .2210	.1940  .2230	
-.0033  .0086	.2010  .2300	.1960  .2250	.1980  .2270	
.0023	.2150	.2090	.2120	

Table 3.1 (Continued)

CELL 14	$D_c = .2530$				$D_s = .2477$			
I	$\tilde{\Phi}$	$\tilde{\Phi}_L$	$\tilde{\Phi}_A$					
.0009	.2080	.2020	.2040					
-.0042  .0077	.1970  .2270	.1910  .2200	.1930  .2220					
-.0043  .0076	.1960  .2260	.1900  .2190	.1920  .2220					
.0007	.2080	.2020	.2040					
CELL 10	$D_c = .2534$				$D_s = .2681$			
I	$\tilde{\Phi}$	$\tilde{\Phi}_L$	$\tilde{\Phi}_A$					
.0026	.2150	.2090	.2110					
-.0032  .0083	.2010  .2300	.1950  .2250	.1970  .2270					
-.0048  .0070	.1980  .2260	.1920  .2210	.1950  .2230					
-.0009	.2080	.2020	.2040					
CELL 5	$D_c = .2309$				$D_s = .2309$			
I	$\tilde{\Phi}$	$\tilde{\Phi}_L$	$\tilde{\Phi}_A$					
-.0026	.2150	.2090	.2110					
.0062  .0103	.2370  .2500	.2310  .2420	.2330  .2440					
-.0057  .0062	.2060  .2370	.2020  .2310	.2040  .2330					
-.0026	.2150	.2090	.2110					
CELL 21	$D_c = .2065$							
I	$\tilde{\Phi}$	$\tilde{\Phi}_L$	$\tilde{\Phi}_A$					
-.0042	.2680	.2590	.2620					
-.0101  .0136	.2480  .3150	.2420  .3090	.2440  .3110					
.0136  .0172	.3150  .3320	.3090  .3200	.3110  .3240					
-.0042	.2680	.2590	.2620					
CELL 20	$D_c = .2230$				$D_s = .2146$			
I	$\tilde{\Phi}$	$\tilde{\Phi}_L$	$\tilde{\Phi}_A$					
-.0014	.2530	.2450	.2480					
-.0086  .0148	.2300  .2970	.2250  .2890	.2270  .2920					
-.0060  .0173	.2370  .3040	.2300  .2960	.2320  .2990					
.0042	.2680	.2590	.2620					
CELL 18	$D_c = .2230$				$D_s = .2134$			
I	$\tilde{\Phi}$	$\tilde{\Phi}_L$	$\tilde{\Phi}_A$					
.0001	.2500	.2410	.2440					
-.0076  .0154	.2260  .2910	.2190  .2840	.2220  .2870					
-.0067  .0158	.2260  .2920	.2210  .2860	.2230  .2880					
.0014	.2530	.2450	.2480					

Table 3.1 (Continued)

CELL	15	$D_c = .2249$		$D_s = .2404$	
	I	$\tilde{\Phi}$	$\tilde{\Phi}_L$	$\tilde{\Phi}_A$	
	.0015	.2540	.2450	.2480	
	-.0070  .0161	.2260  .2900	.2210  .2840	.2230  .2870	
	-.0077  .0154	.2270  .2910	.2200  .2830	.2220  .2860	
	-.0001	.2500	.2410	.2440	
CELL	11	$D_c = .2170$		$D_s = .2161$	
	I	$\tilde{\Phi}$	$\tilde{\Phi}_L$	$\tilde{\Phi}_A$	
	.0039	.2690	.2590	.2620	
	-.0062  .0173	.2370  .3060	.2310  .2960	.2330  .3000	
	-.0083  .0146	.2300  .2970	.2250  .2900	.2270  .2920	
	-.0015	.2540	.2450	.2480	
CELL	6	$D_c = .2231$		$D_s = .2231$	
	I	$\tilde{\Phi}$	$\tilde{\Phi}_L$	$\tilde{\Phi}_A$	
	-.0039	.2690	.2590	.2620	
	.0136  .0171	.3170  .3280	.3090  .3180	.3120  .3220	
	-.0103  .0136	.2500  .3170	.2420  .3090	.2440  .3120	
	-.0039	.2690	.2590	.2620	
CELL	22		$\tilde{\Phi}$	$\tilde{\Phi}_L$	$\tilde{\Phi}_A$
	I				
	-.0031	.3500	.3560	.3540	
	-.0172  -.0172	.3320  .3320	.3200  .3200	.3240  .3240	
	-.0172  -.0172	.3320  .3320	.3200  .3200	.3240  .3240	
	-.0031	.3500	.3560	.3540	

- Leakage

$\times 10^3$

		-65
		-50
	-43	-59
	-38	-47
	-33	-41
	-37	-46
1	-33	-41
	-39	-47
	-43	-59
		-50
		-65

 $(\tilde{\Phi}/\bar{\Phi}) \times 100.$

		95
		97
	98	96
	98	97
	98	98
101	98	97
	99	98
	98	97
	98	96
		97
		95

 $\Sigma_a \times 10^5$

		423
		416
	404	413
	400	417
	397	400
209	407	408
	399	401
	416	414
	414	410
	409	
	418	

 $\nu \Sigma_f \times 10^5$

		936
		912
	912	931
	897	911
	897	904
	899	910
	900	906
	901	914
	906	927
		914
		939

Absorption rates

$\times 10^5$

		205
		207
	199	202
	194	207
	187	196
93	196	202
	186	197
	202	206
	205	200
	204	
		202

 $\bar{\Phi} \times 10^3$

		309
		347
	356	311
	353	350
	346	355
	336	350
319	344	355
	334	351
	347	356
	354	349
	357	310
	346	
	309	

Fig. 3.22 Macrocell 1 parameters (Group 1)

Fig. 3.24 Macrocell 1 parameters (Group 2)

[illegible]

Fig. 3.23 Macrocell 1 parameters (Group 2)

- Leakage	-83
*10 ³	-32
	-34 -83
	-35 -33
	-35 -34 -83
	-35 -35 -33
59	-35 -34 -84
	-35 -35 -33
	-35 -34 -84
	-34 -33
	-33 -83
	-32
	-82

$\nu \Sigma_f \cdot 10^4$	165
	162
	161 164
	160 162
	158 161 164
	160 162
	157 161 163
	161 162
	163 164
	162
	165

$(\bar{\Phi}/\Phi) \cdot 100$	100
	103
	103 99
	103 103
	103 103 100
	102 103 103
119	103 103 100
	103 103 103
	103 103 100
	103 103
	103 199
	103
	100
1 2 3 4 5 6	

$\bar{\Phi} \cdot 10^3$	37
	35
	34 37
	34 35
	33 34 36
	32 34 35
26	33 34 36
	32 34 35
	33 34 36
	33 35
	34 36
	35
	37

$S \cdot 10^4$	837
Source	460
	467 836
	477 462
	475 470 839
	474 471 465
473	478 470 840
	473 472 465
	476 469 841
	471 462
	464 833
	459
	827

$\Sigma_a \cdot 10^3$	1
	28
	27 1
	27 28
	27 27 1
	27 27 28
293	27 27 1
	27 27 28
	27 27 1
	27 28
	27 1
	28
	1

Fig. 3.24 Macrocell 1 parameters (Group 3)

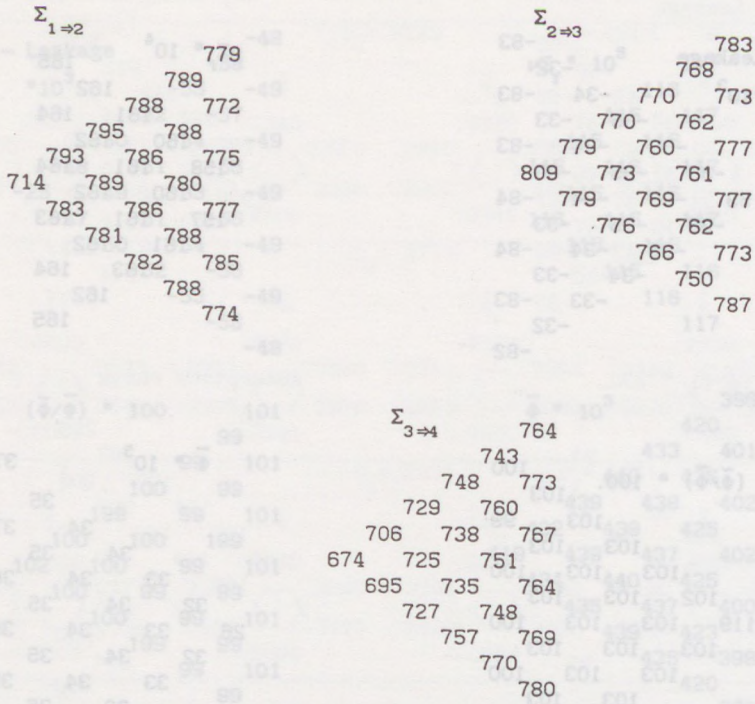


Fig. 3.25 Macrocell 1. Slowing down cross sections

4. ASYMPTOTIC APPROXIMATIONS AND THEIR PLACE IN WWER CORE ANALYSIS

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J. Gado and A. Kereszturi, - Sect. 4.2, 4.3;

V. Pshenin - Sect. 4.1, 4.4, 4.5 (except 4.5.5)

In Chapter 4 the main problems connected with the application of multigroup asymptotic approximation are considered. A brief survey is given of the methods used in the design codes for leakage, slowing down, resonance absorption and thermalization calculations. Short descriptions of the codes based on available reports are also included into the Chapter. Attention is mainly directed to discussing the results of numerical and experimental benchmarking the codes. The solutions of international benchmark problems, the results from comparing of calculated and measured data obtained at critical facilities as well as the results of depletion experiment analysis are considered.

4.1 METHODS OF ASYMPTOTIC PROBLEM SOLVING

4.1.1 Asymptotic approximation in WWER core analysis

The traditional homogenization method used for WWER core analysis is based on the following principles.

1. The transport equation for the real core is replaced by a few-group diffusion equation which is considered as an acceptable mathematical model for an approximate core description.

2. The diffusion equation is written for a lattice that consists of homogeneous cells which are believed to be equivalent in a certain sense to real heterogeneous cells. As a rule it is also supposed that identical cells having different surroundings are considered as being the same ones.

3. In accordance with accepted and not quite strictly founded practice, equivalent homogeneous cells are described by a set of functionals, the functionals being determined by solving an asymptotic problem.

4. The asymptotic problem is formulated as a problem concerning the solution of a homogeneous or nonhomogeneous transport equation for an infinite lattice with the leakage determined by buckling.

5. The asymptotic problem is solved approximately in the design codes. A set of cell diffusion constants is the result of this solution.

6. In fine-mesh simulators the diffusion equations are solved by finite-difference methods usually using one node per elementary cell (in Chaps. 6 and 7 improved nodal type approaches are considered).

As was mentioned above, asymptotic approximation is used at the stage of generating few-group cell constant which are further utilized in the fuel assembly cross section generators or in fine-mesh 2D simulators. It means that the accuracy of asymptotic calculations significantly influences the accuracy in predicting whole core characteristics. At the same time WWER-1000 fuel lattices contain different absorbers and water holes making them nonuniform. Thus, the accuracy in calculating core parameters depends also on the reliability of methods used for taking into account nonuniformity effects.

This problem is considered in detail in Chaps. 5-7. As it will be shown in these Chapters, the application of an improved nodal type balance equation requires solving some additional (besides asymptotic) problems in order to be able compute a full set of needed cell functionals. However, asymptotic functionals in this case play a key role.

Asymptotic approximation in Benoist formulation ((Benoist, 1964) is based on the following principles (see also (Deniz, 1986)).

1. An infinite regular uniform lattice is considered.
2. It is supposed that neutron source $S(\mathbf{r}, \mathbf{v})$ (including fission neutrons) can be represented in the form:

$$S(\mathbf{r}, \mathbf{v}) = s_B(\mathbf{r}, \mathbf{v}) \exp(i\mathbf{B}\mathbf{r})$$

here $s_B(\mathbf{r}, \mathbf{v})$ is a periodic, generally speaking, complex value function with a period equal to the lattice pitch, depending on B as a parameter.

3. Buckling vector B is given and is supposed by most authors to be small in absolute value.

The transport equation for neutron flux in the considered problem has a limited solution of the form:

$$\Psi(\mathbf{r}, \mathbf{v}) = f_B(\mathbf{r}, \mathbf{v}) \exp(i\mathbf{B}\mathbf{r}) \quad (4.1)$$

where $f_B(r, v)$ is also periodic function being a solution of the following equation:

$$\begin{aligned} \frac{v}{v} \nabla f_B(r, v) + i \left(\frac{v}{v} B \right) f_B(r, v) + \Sigma_t(r, v) f_B(r, v) - \\ - \int \Sigma_s(r, v, v') f_B(r, v') dv' = s_B(r, v) \end{aligned} \quad (4.2)$$

For criticality problem the neutron source $s_B(r, v)$ is determined by the correlation

$$s_B(r, v) = \frac{1}{k_{eff}} \int \Sigma_f(r, v, v') f_B(r, v') dv'$$

Neutron flux distribution for zero leakage $\Psi(r, v) = f_0(r, v)$ and corresponding scalar flux

$$\Phi_0(r, v) = \int f_0(r, v) d\Omega$$

are the most important components of the asymptotic solution when traditional balance equations are used. Scalar flux $\Phi_0(r, v)$ is a symmetrical function of coordinates for symmetrical cells.

Diffusion equation parameters for homogeneous cells are determined by averaging with use of some weighting functions (see also Chapter 3). In particular, cross sections for the diffusion equation describing flux distribution averaged over the cell volume are determined by the correlation

$$\bar{\Sigma} = \frac{\langle \Sigma(r, v) \Psi_B(r, v), W(r, v) \rangle_g}{\langle \Psi_B \rangle_g} \quad (4.3)$$

where g is the group number, W is weighting functions.

The diffusion coefficients are expressed through the leakage from the cell:

$$D_g = \frac{\langle (\nabla \Psi_B(r, v), W(r, v)) \rangle_g}{B^2 \langle \Psi_B \rangle_g} \quad (4.4)$$

where B - is the buckling component for a fixed direction, $\langle \dots \rangle$ denotes the scalar product and Ψ_B is the asymptotic problem solution.

Usually the uniform asymptotic problem is solved for $B=0$ to determine

average cross sections and for $B \rightarrow 0$ in order to determine the diffusion coefficients. It is supposed in this case that the dependence of K_{eff} on the B direction may be neglected.

Asymptotic problem is usually solved with use of multigroup approximation. To reduce running time a procedure of preliminary group condensation is some times applied. Calculation of the multigroup cross sections for resonance energy region is a complex problem. It is explained by the fact that a detailed description of the energy dependence of cross sections requires many thousands groups use. Special methods applied in the design codes for reaction rate calculations in this energy region are considered in Sect. 4.2 and partially in Sect. 4.1.3.

The methods used for another energy region important for WWER fuel lattices - thermal are described and analysed in Sects. 4.1.3 and 4.3.

It should be mentioned that in the design codes used at the present time for WWER fuel lattice calculations different approaches are utilized for determining diffusion coefficients. As follows from correlation (4.4) knowledge of f_0 is not generally speaking sufficient for D determination. Nevertheless in some codes the diffusion coefficients are determined by averaging of $1/\Sigma_{tr}$ with weighting function f_0 . The approach in common use is the Benoist (Benoist, 1964) method sometimes with slight modifications. For example, in all versions of the UNIRASOS code special selection of weighting functions was realized to provide equivalence of heterogeneous and homogenized cells.

4.1.2 Methods used for neutrons energy-spatial distributions in WWER fuel lattices

Before giving a brief survey of methods used in the design codes created in the various institutes - TIC participants let us discuss the basic physical features of nowadays and advanced WWER type reactors.

A comparison of reaction rates in various energy regions and produced by some nuclei presented in Table 4.1.1 gives information on the role of different processes in the reactivity balance.

The reaction rate calculations have been performed for the lattices with fuel isotopic content corresponding averaged over the core at zero time point after core refueling. Fuel lattices of standard WWER-1000 with uranium and MOX fuel and WWER-1800U with MOX fuel and tighter pitch lattices (brief descriptions of this project is given, for example, in (Pshenin *et al*, 1990) were considered. It is necessary to note that the use

of MOX fuel in WWERs-1000 can be considered as sufficiently well-founded from the point of view of core physics. At the same time transition to use of MOX fuel and tighter pitch lattices in WWERs, as is suggested in the WWER-1800U pilot project, seems significantly less well-founded and requires a program of wide investigations.

Table 4.1.1 shows that WWER-1000 fuel lattices are characterized by a relatively high proportion of fissions produced by fast neutrons, essential contribution of resonance energy range into total fission and capture reaction rates and predominant contribution of thermal fissions.

The WWER-1800U fuel lattices are distinguished by the shifting of the neutron spectrum into the resonance energy range, increasing capture rate produced by fission products and significant reduction of thermal energy range influence on the reactivity balance. The above mentioned features of WWER-1800 lattices, in particular, require great accuracy of calculations in the resonance energy range. Table 4.1.1 may be useful later on to evaluate the influence of used approximations accuracy on calculations results.

A list of design codes - cross section generators which are considered in the present and the following sections is given in Table 4.1.2. Some reference codes - *MCU*, *PEACO*, *PEANICO*, *SLOGR* will also be mentioned in the text of the present Chapter.

MCU (Maierov and Yudkevich, 1985), (Gomin *et al*, 1991) is the universal code for calculations in a whole energy region based on the Monte-Carlo method (see also Chapt.3).

PEACO (Ishiguro, Takano, 1971), *PEANICO* (Kereszturi, 1981) and *SLOGR* (Sergeev and Karpov, 1985) are the reference codes for calculations in the energy range of resolved resonances based on the method of first collision probabilities and detailed pointwise representation of the resolved resonance cross sections (see Sect. 4.2).

Fast neutron energy region ($\sim 5\text{Kev} < E < 10.5\text{Mev}$). Table 4.1.1 shows that the $5\text{ Kev} \leq E \leq 10\text{ Mev}$ energy region plays a noticeable role in the reactivity balance of WWER fuel lattices giving $\sim 10 - 25\%$ from total fission rate.

The accuracy of reaction rate calculations in the considered energy range depends on the reliability of approaches used for leakage, scattering anisotropy and slowing down description.

Two group structures are used in the codes listed in Table 4.1.2 for describing the epithermal neutron spectrum: 26-group ABBN (Abagyan, 1964) structure and 37-group structure analogous to that used in the well known

MUFT (Bohl and Hemphill, 1961) code. The last structure is used in BETTY-2 only. The real neutron spectrum in fuel lattices of present-day WWERs is very similar to the somewhat shifted fission spectrum being used as weighting spectrum under cross section library generation. Thus the calculational results do not depend in this case on the number of groups in the energy range of fast neutrons.

Table 4.1.1 Reaction rates balance in WWERs fuel lattices.

Energy interval	Reaction type ***	Fuel lattice type / fuel type		
		WWER-1000/UOX	WWER-1000/MOX	WWER-1800MOX
10.5 - 0.821 Mev	R_c / R_f^*	0.0145/0.0775	0.0130/0.0893	0.0179/0.186
0.821 - 4.65 Mev	R_c / R_f	0.0559/0.0167	0.0511/0.0216	0.104 /0.113
4.65 - 0.62 Kev	R_c / R_f	0.548 /0.162	0.599 /0.210	0.802 /0.566
0.625 - 0.0 ev	R_c / R_f	0.381 /0.744	0.337 /0.679	0.0756/0.134
10.5 - 0.0 Mev	R_c^{38} / R_f^{38}	0.455 /0.0677	0.380 /0.0736	0.418 /0.114
10.5 - 0.0 Mev	R_c^{Pu} / R_f^{Pu}	0.167 /0.221	0.379 /0.594	0.453 /0.871
10.5 - 0.0 Mev	R_c^{Am-Cm}	$0.705 \cdot 10^{-3}$	$0.663 \cdot 10^{-2}$	0.0197
10.5 - 0.0 Mev	R_c^{Fp}	0.0600	0.0582	0.0882
A_f / A_{th} ($E_b = 0.625$ ev)		8.95	15.9	318.3
φ^{**}		0.586	0.510	0.120

* - All reaction rates are normalized to a total reaction rate of the considered type.

** - probability of escaping resonance absorption.

*** - R_c^{Fp} , R_c^{Pu} , R_c^{Am-Cm} , R_c^{38} - capture rates produced by fission products, all plutonium isotopes, all americium and curium isotopes and ^{238}U , respectively.

Φ_f , Φ_{th} - fast and thermal fluxes.

MOX - $UO_2 + PuO_2$ fuel; UOX - UO_2 fuel.

A key problem of light water high converters is the value of the void reactivity coefficient which can be positive under some conditions. To provide sufficient accuracy of void effect prediction for tight lattices with MOX fuel it is necessary to use a greater number of energy groups. Such a possibility is provided, in particular, by the MULTIC cross sections library (Nikolaev *et al*, 1984). In this library the energy region of fast neutrons is described by 144 groups and each of them is divided into the number of subgroups. At the present time MULTIC library is used in one of versions of MCU (Maierov and Yudkevich, 1988), (Abagian *et al.*, 1992) and there are no corresponding versions of design codes based on this library.

Table 4.1.2 List of design spectral codes created in the various institutes of the TIC - participants.

Code name	Institute where code		Reference
	was created	is used	
BETTY-2	KFKI Hungary	KFKI Hungary	Gado 1978
NESSEL-4	KKAB FRG	KKAB Germany INRNE Bulgaria	Heinrich 1981
UNIRASOS-2	RRC KI Russia	KIAE Russia	Pshenin <i>et al</i> 1989
RAFORIN	RRC KI Russia	KIAE Russia	Pshenin <i>et al</i> 1989
TVS	RRC KI Russia	KIAE Russia	Pshenin <i>et al</i> 1989
SAPFIR	RRC KI Russia	KIAE Russia	Tebin <i>et al</i> 1985
WIMS-SU	RRC KI Russia	KIAE Russia	Laletin <i>et al</i> 1990
MICROBE	NRI CSFR	NRI CSFR	Zaleski 1989

As has already been mentioned a procedure of preliminary condensation of initial cross section libraries is applied in some spectral codes. In some cases this procedure provides a possibility to reduce processor time spending without loss of accuracy. This approach in a slightly modified form is used in the RAFORIN, UNIRASOS-2 and TVS codes. A brief description is given in the next Section.

The WWER lattices in the fast energy region are slightly heterogeneous. Thus, in several codes (NESSEL-4, UNIRASOS-2, TVS) the cell homogenization in the groups belonging to the $0.8 \text{ Mev} \leq E \leq 10.5 \text{ Mev}$ energy interval is carried out approximately with the use of the constant fluxes ratio. The fluxes ratio is computed by means of cross sections averaged with neutron spectrum corresponding to infinite homogeneous media. In (Gado, Kereszturi, 1986) it is noted that judging from the results of

calculations performed the use of the simplified homogenization procedure in WWER lattices only slightly influences the K_{eff} value.

The relatively high uncertainty of U^{238} cross sections in the considered energy range (see (Abagyan *et al*, 1981)) and the significant contribution of inelastic slowing down and fissions produced by this isotope to the lattice reactivity balance lead to noticeable constants uncertainty of predicted lattice multiplication characteristics.

The application of statistical methods for treating measured data based on the known connection of a priori and a posterior distribution function allows us to reduce constant uncertainty and discrepancies of calculated and measured data. Such an approach was used in (Satmari *et al*, 1978), (Pshenin, 1980) for interpreting measured data obtained at the ZR-6 assembly and known from the literature. It was shown in these papers that the approach used allowed one to improve noticeably the agreement between calculations and measurements for a wide set of fuel lattices. The reliability of the results obtained and the possibility of their practical application is determined partially by the reliability of the initial cross sections covariance matrix. The use of a matrix of simplified shape has to certain degree limited further application of the obtained results.

Resonance energy range ($\sim 1 \text{ eV} < E < 5 \text{ Kev}$). Accurate prediction of reaction rates in the resonance energy range seems to be one of the most complex calculation problems of light water lattices. The accuracy of resonance absorption and fission calculations significantly influences the main lattice parameters under fuel burnup.

According to the Table 4.1.1 a 3% error in resonance capture rate corresponds to $\sim 1.5\%$ error in K_{∞} determining. The accuracy requirements of calculations in the considered energy interval highly increase for WWER lattices with MOX fuel. The great number of resolved resonances of heavy nuclei and fission products demands some thousands of energy groups for a detailed description of cross section energy dependence.

In view of this a direct approach to resonance absorption calculations is not applied in the considered design codes because of the significant processor time needed. As has already been mentioned, such an approach is used for reference calculations in PEANICO, MCU and SLOGR. SLOGR is a module of design oriented code SAPPFIR and is used for the benchmark type calculations.

The approaches utilized in the design codes are usually based on the results of preliminary reference calculations and their further interpolation founded on certain suppositions about the shape of the neutron spectrum inside the group.

The following methods for self-shielded cross section calculations are used in the design codes that are considered:

- interpolation of tabulated dependences of resonance integrals I on dilution cross section σ_{dil} with the use of equivalence theorems (BETTY-2, UNIRASOS-2, WIMS-SU, RAFORIN, TVS);
- formalism of resonance self-shielding factors (Abagyan *et al*, 1964) in a combination with the equivalence theorem (NESSEL-4, MICROBE);
- subgroup method (Nikolaev and Hakhlov, 1967) (SAPFIR, energy range of unresolved resonances);
- generalized subgroup approach (Tebin, 1991) (SAPFIR, energy range of resolved resonances).

Let us consider the main features of the realization of methods listed in different codes.

The following main problems are connected with the interpolation of $I(\sigma_{dil})$ tables (see also Sect.4.2):

- choice of equivalent medium for calculating $I(\sigma_{dil})$ tables;
- choice of fitting parameters (Goldstein's and Bell's factors);
- connection between resonance integrals and group cross sections;

The considering as an equivalent of heterogeneous medium permits one to avoid solving the problem connected with the choice of dilution material the significance of which is mentioned in (Tebin, Yudkevich, 1980). This approach is realized in UNIRASOS-2, RAFORIN and TVS codes. The resonance integrals in these codes are tabulated for the case of a single pin.

The simple, similar to those used in WIMS-D4, approximations for the transition from I_j to σ_j (j - group number) for WWER lattices with relatively small absorption inside the "narrow" group seem to be acceptable from the practical point of view. The accuracy of such approaches for highly enriched tighter pitch lattices with MOX fuel should be specially analysed.

The well known formalism of resonance self-shielding factors based in the resonance energy range on ABBN (Abagyan *et al*, 1981) data is applied in NESSEL-4 and MICROBE. The f-factors including in the ABBN library were computed for homogeneous medium with using a narrow resonance approximation which is not valid for the lowest resonances of ^{238}U and leads to significant calculational errors (see (Kereszturi, 1981)). To reduce these

errors, specially selected λ -factors of ^{238}U are used in *NESSEL-4*. These factors were chosen by the fitting of total resonance integrals to results of Hellstrand measurements (Hellstrand, 1957) and by fitting of calculated ρ^{28} to the measured one. It should be noted that the use of *PEANICO* type codes for f-tables calculations allows one to avoid the problem.

In both of the approaches considered the equivalence theorems with specially selected fitting parameters are used to interpolate $I(\sigma_{d11})$ or $f(\sigma_{d11})$ tables. These parameters are determined in various ways in different codes. Their values correspond to those used in *WIMS-D4*, recommended in (Levin, 1963) or are computed from a condition of the best agreement with the results of reference calculations for the fixed set of variants. The last approach is realized, for example, in *UNIRASOS-2*, *RAFORIN* and *BETTY-2*.

The Goldstein's factors for heavy nuclei in *BETTY-2* are computed on the basis of a special iteration procedure and depend on group number. These factors in *UNIRASOS-2* and *RAFORIN* are supposed independent on group number and are chosen from a condition of the best agreement of total resonance integrals.

The accuracy of the different approximations leading to equivalence correlations was analysed in (Kereszturi, 1981). As has been shown in this paper their total inaccuracy leads to about 1% inaccuracy of the total resonance integral calculation. The accuracy of the equivalence theorem was analysed in (Pshenin and Tebin, 1982), (Kereszturi, 1982). These papers contain the calculation results for different absorbers in combination with various diluters and show that the error of resonance integral calculations does not exceed the uncertainty of cross sections in the resonance energy range.

Mutual resonance overlapping has a noticeable influence (see for example (Kereszturi, 1982)) on resonance absorption in *WWR* lattices. This effect is usually taken into account approximately by iteration procedure. At the first iteration self shielded cross sections are obtained without taking into account the considered effect. At the second iteration mutual the overlapping effect is calculated by correction based on neglecting of the cross section energy dependence of all nuclei besides considered. The accuracy of such approaches is analysed in (Kereszturi, 1982). According to this paper the accuracy of the Askew approach (Askew, 1966) is sufficient for practical calculations of the lattices with ^{238}U and ^{235}U .

To provide sufficient accuracy of calculations of fuel lattices with gadolinium integrated into the fuel rods it is necessary to divide burnable

absorber (BA) rod into some burnable zones. In this case, strictly speaking, the direct use of the equivalence theorem for computing shielded cross sections is not possible. The resonance self-shielding of the odd gadolinium isotopes was analysed in (Rubin, 1989). The data of this paper allow one to conclude that even when the content of Gd_2O_3 in the BA rod is equal to 5-7% the influence of resonance self-shielding on the multiplication characteristics of the fuel assembly is practically negligible. Thus, the simplified approach based on calculations of self shielded cross sections for all burnable zones with the use of averaged over the rod gadolinium isotopes number densities seems acceptable.

The generalized subgroup approach (Tebin and Yudkevich, 1981), (Tebin, 1991) is a further development of the subgroup approach for resonance absorption calculations in thermal reactors lattices. This approach is used as a standard for mass calculations in *SAPFIR*.

This method has the following main advantages:

- possibility of correctly taking into account finite resonance widths that is the most important for low energy region;
- possibility of calculating the systems with complex fuel isotopic composition with the use of subgroup parameters of separate isotopes and not of their mixture;

The latter provides the possibility to generate universal cross section libraries which do not depend on specific system geometry and isotopic composition. As has already been mentioned in Chapter 2, the parameters of the generalized subgroup approach differ from those used in standard subgroup approach included into *ABBN* library.

The accuracy of the generalized subgroup approach was analysed by comparing it with the results of reference calculations using the Monte-Carlo method and the detailed pointwise representation of resolved resonance cross sections. It has been shown in (Osipov and Tebin, 1981) that suggested method provides high accuracy of resonance absorption calculations for a wide set of light water lattices (with ^{235}U , ^{238}U , ^{232}Th as resonance absorbers); the error usually does not exceed ~3% and corresponds to nuclear data uncertainty.

The resonance neutron spectrum in most codes^{*} is calculated on the basis of the group approach with the use of preliminarily prepared scattering matrixes. The scattering matrixes are usually computed by

* Except for *UNIRASOS-2*, *TVS*, *RAFORIN* and *SAPFIR*.

utilising the Fermi spectrum for weighting. Obviously this approach provides sufficient accuracy of calculations for the fuel lattices with slight depression of slowing down density in the group interval.

For highly enriched tight lattices when the resonance neutrons energy interval is divided by $\sim 12\text{--}25$ group the continuous slowing down models or generalized subgroup approach seems more preferable. This conclusion agrees with the inferences of (Bohme *et al*, 1992), (Broeders, 1992).

The Doppler effect significantly influences the WWER core characteristics in stationary and transient regime operation. Usually, the real temperature distribution inside the fuel rod is replaced by constant temperature which is equal to temperature averaged over the rod or corresponds to effective one chosen from a condition of equivalency of resonance absorption.

To check the reliability of recommendations known from the literature for effective temperature choice for WWER fuel rods, special investigations were performed with *PEANICO* (Kereszturi, 1987) and *SAPFIR* (Tebin, private communication) codes. The calculations showed that resonance absorption in the WWER's fuel rod computed with volume averaged constant temperature and the use of real temperature distribution practically coincides.

As it has already been mentioned that some codes based on the method of first collision probabilities and detailed cross section energy dependence representation are used in the institutes of the TIC-participants for semiprecise calculations in the energy range of resolved resonances. One of them - *PENICO* will be described in detail in the next Section. The other code - *SLOGR* (Sergeev and Karpov, 1985), based on nearly the same approximations as *PEACO*, is one of modules of *SAPFIR*. *SLOGR* is also used for cross section libraries generation.

Thermal energy region. As it follows from Table 4.1.1 the thermal energy region gives more than 40% of the total number of absorptions and 70% fissions in present-day WWER lattices. Thus, the accuracy of thermalization calculations practically determines the accuracy of core parameter prediction.

A wide program of theoretical and experimental investigations of thermalization effects was performed in the USSR during the period from the middle fifties to 1972 (see survey in (Mostovoy, 1978)) in connection with developing nuclear energy and WWER reactors, in particular (Kurchatov, 1956, Mostovoy *et al*, 1958 - 1978, Abdullaev *et al*, 1968, Ereemeev *et al*, 1968, Ishmaev *et al*, 1966-1970, Laletin, 1963, Maiorov *et al* 1962 - 1968,

Marchuk et al, 1961 - 1964, Turchin, 1963).

The following problems were investigated within the framework of this program:

- measurement and evaluation of scattering law of slow neutrons in the basic moderator, in particular, in water;
- time-dependent thermalization in various moderators;
- spatial-energy and angular distribution of slow neutrons near the boundary of the media with different temperature, slowing down and absorption capabilities;
- slowing down and thermal neutron spectra in homogeneous and heterogeneous media;
- methods for calculating scattering cross sections and neutron spectra in homogeneous and heterogeneous media;

The investigations performed provided a possibility to create libraries of phonon spectra, codes for transport equation solution in the thermal energy range taking into account thermal motion and chemical bonds based initially on P_1 , P_3 , S_n approximations and then on the Monte-Carlo method. These codes were used to validate the first design codes assigned for WWER lattices calculations and later on as a basis for creating the design codes of the second generation.

Below, a brief survey is given of the methods used for thermalization calculations in the design codes and theoretical investigations performed within the framework of TIC activities in the period after 1972.

The choice of thermal group boundary influences such code characteristics as running time and accuracy of calculations. In most of the codes considered the break point energy is equal to 0.465 or 0.625 ev. In this case the lowest and most important ^{240}Pu , ^{242}Pu resonances are included in the resonance group and their self-shielded cross sections are determined by the methods described above.

The energy break point in BETTY-2 is equal to 1.84 ev. So, to provide sufficient accuracy of ^{240}Pu capture cross section calculations, a special integration procedure (Kereszturi, 1981) is applied in this code for capture rate computation.

Two types of thermalization models are used in the considered design codes - "realistic" based on scattering matrixes use MICROBE, RAFORIN, NESSEL-4, SAPFIR, and differential: UNIRASOS-2, TVS, BETTY-2. The UNIRASOS-2 and TVS codes utilize the two-constant Laletin model (Laletin, 1963), in BETTY-2 the Cadilhac (N. Cadilhac, 1963) model is applied. These models are compared in (Bogachev and Sidorenko, 1975). The results of

benchmark problem solutions given in this report show that the accuracies of both models are nearly the same.

The optimization of group structure is a key problem from the point of view of code speed capability when the "realistic" thermalization model is used and the thermal neutron spectrum must be recalculated with high frequency under burnup calculations. This problem is partially considered in Sect.4.3. The number of thermal groups in *MICROBE* and *RAFORIN* is equal to 24, in *NESSEL-4* it is 10. In *SAPPFIR* well known *THERMOS* group structure is used. To avoid errors connected with insufficient accuracy of ^{239}Pu cross sections the 10 group approximation and the f-factors are used in *NESSEL-4* to obtain shielded cross sections in the group containing the lowest resonance of this isotope.

The description of data files and codes used to generate thermal cross sections libraries are given in Chapter 2, it is unnecessary to give it here.

Spatial flux distributions in all codes except for *WIMS-SU*, and *RAFORIN*, are computed by the first collision probabilities (P_{1j}) method. Some aspects of its application to *WWER* lattices calculations are considered in Sect.4.3. It should be noted that in *SAPPFIR* the first collision probabilities can be calculated in two ways - by the use of deterministic methods or the Monte-Carlo method. The last-named method is applied for calculations of systems with complicated geometry. To reduce processor time, in this case a procedure of P_{1j} preliminary tabulation and their next interpolation is applied.

The surface pseudosources (SPS) method described in (Laletin, 1967, Laletin et al., 1990) is utilized in codes *WIMS-SU* and *RAFORIN*. This method is based on use of Green's functions for the monoenergetic infinite uniform problem. Its application for solving multigroup problem leads to the flat energy current approximation which seems to be more realistic than the flat flux approximation usually used in the P_{1j} method. The SPS method also provides a possibility of reducing running time and this is the most important - correct computing of cell non-traditional functionals needed for improved balance equation application (see Sects. 6 and 7).

The brief survey given in the present section contains short descriptions of the methods used in the design codes for uniform lattice calculations. A detailed exposition of the results of numerical benchmarking the methods used for calculations in the resonance and thermal energy regions is given in Sects. 4.2 and 4.3. The descriptions of models used for depletion calculations are included into Sect. 4.4.

4.2. NUMERICAL ANALYSIS OF METHODS FOR TREATING RESONANCE ABSORPTION

In this Section some approximations are analysed, that are used in engineering calculations of WWERs for the energy range of resolved resonances.

4.2.1. Setup of the problem and the applied programs

In principle, the Monte Carlo method ensures the absolutely exact calculation of resonance absorption in various systems (cf. Chapter 3). However, as a consequence of the enormous amount of computer time needed Monte Carlo programs are generally used to validate approximate methods.

The programs *PEACO* (Ishiguro, 1971) and *PEANICO* (Kereszturi, 1981) were adapted and elaborated for analysing engineering methods used in calculating the resonance range. These codes satisfy both accuracy and computation time requirements. The accuracy of the codes was tested (Kereszturi, 1981) against the results of the Monte Carlo code *MONR1* (cf. Chapter 3).

PEACO makes it possible to solve the integral transport equation for the reactor lattice cell in the energy range of resolved resonances. The method of first flight probabilities is applied in the approximation of isotropic scattering. The energy range may be divided into a large number of intervals (normally about 30000 groups are used), therefore the slowing down of neutrons on the various nuclei is modelled in a very accurate manner.

PEANICO is a generalized version of *PEACO*. In this code the linearly anisotropic scattering in the laboratory system is approximately taken into account (Kereszturi, 1981). In this way the most serious disadvantage of *PEACO* is eliminated. Though the anisotropy of scattering only slightly influences the resonance absorption in WWER lattices, in other lattices this effect may appear to be more significant.

For validating the *PEACO* and *PEANICO* codes a series of calculations was performed by using these codes and *MONR1* with identical nuclear data (Kereszturi, 1981). A description of the investigated test problems can be found in Table 4.2.1, results are given in Table 4.2.2. It can be seen that the results of *PEANICO* (hexagonal cell, anisotropy is accounted for) are in good agreement with the results of the Monte Carlo code *MONR1*.

Applying transport correction leads to discrepancies in lattices of large pitch and the neglecting of anisotropy leads to unacceptable results

in lattices of large pitch and large rod radius. Cylindrization leads to overestimation of the resonance absorption probability by 1% in the investigated tight lattices.

As a conclusion, the PEANICO code is always applicable, whereas the PEACO is applicable in certain conditions for validating engineering codes.

Table 4.2.1 Data of lattices used in the calculations

Notation	Fuel		Cladding	
	r [cm]	Composition [10^{24} cm^{-3}]	r [cm]	Composition [10^{24} cm^{-3}]
TR-1 TR-2 TR-3 TR-4	0.4915	^{235}U $6.2530 \cdot 10^{-4}$ ^{238}U 0.047205	0.57330	Al 0.051503
W3	0.5060	^{16}O 0.046416 ^{235}U $7.0558 \cdot 10^{-4}$ ^{238}U 0.022502	0.54625	Mn 0.001075 Cr 0.01160 Fe 0.038149 Ni 0.005809
Z1 Z2 Z3	0.3800	^{16}O 0.045861 ^{235}U $8.2550 \cdot 10^{-4}$ ^{238}U 0.022105	0.4500	Zr 0.038679 Nb $3.87 \cdot 10^{-4}$
M1	3.1	^{16}O 0.0456 ^{238}U 0.0228	-	-
M2 M3	0.38	^{16}O 0.0456 ^{238}U 0.0228	-	-
M4	0.5	^{238}U 0.0473	-	-
M5	0.188	^{238}U 0.0473	-	-

Table 4.2.1 (Continued) Data of lattices used in the calculations

Notation	Moderator		Lattice	
	r [cm]	H(H ₂ O) [10 ²⁴ cm ⁻³]	Form	Pitch [cm]
TR-1	0.94822	0.03338	Hexagonal	1.8060
TR-2	1.14144	0.03338	Hexagonal	2.1740
TR-3	0.75669	0.03338	Hexagonal	1.4412
TR-4	1.51337	0.03338	Hexagonal	2.8824
W3	0.70558	0.033357	Square	1.2506
Z1	0.57754	0.033357	Hexagonal	1.1000
Z2	0.66680	0.033357	Hexagonal	1.2700
Z3	0.78756	0.033357	Hexagonal	1.5000
M1	5.2504	0.0333	Hexagonal	10.0
M2	2.6252	0.0333	Hexagonal	5.0
M3	0.6668	0.0333	Hexagonal	1.27
M4	3.6753	0.0333	Hexagonal	7.0
M5	0.43368	0.0333	Hexagonal	0.826

Table 4.2.2 Comparison of results of the codes *MONRI*, *PEANICO* and *PEACO*.*)

Code	Lattice Geomet.	Anisotropic	M1	M2	M3	M4	M5
<i>MONRI</i>	Hexagonal	Yes	0.0627±	0.00682±	0.1264±	0.00746±	0.1191±
			0.0003	0.00007	0.0006	0.00005	0.0007
<i>PEANICO</i>	Hexagonal	Yes	-	-	0.1266	-	0.1197
	Cylindr	Yes	0.0620	0.00687	0.1280	0.00736	-
	Cylindr	Trans. Corr.	0.0637	0.00705	0.1281	0.00761	0.1209
<i>PEACO</i>	Hexagonal	No	-	-	0.1261	-	0.1194
	Cylindr	No	0.0595	0.00676	0.1274	0.00706	-

*) resonance absorption probability between 4.65 and 465 eV.

4.2.2 Approximative methods for treating resonance absorption in multi group calculations

Approximative methods for treating resonance absorption, applied in the multi group codes of TIC laboratories, strongly differ from each other. Their validation on the basis of infinite lattice calculations was performed in KFKI, Budapest (Kereszturi, 1981). Details of this analysis are not discussed here. It is worth mentioning that analysis at a given laboratory was necessary since the nuclear data used in the various laboratories differ from each other. The analysis of methodical character should have obviously been based on identical nuclear data. In evaluating the inaccuracies of multi group calculations the results of the methodological analysis should be corrected for the differences in libraries.

As a rule, the majority of engineering calculations are based on equivalence theorems. These theorems connect the multi group constants of the investigated lattice cell with the characteristics of more simple systems (homogeneous medium or isolated rod). Constants parameterized in this manner determined for the simple systems, are included in the multi group libraries.

In the course of multi group calculations the actual parameters of the equivalence theorems and the corresponding constants are determined and then used. In this manner it is possible to avoid the explicit modelling of resonance absorption in heterogeneous lattice cells in the framework of multi group calculations and thus to accelerate them.

The calculation is performed in two steps:

- selection of the equivalent medium,
- calculation of the equivalent system (preparing library constants).

Selection of the equivalent simple system. As a rule, two equivalent simple systems are considered: homogeneous medium or isolated rod. From the equivalence theorems it follows that some quantities (resonance integral, group cross section, group flux) of the lattice cell coincide with the corresponding quantities of the equivalent medium.

If a homogeneous medium is selected as an equivalent system, its composition is given as a mixture of the fuel material and a supplementary scattering material characterized by cross section σ_{ex} . The value of σ_{ex} can be determined on the basis of the Wigner rational approximation for the non-collision probability in the rod:

$$\sigma_{ex} = \frac{a D}{N \bar{I} \left[1 + (a-1)(1-D) \right]},$$

where

N - nuclear density of the absorber isotope (it is assumed that only one isotope has resonances),

$\bar{I}$ - diameter of fuel rod,

a - the Bell factor,

D - the Dancoff-Ginsburg factor.

For the isolated rod $D=1$. Therefore for the isolated rod equivalent with the lattice cell the flux shall be determined for a rod with the real composition, but with the diameter

$$\bar{I}' = \frac{\bar{I}}{D} \left[1 + (a-1)(1-D) \right]$$

Table 4.2.3

Comparison of resonance integrals for equivalent systems

Fuel radii [cm]	Equivalent moderator radii [cm]	D	a	Resonance Integral [10^{-24} cm^2]
0.1	0.13831	0.22187	1.1427	17.4437
0.19	0.27521	0.41124	1.1423	17.4307
0.38	0.66680	0.78233	1.1416	17.4219
0.435	0.87254	0.88316	1.1414	17.4151
0.48	1.36913*	0.96368	1.1412	17.4867
H O M O G E N I O U S M E D I U M				17.4886

* Practically isolated rod

The equivalence theorems are very accurate. It is shown, for example, in Table 4.2.3, where the resonance integrals in the range 4.65 to 600 eV calculated by *PEANICO* are compared for equivalent according to the theorems systems (two-region lattice cell, the moderator is water, the fuel is $^{238}\text{UO}_2$ with the density of 10.2255 g/cm^3). It has to be mentioned that in

these calculations the factors a and D were determined with the maximum possible accuracy. In the case of a homogeneous medium the scattering with the cross section σ_{ex} was modelled by using the scattering law for hydrogen.

It can be seen that the maximum deviation does not reach 0.5%. For WWER lattices an inaccuracy of 1% in the cross section σ_{ex} leads to an inaccuracy of 0.5% in the ^{238}U resonance integral.

Let us now consider the determination of factors a and D .

The Bell factor a plays an important role only if a homogeneous medium is chosen for equivalent system. It is due to the fact that the quantity $\bar{\Gamma}'$ is much less dependent on a than the cross section σ_{ex} . This conclusion was drawn on the basis of calculations by WIMS, NESSEL-4 and CELLAR.

In the WIMS code the Bell factor is calculated for UO_2 by the formulae (Kowalska, 1975).

$$a = \frac{2.71}{2.34} \frac{b+1}{b+1}$$

$$b = \frac{D}{N\bar{\Gamma} \left[5 + 2\sigma_s^{ox} \right]}$$

where σ_s^{ox} - potential scattering cross section of oxygen.

In the BETTY code the Bell factor is determined by adjustment. For the energy groups the values of resonance integrals of isolated rod and homogeneous medium were compared. Bell factors of the various isotopes are included in the group constant library of BETTY-2 (as a function of N).

In the code NESSEL-4¹⁾ the Bell factor is chosen as the constant

$$a = 1.16.$$

As a result, the error in σ_{ex} is about 2% for WWER lattices, leading to an inaccuracy in resonance absorption of about 1%.

In CELLAR the Bell factor was chosen to be $a=1$. This leads to an error of -5.5%. In the code σ_{ex} is determined as

$$\sigma_{ex} = \lambda \frac{D}{N\bar{\Gamma}}$$

¹⁾ More precisely, in NESSEL-4

$$\sigma_{ex} = \frac{1.16D}{N\bar{\Gamma} \left[1 + (1.10-1)(1-D) \right]}$$

Table 4.2.4 Effect of cladding treatment in calculating the Dancoff-Ginsburg factor

Lattice	The calculation Method	D	Error of resonance absorption (%)
Z1	DANCOLL, Intermed. resonance	0.52730	-
	DANCOLL, Narrow resonance	0.54664	2.0
	DANCOLL, Homog. + Narrow res.	0.56565	3.9
	Sauer's method	0.57308	4.7
Z2	DANCOLL, Intermed. resonance	0.70280	-
	DANCOLL, Narrow resonance	0.71665	1.1
	DANCOLL, Homog. + Narrow res.	0.73261	2.5
	Sauer's method	0.73606	2.6

Calculation of the equivalent system. After the equivalent system is determined, calculation of this system is to be performed. Results of these calculations are included (in parameterized or tabulated form) in multi group constant libraries. In the course of these calculations some further approximations are used.

If the homogeneous medium is chosen as the equivalent medium, three different methods are applied in TIC laboratories to calculate resonance absorption in the chosen medium.

1. If the calculations are made using the traditional ABBN library, the results should be evaluated taking into account that the f -factors of the ABBN-library are determined in the narrow resonance approximation for each fuel isotope. ABBN constants are used in the *NESSEL-4* and *CELLAR* codes. As is well known and also shown below, the narrow resonance approximation leads to every inaccurate result for the total resonance absorption in thermal reactors. Therefore in the mentioned codes the total resonance integral of ^{238}U is corrected for the experimental results of Hellstrand (Hellstrand, 1966). The problem of distributing the total resonance integral into energy groups is solved in different ways in the above codes, but it slightly influences the final results.

Table 4.2.5 Effect of approximations used in the calculation of equivalent homogeneous medium on the probability of resonance absorption: $1-p$.

METHOD	$1 - p$	System
Exact result	0.12640	Cell
Narrow resonance approximation for the additional scattering.	0.12663	Equivalent homogeneous medium
Intermediate resonance approximation for oxygen. + the 1 st approximation ^{*)}	0.12646	Equivalent homogeneous medium
Intermediate resonance approximation for + the 1 st approximation ^{*)}	0.12340	Equivalent homogeneous medium
Narrow resonance approximation for ^{238}U and O + the 1 st approximation ^{*)}	0.12083	Equivalent homogeneous medium

^{*)} the 1st approximation = The narrow resonance approximation for the additional scattering.

2. In the *WIMS* code a special procedure is applied. Slowing down on the absorber isotope is calculated exactly, while for the other isotopes it is calculated in the intermediate resonance approximation. The supplementary scattering material of cross section σ_{ex} is calculated in accordance with the scattering law of hydrogen. The approximation of intermediate resonances (at the choice $\lambda=0.94$ (Kowalska, 1975) for oxygen) leads to overestimation of the resonance absorption in *WWR* lattices by about 1%.

3. The third method was applied in generating a new *ABBN*-type library for *NESSEL-4* and *CELLAR* by using the *FEDGROUP* code (Vertes, 1976). In this code the slowing down on the absorber and all other isotopes is calculated in the narrow resonance approximation. This approximation leads to an underestimation of resonance absorption in *WWR* lattices by about 2.5%.

The effect of the considered approximations on the resonance absorption is summarized for WWER lattices in Table 4.2.5 (see also (Kereszturi, 1981)).

If the isolated rod is chosen as an equivalent system, two methods can be distinguished in the calculations.

- The first method is based on determining the total resonance absorption integral of the isolated rod by using the experimental results of (Hellstrand, 1966) (and not performing any calculations). This method is applied in the codes *LASER*, *LEOPARD* and *REMUR*. Of the inaccuracies in the interpretation of the experiments, problems are connected with the lack of determination of the resonance integrals of other isotopes (^{235}U and ^{239}Pu) in isolated rods. As was mentioned above, the uncertainties in the distribution of the resonance integrals in energy groups do not lead to significant errors.
- The second method is based on calculating isolated rods by using the *PEANICO* code. In this case no further approximation is needed. The multi group constant library of the *BETTY-2* code (for resonance isotopes) was prepared in this way.

The mutual screening of resonances of different isotopes was analysed in (Kereszturi, 1982) for homogeneous media. It was pointed out that this effect should be accounted for in calculating WWER lattices. Mutual shielding is well treated by the method of (Askew, 1966). However, its description in (Kidman et al, 1972) contains the error.

2. In the *WIS* code a special procedure is applied. Shown down on Figure 4.2.1, the absorber isotope is calculated exactly, while for the other isotopes it is calculated in the intermediate resonance approximation. The supplementary scattering material of cross section σ_s is calculated in accordance with the scattering law of hydrogen. The approximation of intermediate resonances (at the choice $A=0.94$ (Kereszturi, 1982) for oxygen) leads to overestimation of the resonance absorption in WWER lattices by about 1.5%.

3. The third method was applied in generating a new *WIS*-type library for *WISSEL-4* and *CELLAR* by using the *PEANICO* code (Verter, 1978). In this code the slowing down on the absorber and all other isotopes is calculated in the narrow resonance approximation. This approximation leads to an underestimation of resonance absorption in WWER lattices by about 2.5%.

4.3 NUMERICAL ANALYSIS OF THE METHODS APPLIED IN THE THERMAL ENERGY RANGE

In this Section the results of the numerical investigations are presented, which were performed in the framework of the TIC for studying the effectiveness of various engineering algorithms and codes applicable for calculating lattice characteristics in the thermal energy range. In 4.3.1 the THERMOS-type programs are considered, and then the high speed codes are analysed which are based on more simple algorithms. All the numerical results were obtained for the systems described in Tables 4.3.13-15. The notations used in other Tables are also interpreted in Tables 4.3.13-15.

4.3.1 THERMOS-type programs

The THERMOS code algorithm is well known (cf., for example, Honeck, 1962), therefore it is not described here. Its basic characteristics are as follows.

(a) In the code the Peierls integral equation is solved for the scalar flux ϕ_0 . It is acceptable if an infinite fuel lattice cell without leakage is considered.

(b) The elementary cell (which has an axially infinite size due to assumption (a)) is cylindrized preserving the volume of the moderator (and that of the cell). The cell is calculated in 1D cylindrical geometry. At the cell boundary the so called white boundary condition is applied, which assumes that the neutrons leaving the cell return to it with an isotropic angle distribution.

(c) The cylindric cell is split into cylindrical rings. For calculating first flight collision probabilities (taking into account the boundary condition) various methods are applied.

(d) The scattering is assumed to be isotropic in the laboratory system. This assumption is more or less acceptable since the chemical binding effects and the thermal motion of nuclei reduce the anisotropy of scattering. On the other hand, due to the relatively smooth dependence of the neutron flux on the spatial variable, the neutron flux is assumed to be near to isotropic. For accounting the anisotropy of scattering various corrections are applied.

(e) The slowing down source functions of thermal neutrons are calculated in an approximate manner.

(f) The manner of dividing the thermal energy range into groups and also the methods of calculating group constants (i.e. manner of

integration) effects the results, especially the reaction rates of plutonium isotopes, if their lowest lying resonances are included into the thermal energy range.

Assumption (a) (i.e. neglect of leakage) has not been analyzed in details. However, due to the small contribution of leakage in the thermal energy range this approximation does not seem to be dangerous, if the group constants of the equivalent homogeneous medium are well approximated.

To some extent the effect of leakage on the spectrum of thermal neutrons was analyzed in connection with the more simple code *BETTY-2*.

Approximation (b) (cylindrization with white boundary condition) has been extensively studied in the literature (cf. e.g. Weiss *et al*, 1964). However, the relatively small width of the moderator region in WWR lattice cells required some further investigations.

Comparative calculations were made by using the Monte Carlo code *OMEGA* (Seifert, 1976). The results are presented in Table 4.3.1.

Table 4.3.1 Results of *OMEGA* calculations

Lattice	Hexagonal cell. Mirror boundary condition		Cylindrical cell. White boundary condition.	
	η_f	$\bar{\phi}_m/\bar{\phi}_f$	η_f	$\bar{\phi}_m/\bar{\phi}_f$
Z1	1.7550±0.0005	1.159	1.7652±0.0003	1.139
Z2	1.7014±0.0004	1.169	1.7018±0.0004	1.164

It can be seen that in the limiting case of lattice pitch 11.0 mm the approximation (b) leads to the underestimation of the disadvantage factor by about 2% and the overestimation of η_f with 1%. At the same time for the normal pitch 12.7 mm the inaccuracy is small. The propagated error caused by cylindrization should be accounted for in comparing results of calculations and measurements.

Approximation (c) has also been extensively studied in the literature. Various methods of calculating first flight collision probabilities were considered. In order to evaluate the various methods, comparative calculations were performed in KFKI, Budapest (Gado, 1985). The well known Thie lattices (Thie, 1961) were calculated by applying four methods: (Honeck, 1964), (Bonalmi, 1961 and Jonsson, 1963), (Carlvik, 1966) and Muller *et al*, 1963).

The number of mesh points was varied both in the fuel and the moderator. The methods applied in high speed calculations were also included in this analysis; these were the method of (Kavenoky, 1969) applied in *BETTY-2* (Gado *et al*, 1973) the special method used in *LEOPARD* (Barry, 1963) and the method of *PEACO* (Ishiguro *et al*, 1971). The results of calculations are given in Table 4.3.2.

Table 4.3.2 Disadvantage factors in the Thie lattices according to different algorithms

Method	Number of points	L A T T I C E ^{*)}					
		T1	T2	T3	T4	T5	T6
Bonalumi	1+1	1.1533	1.1508	1.1410	1.1410	1.1427	1.1473
Barry		1.1731	1.1718	1.1582	1.1619	1.1712	1.1806
Carlvik	3+3	1.1603	-	1.1426	-	-	1.1432
Kavenoky		1.1566	1.1508	1.1400	1.1379	1.1370	1.1387
Honeck		1.1623	1.1569	1.1465	1.1449	1.1446	1.1467
Ishiguro <i>et al</i>		1.1566	-	1.1401	-	-	1.1353
Carlvik	5+5	1.1587	-	1.1411	-	-	1.1395
Kavenoky		1.1576	1.1515	1.1404	1.1383	1.1372	1.1389
Honeck		1.1602	1.1542	1.1436	1.1416	1.1507	1.1422
Ishiguro <i>et al</i>		1.1579	-	1.1404	-	-	1.1365
Carlvik	12+12	1.1583	1.1519	1.1408	1.1385	1.1374	1.1387
Kavenoky		1.1582	1.1518	1.1407	1.1385	1.1374	1.1394
Honeck		1.1590	1.1527	1.1413	1.1391	1.1380	1.1392

^{*)} See Table 4.3.14

Comparison of the results show that the Carlvik, Kavenoky, and Ishiguro *et al* methods give the best results. Convergence of the calculations by using the Kavenoky method is better than for the method of Carlvik. The Honeck method also gives good results if the number of mesh points is high enough. The inaccuracy of the Bonalumi-Jonsson method is not very large, but the accuracy of the *LEOPARD* method seems to be unacceptable.

Approximation (d) (i.e. isotropic scattering in the laboratory system) seems to be the most serious one in the *THERMOS*-type codes. Fortunately

this approximation is less important for WWER lattices due to the relatively small amount of moderator.

In all *THERMOS* type programs, approximation (d) is corrected by using the so called "non-complete transport correction" in the moderator where instead of Σ_{s0}^{gg} the quantity $\Sigma_{s0}^{gg} - \bar{\mu} \Sigma_{s1}^{gg}$ is written. If this quantity appears to be negative, $\Sigma_{s0}^{gg} = 0$ is written.

Calculations were performed in KFKI, Budapest, for studying the significance of the transport correction, by using the *THERMOS* and *ANICELL* (Devenyi, 1985) codes. The latter accounts for the linear anisotropy of scattering. Results are given in Table 4.3.3. It can be seen that the transport correction takes into account the anisotropy effects in WWER lattices in a very acceptable manner. Some supplementary calculations were made by using the method of non-complete transport correction and the method of Benoist within the *BETTY-2* code (see below).

Table 4.3.3 Exact and approximate calculations accounting for the anisotropy of scattering

Lattice*	Value	<i>THERMOS</i> Isotropic scattering	<i>ANICELL</i> Isotropic scattering	<i>THERMOS</i> Transport Correct.	<i>ANICELL</i> Anisotrop. scattering
Z1	η_f	1.766	1.767	1.766	1.767
	ϕ_m/ϕ_f	1.103	1.104	1.103	1.102
	$\bar{V}$	2.077	2.065	2.077	2.069
Z2	η_f	1.715	1.715	1.715	1.715
	ϕ_m/ϕ_f	1.134	1.136	1.131	1.132
	$\bar{V}$	1.720	1.714	1.721	1.716
Z3	η_f	1.630	1.630	1.631	1.631
	ϕ_m/ϕ_f	1.170	1.173	1.164	1.168
	$\bar{V}$	1.507	1.504	1.508	1.505

*) See Table 4.3.15

Approximation (e) can be split into two factors: choice of the upper limit of the thermal energy range E^* and the approximation used for the slowing down source of neutrons.

Obviously, the greater the cutoff energy E^* , the less important are

the approximations for the source. The value of E^* is limited by the consideration that it is not reasonable to treat the lowest lying resonance of ^{238}U (at 6.68 eV) in the thermal energy range. At the same time the resonance of the ^{240}Pu isotope (at 1.056 eV) may be treated either in the thermal, or in the epithermal energy range.

Choosing E^* in the range

$$1.5 \text{ eV} < E^* < 4 \text{ eV}$$

is applicable both for plutonium and burned up lattices.

When E^* is chosen in the range

$$0.4 \text{ eV} < E^* < 0.625 \text{ eV},$$

the interference between thermalization and resonance effects becomes significant. In this case the approximations for the slowing down source become substantial even for uranium lattices.

The effects of various approximations of the slowing down source on the lattice parameters were studied in ZES Skoda, Plzen, for $E^*=0.625$ eV and $E^*=1$ eV and also in KFKI, Budapest, for $E^*=0.625$ eV and $E^*=1.84$ eV. Three approximations were considered.

In each model the slowing down source (due to scattering on any nuclei except hydrogen) is calculated by the formula

$$S_k(V) = \begin{cases} \frac{N_k \sigma_{S_0}^k V}{1 - \alpha_k} \left[\frac{1}{(V^*)^2} - \frac{\alpha_k}{V^2} \right] & \left\{ \alpha_k V^* \leq V \leq V^* \right\} \\ 0 & \left\{ 0 \leq V \leq \alpha_k V^* \right\} \end{cases}$$

where

N_k is the nuclear density of isotope k ,

$\sigma_{S_0}^k$ is the isotropic scattering cross section of isotope k at E^* ,

$$\alpha_k = \left(\frac{A_k - 1}{A_k + 1} \right)^2,$$

A_k is the mass number of nucleus k ,

V^* is the neutron velocity corresponding to E^* .

This approximation corresponds to the "billiard ball" model above E^* for neutron scattering. In this model it is neglected by the thermal motion and the chemical binding effects.

Model 1. Traditionally in TIC laboratories the slowing down source due to scattering on hydrogen is calculated by the same model:^{*)}

$$S_H(V) = \frac{N_H \sigma_S^H V}{V^2}$$

$$S_H(V) = \frac{N_H \sigma_S^H V}{V^2}$$

Model 2. In the model proposed in (Lehman, 1974) $S_H(V)$ is calculated taking into account asymptotically the thermal motion and the chemical binding effects in the free gas model with the effective temperature T_{eff} . The parameters of the free gas model correspond to the asymptotic limits of the Nelkin model:

$$S_H(V) = \frac{N_H \sigma_S^H V}{V^2} \operatorname{erf} \left[\sqrt{T/T_{eff}} V \right],$$

Here T is the moderator temperature and

$$T_{eff} = \lambda_0 T + \sum_{i=1}^3 \lambda_i \omega_i \left[\frac{1}{\exp(\omega_i/T) - 1} + \frac{1}{2} \right]$$

(temperature T values are in eV units).

In the Nelkin model:

$$\lambda_0 = 0.0556$$

$$\lambda_1 = 0.4310$$

$$\lambda_2 = 0.1711$$

$$\lambda_3 = 0.3423$$

$$\omega_1 = 0.060 \text{ eV}$$

$$\omega_2 = 0.205 \text{ eV}$$

$$\omega_3 = 0.480 \text{ eV}.$$

Model 3. In the third model $S_H(V)$ is calculated on the assumption that the source can be described by the matrix elements of the scattering matrix from the highest group:

^{*)} In Kurchatov IAE it was used the free gas model taking into account both the thermal motion and the chemical binding effects in asymptotical approximation (cf. (Maierov, 1962), (Marchuk *et al*, 1962), (Maierov, 1965)), (Editor's remark).

$$S_H(V) = N_H \sigma_{S_H} \left[V^* \rightarrow V \right],$$

and the matrix itself is calculated by the model used in the THERMOS calculation otherwise.

Comparative calculations were performed both for homogeneous media and lattice cells. The results are presented in Table 4.3.4. The second method proved to be the most accurate. Integral quantities (like η_f) are generally not sensitive to the choice of source function, but the first model ("billiard ball") underestimates $\bar{V}$ (and consequently overestimates $\bar{\sigma}$ for $1/V$ isotopes) with maximum 1%. The third method gives an opposite error (maximum 2.5%) and its application is not recommended.

Table 4.3.4 Comparison of various models
of slowing down source

Lattice ^{*)}	The Source Model	$\bar{V}$	η_f	f
$\Gamma 1$	1	1.1714	-	-
	2	1.1726	-	-
	3	1.1736	-	-
$\Gamma 2$	1	1.5066	-	-
	2	1.5172	-	-
	3	1.5270	-	-
$\Gamma 3$	1	1.8104	-	-
	2	1.8293	-	-
	3	1.8473	-	-
S1	1	1.963	1.9356	0.8970
	2	1.979	1.9353	0.8970
	3	2.029	1.9345	0.8967
S2	1	1.296	1.9473	0.6811
	2	1.300	1.9472	0.6812
	3	1.300	1.9471	0.6811

^{*)} See Tables 4.3.13, 4.3.15.

The last approximation (f) is connected with choosing the multi group structure in the thermal energy range. As the generally applied group structures give a satisfactorily detailed picture, their choice was not studied for cases when the number of groups is high enough. In the study

(Kereszturi, 1981) correspondingly only the 35-group structure of LASER was investigated. For this purpose the thermalization equation was solved for various homogeneous media in the free gas model. In this case it is easy to obtain the exact solution. The calculations were performed in the 35-group structure with point wise cross sections. It turned out that the group width ΔV_1 is considered as a weighting function of integration.

More exactly,

(1) The 35-group calculation of the neutron spectrum is not sensitive to the choice of ΔV_1 .

(2) Reaction rates R^x are usually integrated by the formula

$$R^x = \sum_i \phi_1 \sigma_1^x \Delta V_1,$$

where ΔV_1 is chosen as

$$\Delta V_1 = \begin{cases} 2V_1 & i=1 \\ 2 \left[V_i - \sum_{j=1}^{i-1} \Delta V_j \right] & i \geq 2 \end{cases}$$

However, in the case of using point wise cross sections, the value of the ^{240}Pu capture rate significantly deviates from the exact value (4%, cf. Table 4.3.5). It is worth mentioning that by applying multi group constants rather than point wise cross sections the problem is less important, but the accuracy of determining the capture rate for ^{240}Pu remains problematic.

Table 4.3.5 Effect of integration methods on integral quantities

M E D I U M	$\bar{V}$			$^{239}\sigma_a 10^2$			$^{240}\sigma_a 10^2$		
	Method*			Method*			Method*		
	1	2	3	1	2	3	1	2	3
$\Gamma 1$	1.4589	1.4580	1.4579	-	-	-	-	-	-
$\Gamma 2$	1.5702	1.5642	1.5723	6.2943	6.2728	6.2749	3.101	2.9465	3.0997
$\Gamma 3$	1.4659	1.4604	1.4687	6.5341	6.5119	6.5125	1.580	1.5238	1.5738
$\Gamma 4$	1.5753	1.5704	1.5782	6.3298	6.2992	6.3064	1.962	1.8827	1.9527

* (1) - Exact solution

(2) - Classical method

(3) - Method (Kereszturi, 1981)

**) See Table 4.3.13

On the basis of the above considerations it is possible to conclude that the *THERMOS*-type codes may be applied with great accuracy for the calculation of the thermal neutron flux in regular fuel lattices. The summary of inaccuracies for WWER lattices is given in Table 4.3.6.

Table 4.3.6 Inaccuracy of various quantities calculated by THERMOS

Approximation ↓		**) Lattice								
		Z1			Z2			Z3		
		$\bar{\phi}_m / \bar{\phi}_f$	$\bar{V}$	η_f	$\bar{\phi}_m / \bar{\phi}_f$	$\bar{V}$	η_f	$\bar{\phi}_m / \bar{\phi}_f$	$\bar{V}$	η_f
Cylindrization		-1.8%	-0.3	.1%	-0.4%	0	0	0	0	0
Transfer	1 *	0	0	0	0	0	0	0	0	0
Kernel	2 *	.1%	0	0	0.6%	0	0	0.3%	0	0
Calcul.	3 *	-0.5%	-0.1%	0	-0.5%	0	0.1%	-0.7%	0.1%	0.2%
Slow. down Source	T_{eff}	-	-	-	-	-	-	-	-	-
	Bill. Ball	0.1%	-0.8%	0	0.1%	-0.6%	0	0.1%	0.5%	0
In sum: (Honeck) Billiard Ball appr. Cylindrization		-0.5%	~-1.2%	.1%	0.3%	-0.6%	0	0.4%	0.5%	0

*) Methods: **) See Table 4.3.15

1. Carlvik
2. Honeck
3. Bonalumi-Jonsson

4.3.2 High speed engineering programs

In the high speed thermalization programs some general assumptions are used:

- (a) The thermalisation effects are accounted for only the basic moderator (in the case of WWER lattices for water), while these effects are neglected for the other isotopes (e.g. for oxygen in fuel).
- (b) It is assumed that the thermalization source differs from zero only in the moderator region (in accordance with assumption (a)). There it is constant in space and isotropic in the laboratory system. As a consequence, the disadvantage factor for each group can be separately calculated before the thermalization calculation.
- (c) Instead of the integral thermalization equation a second order ordinary differential equation is solved and the characteristics of the scattering

matrix of water are described by using auxiliary functions.

As a consequence of assumptions (a) and (b) the elementary lattice cell can be homogenized by using the pre-calculated disadvantage factors, and the neutron spectrum is calculated for this equivalent medium.

The approximate differential equations vary with the different codes. In the *LEOPARD* code the Wigner-Wilkins model (Wigner *et al*, 1944) is applied, in *BETTY-2* Cadilhac's "secondary model" (Cadilhac, 1963) is utilized, while in *UNIRASOS* the simplified option of the Laletin model (Laletin, 1963) is made use of. The differences between these models are partially known from the literature (e.g. Williams, 1966), and were partially analyzed in (Gado, 1980). The differences can be summarized as follows.

As a basis of discussion the Cadilhac model is chosen. This model determines the connection between the slowing down density $q(E)$ and the neutron spectrum $\phi(E)$ by the formula

$$\frac{d\phi(E)/M(E)}{dE} = j(E)q(E) - \frac{d}{dE} k(E) \frac{dq(E)}{dE} \quad (4.3.1)$$

where $M(E) = \frac{E}{T^2} \exp(-E/T)$ - is the Maxwellian distribution.

$$q(E) = \int_0^E dE' \int_E^\infty dE'' \Sigma_s(E'' E') \phi(E'') dE'' - \int_E^\infty dE' \int_0^E dE'' \Sigma_s(E'' E') \phi(E'')$$

and $j(E)$ and $k(E)$ are functions characterizing the approximate thermalization model.

Equation (4.3.1) is solved together with the balance equation

$$\Sigma_a(E) \phi(E) = -\frac{dq(E)}{dE} \quad (4.3.2)$$

where $\Sigma_a(E)$ is the macroscopic absorption cross section.

In the *BETTY-2* program the basic concept of Cadilhac is used: the functions $j(E)$ and $k(E)$ are adjusted to *THERMOS* calculations and the tabulated functions for various materials and temperatures are stored in the multi group constant library (cf. Chapter 2).

The models used in other high speed programs can be interpreted as special sub cases of the Cadilhac model.

- The traditional model of generalized heavy free gas is obtained when choosing

$$j(E) = \left[\xi \Sigma_s \text{ETM}(E) f(E) \right]^{-1}$$

$$k(E) = 0$$

where Σ_s and $\xi\Sigma_s$ are the scattering and slowing down cross sections above the thermal energy range. When choosing further

$$f(E) = 1$$

the heavy free gas model is obtained. These models are not used in TIC laboratories.

- In the *UNIRASOS* code the functions $j(E)$ and $k(E)$ are chosen as

$$j(E) = \left[\xi\Sigma_s \text{ETM}(E) \right]^{-1},$$

$$k(E) = \gamma \left[\xi\Sigma_s M(E) \right]^{-1},$$

where γ is a parameter used for adjusting to *THERMOS* calculations. In the limiting cases of $\gamma=0$ and $\gamma=1$ the equations of the heavy free gas model and the simplified Laletin model are obtained.

- In the *LEOPARD* code the Wigner-Wilkins model is applied. This model is based on the approximate degenerated kernel of the transport equation (for the differential scattering cross section), when the Cadilhac model is exact and the functions $j(E)$ and $k(E)$ can be calculated by the formulae

$$j(E) = \left[\Sigma_s \text{ETM}(E) f(E) \right]^{-1}$$

$$k(E) = \left[\Sigma_s M(E) g(E) \right]^{-1}$$

where

$$f(E)^{-1} = \Sigma_s \left[\frac{1}{E_s(E)} - E \frac{d}{dE} \frac{1}{\Sigma_s(E)} \right]$$

and

$$g(E)^{-1} = \frac{\Sigma_s(E)}{\Sigma_s}$$

(This model concerns hydrogen gas, therefore $\xi=1$.)

The non-physical choices

$$f(E) = 1 \text{ and } g(E) = 0$$

$$f(E) = 1 \text{ and } g(E) = 1/\gamma$$

correspond to the models of heavy free gas and that applied in *UNIRASOS*, respectively. These models are not equivalent with each other under any circumstances.

For constant scattering cross section

$$\Sigma_s(E) = \Sigma_s$$

the simplified option of Laletin's model is obtained.

According to calculational experience, the Wigner-Wilkins model gives satisfactory results for thermalization studies. This fact can be explained by compensation of errors. Application of the model does not require any further work for library preparation since $\Sigma_s(E)$ can be directly calculated in the framework of the model.

As a conclusion of the above consideration one may state that from among the mentioned high speed thermalization codes *BETTY-2* should give the best results. Results from calculations by these high speed thermalization codes are compared with each other and *THERMOS* calculations in Section 4.3.3.

4.3.3 Analysis of approximations used in high speed thermalization codes

The general approximation used in the high speed thermalization codes and the various approximations to the thermalization model are described above. These approximations were analysed in KFKI, Budapest (Kereszturi, 1981). Below, the most important conclusions of this analysis are discussed.

The first problem is the numerical method utilized for integrating the differential equations. It was investigated only for the *BETTY-2* code (Kereszturi, 1981). Calculations were performed in an analogous way to the *THERMOS* investigations and practically the same accuracy was reached as by the 35-group *THERMOS* calculations.

The high speed of the investigated codes is partially due to the application of approximate thermalization equations. These approximations were validated in comparative calculations performed by using *BETTY-2* (where the Laletin and Wigner-Wilkins models were also included, although the numerical method of *BETTY-2* was always applied) and *THERMOS*. Library constants were identical and the application of the Nelkin model in the *THERMOS* code corresponded to the adjustment of functions $j(E)$ and $k(E)$ of the *BETTY-2* code. The calculations were carried out for various homogeneous media. The results are presented in Table 4.3.7.

Table 4.3.7 Comparison of various approximate scattering models

Medium	$\bar{V}$				$^{239}\sigma_a 10^2$			
	1	2	3	4	1	2	3	4
$\Gamma 1$	1.1736	1.1741	1.1659	1.1732	-	-	-	-
$\Gamma 2$	1.5270	1.5263	1.4602	1.5177	-	-	-	-
$\Gamma 3$	1.8473	1.8438	1.7358	1.8194	-	-	-	-
$\Gamma 4$	1.6669	1.6638	1.5715	1.6426	6.3029	6.4022	6.2799	6.3421
$\Gamma 5$	1.5371	1.5351	1.4674	1.5257	6.5576	6.6550	6.5189	6.5939
$\Gamma 6$	1.6761	1.6707	1.5768	1.6485	6.3288	6.4393	6.3152	6.3792

Medium	$^{240}\sigma_a 10^2$				
	1	2	3	4	
$\Gamma 1$	-	-	-	-	/1/ THERMOS \Nelkin\ /2/ Cadilhac /3/ Wigner-Wilkins /4/ Laletin
$\Gamma 2$	-	-	-	-	
$\Gamma 3$	-	-	-	-	
$\Gamma 4$	3.2278	3.2770	3.0968	3.0744	
$\Gamma 5$	1.6279	1.6119	1.5725	1.5450	
$\Gamma 6$	2.0470	2.0297	1.9519	1.9359	

Choosing the Nelkin model as a basis, the following conclusions can be drawn.

- For the Cadilhac model in the case of $1/V$ absorption the results coincide with the results of the Nelkin model. In the presence of plutonium isotopes, however, the effective cross sections of the plutonium isotopes are obtained with an inaccuracy of 1.5%, while the $1/V$ absorption remains accurate up to 0.1-0.3%.
- For the Wigner-Wilkins model at mass number 1, the $1/V$ absorption highly deviates from the value in the Nelkin model (-6.8%), but the plutonium cross sections are obtained with an accuracy of 1 to 4%.
- The results of the simplified Laletin model lie between the Cadilhac and Wigner-Wilkins model, but the optimal choice of the parameter γ may improve the results.

Assumption (a) of Section 4.3.2 can be investigated by using such THERMOS calculations, where thermalization is taken into account for water and the thermalization source is present also only in the moderator region. Calculations of this kind were performed for various lattices. The results are given in Table 4.3.8.

Table 4.3.8 Effect of neglecting thermalization in the fuel

Lattice	Thermalization inside fuel	η_f	$\bar{\phi}_m / \bar{\phi}_f$	$\bar{\phi}_c / \bar{\phi}_f$
S1	Yes	1.7360	1.2066	1.1026
	No	1.7355	1.2079	1.1037
S2	Yes	1.3264	1.5006	1.1410
	No	1.3257	1.5012	1.1414
P1	Yes	1.4698	1.3000	1.1607
	No	1.4733	1.3005	1.1611
P2	Yes	1.2272	1.4768	1.1538
	No	1.2271	1.4773	1.1542

It can be seen that if neglected thermalization in the fuel is it does not affect the disadvantage factors and η_f of the uranium lattices, but in the case of tight plutonium lattices the effect in η_f may reach 0.25%.

The influence of assumption (b) of Section 4.3.2 proved to be even less significant. Comparative calculations were made by using the BETTY-2 code and its improved version, which permits the variation of the thermalization source in the lattice cell. Results are presented in Table 4.3.9 and, as can be seen, the results practically coincide with each other.

Table 4.3.9 Effect of neglecting spatial dependence of thermalisation source

L A T T I C E						
C O D E	Z1			Z2		
	Parameter			Parameter		
	ϕ_m/ϕ_f	$\bar{V}$	η_f	ϕ_m/ϕ_f	$\bar{V}$	η_f
BETTY-2	1.1019	2.1220	1.7651	1.1329	1.7463	1.7140
Modified BETTY-2	1.1019	2.1215	1.7651	1.1330	1.7459	1.7140
C O D E	Lattice Z3			Description of the Z1-Z3 cells is given in the Table 4.3.15		
	Parameter					
	ϕ_m/ϕ_f	$\bar{V}$	η_f			
BETTY-2	1.1703	1.5220	1.6287			
Modified BETTY-2	1.1703	1.5218	1.6289			

In order to calculate the transport kernel the following methods are applied in the investigated codes:

- method (Kavenoky, 1969) in BETTY-2,
- method of Bonalumi-Jonsson in UNIRASOS,
- modified method of Amouyal-Benoist in LEOPARD (Barry, 1963).

These methods were compared in Table 4.3.2. Method described in (Kavenoky, 1969) is very accurate, but the methods of (Bonalumi, 1961 and Jonsson, 1963) and especially (Barry, 1963) lead to significant inaccuracies. In the investigated codes the non-complete transport correction is utilized to account for the anisotropy of scattering (in the BETTY-2 code the Benoist method (Benoist, 1964) is also available). It is not trivial that this correction leads to the same results when applied for group-wise disadvantage factors, as in the case of THERMOS. Results without and with correction for the BETTY-2 and THERMOS codes are compared in Table 4.3.10.

Table 4.3.10 Comparison of lattice calculations
by THERMOS and BETTY-2 codes

Lattice	CODE	Transp. Correction	η_f	$\bar{\phi}_m / \bar{\phi}_f$	$^{235}\sigma_a$	$^{238}\sigma_a$	$^{240}\sigma_a$
S1	T	No	1.7351	1.2135	286.75	1.2670	-
	T	Yes	1.7355	1.2079	286.77	1.2670	-
	C	No	1.7352	1.2102	283.54	1.2560	-
	C	Yes	1.7354	1.2044	283.41	1.2554	-
	C	B*	1.7363	1.1965	283.02	1.2539	-
S2	T	No	1.3120	1.5527	437.09	1.8385	-
	T	Yes	1.3257	1.5012	437.01	1.8399	-
	C	No	1.3069	1.5526	429.66	1.8133	-
	C	Yes	1.3211	1.4954	429.52	1.8127	-
	C	B*	1.3247	1.4850	429.33	1.8120	-
P1	T	No	1.4723	1.3118	350.72	1.5216	499.3
	T	Yes	1.4733	1.3005	350.45	1.5208	499.4
	C	No	1.4720	1.3086	346.88	1.5077	496.8
	C	Yes	1.4723	1.2970	346.36	1.5056	498.6
	C	B*	1.4703	1.2832	344.94	1.5001	506.6
P2	T	No	1.2144	1.5296	464.33	1.9454	332.1
	T	Yes	1.2271	1.4773	464.08	1.9441	331.5
	C	No	1.2116	1.5266	456.04	1.9156	323.6
	C	Yes	1.2239	1.4706	454.71	1.9105	329.7
	C	B*	1.2271	1.4532	453.93	1.9074	334.2

* On Benoist formulae.

As can be seen, the transport correction leads to the same effects in both cases. The formula of Benoist overestimates this correction.

The BETTY-2 code gives a possibility to investigate the influence of thermal leakage on the neutron spectrum. In the code the diffusion coefficient is calculated according to the formula of Benoist (Benoist, 1964):

$$D^g = \frac{1}{3} \frac{\sum_i \sum_j V_i \varphi_i^g \lambda_j^g P_{ij}^g}{\sum_i V_i \varphi_i^g},$$

where V_i - volume of the subregion,

φ_i - average flux in subregion i for group g ,

P_{ij} - first flight collision probability,

$\lambda_j = 1/\Sigma_{trj}^g$ everywhere except in the moderator, where $\lambda_0 = 1/\Sigma_{trj}^g$.

The supplementary absorption term DB^2 approximately accounts for the leakage. The corresponding results are given in Table 4.3.11. It can be seen that the effect is negligibly small for real cases.

Table 4.3.11 Effect of leakage on some thermal characteristics of lattices

Lattice	B^2 [cm^{-2}]	η_f	$\bar{\phi} / \bar{\phi}$	$\bar{V}$
P1	0	1.4723	1.2970	1.7244
	0.00631	1.4710	1.2968	1.7294
P2	0	1.2239	1.4706	1.3013
	0.00537	1.2237	1.4702	1.3037

The inaccuracies of various approximate thermalization calculations are summarized in Table 4.3.12 for ZR-6 lattices. For the BETTY-2 code the assumption on the thermalization source is significant, but the other assumptions lead to negligible errors. In the case of codes LEOPARD and UNIRASOS the thermalization models and also the calculation of first flight collision probabilities contribute to the inaccuracy of the calculations.

Table 4.3.12 Summary of inaccuracies in various quantities

Source of inaccuracy	L A T T I C E								
	Z1			Z2			Z3		
	P A R A M E T E R								
	$\bar{\phi}_m / \bar{\phi}_f$	$\bar{V}$	η_f	$\bar{\phi}_m / \bar{\phi}_f$	$\bar{V}$	η_f	$\bar{\phi}_m / \bar{\phi}_f$	$\bar{V}$	η_f
Thermalis. Model:	0	+1.3%	0	+0.2%	+0.8%	0	+0.6%	+0.5%	0
Cadilhac	0	-0.3%	0	0	-0.2%	0	0	0	0
Wigner-Wilkins		-9%			-6%		-0.6%		
Laletin		-2%			-1.5%		0		
No Thermalisation in Fuel	+0.1%	-0.5%	0	+0.1%	-0.2%	0	+0.1%	-0.1%	0
Constant Source Inside Moderator	0	0	0	0	0	0	0	0	0

Table 4.3.13 Data of homogeneous media used in comparative calculations of Section 4.3.

Homogeneous media

Notation	PARAMETERS		
	$\Sigma_a^{2200} / * /$ [cm ⁻¹]	N / ²³⁹ Pu/ [10 ²⁴ cm ⁻³]	N / ²⁴⁰ Pu/ [10 ²⁴ cm ⁻³]
Γ1	0.02	0	0
Γ2	0.2	0	0
Γ3	0.4	0	0
Γ4	0.2	10 ⁻⁴	0
Γ5	0.2	0	2.5*10 ⁻⁵
Γ6	0.2	10 ⁻⁴	2.5*10 ⁻⁵

/*/ for 1/V absorber.

Table 4.3.14 Data of the lattices used in comparative calculations of Section 4.3.

Thie lattices

Notation	Fuel			Moderator		
	Parameter			Parameter		
	r [cm]	Σ_t [cm ⁻¹]	Σ_s [cm ⁻¹]	r [cm]	Σ_t [cm ⁻¹]	Σ_s [cm ⁻¹]
T1	0.381	0.780	0.387	0.859825	1.0618	1.053
T2	-"	-"	-"	-"	0.70787	0.702
T3	-"	-"	-"	0.644869	1.0618	1.053
T4	-"	-"	-"	-"	0.70787	0.702
T5	-"	-"	-"	-"	0.35393	0.351
T6	-"	-"	-"	-"	0.070787	0.0702

Table 4.3.15 Data of lattices used in comparative
calculations of Section 4.3

Notation	Fuel			Reactor lattices Cladding		
	r [cm]	Material [10^{24} cm^{-3}]		r [ccm]	Material [10^{24} cm^{-3}]	
Z1-Z3	0.38	^{16}O ^{235}U ^{238}U	0.045861 8.2550×10^{-4} 0.022105	0.45	Zr Nb	0.038679 3.87×10^{-4}
S1	0.453390	^{16}O	0.044925	0.4965	Mn	0.001400
		^{235}U	0.001305		Cr	0.013850
S2		^{238}U	0.021157		Fe	0.051585
					Ni	0.007692
P1	0.641350	^{16}O	0.042580	0.7175	Z i r c a l l o y	0.043248
		^{235}U	1.4857×10^{-4}			
		^{238}U	0.020718			
P2		^{239}Pu	3.0405×10^{-4}			
		^{240}Pu	9.9571×10^{-5}			
		^{241}Pu	1.7287×10^{-5}			
		^{242}Pu	2.7965×10^{-6}			

Table 4.3.15 (Continued)

Notation	Moderator		Lattice	
	r [cm]	$\text{N}/\text{H}_2\text{O}/$ [10^{24} cm^{-3}]	Form	Pitch [cm]
Z1	0.57754	0.33357	Hexagonal	1.10
Z2	0.66680	0.33357	Hexagonal	1.27
Z3	0.78756	0.33357	Hexagonal	1.50
S1	0.74517	0.033431	Square	1.3208
S2	0.49037	0.033431	Square	2.6416
P1	1.06688	0.033341	Hexagonal	2.0316
P2	1.7604	0.033341	Hexagonal	3.3529

4.4 DESIGN CODES METHODS AND CROSS SECTIONS LIBRARIES

The present section contains short descriptions of methods used in the design codes created in the institutes of the members of TIC and assigned for fuel lattices burnup calculations. For more detailed information about the codes the reader is referred to Table 4.1.2. It should be mentioned that here we do not consider codes adopted by the TIC participants.

The descriptions of the codes given below with use of unified format contain the following information:

1. the code assignment and treated configurations;
2. group structure;
3. used files of evaluated nuclear data;
4. approximations used for reaction rate calculations in the resonance energy range;
5. approximations used for thermal neutron spectrum calculations and energy break point between epithermal and thermal energy ranges;
6. number of actinoids and fission products taken into account in burnup calculations;
7. the approaches utilized for spatial neutron fluxes distribution calculations in treated configurations;
8. the code features.

BETTY-2

1. The code is assigned for elementary cell and supercell burnup calculations.
2. 70-groups (35 epithermal and 35 thermal) with energy break point at 1.84 eV.
3. Cross sections library is based on ENDF/B-IV data.
4. Self-shielded cross sections are computed by interpolation of I (σ_{dil}) tables based on the equivalence theorem by taking into account the effect of mutual overlapping of resonances. The Goldstein factors are obtained for each group by means of a special iteration procedure with use of pretabulated resonance integrals and group fluxes. The Bell factors are represented as a function of fuel rod diameter and the Dancoff factor and determined by interpolation. Resonance neutron spectrum is calculated using scattering matrixes.

5. Thermal neutron spectrum is computed on the basis of the Cadilnac differential thermalization model and 35-group cross sections energy dependencies representation.
6. 18 actinoids and 164 fission products.
7. Calculations of the flux spatial distribution are based on P_{1j} method.
8. Special technique for determining Goldstein and Bell factors.

MICROBE

1. The code is assigned for burnup calculations of elementary cells, supercells and fuel assemblies on the basis of preliminary homogenization of fuel cells and the 1D approximation.
2. 48 groups (24 epithermal and 24 thermal) with energy break point at 0.465 ev.
3. Cross sections library is based on ENDF/B-IV data.
4. Self-shielded cross sections are computed by f-table interpolation on the basis of the equivalence theorem. The resonance neutron spectrum is calculated using scattering matrixes.
5. Thermal neutron spectrum is computed with use of scattering matrixes. Scattering matrixes for hydrogen were prepared using the Coppel-Young model.
6. Burnup model description is not available in literature.
7. Spatial fluxes distributions are calculated by the P_{1j} method.
8. Special iteration procedure is used for thermal spectrum calculation to significantly reduce running time.

NESSEL-4

1. The code is assigned for burnup calculations of elementary cells, supercells and fuel assemblies on the basis of preliminary homogenization of fuel cells and the 1D approximation.
2. 34 groups (24 epithermal and 10 thermal) with energy break point at 0.465 ev.
3. Cross section library for epithermal groups is based on ABBN data. Thermal cross sections library was prepared using ENDF/B-IV data.
4. Self-shielded cross sections are determined by f-table interpolation on the basis of the equivalence theorem. Goldstein factors depending on group number were obtained by fitting to the

results of Hellstrand measurements. Resonance neutron spectrum are calculated using scattering matrixes.

5. Thermal neutron spectrum is computed using scattering matrixes.
6. 8 actinoids, 6 fission products and 9 pseudo products.
7. Spatial neutron fluxes distributions are computed using the P_{1j} method.
8. The code can be used as cross section generator for diffusion and transport codes based on the S_n - method.

UNIRASOS-2

1. The code is used for cell burnup calculations.
2. 14 group (2 fast, 12 resonance), 101 energy points for thermal energy region with energy break point at 0.625 ev. Micro cross sections in 2 fast groups are represented as a function of some parameters characterizing fast neutron spectrum to provide equivalence of 2-group and 12-group description of considered energy range.
3. Cross sections library is based on ABBN (energy range of fast neutrons and unresolved resonances), LIPAR (energy range of resolved resonances) and KORT (thermal energy range) data.
4. Self-shielded resonance integrals are computed by interpolation of the $I(\sigma_{d11})$ tables on the basis of the equivalence theorem with taking into account mutual overlapping of resonances. Data of $I(\sigma_{d11})$ tables were obtained with reference code for a single pin case. The Goldstein factors do not depend on group number and were obtained by fitting to results of reference calculations. Resonance neutron spectrum is computed for homogeneous media on the basis of continuous slowing down methods (Yamamura, Sekija, 1971).
5. Thermal neutron spectrum calculations are based on Laletin two-constant differential model (Laletin¹⁹⁶³).
6. 19 actinoids and 95 fission products.
7. Calculations on distributions of spatial neutron fluxes are based on the P_{1j} method.
8. Low running times.

RAFORIN

1. The code is assigned for the cells and supercells burnup calculations. The supercell calculations can be performed using preliminary homogenization and 1D approximation or on the basis of the 2D "cluster" approach.
2. 38 group (2 fast, 12 resonance and 24 thermal) with energy break point at 0.625 ev. The same approach is used for reaction rate calculations in the fast groups as in *UNIRASOS-2*. It is supposed that the fission spectrum depends on fission energy and, therefore, is a function of fuel isotopic composition. The 48-group (with 12 fast groups) version of the code is also available.
3. Cross section library is based on the same evaluated nuclear data files as *UNIRASOS-2*.
4. The approaches realized for reaction rates calculations in the uniform fuel lattice are practically, with some exceptions (^{240}Pu lowest resonance treatment, the way of $I(\sigma_{dil})$ tables computing), identical to those used in *UNIRASOS-2*. In the supercell, the resonance neutron spectrum is computed using preliminary homogenization of fuel cells and scattering matrixes for description of neutron slowing down.
5. Thermal neutron spectrum is computed using scattering matrixes.
6. 19 actinoids, 95 fission products and all Gd isotopes.
7. Spatial neutron distributions are computed using surface pseudo sources method.
8. The code provides a possibility to obtain sets of functionals needed for elementary cell description used in diffusion and nodal type approaches.

TVS

1. The code is assigned for fuel assembly burnup calculations taking into account real 2D geometry.
2. The same as in *UNIRASOS-2*.
3. The same as in *UNIRASOS-2*.
4. The approaches used for resonance absorption calculations are identical to those used in *UNIRASOS-2*. Special modules included into the code allow one to calculate resonance absorption in the fuel or BA rod with nonuniform absorber distribution (Rubin, 1989).

5. The same as in UNIRASOS-2.
6. 19 actinoids, 95 fission products, all gadolinium isotopes. Number of burnable zones can be varied from 1 to 15.
7. Spatial distribution of fluxes in the elementary cells are computed using the P_{1j} method. Four-group diffusion approach is used for calculations of spatial distribution of fluxes in a whole assembly.
8. Low running time.

SAPFIR

1. Design oriented code package is assigned for burnup calculations of core fragments of different type reactors. For WWER type reactors, the code package allows one to perform multigroup calculations of supercell and a whole fuel assembly.
2. 63 group. (23 epithermal and 40 thermal groups) with energy break point at 1.0 ev. In the resonance energy region each group is divided into a number of subgroups. Subgroup fluxes are computed for all zones of considered configuration.
3. Cross section library is based on ABBN, LIPAR and KORT data.
4. Generalized subgroup approach is used for calculations in the resonance energy range. The code package also includes a module that solves the space and energy dependent transport equation on a very fine energy mesh (some thousand energy groups) in the energy range of resolved resonances.
5. Thermal neutron spectrum is calculated using 40-group approximation and scattering matrixes.
6. 14 actinoids, 30 fission products, one pseudo product and all gadolinium isotopes.
7. Calculations of spatial fluxes distributions are based on the P_{1j} method. The first collision probabilities can be computed by deterministic or Monte-Carlo methods. To reduce running time a procedure of their preliminary tabulation and further interpolation is applied.
8. Strict modular structure, different possibilities for resonance absorption and calculation of first collision probabilities.

4.5 ANALYSIS OF NUMERICAL AND EXPERIMENTAL BENCHMARKS WITH DESIGN CODES

4.5.1 Analysis of numerical benchmarks

Analysis of numerical benchmarks is a necessary and important feature of design code verification. When design and reference codes are based on identical files of evaluated nuclear data, reliable estimation of physical approximations used in the design codes becomes possible.

The present section gives results of calculations obtained with design codes described in Sect. 4.4, the *MCU* code and some codes created in FRG, Japan, the USA and other countries. A wide set of zero leakage numerical benchmarks including more than 20 cells is considered. This set includes UO_2 , U_m , PuO_2 - UO_2 , Pu_m - U_m cells with enrichment and moderator-fuel volume ratio varying in a wide limits. Most of the results discussed in the present Section have been taken from (Becker et al., 1990).

It should be noted that, as follows from Sect. 4.4, some TIC design codes and the *MCU* code use different files of evaluated nuclear data. This causes problems in interpreting observed deviations but nevertheless provides a possibility to reveal the main trends of design code errors.

The authors faced serious problems when writing the present Section: on the one hand there were the great number of papers devoted to the problem of spectral code validation prepared in the framework of TIC activities, on the other hand, the full sets of benchmark solutions have been obtained with only a few codes. Apart from this, all codes are being continuously modified by their authors. The last factor leads to the rapid "aging" of calculation results. Thus, some of the results discussed below may not probably relate to the newest versions of the codes.

The set of numerical benchmarks was defined in (Badalov and Cononov, 1988) to test the validity of design codes.

The suggested set of benchmarks consists of 12 zero-leakage, three zone (fuel, clad, moderator) cell configurations. The cells considered are divided into three groups: "wide", "intermediate" and "tight" with moderator/fuel volume ratio equals to 1.82, 1.00 and 0.5 respectively.

The volume ratio of "wide" cells is close to the effective volume ratio in the core of a WWER-1000 type reactor and so are interesting from the practical point of view. The cells with smaller volume ratio are interesting mainly as strict test for approaches used in design codes for calculations in the epithermal energy range.

In each of three groups of cells four types of fuel are considered -

UO_2 , U_m , $UO_2 + PuO_2$, $U_m + Pu_m$. The isotope composition of Pu in all cells with mixed fuel corresponds to the composition in a spent fuel of WWER-1000. Contents of Pu fissile isotopes changes from 2.6 at.% to 10 at.% (in a "tight" cell).

All cell characteristics needed for calculations are given in Table 4.5.1.

Results of calculations obtained with UNIRASOS-2, RAFORIN, NESSEL-4, SAPPFIR* and MCU are given in Tables 4.5.2-4.5.3. It should be noted that because UNIRASOS-2 is a module of assembly cross section generator TVS the results obtained with UNIRASOS-2 for uniform fuel lattices and given in the present and the following sections may also be considered as TVS results. Before discussing the results obtained let us note that in MCU pointwise presentation (in particular, for U and Pu isotopes) of cross sections in energy range of resolved resonances was used to provide the necessary accuracy of computed cell parameters.

Calculated values of multiplication factor K_∞ and conversion ratio CR are compared in Table 4.5.2. The conversion ratio is determined as:

$$CR = \frac{R_c^{238} + R_c^{240}}{R^{235} + R^{239} + R^{241}}$$

where R^i , R^i represent the capture and absorption rates produced by isotope "i".

*) The SAPPFIR results were kindly presented to the authors by V. Tebin.

Table 4.5.1. Benchmark dimensions and compositions.

P a r a m e t e r	Cell type / dimensions and composition											
	"Wide"				"Intermediate"				"Tight"			
	UO ₂	UO ₂ + PuO ₂	U	U+Pu	UO ₂	UO ₂ + PuO ₂	U	U+Pu	UO ₂	UO ₂ + PuO ₂	U	U+Pu
R _{fuel}	0.387				0.387				0.387			
R _{clad}	0.455				0.455				0.455			
R _{moder.}	0.693				0.597				0.531			
V _m /V _f	1.82				1.00				0.50			
Enrichm. %	3.9	5.0	2.0	2.6	5.9	7.5	3.0	3.8	7.9	10.0	4.0	5.1
Moderat.	¹ H: $\rho=0.0668$; ¹⁶ O: $\rho=0.0334$											
Clad	Zr: $\rho=0.0425$											
Fuel												
⁵ U * 10 ²	8.5	-	8.5	-	12.8	-	12.8	-	16.5		16.5	-
⁸ U * 10 ²	2.05	1.99	4.09	4.03	2.00	1.92	4.05	3.97	1.97	1.85	4.01	3.89
⁹ Pu * 10 ⁴	-	8.5	-	8.5	-	12.8	-	12.8	-	-		
⁴⁰ Pu * 10 ⁴	-	2.8	-	2.8	-	4.2	-	4.2	-	5.6	-	5.6
⁴¹ Pu * 10 ⁴	-	2.1	-	2.1	-	3.2	-	3.2	-	5.6	-	5.6
⁴² Pu * 10 ⁵	-	7.0	-	7.0	-	11.0	-	11.0	-	14.0	-	14.0
O * 10 ²	4.26	4.26	-	-	4.26	4.26	-	-	4.26	4.26	-	-

All concentrations ρ are given in $10^{24} / \text{cm}^3$, radiuses (R) - in cm.

Temperatures of fuel, clad and moderator are equal to 293^0K .

Table 4.5.2. Integral parameter results.

Cell type fuel type	Param.	MCU		Deviation from MCU (%)			
		Value	Stat. error %	UNIRA SOS2	RAFORIN	NESSSEL-4	SAPFIR
"Wide" UO ₂	K _∞	1.458	0.1	-0.3	-0.3	-0.3	-0.1
	CR	0.317	1.2	-0.1	-0.6	-0.6	-0.6
"Wide" U	K _∞	1.278	0.2	-0.2	0.0	-0.2	-0.3
	CR	0.560	0.7	-0.9	-1.2	-0.9	0.0
"Interm." UO ₂	K _∞	1.421	0.3	-0.2	-0.1	-0.6	0.1
	CR	0.370	0.8	-1.4	-1.6	-0.3	-0.8
"Interm." U	K _∞	1.241	0.2	-0.6	-0.1	-0.2	-0.6
	CR	0.643	0.6	-0.8	-2.1	-0.8	0.5
"Tight" UO ₂	K _∞	1.301	0.3	-0.9	-0.9	-0.5	-0.2
	CR	0.473	1.1	-0.6	-1.7	0.3	0.0
"Tight" U	K _∞	1.113	0.4	+0.2	0.7	0.4	-0.5
	CR	0.844	1.1	-3.1	-4.7	-2.6	-1.1
"Wide" UO ₂ +PuO ₂	K _∞	1.346	0.1	0.2	-0.5	2.7(+0.3)	-1.0
	CR	0.448	0.3	-5.5	-1.1	6.0(-3.2)	-0.4
"Wide" U+Pu	K _∞	1.249	0.1	-0.2	-0.3	2.5(-0.2)	-1.5
	CR	0.614	1.0	-4.1	-2.1	6.2(-1.5)	0.2
"Interm." UO ₂ +PuO ₂	K _∞	1.260	0.1	-0.2	-0.7	2.3(-0.7)	-0.8
	CR	0.580	1.0	-2.9	-0.1	3.8(-0.1)	-3.1
"Interm." U+Pu	K _∞	1.159	0.1	-0.6	-0.5	3.2(-1.2)	-1.3
	CR	0.805	1.0	-1.9	-0.9	6.5(+1.8)	-1.1
"Tight" UO ₂ +PuO ₂	K _∞	1.259	0.1	-1.1	-0.3	-2.3	-0.8
	CR	0.644	1.0	+0.8	-0.2	3.9	+0.9
"Tight" U+Pu	K _∞	1.131	0.2	-1.0	0.6	-2.6	-0.9
	CR	0.954	0.8	+1.2	-2.2	6.4	+1.0

Table 4.5.2 shows that all codes give relatively close values of K_{∞} for cells with uranium fuel. Calculated values of K_{∞} obtained with design codes for practically all cells are lower than obtained with MCU. Maximum deviation from MCU results equals 0.9% and was achieved in "tight" cell.

Maximum deviation of CR equal to 4.7% gives RAFORIN in the case of a

tight cell with U_m fuel. This code also tends to underestimate K_{eff} when the moderator-fuel volume ratio is decreased.

As is seen from Table 4.5.2 agreement of K_{∞} and CR for cells with mixed fuel is noticeably worse in comparison with the observed for cells with uranium fuel. It should be noted that calculations with *NESSEL-4* and *MCU* are based on different nuclear data for uranium and plutonium isotopes in thermal and resolved resonance energy region. At the same time *MCU*, *SAPFIR*, *UNIRASOS-2* and *RAFORIN* utilize practically identical nuclear data. The influence of nuclear data scattering on calculational results is partially illustrated by *NESSEL-4* K_{∞} and CR. The values of these parameters given in brackets were obtained by using the same values of infinite dilution capture cross section of ^{240}Pu as in *MCU*.

Maximum deviations of K_{∞} and CR obtained with *UNIRASOS-2*, *RAFORIN* and *SAPFIR* from *MCU* results for cells with mixed fuel are equal to 1.1 and 5.5, 0.7 and 2.2, 1.3 and 3.1%, respectively.

One-group capture and fission reaction rates produced by some isotopes are presented in Table 4.5.3. All reaction rates are normalized to total absorption rate in the cell.

Table 4.5.3 shows that for cells with uranium fuel, the deviations of K_{∞} and CR obtained with *UNIRASOS-2* and *RAFORIN* results from the relatively small differences in reaction rates produced by $^{235,238}\text{U}$ which do not exceed the statistical errors of *MCU* results.

The agreement of the *NESSEL-4* reaction rates with *MCU* data are worse. Systematic increase of R_f^{35} and R_c^{38} deviations with reduction of the moderator/fuel volume ratio is typical for this code. Probably this trend is partially connected with differences in the nuclear data used.

As follows from Table 4.5.3, deviations of *UNIRASOS-2* K_{∞} and CR for cells with mixed fuel are explained mainly by disagreement in R_c^{39} and R_c^{40} . This code also noticeably underpredicts R_c^{38} in the "tight" cell. The error of R_c^{40} calculation by *UNIRASOS-2* is connected with the use of ABBN group structure and approximation of "effective" resonance used in this code. Group intervals in ABBN were chosen so that the boundary between 23^{rd} and 24^{th} group divides the lowest and the most important resonance into parts. The inaccuracy mentioned above can be avoided by rather simple modifications of algorithm used for self-shielded cross sections and spectrum calculations.

In conclusion, it should be noted that the neglecting of resonance self-shielding for ^{242}Pu in *NESSEL-4* leads to significant errors in K_{∞} and CR for "tight" and "intermediate" cells.

Table 4.5.3. Comparison of one-group reaction rates.

Cell	Isotope	Code name / calculation result									
		RAFORIN		UNIRASOS-2		SAPFIR		NESSEL-4		MCU	
		R_c	R_f	R_c	R_f	R_c	R_f	R_c	R_f	R_c	R_f
1	^{235}U	0.117	0.569	0.119	0.570	0.118	0.572	0.120	0.569	0.117	0.568
	^{238}U	0.217	0.022	0.217	0.023	0.226	0.023	0.217	0.024	0.218	0.023
	^{16}O	0.003	-	0.003	-	0.001	-	0.000	-	-	-
2	^{238}U	0.164	0.022	0.164	0.022	0.163	0.023	0.163	0.022	0.164	0.022
	^{239}Pu	0.168	0.334	0.177	0.338	0.170	0.335	0.163	0.320	0.165	0.339
	^{240}Pu	0.123	0.002	0.114	0.002	0.125	0.002	0.132	0.002	0.125	0.002
	^{241}Pu	0.037	0.104	0.037	0.105	0.036	0.103	0.034	0.104	0.037	0.103
	^{242}Pu	0.012	0.000	0.012	0.0003	0.012	-	0.020	0.000	0.012	0.000
	^{16}O	0.003	-	0.003	-	0.001	-	-	-	-	-
3	^{235}U	0.136	0.545	0.138	0.546	0.136	0.546	0.135	0.533	0.135	0.544
	^{238}U	0.248	0.031	0.249	0.031	0.252	0.032	0.244	0.032	0.252	0.032
	^{16}O	0.003	-	0.003	-	-	-	-	-	-	-

Cell type : 1 "Wide" UO_2 4 "Interm." $\text{UO}_2 + \text{PuO}_2$ 2 "Wide" $\text{UO}_2 + \text{PuO}_2$ 5 "Tight" UO_2 3 "Interm." UO_2 6 "Tight" $\text{UO}_2 + \text{PuO}_2$ R_c - capture rate; R_f - fission rate.

Table 4.5.3 (Continued).

Cell	Isotope	Code name / calculation result									
		RAFORIN		UNIRASOS-2		SAPFIR		NESSEL-4		MCU	
		R _c	R _f	R _c	R _f	R _c	R _f	R _c	R _f	R _c	R _f
4	²³⁸ U	0.201	0.031	0.202	0.030	0.202	0.032	0.195	0.031	0.202	0.030
	²³⁹ Pu	0.153	0.291	0.162	0.294	0.155	0.294	0.146	0.273	0.153	0.298
	²⁴⁰ Pu	0.137	0.004	0.135	0.004	0.140	0.004	0.143	0.004	0.138	0.004
	²⁴¹ Pu	0.035	0.105	0.036	0.106	0.034	0.103	0.031	0.104	0.035	0.101
	²⁴² Pu	0.019	0.001	0.019	0.001	0.018	0.001	0.034	0.000	0.018	0.000
	¹⁶ O	0.003	0.000	0.003	-	-	-	-	-	-	-
5	²³⁵ U	0.152	0.481	0.152	0.481	0.151	0.484	0.147	0.462	0.150	0.483
	²³⁸ U	0.294	0.042	0.298	0.042	0.300	0.043	0.284	0.042	0.299	0.043
	¹⁶ O	0.003	-	0.003	-	0.002	-	-	-	-	-
6	²³⁸ U	0.234	0.041	0.234	0.039	0.242	0.040	0.230	0.040	0.242	0.040
	²³⁹ Pu	0.136	0.268	0.139	0.268	0.139	0.271	0.128	0.245	0.138	0.273
	²⁴⁰ Pu	0.116	0.008	0.126	0.008	0.119	0.008	0.119	0.007	0.116	0.008
	²⁴¹ Pu	0.035	0.114	0.035	0.113	0.024	0.111	0.030	0.112	0.034	0.110
	²⁴² Pu	0.022	0.001	0.021	0.001	0.020	0.001	0.040	0.001	0.020	0.001
	¹⁶ O	0.003	-	0.003	-	-	-	-	-	-	-

Such modifications were realized in the *RAFORIN* code and, as seen from Table 4.5.2, allowed us to increase the accuracy of K_{∞} and CR calculations in the considered cells. Table 4.5.3 also shows that *RAFORIN* $R_{c,f}^{39}$ is in better agreement with *MCU* data for cells with a soft spectrum. The last feature is connected with differences in thermalization models and approaches used in these codes for spatial flux distributions in the cell.

In conclusion, it should be noted that the neglecting of resonance self-shielding for ²⁴²Pu in *NESSEL-4* leads to significant errors in K_{∞} and CR for "tight" and "intermediate" cells.

Two benchmarks for the ZR-6 lattices have been formulated to simplify the interpretation of measurements at ZR-6. These benchmarks consist of two zero-leakage cell configurations with UO_2 fuel enriched to 1.6 and 3.6% and an outer radius corresponding to lattice pitch of 1.27 cm. Calculations have been performed for room temperature and zero boron acid concentration. Compositions and dimensions of the cells correspond to those given in (Szatmary et al. 1985).

Multiplication factors and two-group cross sections averaged over the cell volume are compared in Table 4.5.4. The UNIRASOS-2 and NESSEL-4 values for both cells are in excellent agreement with Monte-Carlo values. Cross sections obtained with UNIRASOS-2 also agree well with Monte-Carlo values. The RAFORIN and SAPPFIR K_∞ are 0.2-0.3% lower. This disagreement for the cell with a fuel enrichment of 1.6% is somewhat more than the MCU statistical error. The RAFORIN cross sections are in good agreement with MCU data. Their deviation is close to that obtained with UNIRASOS-2 and do not exceed MCU statistical error.

The group structure of NESSEL-IV and SAPPFIR does not allow the cross sections to be condensed into a group with cut off energy 0.625 eV. That is why they are omitted from Table 4.5.4.

The temperature effect plays an important role in the reactivity balance of WWER cores under stationary and transient regimes. To verify the accuracy of its calculations with design codes special benchmarks have been formulated and solved with MCU, SAPPFIR, UNIRASOS-2 and RAFORIN.

The considered cell is a zero-leakage version of WWER-1000 fuel lattice with fuel enrichment 3.6%. Calculations have been carried out for fuel temperature equal to 300, 550, and 1000°K. Moderator and clad temperatures were varied from 300 to 550°K. To separate temperature effects the moderator density was kept constant equal to a value of 1.0 g/cm³.

Table 4.5.5 shows that the UNIRASOS-2 K_∞ values are in good agreement with the K_∞ values obtained with MCU. They practically coincide when the fuel temperature is equal to 300 and 550°K and differ by 0.2% at 1000°K. The RAFORIN and SAPPFIR systematically underpredict K_∞ by ~0.3%. Comparison of the temperature effect values determined as

* Results included in Tables 4.5.4 and 4.5.5 were obtained by G. A. Bogachev.

$$\frac{\delta K_{\infty}(T)}{K_{\infty}} = \frac{K_{\infty}(300^{\circ}) - K_{\infty}(T)}{K_{\infty}(300^{\circ})}$$

shows that the *RAFORIN* and *SAPFIR* results are in good agreement with *MCU* data.

The deviations of $\delta K/K$ values hardly exceed the *MCU* statistical error. *UNIRASOS-2* slightly underpredicts the temperature effect. The accuracy of all three codes from practical point of view seems sufficient.

Table 4.5.4. Integral parameter results for ZR-6 cells.

Code name	Fuel enrich.	K_{∞}	$\Sigma_a^{\text{fast}} \cdot 10^3$	$\Sigma_f^{\text{fast}} \cdot 10^3$	$\Sigma_R^{\text{fast}} \cdot 10^2$	$\nu \Sigma_f^{\text{th}} \cdot 10$	$\Sigma_a^{\text{th}} \cdot 10^2$
<i>MCU</i>		1.200 (0.002)	8.833	4.943	—	1.069	7.420
<i>UNIRASOS-2</i>	1.6%	1.201	8.808	4.937	2.333	1.074	7.442
<i>SAPFIR</i>		1.197	—	—	—	—	—
<i>RAFORIN</i>		1.196	8.849	4.945	2.333	1.062	7.345
<i>NESSSEL-4</i>		1.200	—	—	—	—	—
<i>MCU</i>		1.417 (0.003)	1.041	7.877	2.209	2.043	1.185
<i>UNIRASOS-2</i>	3.6%	1.418	1.051	7.982	2.211	2.071	1.197
<i>SAPFIR</i>		1.413	—	—	—	—	—
<i>RAFORIN</i>		1.416	1.041	7.930	2.216	2.042	1.185
<i>NESSSEL-4</i>		1.415	—	—	—	—	—

* - boundary energy 0.625 ev.

Σ_a^{fast} , Σ_a^{th} - macro cross sections in the fast and the thermal group, respectively.

Table 4.5.5 K_{∞} temperature dependence for the cell
of ZR-6 1.27/3.6/0.0 lattice.

T_f (°K)	T_c (°K)	T_m (°K)	Code name / K_{∞}			
			MCU	SAPFIR	UNIRASOS-2	RAFORIN
300	300	300	$1.409^{+0.001}$	1.403	1.410	1.404
550	550	550	$1.396^{+0.001}$	1.391	1.395	1.391
1000	550	550	$1.384^{+0.001}$	1.378	1.381	1.378

The NB cells were suggested as a numerical benchmark in (Williams et al, 1985). Integral parameter values for NB cells are compared in Table 4.5.6.

The NB-1 cell is a zero leakage version of the well known BAPL-1 lattice, NB-2 corresponds to low enriched (Mass Pu/Mass U $\approx$ 2%) mixed oxide lattice, NB-4 exhibits infinite PWR lattice and NB-5 is a cell of high conversion HiC-13 lattice characterized by extremely low (0.43) moderator/fuel volume ratio and hard neutron spectrum.

As can be seen from Table 4.5.6, the MCU K_{∞} values are in a good agreement with the results of Monte-Carlo calculations based on ENDF/B-V data. The maximum deviation equal to 0.3 is achieved in the NB-5 cell. Taking into account statistical errors of both calculations it is possible to conclude that the results for all the cells practically coincide.

The values of ρ^{28} , δ^{25} and MCR obtained with MCU and given in (Williams et al., 1985) are also in good agreement. At the same time MCU tends to underpredict δ^{28} as regards data of (Williams, 1985). One of the possible reasons for this is briefly discussed below.

Deviations of the UNIRASOS-2 and SAPFIR K_{∞} values achieve their maximum values equal to $\sim$ 1% in NB-5 cell. Table 4.5.6 shows that both codes provide good agreement with Monte-Carlo results in ρ^{28} and CR. Disagreements in this parameters doesn't exceed $\sim$ 1%. Both codes UNIRASOS-2 and SAPFIR noticeably underestimate δ^{25} by (2%). Apparently that the last in a combination with δ^{28} underestimation is the main reason of K_{∞} underprediction in NB-5 cell.

Table 4.5.6 Comparison of integral parameters for NB lattices.

Cell number, V_m/V_f	Parameter	Code name / calculation results							
		Monte Carlo ENDF-5	EPRI CELL	C A S M O	U N I R A S O S 2	MCU	S A P F I R	R A F O R I N	NESSEL 4
NB-1 $V_m/V_f = 1.43$	K_∞	1.147	-0.2	-0.2	-0.3	0.0	-0.4	-0.3	-0.5
	ρ^{28}	1.363	-0.2	-1.5	2.1	0.3	1.0	-0.3	2.1
	δ^{25}	0.0803	1.4	2.2	1.6	0.6	0.0	1.1	1.1
	δ^{28}	0.0722	-2.4	1.9	-5.1	-2.6	-1.9	-1.9	0.0
	CR	0.798	-0.3	-1.6	0.0	-0.4	0.5	0.1	0.8
NB-2 $V_m/V_f = 2.53$	K_∞	1.175	-0.4	-	0.6	-0.2	0.8	0.1	-0.5
	ρ^{28}	2.612	0.0	-	0.0	1.3	-1.4	1.3	1.9
	δ^{25}	0.151	0.7	-	0.0	-0.7	-0.3	4.6	0.0
	δ^{28}	0.297	0.0	-	-7.4	-7.0	-3.7	1.7	-3.4
	CR	2.148	0.0	-	-1.4	-1.3	-0.8	0.2	0.0
NB-4 $V_m/V_f = 1.26$	K_∞	1.342	-0.1	-0.2	0.6	0.1	0.2	0.5	-0.7
	ρ^{28}	2.654	-0.8	0.8	-2.1	-0.4	1.0	-4.4	3.9
	δ^{25}	0.159	-1.3	-0.1	-5.0	-1.7	-2.5	-5.6	-0.6
	δ^{28}	0.062	-0.8	3.0	-4.8	-0.8	-1.6	-1.6	2.3
	CR	0.549	-0.2	-1.3	-2.2	-0.1	0.2	-2.5	1.8
NB-5 $V_m/V_f = 0.43$	K_∞	1.146	-0.3	-	-0.9	-0.3	-1.0	0.1	0.0
	ρ^{28}	8.503	0.4	-	0.6	-0.1	0.5	-3.1	1.9
	δ^{25}	0.548	0.4	-	-2.6	-0.3	-2.0	-3.0	-4.7
	δ^{28}	0.133	-0.8	-	-8.0	-5.4	-2.2	-5.5	-1.5
	CR	1.006	0.0	-	-0.3	-0.2	0.8	-2.0	-3.1

All deviations are given in % as regards Monte-Carlo results presented in (Williams et al., 1985).

V_m/V_f - moderator/fuel volume ratio.

RAFORIN and *NESSEL-4* K_{∞} agree rather well with data of (Williams et al., 1985). The maximum deviations are 0.5 and 0.7%, respectively. As it follows from Table 4.5.6, *NESSEL-4* systematically overpredicts (by 2-4%) resonance absorption by ^{238}U as regards Monte-Carlo results. As a result this code systematically understates the K_{∞} value. *RAFORIN* as distinct from *NESSEL-4* tends to underpredict resonance absorption by ^{238}U . At the same time, as was already mentioned, *RAFORIN* also tends to underpredict the fission rate produced by this isotope. So, the observed deviation of K_{∞} for NB-5 cell is the result of partial compensation of mentioned above inaccuracies.

It should be noted that the above described *RAFORIN* results for NB cells as well as all the results which will be discussed below have been obtained using combined a fission spectrum based on ENDF/B-V data. All the results obtained earlier in order to simplify their interpretation were obtained for the ^{235}U fission spectrum which is also utilized in *MCU*. Calculations have shown that the use of ENDF/B-V spectra provides a means of reducing the difference between the calculated and measured values of δ^{28} and only slightly influences K_{∞} of uranium-water lattices. Variation of K_{∞} due to the use of combined fission spectrum based on ENDF/B-V data instead of the ^{235}U spectrum from ABBN in the lattices with MOX fuel is about 0.2-0.3%.

Summarizing the results of *UNIRASOS-2*, *RAFORIN*, *SAPFIR* and *NESSEL-4* numerical benchmarking it is possible to conclude that:

- all the above listed codes provide satisfactory agreement with the results of Monte-Carlo calculations for WWER-1000 fuel lattices with uranium fuel;

- reducing moderator/fuel volume ratio leads to some lowering of accuracy of integral parameter calculations;

- errors of integral parameter calculations of the cells with mixed fuel are appreciably greater than corresponding errors in the cells with uranium fuel. To reduce these errors special attention should be paid to improving the approaches used for calculations in the resonance energy range.

4.5.2. Analysis of numerical benchmarks on fuel lattice burnup

Analysis of benchmarks on fuel lattice burnup is the second and important stage of design code numerical benchmarking. Such analysis seems rather complex. The following factors influence calculation results and must be taken into account when they are interpreted:

- scattering of nuclear data for fission products, U and Pu isotopes;
- differences in fission product chains;
- differences in approaches used for taking into account self-shielding of Pu isotopes lowest resonances and resonances of fission product.

Besides this, there are very few reference solutions of such benchmarks. Nevertheless analysis of such benchmarks in combination with analysis of measurement data allow one to estimate the accuracy of burnup calculations with design codes.

Some benchmarks on water moderated lattice burnup have been formulated and solved within the framework of TIC activities. The solution results of two of them are briefly discussed below. These benchmarks were defined initially within the TIC and then considered in the framework of IAEA Coordinated Research Program activities (IAEA, 1988).

Table 4.5.7 and Figs.4.1-4.2 compare results of cell burnup calculations. The composition and dimensions of the considered cells which are zero-leakage versions of WWER-1000 lattice with fuel enrichment of 3.6% are given in (IAEA, 1988). Full analysis of the results obtained with NESSEL-4 (Becker, 1990), EXCELL (Jagannathan, 1989), TVS (Pshenin et al. 1989), CASMO-HEX (Antilla, 1989), RSYST (Lutz, 1990), KARATE (Hegyí, Maraczy, 1991), MICROBE (Zalesky, 1991) and WIMS-D4 (Kulikowska, Sadovska, 1989) is given in (Pshenin et al., 1992).

Computed values of K_{∞} are compared in Table 4.5.7. The lowest value at zero burnup point is predicted by KARATE, the highest by MICROBE. Variation of K_{∞} determined as the ratio of standard deviation to average value changes in the limits 0.007-0.003 slightly decreasing with burnup growth. Comparison of reactivity loss as a function of burnup shows that the highest values of this parameter are calculated with RAFORIN and TVS. Variation of this parameter at all burnup points does not exceed 0.005.

Concentrations of ^{235}U and ^{239}Pu are compared in Figs.4.1-4.2. These figures show that at final burnup point scattering of ^{235}U and ^{239}Pu concentrations is about 4%. The lowest value of ^{235}U concentration is given by RAFORIN, which partially explains the slight understating of K_{∞} by this

code at high burnups.

Scattering of higher Pu isotopes is significantly greater in comparison with that indicated for ^{239}Pu and reaches ~15% for ^{242}Pu at final burnup point. Observed uncertainties of calculational prediction of most important cell parameters taking into account differences in nuclear data used seems satisfactory. The above mentioned uncertainties are close to those indicated in (Fisher, 1989) for codes utilized in some organizations performing PWR core analysis.

Table 4.5.7. K_{∞} of the fuel cell as a burnup function.*)

Code name	W (Mwd / kg U) , K_{∞}					
	0.0	2.0	5.0	10.0	15.0	20.0
NESSEL-4	1.350	1.275	-	1.188	1.135	1.100
WIMS-D4	1.351	-	1.250	1.193	1.145	1.103
EXCELL	1.368	1.291	1.253	1.196	1.147	1.105
RSYST	1.358	1.282	1.249	1.192	1.144	1.101
CASMO-HEX	1.364	1.288	1.252	1.197	1.148	1.107
TVS	1.364	1.286	1.250	1.190	1.142	1.098
KARATE	1.347	1.274	1.240	1.185	1.138	1.096
MICROBE	1.373	-	-	-	-	-
RAFORIN	1.350	1.292	1.255	1.192	1.140	1.095
$\bar{K}_{\infty}$	1.360	1.284	1.250	1.191	1.143	1.100
$S/\bar{K}_{\infty}$	0.007	0.005	0.004	0.003	0.003	0.004

*) S - standard deviation.

fig4-1

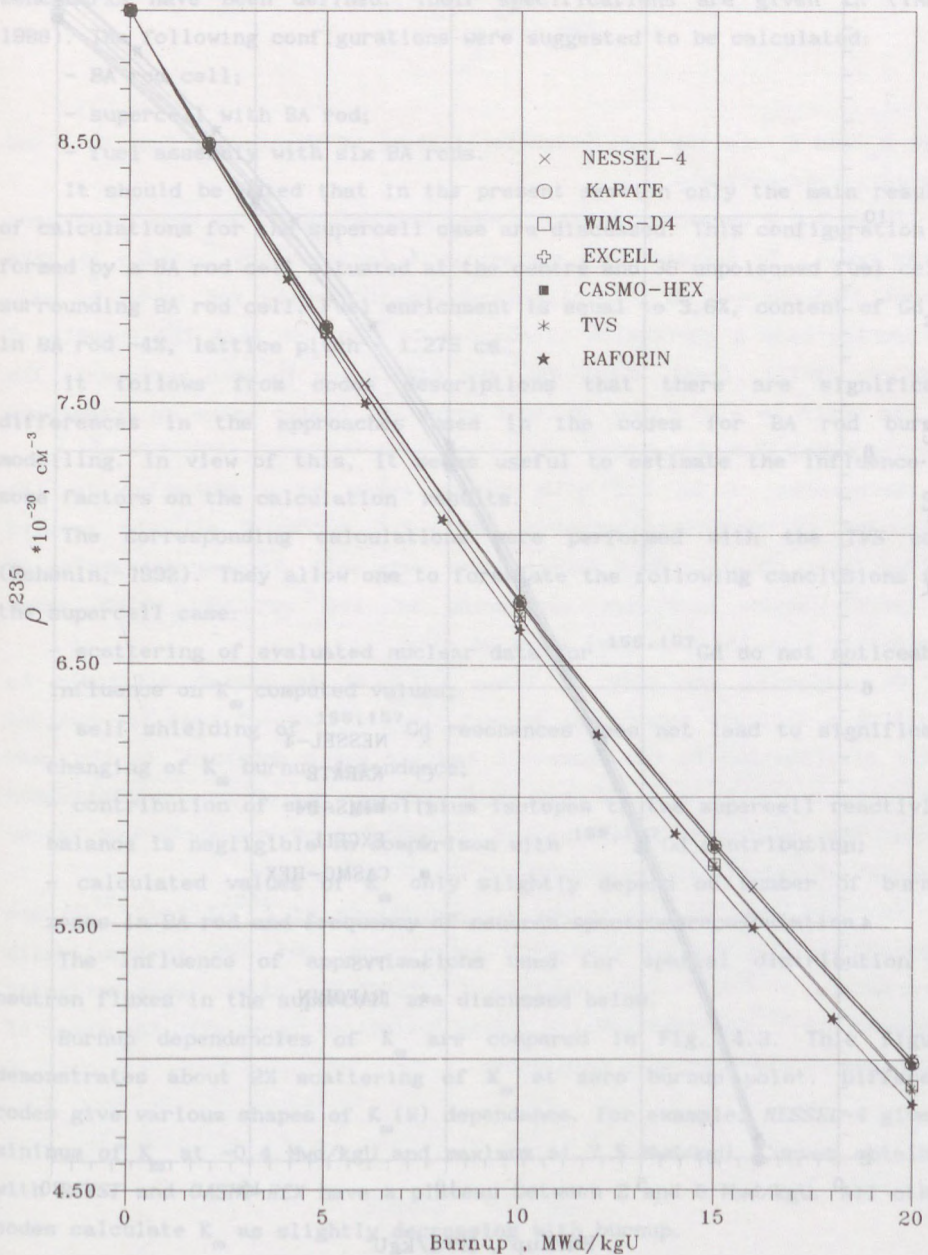
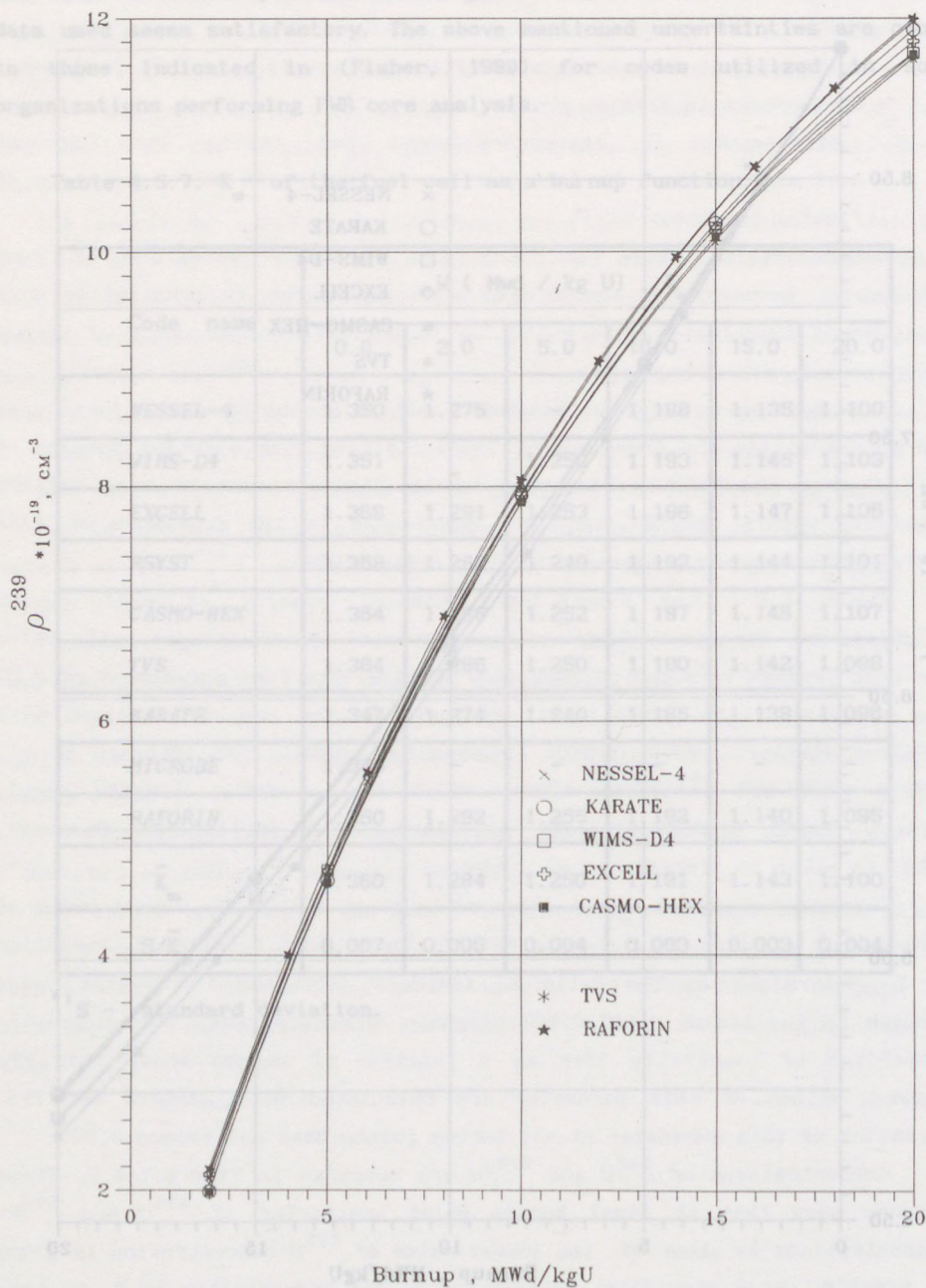
Fig. 4.1 Burnup dependence of ^{235}U number density in the fuel rod.

fig4-2

Fig. 4.2 Burnup dependence of ^{239}Pu number density in the fuel rod.



Burnup calculations of fuel lattices containing burnable absorber rods with gadolinium need serious modifications of spectral codes to provide an acceptable accuracy when computing lattice parameters. In connection with investigations being performed now and aimed at analysing different aspects of IFBA type burnable absorbers used in new generation WWER, three benchmarks have been defined. Their specifications are given in (IAEA, 1988). The following configurations were suggested to be calculated:

- BA rod cell;
- supercell with BA rod;
- fuel assembly with six BA rods.

It should be noted that in the present section only the main results of calculations for the supercell case are discussed. This configuration is formed by a BA rod cell situated at the centre and 36 unpoisoned fuel cells surrounding BA rod cell. Fuel enrichment is equal to 3.6%, content of Gd_2O_3 in BA rod ~4%, lattice pitch - 1.275 cm.

It follows from codes descriptions that there are significant differences in the approaches used in the codes for BA rod burnup modelling. In view of this, it seems useful to estimate the influence of some factors on the calculation results.

The corresponding calculations were performed with the TVS code (Pshenin, 1992). They allow one to formulate the following conclusions for the supercell case:

- scattering of evaluated nuclear data for $^{155,157}Gd$ do not noticeably influence on K_{∞} computed values;
- self shielding of $^{155,157}Gd$ resonances does not lead to significant changing of K_{∞} burnup dependence;
- contribution of even gadolinium isotopes to the supercell reactivity balance is negligible in comparison with $^{155,157}Gd$ contribution;
- calculated values of K_{∞} only slightly depend on number of burnup zones in BA rod and frequency of neutron spectrum recalculation.

The influence of approximations used for spatial distribution of neutron fluxes in the supercell are discussed below.

Burnup dependencies of K_{∞} are compared in Fig. 4.3. This figure demonstrates about 2% scattering of K_{∞} at zero burnup point. Different codes give various shapes of $K_{\infty}(W)$ dependence. For example, NESSEL-4 give a minimum of K_{∞} at ~0.4 Mwd/kgU and maximum at 7.5 Mwd/kgU. Curves obtained with RSYST and CASMO-HEX have a plateau between 2 and 6 Mwd/kgU. All other codes calculate K_{∞} as slightly decreasing with burnup.

Taking into account the conclusions above, it appears that the

mentioned disagreement is connected mainly with approximations used for calculating the spatial distribution of fluxes.

The BA rod worths are compared in Table 4.5.8. Rod worth is determined as

$$RW = \frac{\overset{\text{f.c. s.c.}}{(K_{\infty}^{\text{f.c.}} - K_{\infty}^{\text{s.c.}})}}{K_{\infty}^{\text{f.c.}}}$$

where $K_{\infty}^{\text{f.c.}}$ and $K_{\infty}^{\text{s.c.}}$ are the multiplication factors of unpoisoned fuel cell and supercell, respectively.

Table 4.5.8 demonstrates significant scattering of the results at zero burnup point. To compare them correctly it is necessary to take it into account that Xe and Sm poisoning leads to increasing rod worth by ~4%. Introducing such a correction allows one to conclude that the results of NESSEL-4, EXCELL, RSYST, CASMO-HEX, and KARATE are in good agreement. The TVS rod worth is ~15% lower, MICROBE gives ~6% higher value in comparison with the codes listed above.

Decreasing of BA rod with burnup leads to a reduction in the scattering of calculation results. At $W=2.0$ Mwd/kg U all the results besides those obtained with EXCELL agree very well. Further decreasing of rod worth again increases scattering of the results, which seems permissible from the practical point of view.

On analyzing the data of Table 4.5.8 it is rather difficult to establish a definite connection between type of approach used for spatial fluxes distribution in the supercell and rod worth obtained. At the same time comparison with measured data shows that the use of more sophisticated methods than diffusion approach lead to reducing of rod worth and better agreement of calculated and measured critical parameters.

Averaged over BA rod volume concentrations of ^{155}Gd and ^{157}Gd are compared in Figs.4.4-4.5. These figures show that TVS systematically overpredicts ^{155}Gd concentration. NESSEL-4 also systematically underpredicts ^{157}Gd concentration. These deviations agree with the shape of K_{∞} dependence obtained with both codes.

fig4-3

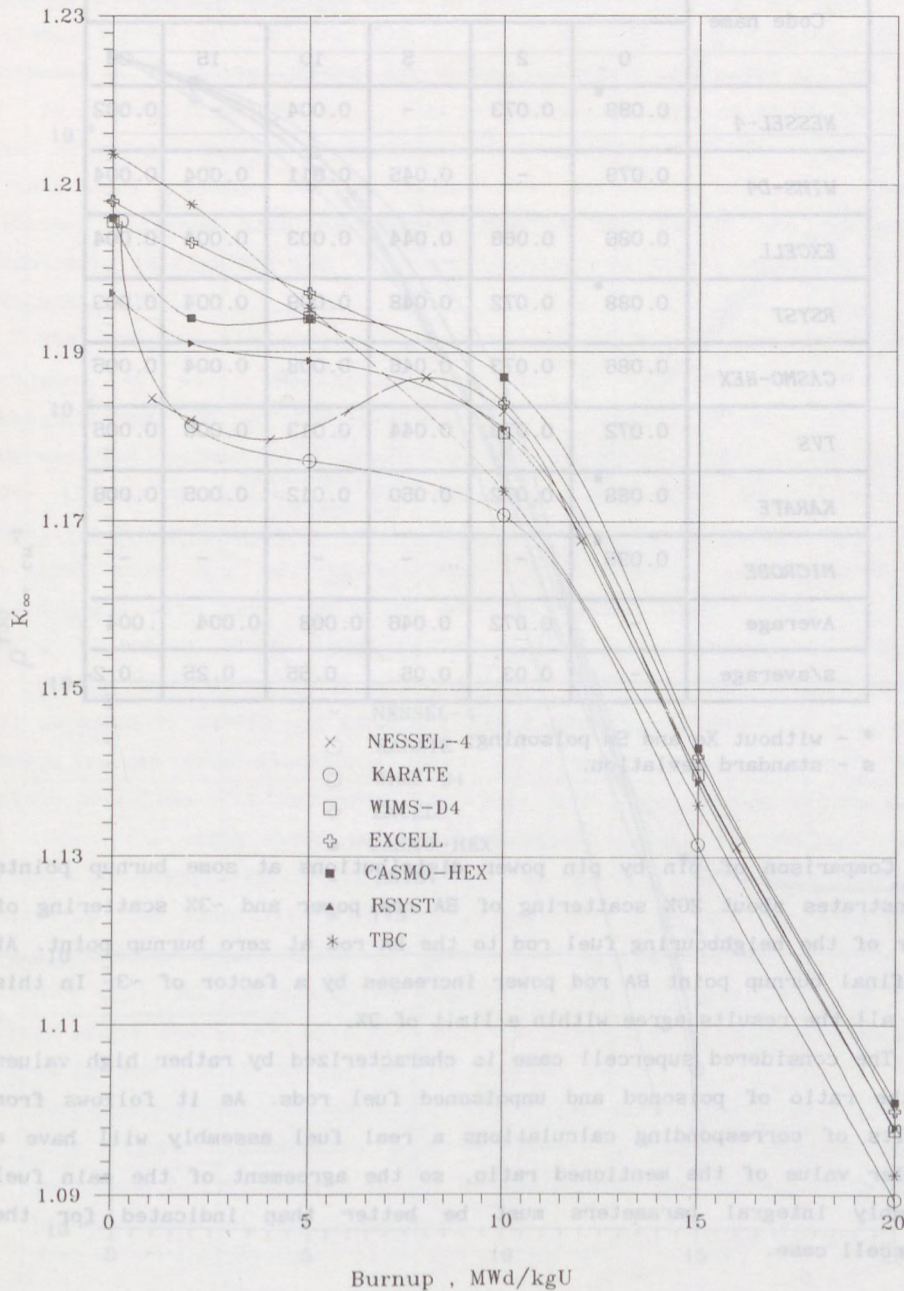
Fig 4.3 Burnup dependence of K_{∞} for the supercell with gadolinium BA rod.

Table 4.5.8. Gadolinium rod worth as a function of burnup.

Code name	W (Mwd /kg U, BA rod worth)					
	0	2	5	10	15	20
NESSEL-4	0.089*	0.073	-	0.004	-	0.002
WIMS-D4	0.079	-	0.045	0.011	0.004	0.004
EXCELL	0.086	0.068	0.044	0.003	0.004	0.004
RSYST	0.088*	0.072	0.048	0.009	0.004	0.003
CASMO-HEX	0.086	0.073	0.046	0.008	0.004	0.005
TVS	0.072	0.073	0.044	0.013	0.005	0.005
KARATE	0.088*	0.072	0.050	0.012	0.005	0.006
MICROBE	0.095*	-	-	-	-	-
Average	-	0.072	0.046	0.008	0.004	.004
s/average	-	0.03	0.05	0.55	0.25	0.2

* - without Xe and Sm poisoning;

s - standard deviation.

Comparison of pin by pin power distributions at some burnup points demonstrates about 20% scattering of BA rod power and ~3% scattering of power of the neighbouring fuel rod to the BA rod at zero burnup point. At the final burnup point BA rod power increases by a factor of ~3. In this case all the results agree within a limit of 3%.

The considered supercell case is characterized by rather high values of the ratio of poisoned and unpoisoned fuel rods. As it follows from results of corresponding calculations a real fuel assembly will have a smaller value of the mentioned ratio, so the agreement of the main fuel assembly integral parameters must be better than indicated for the supercell case.

fig4-4

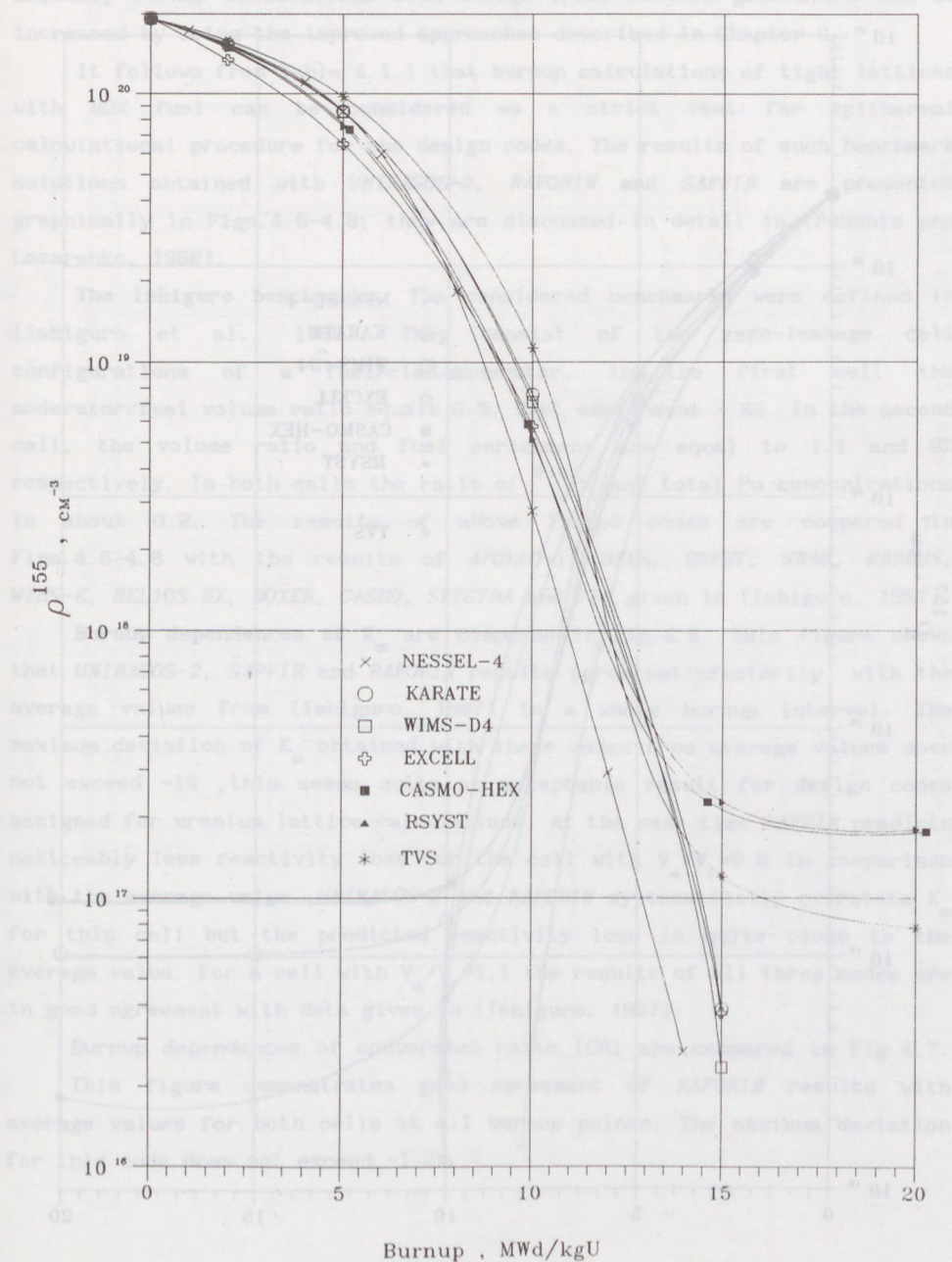
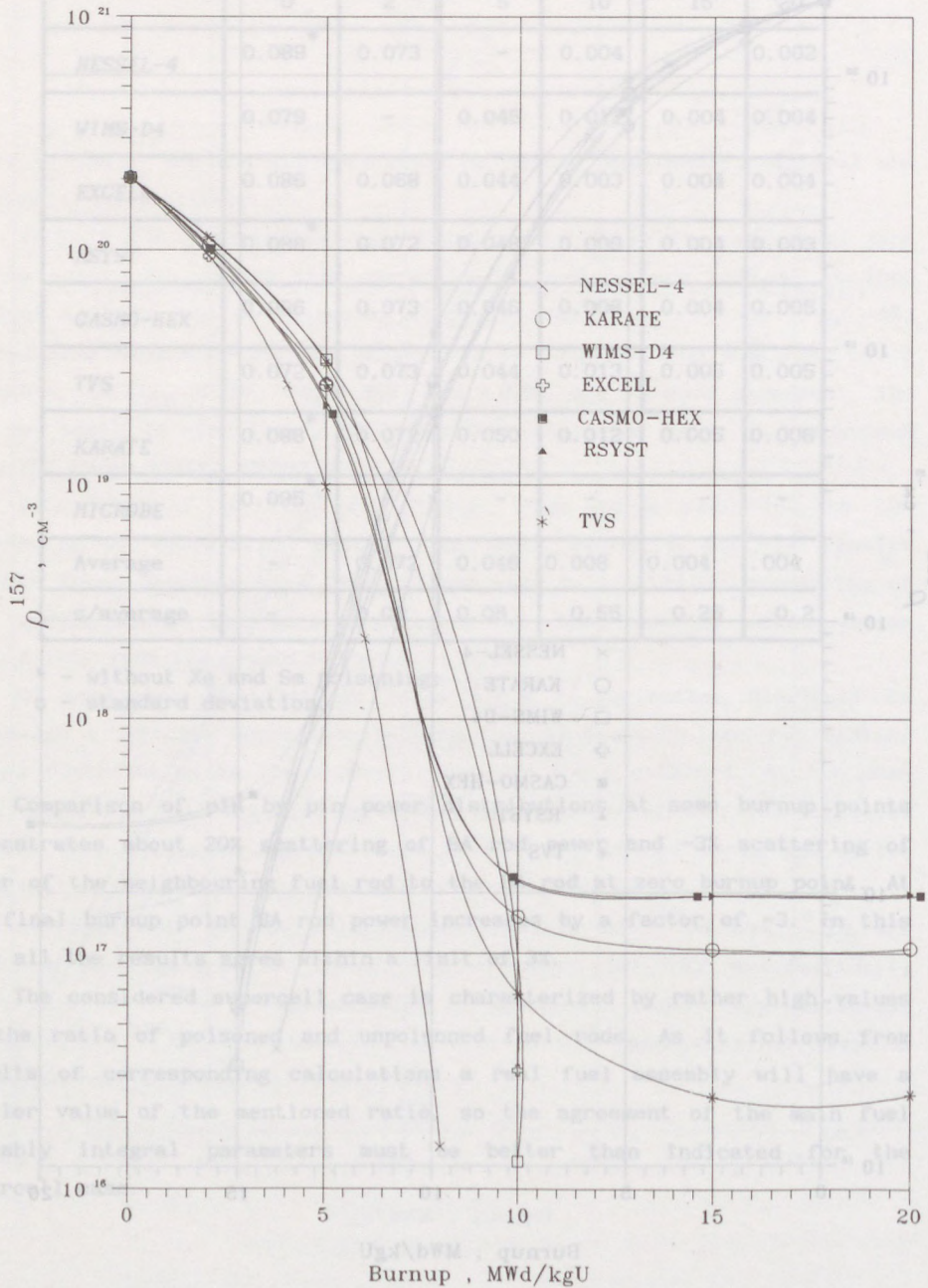
Fig. 4.4 Burnup dependence of ^{155}Gd number density in BA rod.

fig4-5

Fig. 4.5 Burnup dependence of ^{157}Gd number density in BA rod.

Preliminary sensitivity analysis performed with 3D simulator BIPR-7 makes it possible to conclude that the above indicated scattering of calculation results for fuel lattices with gadolinium does not lead to noticeable uncertainty of WWER-1000 core main parameters. Accuracy of fuel assembly burnup calculations with design cross section generators can be increased by using the improved approaches described in Chapter 6.

It follows from Table 4.1.1 that burnup calculations of tight lattices with MOX fuel can be considered as a strict test for epithermal calculational procedure for the design codes. The results of such benchmark solutions obtained with *UNIRASOS-2*, *RAFORIN* and *SAPFIR* are presented graphically in Figs.4.6-4.8; they are discussed in detail in (Pshenin and Lazarenko, 1988).

The Ishiguro benchmarks. The considered benchmarks were defined in (Ishiguro et al., 1986). They consist of two zero-leakage cell configurations of a fuel/clad/moderator. In the first cell the moderator/fuel volume ratio equals 0.5, fuel enrichment - 8%. In the second cell, the volume ratio and fuel enrichment are equal to 1.1 and 8% respectively. In both cells the ratio of ^{240}Pu and total Pu concentrations is about 0.2. The results of above listed codes are compared in Figs.4.6-4.8 with the results of *APOLLO-1*, *GELS*, *RSYST*, *SRAC*, *KARBUS*, *WIMS-E*, *HELIOS.HX*, *BOXER*, *CASMO*, *SPECTRA* and *VIM* given in (Ishiguro, 1987).

Burnup dependences of K_{∞} are compared in Fig.4.6. This figure shows that *UNIRASOS-2*, *SAPFIR* and *RAFORIN* results agree satisfactorily with the average values from (Ishiguro, 1987) in a whole burnup interval. The maximum deviation of K_{∞} obtained with these codes from average values does not exceed ~1%, this seems quite an acceptable result for design codes assigned for uranium lattice calculations. At the same time *SAPFIR* predicts noticeably less reactivity loss for the cell with $V_m/V_f=0.6$ in comparison with the average value. *UNIRASOS-2* and *RAFORIN* systematically overstate K_{∞} for this cell but the predicted reactivity loss is quite close to the average value. For a cell with $V_m/V_f=1.1$ the results of all three codes are in good agreement with data given in (Ishiguro, 1987).

Burnup dependences of conversion ratio (CR) are compared in Fig.4.7.

This figure demonstrates good agreement of *RAFORIN* results with average values for both cells at all burnup points. The maximum deviation for this code does not exceed ~1.2%.

fig4-6

Fig. 4.6 Burnup dependence of K_{∞} for the tight lattices with MOX fuel.

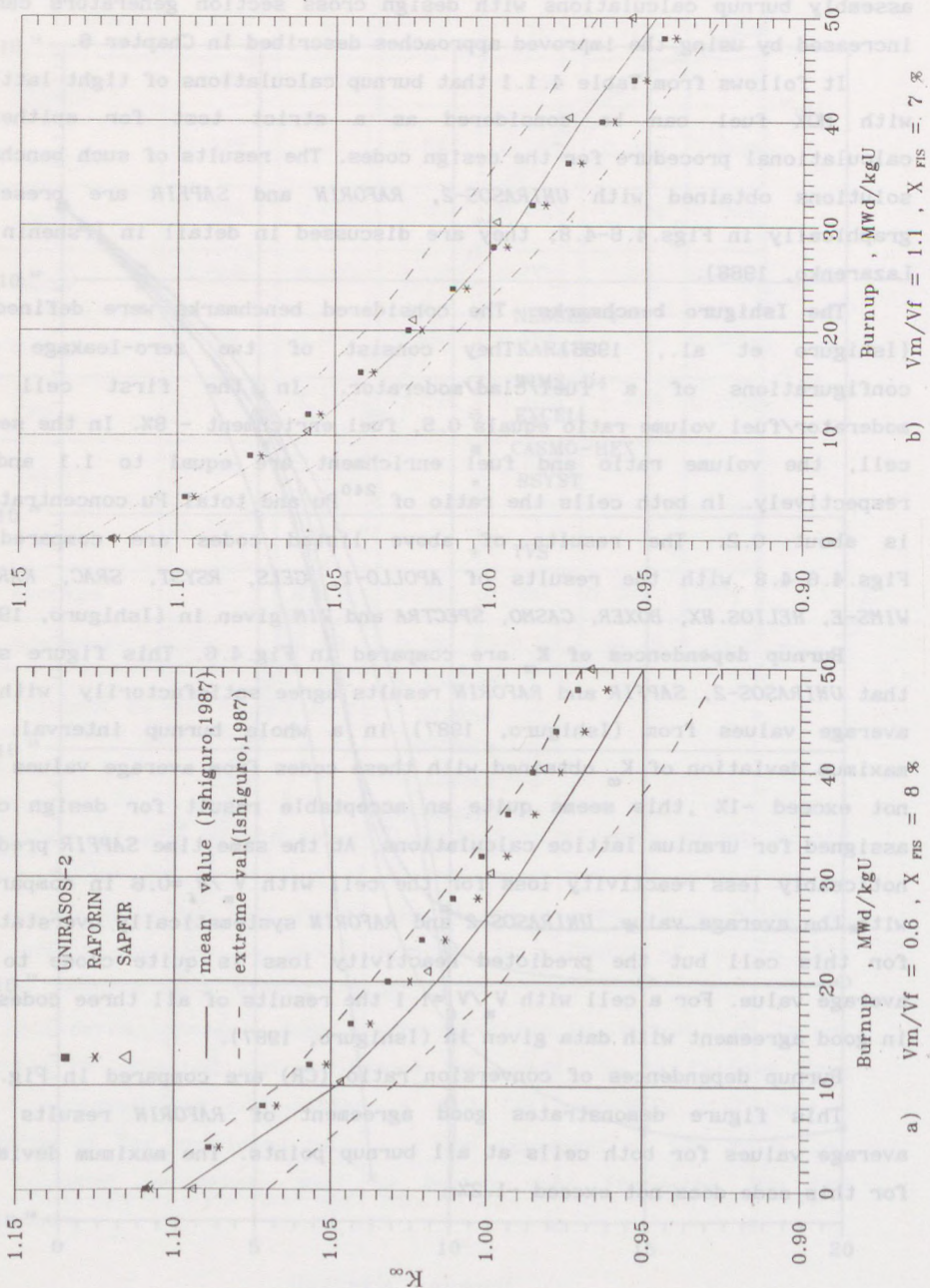
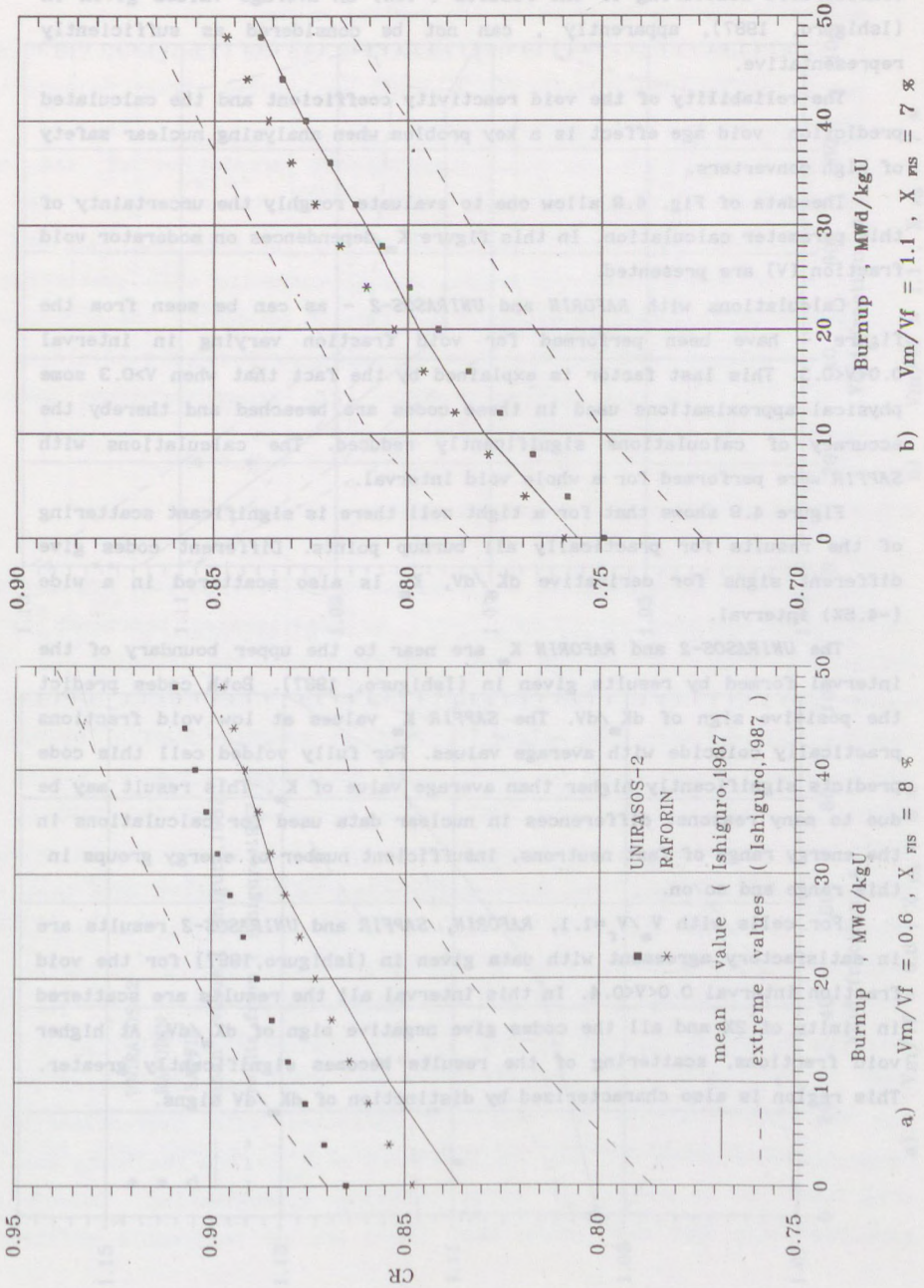


fig4-7

Fig. 4.7 Burnup dependence of conversion ratio (CR) for the tight lattices with MOX fuel



The corresponding deviation for UNIRASOS-2 in the tight cell ($V_m/V_f=0.6$) at zero burnup point is ~3.5% and it noticeably decreases with burnup growth. For cells with greater volume ratio CR predicted by this code agree well with average values. It is necessary to note that owing to considerable scattering of the results (~10%) CR average values given in (Ishiguro, 1987), apparently, can not be considered as sufficiently representative.

The reliability of the void reactivity coefficient and the calculated prediction void age effect is a key problem when analysing nuclear safety of high converters.

The data of Fig. 4.8 allow one to evaluate roughly the uncertainty of this parameter calculation. In this figure K_∞ dependences on moderator void fraction (V) are presented.

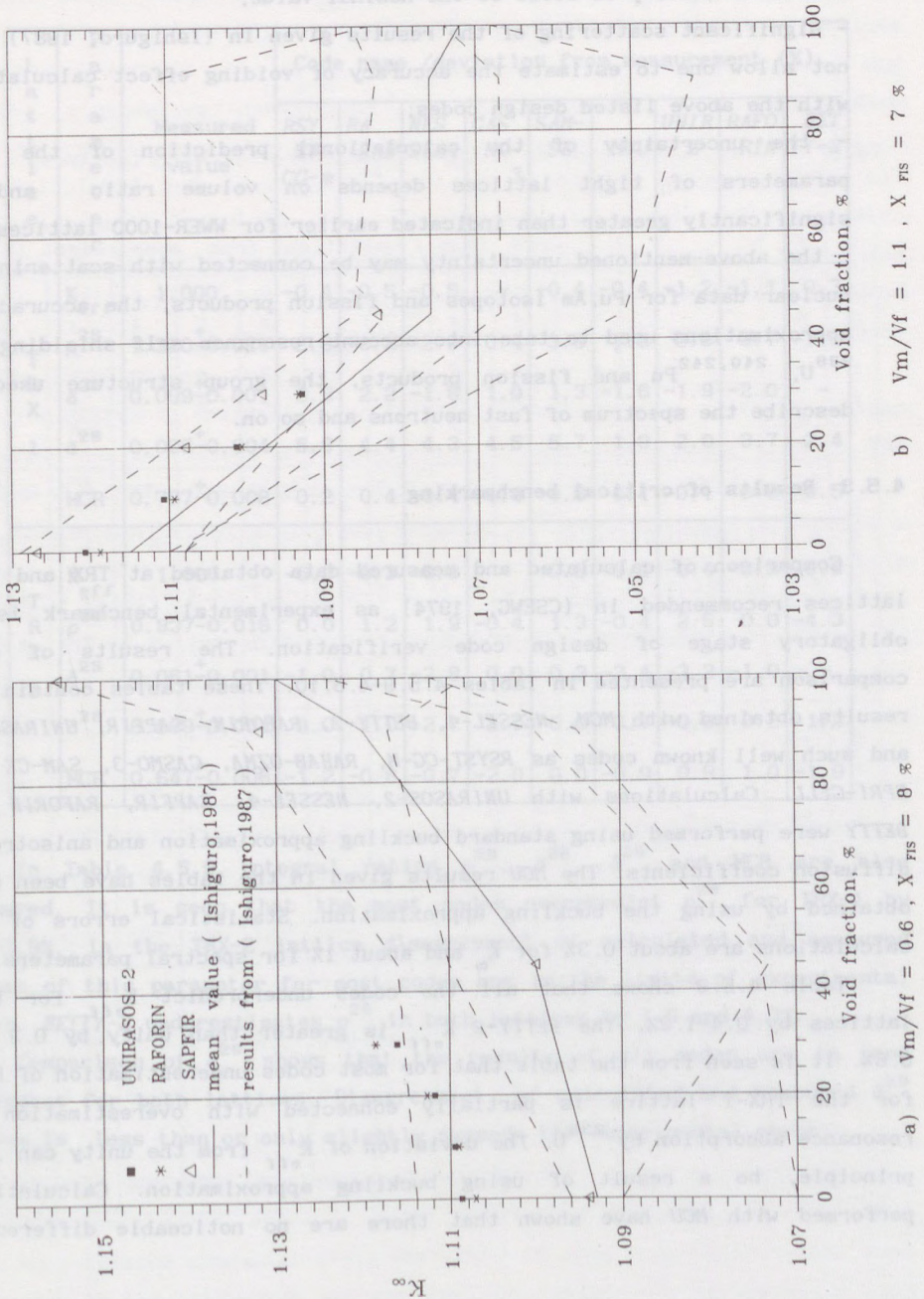
Calculations with RAFORIN and UNIRASOS-2 - as can be seen from the figure - have been performed for void fraction varying in interval $0.0 < V < 0.3$. This last factor is explained by the fact that when $V > 0.3$ some physical approximations used in these codes are breached and thereby the accuracy of calculations significantly reduced. The calculations with SAPPFIR were performed for a whole void interval.

Figure 4.9 shows that for a tight cell there is significant scattering of the results for practically all burnup points. Different codes give different signs for derivative dK_∞/dV , K_∞ is also scattered in a wide (~4.5%) interval.

The UNIRASOS-2 and RAFORIN K_∞ are near to the upper boundary of the interval formed by results given in (Ishiguro, 1987). Both codes predict the positive sign of dK_∞/dV . The SAPPFIR K_∞ values at low void fractions practically coincide with average values. For fully voided cell this code predicts significantly higher than average value of K_∞ . This result may be due to many reasons: differences in nuclear data used for calculations in the energy range of fast neutrons, insufficient number of energy groups in this range and so on.

For cells with $V_m/V_f=1.1$, RAFORIN, SAPPFIR and UNIRASOS-2 results are in satisfactory agreement with data given in (Ishiguro, 1987) for the void fraction interval $0.0 < V < 0.4$. In this interval all the results are scattered in limits of 2% and all the codes give negative sign of dK_∞/dV . At higher void fractions, scattering of the results becomes significantly greater. This region is also characterized by distinction of dK_∞/dV signs.

fig4-8

Fig. 4.8 Dependence of K_{∞} on void fraction for zero burnup point .

Thus the results from solving benchmarks on tight lattice burnup make it possible to conclude that:

- the *RAFORIN*, *SAPFIR* and *UNIRASOS-2* results are in satisfactory agreement with the results obtained with modern spectral codes when the moderator density is close to the nominal value;
- significant scattering of the results given in (Ishiguro, 1987) does not allow one to estimate the accuracy of voiding effect calculations with the above listed design codes;
- the uncertainty of the calculational prediction of the main parameters of tight lattices depends on volume ratio and is significantly greater than indicated earlier for WWER-1000 lattices;
- the above-mentioned uncertainty may be connected with scattering of nuclear data for Pu, Am isotopes and fission products, the accuracy of approximations used to take into account resonance self shielding for ^{238}U , $^{240,242}\text{Pu}$ and fission products, the group structure used to describe the spectrum of fast neutrons and so on.

4.5.3 Results of critical benchmarking

Comparison of calculated and measured data obtained at TRX and BAPL lattices recommended in (CSEWG, 1974) as experimental benchmark is an obligatory stage of design code verification. The results of such comparison are presented in Tables 4.5.9-4.5.10. These tables contain the results obtained with *MCU*, *NESSEL-4*, *BETTY-2*, *RAFORIN*, *SAPFIR*, *UNIRASOS-2* and such well known codes as *RSYST-CG-M*, *RAHAB-OZMA*, *CASMO-3*, *SAM-CE* and *EPRI-CELL*. Calculations with *UNIRASOS-2*, *NESSEL-4*, *SAPFIR*, *RAFORIN* and *BETTY* were performed using standard buckling approximation and anisotropic diffusion coefficients. The *MCU* results given in the tables have been also obtained by using the buckling approximation. Statistical errors of *MCU* calculations are about 0.3% for K_{∞} and about 1% for spectral parameters.

Table 4.5.9 shows that all the codes underpredict K_{eff} for both lattices by 0.4-1.2%. The *BETTY-2* K_{eff} is greater than unity by 0.3 and 0.6%. It is seen from the table that for most codes underestimation of K_{eff} for the TRX-1 lattice is partially connected with overestimation of resonance absorption by ^{238}U . The deviation of K_{eff} from the unity can, in principle, be a result of using buckling approximation. Calculations performed with *MCU* have shown that there are no noticeable differences

between K_{eff} obtained using the mentioned approximation and detailed modelling of real 2D geometry of the assembly.

Table 4.5.9. Comparison of integral parameters for TRX-12 lattices.

Lattice	Parameter	Measured value	Code name /deviation from measurement (%)								
			RSY ST- CG-m	RA HAB	NES SEL4	CAS MO- 3	SAM- SE	MCU	UNIR 2	RAFO RIN	BET TY-2
TRX-1	K_{eff}	1.000	-0.4	-0.5	-0.5	-	-0.4	-0.4	-1.2	-1.1	0.3
	ρ^{28}	$1.320^{+0.021}$	2.8	-0.2	2.9	0.4	3.8	1.5	3.9	0.7	-1.5
	δ^{25}	$0.099^{+0.001}$	0.5	2.2	-1.6	1.0	1.3	-1.6	-1.9	-2.0	-
	δ^{28}	$0.095^{+0.004}$	5.8	4.4	4.3	4.5	5.7	1.9	2.0	3.7	2.4
	MCR	$0.797^{+0.008}$	0.2	0.4	-0.4	-1.8	0.6	0.1	-0.1	0.9	0.5
TRX-2	K_{eff}	1.000	-0.3	-0.3	-0.3	-	-0.8	-0.1	-0.4	-0.9	0.6
	ρ^{28}	$0.837^{+0.016}$	0.0	1.2	1.9	-0.4	1.3	-0.4	2.5	0.0	-4.3
	δ^{25}	$0.061^{+0.001}$	-1.0	0.7	-2.8	0.0	0.3	-3.4	-3.2	-1.0	-
	δ^{28}	$0.069^{+0.004}$	3.0	1.0	-2.7	2.0	0.0	3.7	-0.9	3.2	1.3
	MCR	$0.647^{+0.006}$	-1.2	-0.8	-0.7	-2.0	0.0	-0.9	0.9	1.0	-1.9

In Table 4.5.9 integral ratios ρ^{28} , δ^{28} , δ^{25} and MCR are also compared. It is seen that the most codes overpredict ρ^{28} for TRX-1 by 0.4-3.9%. In the TRX-2 lattice disagreement of calculated and measured values of this parameter for most codes are in the limits of experimental error. BETTY-2 underestimates ρ^{28} in both lattices by 1.5 and 4.3%.

Comparison of δ^{28} shows that the results of all codes are in good agreement for both lattices. Disagreement of calculated and measured δ^{28} values is less than or only slightly exceeds the experimental error.

Table 4. 5.10. Comparison of integral parameters for BAPL lattices.

L a t t i c e	P a r a m e t e r	Measured value	Code name / deviation from measurement (%)									
			R S Y T	R A H A B	C A S M O 3	EPRI CELL	MCU	U N I R 2	N E S S 4	R A F O R.	S A P F I R	B E T T Y 2
B A P L 1	K_{eff}	1.000	0.1	0.1	0.1	0.3	-0.3	-0.3	-0.1	0.0	0.0	-0.3
	ρ^{28}	$1.390^{+0.01}$	2.1	1.7	-0.7	1.7	1.4	2.2	1.2	-0.1	-1.2	2.6
	δ^{25}	$0.084^{+0.00}$	0.1	1.0	0.1	0.0	-0.8	-1.7	-2.4	-1.8	-3.2	-4.1
	δ^{28}	$0.078^{+0.00}$	-0.6	-2.4	-0.5	-2.3	-1.2	-5.1	-2.1	-3.3	-7.9	-3.1
	MCR	-	.813	.810	-	-	.813	.807	.806	.803	.811	.823
B A P L 2	K_{eff}	1.000	0.0	0.1	-	0.3	0.9	-0.1	-0.1	0.0	0.0	-0.1
	ρ^{28}	$1.120^{+0.01}$	-	4.6	2.8	4.7	2.7	5.0	4.6	2.9	4.2	5.4
	δ^{25}	$0.068^{+0.00}$	-	1.6	1.0	0.0	-2.1	-1.0	-1.5	-1.4	2.5	-3.5
	δ^{28}	$0.070^{+0.00}$	-	-7.0	-4.6	-6.7	-5.7	-8.5	-6.1	-7.1	-13.	-6.6
	MCR	-	-	.737	-	-	.733	.734	.734	.731	.738	.748
B A P L 3	K_{eff}	1.000	0.1	0.2	-	0.4	0.2	0.2	0.0	0.1	0.0	0.2
	ρ^{28}	$0.906^{+0.02}$	-	0.4	0.0	0.9	-0.6	1.2	1.5	-0.3	0.8	1.4
	δ^{25}	$0.052^{+0.00}$	-	2.1	1.5	2.5	-1.5	-1.0	-1.1	-0.6	-2.4	-3.5
	δ^{28}	$0.057^{+0.00}$	-	-6.3	-3.8	-8.2	-3.6	-7.0	-4.8	-5.2	-11.	-5.2
	MCR	-	-	.657	-	-	.656	.654	.658	.654	.658	.666

Calculated values of MCR obtained with *MCU*, *UNIRASOS-2* and *RAFORIN* agree with measured values in the limits of measurement error. *BETTY-2* slightly underestimates this parameter for the TRX-2 lattice.

The calculation results for BAPL lattices are presented in Table 4.5.10, which shows that K_{eff} computed with *UNIRASOS-2*, *NESSEL-4* and *BETTY-2* deviates from unity by not more than 0.3%. For all three lattices *SAPFIR* and *RAFORIN* give K_{eff} very close to unity. The *UNIRASOS-2* and *BETTY-2* eigenvalues demonstrate a slight tendency to underpredict criticality with reduction of moderator fuel volume ratio.

Calculated and measured ρ^{28} are in acceptable agreement for all lattices besides BAPL-2 for which all the codes overpredict this parameter by 2.8-5.4%. Comparing deviations for BAPL-2 on the one hand and BAPL-1 and BAPL-3 on the other hand it seems possible to conclude that ρ^{28} measured value is erroneous or does not correspond to the cutoff energy of 0.625 eV used in calculations.

The *NESSEL-4*, *UNIRASOS-2* and *RAFORIN* δ^{25} values are slightly less than measured and deviations are very close to the measurement errors. The *BETTY-2* δ^{25} differ from the measured ones by 3.5-4.1%.

Comparison of calculated and measured δ^{28} show that for all codes a trend to underpredict this parameter is observed. The lowest values of this parameter which are up to 12.7 % lower than measured are obtained with *SAPFIR*. It is rather difficult to explain such differences taking into account the *MCU* results and the fact that both codes use ABBN data and the results given in Table 4.5.3.

Summarizing one can conclude that:

- *MCU*, *NESSEL-4*, *UNIRASOS-2* and *RAFORIN* underpredict K_{eff} for TRX lattices;
- the same tendency is typical for modern codes based on ENDF-B/V and JEF-1 data;
- all design codes provides good accuracy of K_{eff} calculations for BAPL lattices;
- accuracy of integral parameter calculations by most design codes are close to the accuracy provided by codes based on the above mentioned data files.

BETTIS, WINFRITH and BNL lattices. In addition to the TRX and BAPL criticals considered above a great number of measurements of water moderated lattice characteristics performed in many laboratories have been described in the literature and are used for design code verification. The

results of such measurements, for example, are generalized in (Straubridge, Barry, 1965), (Bernocely, Martinelly, 1977).

These papers contain the data obtained for those lattices characterized by variation of their parameters in a wide limits. Comparisons using such measurements allow one to discern many consistent trends in the calculation results because of nuclear data or approximations used in the design codes. At the same time these measurements are not included in category of the benchmarks and so must be carefully analysed to exclude erroneous or doubtful data. The results of such analyses are discussed in (Becker, 1988, Jozefowich, 1977).

A set of criticals recommended initially for verification and intercomparison included most of the criticals described in (Bernoceli, Martinelly, 1977), (Andrianov *et al*, 1964), (Liikala *et al*, 1972). It should be mentioned that one of the main requirements under the selection of criticals was the presence of the data on material buckling and integral ratios (δ^{25} , δ^{28} , ρ^{28} , MCR).

The procedure of selection included

- comparison of results obtained with different codes,
- comparison of the code results with measurements data (see (Becker, 1981), (Pshenin *et al*, 1989);
- estimation of the sensitivity of measured parameters to the uncertainty of dimensions and compositions;
- 2D diffusion and transport calculations to determine a dimension of asymptotic region in the assembly (Becker, 1988).

The analyses performed have led to the necessity for excluding some criticals. The calculational results for 13 selected criticals are discussed below. These criticals are numerated in accordance with the standard accepted in (Becker, 1981).

Calculated K_{eff} values are compared in Table 4.5.11 which shows that the maximum deviations of K_{eff} computed by UNIRASOS-2, NESSEL-4, RAFORIN, SAPFIR, BETTY and MICROBE from unity are equal to 0.9, 1.3, 1.1, 0.8, 1.5 and 1.8%, respectively.

To discern trends in calculation results the deviations of K_{eff} from unity are presented in Figs. 4.9-4.11 as functions of different parameters - leakage, volume ratio, and resonance absorption by ^{238}U .

Table 4.5.11. Computed K_{eff} for BETTIS, WINFRITH and BNL criticals.

Lattice	Code name / K_{eff}						
	MCU	NESSEL4	UNIRASOS 2	BETTY2	RAFORIN	MICROBE	SAPFIR
BETTIS							
3/1	-	0.9959	0.9933	0.9953	0.9969	1.0000	0.999
3/2	-	0.9995	0.9990	1.0011	1.0000	1.0017	1.008
3/2	-	0.9999	1.0009	1.0015	0.9993	1.0012	1.007
3/4	-	0.9984	0.9974	0.9968	0.9993	0.9979	0.998
3/5	-	0.9990	1.0001	0.9985	1.0000	0.9977	1.000
WINFRITH							
4/1	0.998(4)	1.0010	1.0053	1.0028	1.0081	1.0114	0.995
4/2	1.002(4)	1.0029	1.0037	1.0153	1.0060	0.9920	0.996
4/3	1.003(4)	1.0023	1.0008	0.9983	1.0052	1.0180	1.003
BNL							
6/1	-	0.9905	1.0046	0.9930	0.9980	-	0.997
6/2	-	0.9872	1.0008	0.9978	0.9934	-	0.992
6/3	-	0.9869	1.0018	0.9968	0.9926	-	0.997
6/4	-	0.9884	1.0075	1.0015	0.9945	-	1.002
6/5	-	0.9846	1.0093	1.0011	0.9894	-	1.003

Figure 4.9 shows that there are no consistent trends in K_{eff} dependence on leakage. At the same time scattering of the results for the lattices with large leakage is significantly greater.

The dependences of $K_{eff} - 1$ on volume ratio are presented in Fig. 4.10. As in the previous case, it is also difficult here to establish stable trends in K_{eff} behaviour. UNIRASOS-2 appears to slightly overestimate the K_{eff} value with volume ratio growth.

Figure 4.11 illustrates K_{eff} dependences on ρ^{28} . It is seen from this figure that the results practically do not depend on resonance absorption by ^{238}U in a wide range ($\sim 0.6 < \rho^{28} < \sim 5.0$).

Thus, to summarize one can conclude on the lack of evident trends in accuracy of eigenvalue prediction by all the design codes considered.

fig4-9

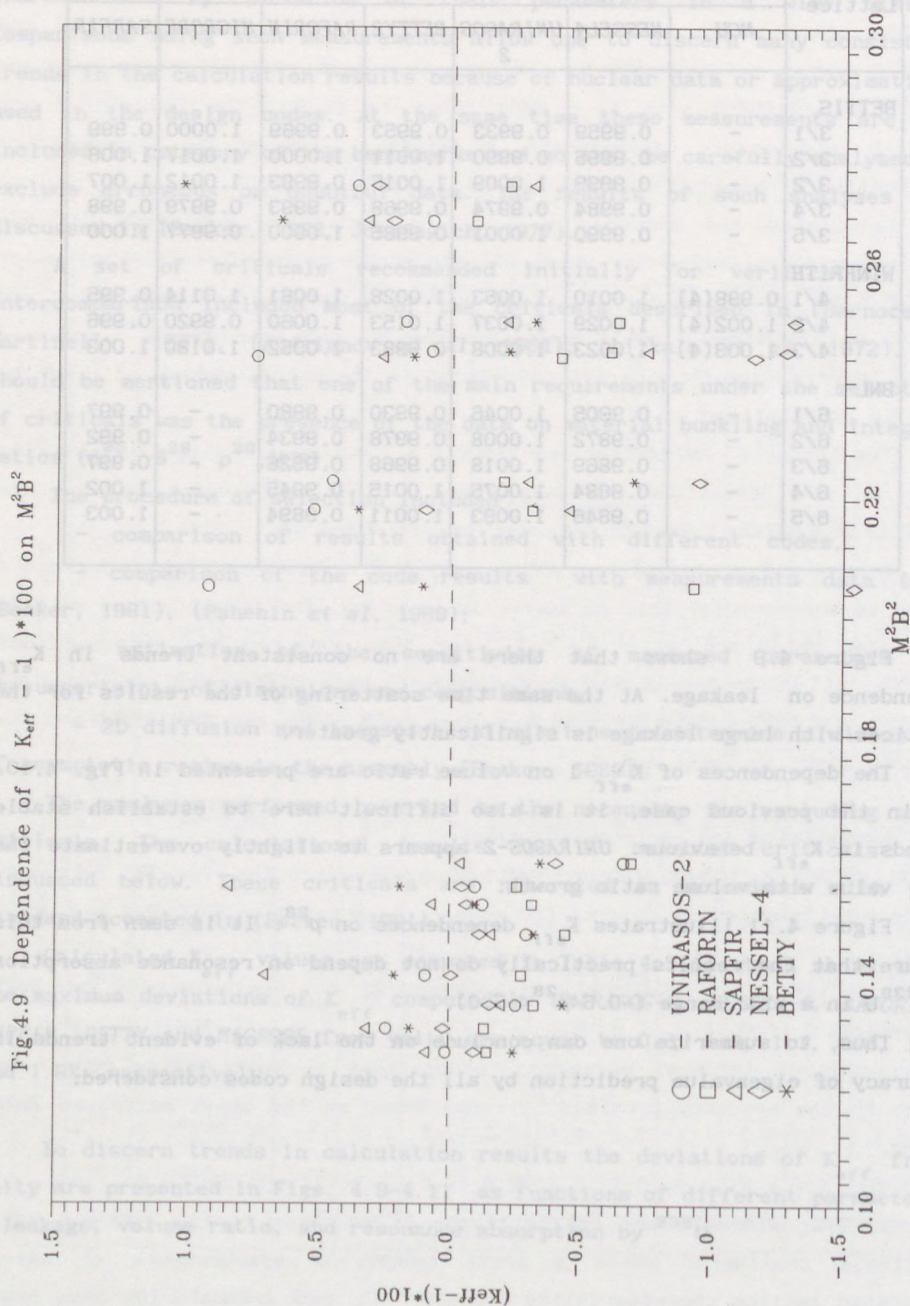


fig4-10

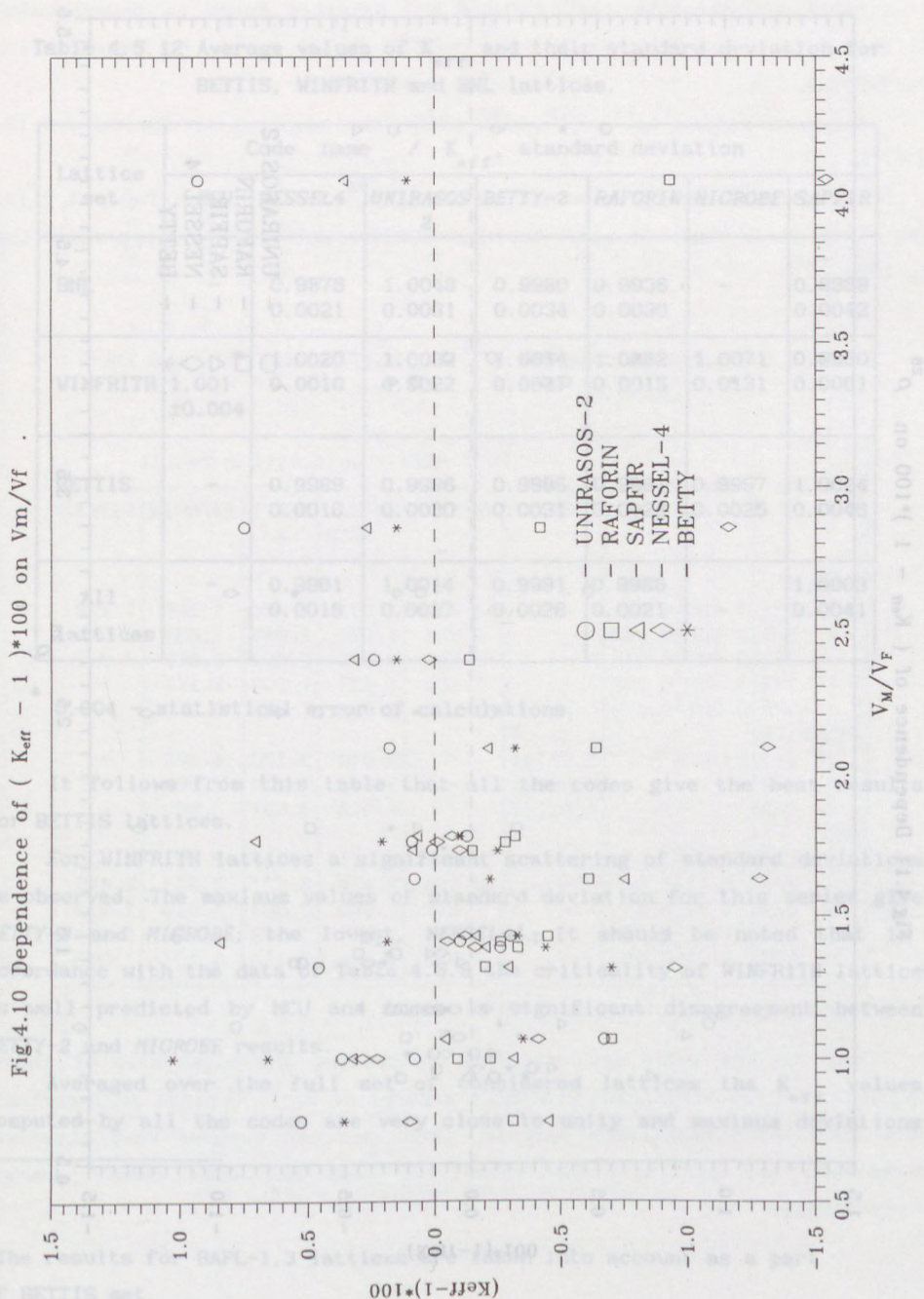


fig4-11

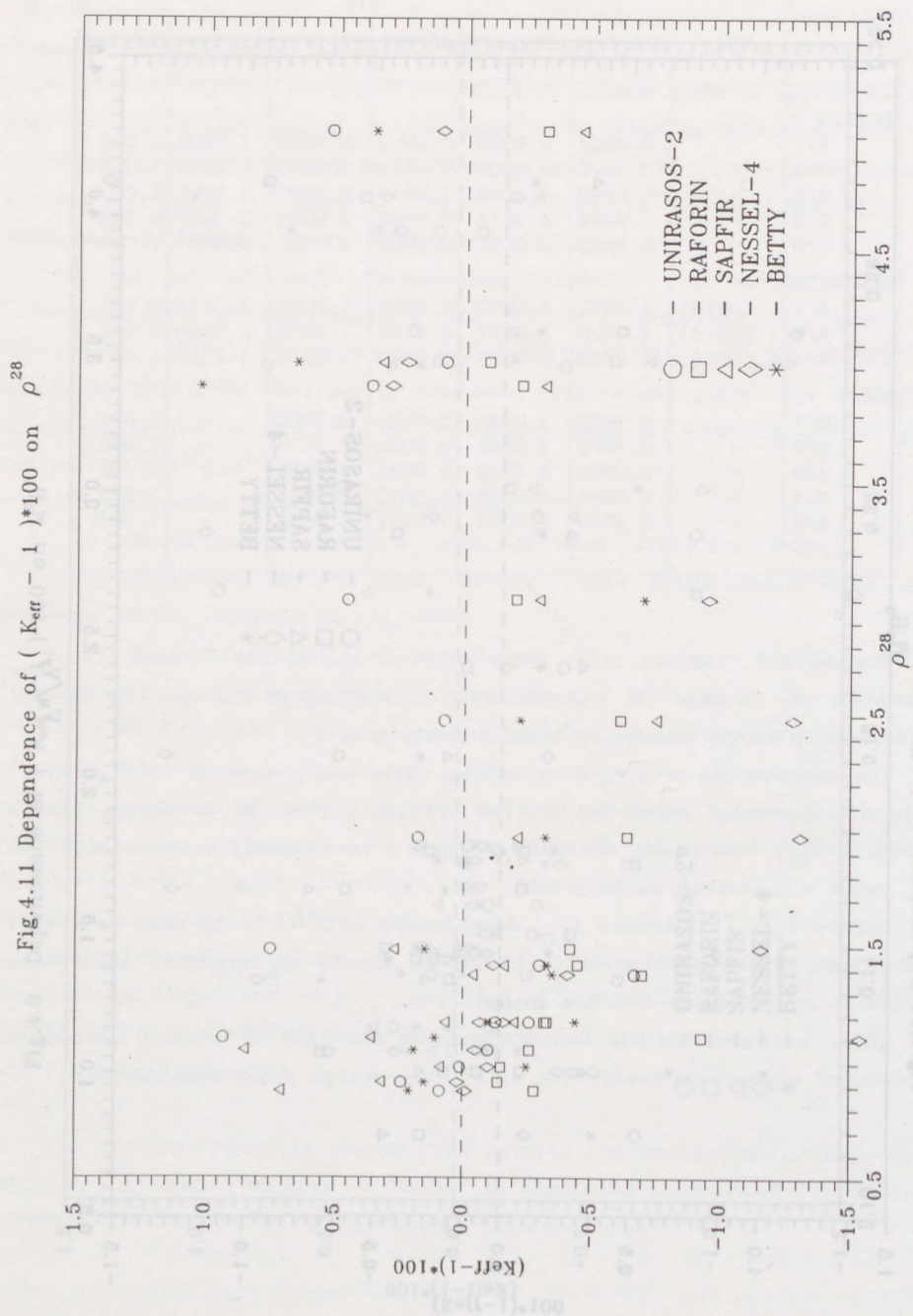


Table 4.5.12 generalizes the results of K_{eff} calculations. The average values of K_{eff} and their standard deviations are given in this table.*

Table 4.5.12 Average values of K_{eff} and their standard deviation for BETTIS, WINFRITH and BNL lattices.

Lattice set	Code name / K_{eff} , standard deviation						
	MCU	NESSEL4	UNIRASOS 2	BETTY-2	RAFORIN	MICROBE	SAPFIR
BNL	-	0.9875 0.0021	1.0048 0.0031	0.9980 0.0034	0.9936 0.0030	-	- 0.9988 0.0042
WINFRITH	* 1.001 ± 0.004	1.0020 0.0010	1.0032 0.0022	1.0054 0.0087	1.0062 0.0015	1.0071 0.0131	0.9980 0.0061
BETTIS	-	0.9989 0.0016	0.9986 0.0030	0.9986 0.0031	0.9991 0.0022	0.9997 0.0025	1.0024 0.0046
All lattices	-	0.9961 0.0016	1.0014 0.0027	0.9991 0.0026	0.9986 0.0021	-	1.0003 0.0041

* 0.004 - statistical error of calculations.

It follows from this table that all the codes give the best results for BETTIS lattices.

For WINFRITH lattices a significant scattering of standard deviations is observed. The maximum values of standard deviation for this series give BETTY-2 and MICROBE; the lowest, NESSEL-4. It should be noted that in accordance with the data of Table 4.5.9 the criticality of WINFRITH lattices is well predicted by MCU and there is significant disagreement between BETTY-2 and MICROBE results.

Averaged over the full set of considered lattices the K_{eff} values computed by all the codes are very close to unity and maximum deviations

* The results for BAPL-1,3 lattices are taken into account as a part of BETTIS set.

for most of them are within the limits of uncertainty due to the error of buckling measurements. The maximum value of standard deviation gives SAPPFIR (0.0041), the minimum - NESSEL-4 (0.0016).

Table 4.5.10 shows that RAFORIN and NESSEL-4 tends to underpredict slightly the eigenvalue and the opposite trend seems to characterize UNIRASOS-2.

Integral ratios (ρ^{28} , δ^{28} , δ^{25} , MCR) are compared in Tabs. 4.5.13-4.5.16.

The calculated and measured values of ρ^{28} are given in Table 4.5.13. The table shows that all codes besides SAPPFIR significantly overpredict (up to 15%) ρ^{28} .

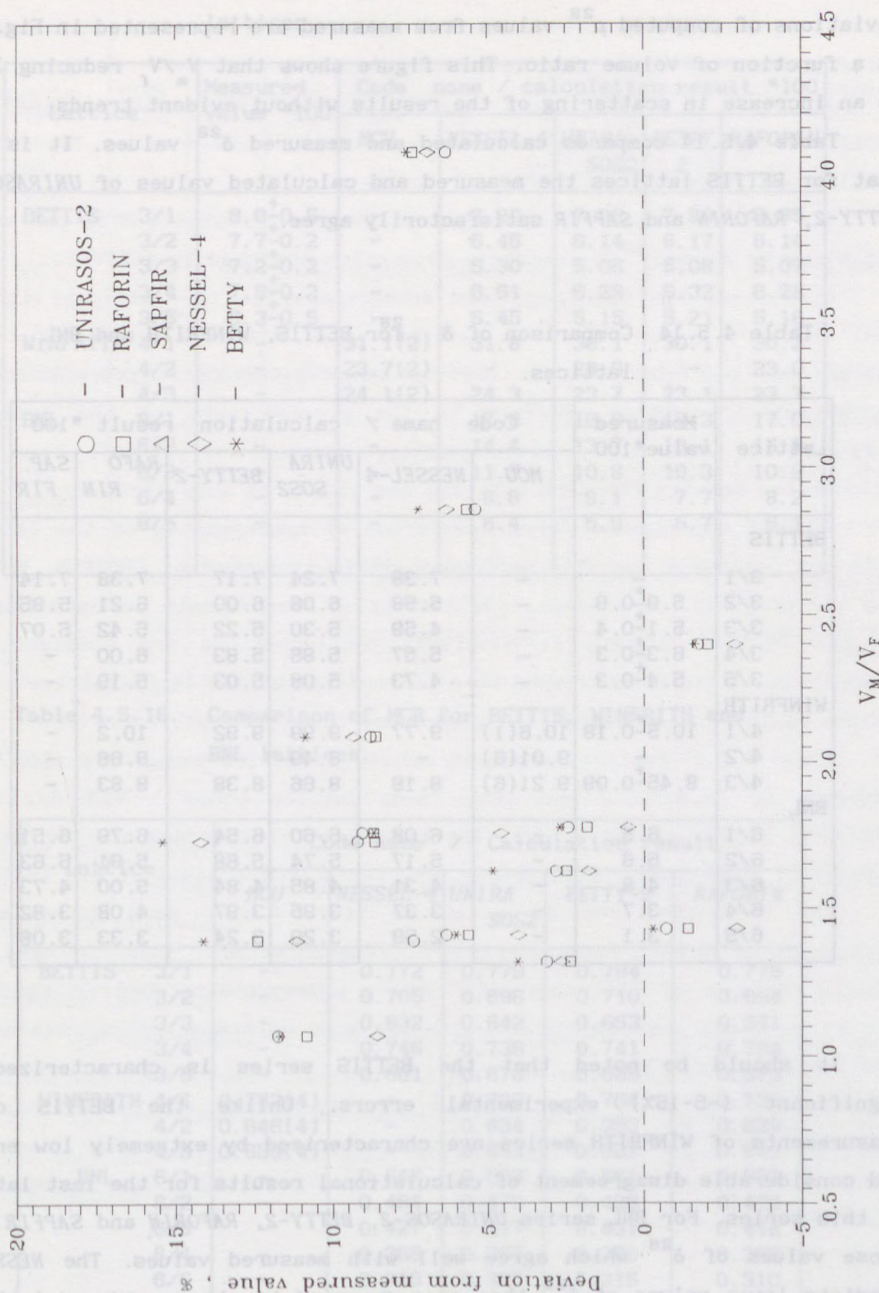
Table 4.5.13. Comparison of ρ^{28} for BETTIS, WINFRITH and BNL lattices.

Lattice	Measured value	Code name / calculation result						
		MCU	NESSEL4	UNIRA SOS2	BETTY 2	RAFORIN	SAPFIR	
BETTIS	3/1	1.190 ⁺ 0.04	-	1.292	1.330	1.360	1.299	1.274
	3/2	0.994 ⁺ 0.013	-	1.034	1.057	1.084	1.035	0.983
	3/3	0.807 ⁺ 0.014	-	0.844	0.880	0.902	0.866	0.817
	3/4	1.040 ⁺ 0.050	-	1.156	1.177	1.205	1.157	-
	3/5	0.901 ⁺ 0.020	-	1.029	0.984	1.016	0.970	-
WINFRITH			*					
	4/1	-	5.06(4)	-	5.018	5.120	4.862	-
	4/2	-	3.96(3)	-	3.919	1.430	3.809	-
	4/3	-	4.03(3)	-	4.018	4.037	3.909	-
BNL								
	6/1	2.92 ⁺ 0.09	-	2.997	3.001	3.038	2.951	3.000
	6/2	2.41 ⁺ 0.04	-	2.453	2.478	2.527	2.441	2.446
	6/3	1.81 ⁺ 0.06	-	1.979	1.969	2.007	1.945	1.938
	6/4	1.41 ⁺ 0.02	-	1.499	1.486	1.512	1.476	1.454
	6/5	1.04 ⁺ 0.02	-	1.112	1.106	1.119	1.107	1.073

* should be considered as 5.06⁺0.04

Most of the codes are well able to predict the eigenvalue of these lattices. On the other hand resonance absorption by ^{238}U plays an important role in lattice reactivity balance. Thus, one can suppose that observed deviations are partially the result of real and used cutoff energy unconformity.

Fig. 4.12 Deviation of calculated ρ^{28} from measured one as a function of V_M/V_F .



This statement is confirmed by *SAPFIR* results which have been obtained using a variable value of cutoff energy which was computed directly. Deviations of computed ρ^{28} values from measured are represented in Fig. 4.12 as a function of volume ratio. This figure shows that V_m/V_f reducing leads to an increase in scattering of the results without evident trends.

Table 4.5.14 compares calculated and measured δ^{28} values. It is seen that for BETTIS lattices the measured and calculated values of *UNIRASOS-2*, *BETTY-2*, *RAFORIN* and *SAPFIR* satisfactorily agree.

Table 4.5.14 Comparison of δ^{28} for BETTIS, WINFRITH and BNL lattices.

Lattice	Measured value*100	Code name / calculation result *100					
		MCU	NESSEL-4	UNIRASOS2	BETTY-2	RAFORIN	SAPFIR
BETTIS							
3/1	$\bar{+}$	-	7.38	7.24	7.17	7.38	7.14
3/2	5.9 ± 0.9	-	5.58	6.08	6.00	6.21	5.85
3/3	5.1 ± 0.4	-	4.59	5.30	5.22	5.42	5.07
3/4	6.3 ± 0.3	-	5.57	5.88	5.83	6.00	-
3/5	5.4 ± 0.3	-	4.73	5.08	5.03	5.19	-
WINFRITH							
4/1	10.5 ± 0.18	10.6(1)	9.77	9.99	9.92	10.2	-
4/2	$\bar{-}$	9.01(6)	-	8.49	-	8.68	-
4/3	8.45 ± 0.09	9.21(6)	8.18	8.66	8.38	8.83	-
BNL							
6/1	6.5	-	6.08	6.60	6.54	6.79	6.51
6/2	5.6	-	5.17	5.74	5.68	5.91	5.63
6/3	4.8	-	4.31	4.85	4.84	5.00	4.73
6/4	3.7	-	3.37	3.95	3.97	4.08	3.82
6/5	3.1	-	2.59	3.20	3.24	3.33	3.08

It should be noted that the BETTIS series is characterized by significant (~5-15%) experimental errors. Unlike the BETTIS case, measurements of WINFRITH series are characterized by extremely low errors and considerable disagreement of calculational results for the last lattice of this series. For BNL series *UNIRASOS-2*, *BETTY-2*, *RAFORIN* and *SAPFIR* give close values of δ^{28} which agree well with measured values. The *NESSEL-4* predicts lower values of δ^{28} than ones measured in all considered lattices that is in good agreement with data of numerical benchmarking (see Table 4.5.3).

Table 4.5.15 Comparison of δ^{25} for BETTIS, WINFRITH and BNL lattices.

Lattice		Measured value *100	Code name / calculation result *100				
			MCU	NESSEL-4	UNIRA SOS2	BETTY 2	RAFORIN
BETTIS	3/1	8.0 ⁺ _{-0.5}	-	8.20	7.86	7.89	7.85
	3/2	7.7 ⁺ _{-0.2}	-	6.46	6.14	6.17	6.14
	3/3	7.2 ⁺ _{-0.2}	-	5.30	5.06	5.08	5.07
	3/4	7.8 ⁺ _{-0.2}	-	6.61	6.28	6.32	6.28
	3/5	6.3 ⁺ _{-0.5}	-	5.45	5.15	5.21	5.16
WINFRITH	4/1	-	31.1(2)	31.8	30.1	30.1	30.2
	4/2	-	23.7(2)	-	23.0	-	23.0
	4/3	-	24.1(2)	24.3	23.7	23.1	23.7
BNL	6/1	-	-	17.8	16.9	16.3	17.0
	6/2	-	-	14.4	13.7	13.1	13.8
	6/3	-	-	11.5	10.8	10.3	10.9
	6/4	-	-	8.6	8.1	7.7	8.2
	6/5	-	-	6.4	5.9	5.7	6.1

Table 4.5.16. Comparison of MCR for BETTIS, WINFRITH and BNL lattices.

Lattice		Code name / Calculation result				
		MCU	NESSEL-4	UNIRA SOS2	BETTY-2	RAFORIN
BETTIS	3/1	-	0.772	0.779	0.794	0.775
	3/2	-	0.705	0.696	0.710	0.694
	3/3	-	0.632	0.642	0.653	0.641
	3/4	-	0.746	0.736	0.741	0.734
	3/5	-	0.661	0.676	0.689	0.676
WINFRITH	4/1	0.752(4)	-	0.739	0.764	0.731
	4/2	0.646(4)	-	0.634	0.353	0.629
	4/3	0.653(4)	-	0.653	0.657	0.645
BNL	6/1	-	0.547	0.538	0.561	0.538
	6/2	-	0.484	0.479	0.495	0.479
	6/3	-	0.427	0.417	0.431	0.418
	6/4	-	0.366	0.357	0.368	0.358
	6/5	-	0.315	0.307	0.315	0.310

Calculated and measured values of δ^{25} are compared in Table 4.5.15. Because δ^{25} strongly depends on cutoff energy it seems that observed deviations for BETTIS lattices indicate discrepancy between real values of cutoff energy and those used in calculations.

Table 4.5.16 compares calculated MCR values. The results obtained with NESSEL-4, UNIRASOS-2 and RAFORIN agree within ~2.5% limits. The BETTY-2 results are higher by ~1.5% for all lattices.

The last mentioned results agree with data of Table 4.5.13 and may be explained by higher ^{238}U resonance absorption computed by BETTY-2.

As already has been mentioned measurements at the lattices with MOX fuel that are known from the literature were initially included into the recommended set of criticals were excluded later for different reasons (nonasymptotic neutron spectrum in the greater part of the assembly, influence of fuel micro heterogeneity, presence of ^{241}Am). Thus, the calculation results for such lattices are absent in this section.

PROTEUS experiment. Three new series of measurements at the lattices with MOX fuel were recently performed within framework of PROTEUS, EPICURE and VIP programs. At present, the results of measurements performed at one of the PROTEUS (Chawla et al., 1984) configurations are available for comparison. These measurements were carried out at the tight lattice with a volume ratio $V_m/V_f=0.5$ and highly enriched (6%) MOX fuel.

Table 4.5.17 compares measured values of lattice parameters with those computed by UNIRASOS-2 and some known lattice codes - WIMS-81, SRAC, EPRI-CPM, HELIOS.HX and others. The results of these codes and the lattice parameters needed for calculations were taken from (Chawla et al. 1984).

The UNIRASOS-2 results given in Table 4.5.17 were corrected in accordance with the recommendations of (Chawla et al., 1984) to take into account effects of "heterogeneity" and a nonasymptotic neutron spectrum. The table shows that UNIRASOS-2 provides good agreement of calculated and measured integral ratios.

The values of K_{eff} calculated with this code are in satisfactory agreement with predicted by most other codes and are noticeably lower than unity. This deviation seems due both to the inaccuracy of the approximations used and experimental procedure.

Table 4.5.17. Integral ratios for PROTEUS experiments.

Parameter	Measured value; experim. error, %	Code name, calculation / measurement									
		WIMS -STd	WIMS 81	GRU-CAN	KAR-BUS	SPEC-TRA	EPRI-CPM	SRAC /J2	HELIOS -HX	BOXER	UNIRA SOS-2
$\frac{F_5}{F_9}$	0.988 (2.0)	-	-	-	-	-	1.016	1.002	0.964	1.011	1.013
$\frac{C_8}{F_9}$	0.0691 (2.2)	1.002	0.951	1.042	1.005	0.983	0.933	0.967	0.964	1.036	0.997
$\frac{F_8}{F_9}$	0.00987 (2.5)	0.974	0.992	0.979	0.999	0.941	1.003	1.010	0.993	1.113	0.973
$\frac{F_1}{F_9}$	1.780 (4.5)	-	-	-	-	-	1.033	0.953	0.970	0.889	0.974
K_∞	1.045 (1.1)	0.986	1.009	0.995	0.992	1.001	1.012	1.005	0.996	-	1.001
M^2	$53 \cdot \text{cm}^{-2}$	-	-	-	-	-	-	-	-	-	55.0

F_i, C_i - fission and capture rates produced by "i" isotope.

Thus one can conclude that:

- all considered design codes accurately predict the eigenvalues of BETTIS series criticals;
- significant disagreement of the results is observed for some BNL and WINFRITH lattices;
- the discrepancy of calculated and measured ρ^{28} and δ^{25} is mainly due to differences between the real and used values of cutoff energy.
- limited number of available measurements at tight lattice with MOX fuel does not allow one to make certain conclusions about the accuracy of their calculation.

4.5.4 Comparison of calculated and measured data obtained at unperturbed ZR-6 cores

It can be seen from the title of the present section that the results related to "clean" ZR-6 cores are discussed. All the calculations were carried out using the standard buckling approximation. To analyse the accuracy of this approach some configurations were also calculated with 1D diffusion and transport codes. The results of such calculations are given and discussed in (Becker, 1988). Let us adduce here some conclusions formulated in these works which will be useful for further discussion of the results.

1. Experimental errors of material buckling measurements lead to 0.1-0.5 uncertainty of K_{eff} calculations. The maximum uncertainty is inherent to lattices with fuel enrichment 3.6 and 4.4 %.

2. Transport calculations give K_{eff} higher by 0.2-2.0% than diffusion one.

3. Discrepancies of K_{eff} computed using buckling and 1D approximations for TRX and BAPL lattices are significantly less in comparison with discrepancies observed for most ZR-6 lattices.

These conclusions suggest that K_{eff} computed using buckling approximation can not be considered as fully representative. At the same time buckling approximation is sufficient for calculation of spectral characteristics. From the practical point of view the results of 2D calculations discussed in Chapter 6 give more objective and important information on the accuracy of eigenvalue calculations.

Computed eigenvalues are compared in Table 4.5.18. It is necessary to note that *NESSEL-4*, *UNIRASOS-2*, *SAPFIR* and *RAFORIN* results were obtained using the average material bucklings recommended in (Szatmary et al., 1985), (Szatmary et al., 1991). The results of *BETTY-2* are based on buckling values taken from (Vidovszky and Hegyi, 1988) and those obtained for a specific configuration. Table 4.5.18 shows that there are some common trends for *UNIRASOS-2*, *NESSEL-4*, *RAFORIN* and *SAPFIR*.

To analyse the dependence of K_{eff} on moderator/fuel volume ratio let us consider the lattices with fuel enrichment equal to 3.6% without boron in the moderator.

Tabl. 4.5.18. Eigenvalues for uniform ZR-6 lattices.

Lattice	T°C	B_{rec}^a (m ⁻²)	δK_{eff}^b (%)	Code name / K_{eff}				
				NESS SEL4	UNIRA SOS2	RAFO RIN	SAP FIR	^c BETTY-2
12.7/1.6/0.0	20	50.57	0.41	0.988	0.987	0.984	0.987	0.983
12.7/1.6/1.85	20	33.32	0.48	0.986	0.987	0.982		
12.7/3.6/0.0	20	98.26	0.32	1.008	1.002	1.000	0.993	1.019 99.57
12.7/3.6/0.0	80	96.55	0.43		0.991	0.990		1.008 97.28
12.7/3.6/0.0	130	90.27	0.32		0.988	0.989		1.001 89.94
12.7/3.6/4.0	20	76.03	0.04	0.999	0.996	0.992		
12.7/3.6/4.0	80	72.07	0.07		0.998	0.997		
12.7/3.6/4.0	130	67.63	0.07		0.994	0.997		
12.7/3.6/5.8	20	64.95	0.10		1.000	0.995		1.002 64.45
12.7/3.6/5.8	80	61.69	0.07		1.001	1.000		1.002 60.99
12.7/3.6/5.8	130	59.02	0.05		0.993	0.998		1.002 58.26
12.7/3.6/7.2	20	56.54	0.13	1.004	1.004	0.999		
12.7/4.4/0.0	20	112.58	0.50	0.995	0.988	0.986	0.977	1.018 108.6
12.7/4.4/0.0	80	105.11	0.24			0.993		1.008 105.1
12.7/4.4/0.0	130	96.61	0.22			0.998		1.015
12.7/4.4/0.64	20	106.60	0.58	1.002	0.995	0.993		1.002
12.7/4.4/7.2	20	69.03	0.33	1.010	1.009	1.005		
15.0/3.6/0.0	20	120.36	0.19		0.993	0.990		1.008 120.7
15.0/3.6/4.0	20	70.25	0.25		1.010	1.002		1.013 69.36
15.0/4.4/0.0	20	136.80	0.26		0.984	0.981		0.993 138.9
15.0/1.6/0.0	20	48.90	0.17		1.003	0.996		
11.0/3.6/0.0	20	65.27	0.21	0.992	0.987	0.985	0.975	1.009 64.35
11.0/3.6/0.0	80	64.02	0.19		0.977	0.976		1.003 63.15
11.0/3.6/0.0	130	59.76	0.13		0.972	0.972		0.981 58.99
11.0/3.6/0.96	20	62.14	0.13		0.988	0.988		0.995 61.79
11.0/3.6/1.41	20	61.70	0.21	0.991	0.986	0.983		

^a Recommended material buckling.

^b K_{eff} uncertainty corresponding to buckling experimental error.

^c The last column contains buckling values used in calculations with BETTY-2.

Comparison of eigenvalues shows that all listed codes significantly understate K_{eff} for lattices with a pitch of 1.1 cm. At the same time, UNIRASOS-2 and RAFORIN results for wide lattices (with pitch 1.5cm) do not allow one to conclude that K_{eff} is a function of moderator/fuel volume ratio.

The BETTY-2 K_{eff} values are by ~0.5-1% higher in comparison with NESSEL-4, SAPFIR, RAFORIN and UNIRASOS-2 results for all three lattices (taking into account the bucklings differences). It should be mentioned that the last does not correlate with data of Tables 4.5.10-4.5.11.

The dependence of K_{eff} on fuel enrichment can be analysed by consideration of the lattices with pitch 1.27 and 1.5 cm.

Table 4.5.18 demonstrates significant underprediction of K_{eff} values by all the codes for 12.7/1.6/0.0 lattice. As can be seen from the table this lattice is characterized by noticeable K_{eff} uncertainty caused by buckling error. This uncertainty however is less by a factor ~ 2.5 than observed deviations of K_{eff} from unity.

Low and highly enriched ($x=4.4\%$) lattices are also characterized by small radius of test zone. Thus, the obtained values of K_{eff} seem to be partially connected with the inaccuracy of asymptotic approximation. To check this assumption 2D calculations based on various approaches have been performed. Computed in this way K_{eff} values are by $\sim 0.5\%$ higher than those given in the table, thereby confirming made assumption.

It should also be noted that low enriched lattice is characterized by significant ($\sim 0.3\%$) uncertainty of K_{eff} caused by the $\sim 1\%$ enrichment uncertainty. Table 4.5.18 shows that all codes besides BETTY-2 underestimate the eigenvalue for the 12.7/4.4/0.0 lattice.

Simple estimations show that use of the buckling equal to 108.6 m^{-2} corresponding to (Vidovszky and Hegyi, 1988) leads to good agreement of NESSEL-4 and BETTY-2 results. The UNIRASOS-2 and RAFORIN K_{eff} in this case becomes close to unity. Unfortunately, the results obtained with UNIRASOS-2, RAFORIN and BETTY-2 are only available for lattices with a pitch equal to 1.5 cm. It is seen that for such lattices significant disagreement of the RAFORIN and BETTY-2 results is observed. Underprediction of K_{eff} by RAFORIN for these lattices characterized by small radius of test zone can probably be explained by the inaccuracy of asymptotic approximation. Nevertheless comparison with the results of 2D and reference zero leakage calculations seems to be useful.

Taking into account the problem connected with uncertainty of the result interpretation for the small test zones let us limit ourselves by considering the 3.6% enriched lattices to analyze accuracy of predicting boron poisoning and temperature effects.

Table 4.5.18 shows that NESSEL-4, UNIRASOS-2 and RAFORIN give a similar irregular shape of K_{eff} dependence on boron acid concentration. These codes predict $\sim 0.8\%$ difference between K_{eff} for lattices with zero and 0.4 g/l boron acid concentration. The results of all the above listed codes are in satisfactory agreement for the maximum boron concentration. In this case the K_{eff} obtained are quite close to unity.

Table 4.5.18 demonstrates systematic decreasing of K_{eff} obtained with *RAFORIN*, *UNIRASOS-2* and *BETTY-2* for the 12.7/3.6/0.0 lattice with increasing temperature. Such K_{eff} behaviour does not correlate with data given in the Table 4.5.7 and may be connected with correction introduced to take into account the flux perturbation by intermediate spacer grid placed in the core. As follows from (Szatmary et al., 1991) this correction significantly increases with temperature growth. Two-dimensional calculations with axial buckling corresponding to uncorrected value of moderator level give K_{eff} values which practically do not depend on temperature. It is necessary to note that the mentioned above trend is not observed for lattices poisoned by boron.

Calculated and measured δ^{28} are compared in Table 4.5.19. The agreement of calculated and measured values is rather good for low enriched lattices and tighter pitch lattices. In this case the results of all the codes are practically within the limits of experimental error. The calculation results agree well with measured values for 3.6 and 4.4% enriched lattices with unpoisoned moderator. Poisoning of the moderator by boron leads to significant underestimation of δ^{28} by all codes. It should be mentioned that the *MCU* results are very close to those obtained with design codes. Because all codes are based on ABBN data in the energy region of fast neutrons it seems very difficult to explain the observed deviations which are about twice greater than those given in Table 4.5.10 for BAPL lattices.

Table 4.5.19 Comparison of calculated and measured δ^{28}

Lattice	Measured vaue	Code name / calculated value				
		<i>MCU</i>	<i>NESSEL</i> 4	<i>UNIRA</i> <i>SOS2</i>	<i>RAFO</i> <i>RIN</i>	<i>MICRO</i> <i>BE</i>
12.7/1.6/0.0	0.0667 ⁺ 0.0039	0.061 ⁺ 0.006	0.0626	0.0621	0.0632	0.0629
12.7/1.6/1.8	0.0673 ⁺ 0.0039	0.062 ⁺ 0.006	0.0650	0.0647	0.0660	0.0658
12.7/3.6/0.0	0.0543 ⁺ 0.0013	0.054 ⁺ 0.002	0.0547	0.0545	0.0553	0.0547
12.7/3.6/4.0	0.0671 ⁺ 0.0028		0.0574	0.0574	0.0586	0.0579
12.7/3.6/7.2	0.0671 ⁺ 0.0021	0.059 ⁺ 0.003	0.0593	0.0596	0.0607	0.0603
12.7/4.4/0.0	0.0557 ⁺ 0.0014	0.053 ⁺ 0.002	0.0536	0.0534	0.0542	0.0533
12.7/4.4/7.2	0.0656 ⁺ 0.0016	0.056 ⁺ 0.002	0.0580	0.0574	0.0584	0.0580
11.0/3.6/0.0	0.0853 ⁺ 0.0027	0.084 ⁺ 0.003	0.0844	0.0841	0.0853	0.0856
11.0/3.6/1.4	0.0819 ⁺ 0.0029		0.0851	0.0847	0.0862	0.0865

Different spectral indexes are compared in Tables 4.5.20-4.5.23. The spectral index for position 1 is determined as the double ratio of activations $SI(N/M) = A_{n1}/A_{m1}$

$$A_{n1} = \int_0^{\infty} \sigma_n(E) \bar{\Phi}_1(E) dE / \int_0^{\infty} \sigma_n(E) \bar{\Phi}_{th}(E) dE$$

where N, M - detector materials, $\bar{\Phi}_1$, $\bar{\Phi}_{th}$ investigated and thermal column spectra.

Spectral indexes $SI(Pu/Dy)$ are compared in Table 4.5.20. This table demonstrates satisfactory agreement of measured and calculated values obtained with most codes. The maximum deviations for *MCU*, *NESSEL-4*, *RAFORIN*, and *UNIRASOS-2* do not exceed ~6%. The deviations of SI in the moderator calculated with these codes depend on fuel enrichment. They are negative for low enriched lattices and are reduced in absolute value with enrichment growth becoming positive (or practically zero) for 4.4% enriched lattices. The deviations of *BETTY-2* results are somewhat greater. This code systematically underestimates the considered spectral index for both detector positions.

Calculated and measured values of $SI(Mn/Dy)$ are given in Table 4.5.21. As it follows from this table *MCU*, *NESSEL-4*, *BETTY-2* and *RAFORIN* results satisfactory agree with measured data. The *UNIRASOS-2* results are significantly lower than measured value for both detector positions. The last is connected only with the simplified approach used in this code for Mn activation calculation in the resonance energy region.

Table 4.5.22 compares values of $SI(Pu/U)$. As in the previous cases the *MCU*, *RAFORIN* and *NESSEL-4* results are in satisfactory agreement with measured values. The *BETTY-2* systematically underpredicts the value of SI in the moderator by 3-9%. This code, like *UNIRASOS-2*, also noticeably underpredicts SI in the tighter pitch lattice.

Spectral indexes $SI(U/Dy)$ are given in Table 4.5.23. This table shows that all the codes give close values of SI which agree rather well with measured data. In this case the maximum deviations do not exceed ~3%, i.e. about twice greater than experimental error.

Table 4.5.20. Comparison of calculated and measured SI(Pu/Dy).

Lattice	P ^o s.	Measured value	Code name / calculated value				
			MCU	NES SEL4	UNIRA SOS2	BETTY 2	RAFO RIN
12.7/1.6/0.0	1	1.354 ⁺ 0.02	1.36 ⁺ 0.01	1.399	1.347	1.326	1.392
	2	1.387 ⁺ 0.02	1.34 ⁺ 0.01	1.375	1.317	1.294	1.348
12.7/1.6/1.85	1	1.390 ⁺ 0.02	1.39 ⁺ 0.02	1.425	1.372	1.347	1.419
	2	1.430 ⁺ 0.02	1.36 ⁺ 0.01	1.392	1.341	1.314	1.374
12.7/3.6/0.0	1	1.648 ⁺ 0.02	1.63 ⁺ 0.01	1.676	1.610	1.579	1.669
	2	1.568 ⁺ 0.02	1.55 ⁺ 0.01	1.598	1.529	1.493	1.565
12.7/3.6/7.2	1		1.72 ⁺ 0.01		1.700		1.765
	2		1.63 ⁺ 0.01		1.612		1.654
12.7/4.4/0.0	1	1.716 ⁺ 0.03	1.71 ⁺ 0.02	1.772	1.703		1.765
	2	1.548 ⁺ 0.03	1.61 ⁺ 0.02	1.673	1.599		1.635
12.7/4.4/7.2	1	1.901 ⁺ 0.03	1.80 ⁺ 0.01	1.863	1.791	1.765	1.858
	2	1.686 ⁺ 0.02	1.68 ⁺ 0.01	1.759	1.681	1.646	1.721
11.0/3.6/0.0	1		2.00 ⁺ 0.01		2.013		2.059
	2		1.90 ⁺ 0.01		1.906		1.939

Table 4.5.21. Comparison of calculated and measured SI(Mn/Dy)

Lattice	P ^o s.	Measured value	Code name / calculated value				
			MCU	NES SEL4	UNIRA SOS2	BETTY 2	RAFO RIN
12.7/1.6/0.0	1	1.195 ⁺ 0.016	1.17 ⁺ 0.01	1.193	1.119	1.196	1.218
	2	1.200 ⁺ 0.013	1.16 ⁺ 0.01	1.173	1.100	1.174	1.188
12.7/1.6/1.85	1	1.232 ⁺ 0.016	1.18 ⁺ 0.01	1.206	1.131	1.210	1.232
	2	1.166 ⁺ 0.013	1.16 ⁺ 0.01	1.185	1.112	1.186	1.202
12.7/3.6/0.0	1	1.419 ⁺ 0.019	1.35 ⁺ 0.01	1.371	1.283	1.364	1.408
	2	1.378 ⁺ 0.031	1.29 ⁺ 0.01	1.308	1.224	1.294	1.327
12.7/4.4/0.0	1	1.411 ⁺ 0.018	1.41 ⁺ 0.01	1.442	1.350	1.440	1.482
	2	1.406 ⁺ 0.018	1.34 ⁺ 0.01	1.357	1.271	1.347	1.372
12.7/4.4/7.2	1	1.533 ⁺ 0.021	1.47 ⁺ 0.01	1.500	1.412	1.498	1.556
	2	1.406 ⁺ 0.019	1.38 ⁺ 0.01	1.406	1.323	1.396	1.434

^o) Detector position:

1-detectors are situated in the fuel rod.

2-detectors are situated in the moderator.

Table 4.5.22 Comparison of calculated and measured SI(Pu/U).

Lattice	P o s.	Measured value	Code name / calculated value				
			MCU	NES SEL4	UNIRA SOS2	BETTY 2	RAFO RIN
12.7/1.6/0.0	1	1.298 ⁺ 0.014	1.283 ⁺ 0.01	1.312	1.287	1.241	1.294
	2	1.279 ⁺ 0.014	1.264 ⁺ 0.01	1.289	1.265	1.218	1.268
12.7/1.6/1.8	1	1.292 ⁺ 0.017	1.299 ⁺ 0.01	1.331	1.304	1.245	1.313
	2	1.290 ⁺ 0.017	1.283 ⁺ 0.01	1.299	1.283	1.232	1.287
12.7/3.6/0.0	1	1.491 ⁺ 0.092	1.455 ⁺ 0.01	1.483	1.444	1.418	1.470
	2	1.485 ⁺ 0.079	1.396 ⁺ 0.01	1.420	1.400	1.364	1.416
12.7/3.6/7.2	1	1.569 ⁺ 0.028	1.509 ⁺ 0.01	1.557	1.494	1.469	1.526
	2	1.456 ⁺ 0.025	1.455 ⁺ 0.01	1.489	1.451	1.414	1.472
12.7/4.4/0.0	1	1.489 ⁺ 0.011	1.500 ⁺ 0.01		1.490		1.524
	2	1.371 ⁺ 0.012	1.420 ⁺ 0.01		1.439		1.460
12.7/4.4/7.2	1	1.596 ⁺ 0.021		1.609	1.534	1.529	1.575
	2	1.522 ⁺ 0.018		1.528	1.486	1.464	1.512
11.0/3.6/0.0	1	1.703 ⁺ 0.017	1.626 ⁺ 0.01	1.706	1.608	1.585	1.664
	2	1.659 ⁺ 0.016	1.570 ⁺ 0.01	1.632	1.574	1.538	1.620
11.0/3.6/1.41	1	1.700 ⁺ 0.017		1.713	1.613	1.591	1.671
	2	1.619 ⁺ 0.019		1.639	1.579	1.545	1.628

Table 4.5.23. Comparison of calculated and measured SI(U/Dy).

Lattice	P o s.	Measured value	Code name / calculated value				
			MCU	NES SEL4	UNIRA SOS2	BETTY2	RAFO RIN
12.7/1.6/0.0	1	1.044 ⁺ 0.014	1.06 ⁺ 0.01	1.067	1.047	1.068	1.076
	2	1.085 ⁺ 0.014	1.06 ⁺ 0.01	1.067	1.041	1.063	1.064
12.7/1.6/1.8	1	1.076 ⁺ 0.018	1.07 ⁺ 0.02	1.071	1.053	1.082	1.081
	2	1.109 ⁺ 0.017	1.06 ⁺ 0.02	1.071	1.045	1.066	1.068
12.7/3.6/0.0	1	1.109 ⁺ 0.011	1.12 ⁺ 0.01	1.130	1.114	1.114	1.135
	2	1.098 ⁺ 0.011	1.11 ⁺ 0.01	1.126	1.092	1.095	1.105
12.7/4.4/0.0	1	1.153 ⁺ 0.016	1.14 ⁺ 0.02	1.140	1.143	1.135	1.158
	2	1.129 ⁺ 0.016	1.13 ⁺ 0.02	1.133	1.111	1.109	1.119
12.7/4.4/7.2	1	1.192 ⁺ 0.017	1.17 ⁺ 0.01	1.158	1.167	1.154	1.179
	2	1.108 ⁺ 0.017	1.14 ⁺ 0.01	1.151	1.131	1.124	1.137

*) Detector position:

- 1-detectors are situated in the fuel rod.
- 2-detectors are situated in the moderator.

Table 4.5.24. Comparison of calculated and measured disadvantage factors.

Lattice	Detector	Measured value	Code name / calculated value				
			MCU	NES SEL4	UNIRA SOS2	BETTY 2	RAFO RIN
12.7/1.6/0.0	U	1.154 ⁺ _{-0.01}	1.09 ⁺ _{-0.01}	1.116	1.106	1.122	1.117
	Pu	1.137 ⁺ _{-0.01}	1.08 ⁺ _{-0.01}	1.093	1.088	1.101	1.095
12.7/1.6/1.85	U	1.166 ⁺ _{-0.02}	1.11 ⁺ _{-0.01}	1.115	1.105	1.111	1.116
	Pu	1.164 ⁺ _{-0.01}	1.09 ⁺ _{-0.01}	1.092	1.087	1.100	1.093
12.7/3.6/0.0	U	1.217 ⁺ _{-0.01}	1.22 ⁺ _{-0.01}	1.206	1.183	1.213	1.201
	Pu	1.171 ⁺ _{-0.00}	1.17 ⁺ _{-0.01}	1.154	1.147	1.167	1.157
12.7/3.6/7.2	U	1.206 ⁺ _{-0.02}	1.20 ⁺ _{-0.02}	1.199	1.173	1.202	1.190
	Pu	1.119 ⁺ _{-0.03}	1.15 ⁺ _{-0.02}	1.147	1.139	1.158	1.148
12.7/4.4/0.0	U	1.195 ⁺ _{-0.01}	1.25 ⁺ _{-0.01}	1.238	1.208	1.241	1.230
	Pu	1.100 ⁺ _{-0.01}	1.19 ⁺ _{-0.01}	1.176	1.168	1.186	1.178
12.7/4.4/7.2	U	1.202 ⁺ _{-0.02}	1.24 ⁺ _{-0.01}	1.230	1.197	1.229	1.218
	Pu	1.147 ⁺ _{-0.01}	1.19 ⁺ _{-0.01}	1.168	1.159	1.176	1.168
11.0/3.6/0.0	U	1.143 ⁺ _{-0.01}	1.17 ⁺ _{-0.01}	1.170	1.138	1.159	1.149
	Pu	1.114 ⁺ _{-0.01}	1.13 ⁺ _{-0.01}	1.119	1.114	1.125	1.119
11.0/3.6/1.41	U	1.179 ⁺ _{-0.01}		1.168	1.137	1.158	1.148
	Pu	1.123 ⁺ _{-0.01}		1.118	1.113	1.124	1.118

Disadvantageous factors for uranium and plutonium detectors are compared in Table 4.5.24, which shows that agreement of calculated and measured disadvantageous factors for plutonium detector is worse than for an uranium detector. The deviations for this detector reach ~9%. At the same time all the calculated values including those obtained with MCU agree within the limits of ~3%. The last value correlates with the above described results from comparing spectral indexes, thereby showing that agreement of calculated and measured values for plutonium detectors is worse than for the uranium one.

A comparison of calculated and measured values of ρ^{28} and δ^{25} give information that is most important from the practical point of view concerning the accuracy of calculations of reaction rates produced by ^{235}U and ^{238}U . The interpretation of such measurements, as it has been already mentioned in Sect.4.5.3, is made difficult by uncertainties of cutoff energy and perturbations of neutron spectrum introduced by cadmium coat. So, in (Szatmary et al., 1985) instead of the mentioned parameters spectral indexes $\text{SI}(\text{Np/Dy})$ and $\text{SI}(\text{Ce/Dy})$ connected with ρ^{28} and δ^{25} by simple correlations are recommended for comparison.

Calculated and measured values of $\text{SI}(\text{Np/Dy})$ and $\text{SI}(\text{Ce/Dy})$ are compared in Tables 4.5.25-4.5.26.

It follows from Table 4.5.25 that the results of *NESSEL-4*, *RAFORIN* and *BETTY-2* satisfactorily agree between themselves. The scattering of calculated values is about 5%. Their comparison with measurement data shows that for all lattices disagreement is by a factor of 2-3 greater than the experimental error. The maximum deviations are ~10% in 4.4% enriched lattices. It is necessary to note that all codes give in this case the same sign of deviation. This deviation seems to be caused mainly by inaccuracy of ^{238}U resonance absorption calculation which, as has been shown in the previous sections, does not usually exceed ~3%. It thus seems difficult to give a reasonable explanation of the results obtained.

In conclusion let us note that a limited set of measurements unfortunately does not allow one to reveal any trends in disagreement behaviour.

Table 4.5.25 Comparison of calculated and measured
SI(Np/Dy).

Lattice	Measured value	Code / calculated value		
		<i>NESSEL-4</i>	<i>RAFORIN</i>	<i>BETTY-2</i>
12.7/1.6/0.0	2.544 ⁺ 0.040	2.423	2.521	2.521
12.7/3.6/0.0	4.014 ⁺ 0.064	3.785	3.938	4.023
12.7/4.4/0.0	4.331 ⁺ 0.107	4.494	4.514	4.580
12.7/4.4/7.2	5.434 ⁺ 0.134	4.975	5.028	5.058

Table 4.5.26 Comparison of calculated and measured
SI(Ce/Dy).

Lattice	Measured value	Code / calculated value		
		<i>NESSEL-4</i>	<i>RAFORIN</i>	<i>BETTY-2</i>
12.7/1.6/0.0	1.141 ⁺ 0.022	1.121	1.128	1.113
12.7/3.6/0.0	1.179 ⁺ 0.011	1.168	1.184	1.163
12.7/4.4/0.0	1.164 ⁺ 0.025	1.191	1.207	1.223
12.7/4.4/7.2	1.315 ⁺ 0.028	1.218	1.232	1.251

Calculated and measured $SI(Ce/Dy)$ are compared in Table 4.5.26. The table demonstrates good agreement for all lattices except to 12.7/4.4/7.2. In this case the spectral index is underpredicted by all codes.

Summarizing the results of comparison with measured data obtained at uniform ZR-6 configurations it seems possible to conclude that:

- there are trends of K_{eff} behaviour common for all codes; these trends are most probably due to inaccuracy of the bucklings used and the asymptotic approximation;
- accuracy of the calculational prediction of spectral characteristics can be considered as satisfactory in most cases;
- the results of 2D calculations which are considered in the following Chapters give information concerning the accuracy of calculational prediction of fuel lattices multiplication characteristics that is more objective and important from practical point of view.

4.5.5 Bucklings and reaction rate distributions in the macrocells of X_n and K91 type

The measurements at ZR-6 assembly can be divided into two groups. In the first group of measurements unperturbed lattices were investigated, in the second - perturbed. The results of these measurements treated by RFIT (Szatmary, 1977) are presented in Volume 1 and 3 of the Final Report of the TIC. The following types of lattice perturbations which are typical for WWER-1000 core were studied: perturbations caused by absorbers or water holes replacing the withdrawn absorbers and perturbations imitating assembly structure of the core. In the case of "point" perturbations every n^2 -th fuel rod is substituted by pointwise perturbation of type X (absorber or water hole). Corresponding cores may be considered as consisting of macrocell of type X_n . Six types of absorbers marked as $X=A, B, C, D, F, G$ have been studied. Water hole is marked as E. The material content and dimensions of absorber rods are given in Table 2.2.3 of Volume 1 of the Final Report of TIC. Lattices imitating assembly structure of the core are marked as K_m where m is a number of the fuel rods in the assembly.

In the previous section calculated and measured bucklings and rod by rod power distributions are compared for a case of regularly perturbed lattices containing macrocells. Consideration of such configurations is important for code verification. It is explained by the following reasons:

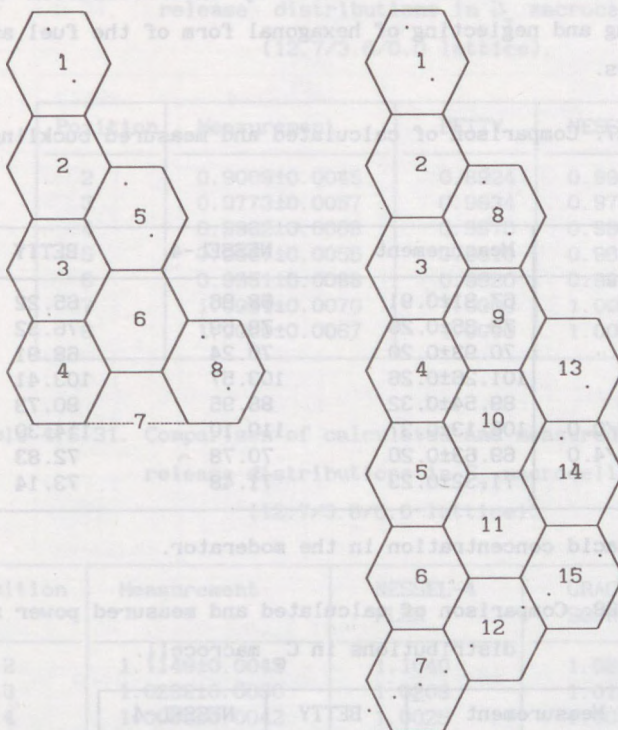
- the concept of macrocell is general basis of spectral calculations, so comparison of the results for the configurations formed by the macrocells provides a possibility to validate this concept in a "clean" conditions;
- the main types of nonuniform lattices typical for WWER-type reactors have been studied in the experiments at such configurations (absorbers or water holes, assembly structure).

The reaction rates distributions in the regularly perturbed lattices of X_n type, as well as in K91 type lattices imitating assembly structure, can be presented in a first approximation as the product of two functions:

- intra macrocell distribution which is periodical function;
- macrodistribution (Bardos, 1978, Gado, 1979).

Evaluated measured bucklings and intra macrocell distribution of reaction rates can be directly compared with the results of macrocell calculations based on asymptotic approximation. The comparison of measured and calculated data obtained with NESSEL-4 and BETTY are given in Tables 4.5.27-33. Numbering of the cells in the macrocells of X_7 and X_3 type is

illustrated by the figure.



The results given in these tables make it possible to conclude that:

1. The most part of bucklings calculated with NESSEL-4 (with the exception of bucklings for K91/0.0 and 12.7/3.6/0.0 lattices) are in a good agreement with measured one (see Table 4.5.27). The BETTY results agree with measurements slightly worse. In this case the maximum deviation achieves 3.5%.

2. The reaction rates in the fuel rods situated in the asymptotic region of macrocells of X_n and K91 type calculated with NESSEL-4 and BETTY are in the main in a good agreement with measured ones. Marked disagreements of the reaction rates is observed only for the fuel rods situated near perturbations and the boundary of the fuel assembly:

- the deviations of reaction rates obtained with NESSEL-4 and BETTY for E_n lattices achieve 1.5% and 3.0%, respectively;
- the deviations for the fuel rods situated near strong absorbers (B_4C and Eu_2O_3) are less and do not exceed 1% for both codes;
- underestimation of reaction rates up to 6-7% is observed for the fuel

rods situated near water gap in the configuration modeling fuel assembly structure. This underestimation is caused by underestimation of neutron spectrum softening and neglecting of hexagonal form of the fuel assembly in the spectral codes.

Table 4.5.27. Comparison of calculated and measured bucklings.

Lattice	Measurement	NESSEL-4	BETTY
F-7/1.8 *	67.91±0.91	68.96	65.22
F-7/0.0	78.35±0.20	79.59	76.32
D-7	70.93±0.20	70.24	68.91
E-7/0.0	101.26±0.26	103.57	103.41
E-7/1.8	89.54±0.32	88.95	90.73
K91/H ₂ O/0.0	106.13±0.37	110.10	114.30
K91/H ₂ O/4.0	69.63±0.20	70.78	72.83
C-5	71.32±0.23	71.48	73.14

* - boron acid concentration in the moderator.

Table 4.5.28. Comparison of calculated and measured power release distributions in C₅ macrocell.

Position	Measurement	BETTY	NESSEL-4
2	0.9187±0.0037	0.9401	0.9338
3	0.9961±0.0045	0.9946	0.9938
4	0.9880±0.0036	0.9871	0.9867
5	1.0000±0.0043	1.0000	1.0000

Table 4.5.29. Comparison of calculated and measured power release distributions in E₃ macrocell.

Pozition	Measurement	BETTY	NESSEL-4
2	1.0046±0.0039	1.0262	1.0386
3	1.0000±0.0043	1.0000	1.0000

Table 4.5.30. Comparison of calculated and measured power release distributions in D_7 macrocell (12.7/3.6/0.0 lattice).

Pozition	Measurement	BETTY	NESSEL-4
2	0.9009±0.0045	0.8924	0.8941
3	0.9773±0.0057	0.9634	0.9734
4	0.9962±0.0068	0.9970	0.9967
5	0.9667±0.0055	0.9610	0.9601
6	0.9951±0.0088	0.9920	0.9910
7	1.0051±0.0070	1.0003	1.0002
8	1.0000±0.0067	1.0000	1.0000

Table 4.5.31. Comparison of calculated and measured power release distributions in E_7 macrocell (12.7/3.6/0.0 lattice).

Pozition	Measurement	NESSEL-4 FLEX	GRACE SOPHIE
2	1.1149±0.0045	1.1040	1.0893
3	1.0232±0.0050	1.0209	1.0199
4	1.0062±0.0042	1.0025	1.0023
5	1.0339±0.0052	1.0315	1.0308
6	-	1.0064	1.0065
7	1.0150±0.0045	0.9998	0.9998
8	1.0000±0.0051	1.0000	1.0000

Table 4.5.32. Comparison of calculated and measured power release distributions in E_7 macrocell (12.7/3.6/1.8 lattice).

Pozition	Measurement	NESSEL-4 FLEX	GRACE SOPHIE
2	1.1161±0.0030	1.1014	1.0849
3	1.0317±0.0037	1.0203	1.0189
4	1.0158±0.0043	1.0022	1.0022
5	1.0366±0.0051	1.0292	1.0319
6	1.0256±0.0054	1.0060	1.0060
7	1.0127±0.0030	0.9999	0.9998
8	1.0000±0.0047	1.0000	1.0000

Table 4.5.33. Comparison of calculated and measured power release distributions in 12.7/3.6-K91-4.0 macrocell.

Pozition	Measurement	NESSEL-4	BETTY
1	1.0000±0.0080	1.0000	1.0000
2	1.0171±0.0077	1.0076	1.0065
3	1.0467±0.0082	1.0322	1.0324
4	1.0965±0.0086	1.0874	1.0934
5	1.2306±0.0094	1.2539	1.2606
6	1.5398±0.0079	1.5985	1.6954
7	-	-	-
8	1.0346±0.0067	1.0246	1.0229
9	1.0804±0.0075	1.0662	1.0660
10	1.1717±0.0080	1.1784	1.1869
11	1.4154±0.0068	1.4592	1.4889
12	-	-	-
13	1.1668±0.0082	1.1584	1.1700
14	1.3866±0.0065	1.3658	1.4077
15	-	-	-
16	-	-	-

Microparameters in macrocells Disadvantage factors $\delta_{H_2O}^x$, spectral indexes $SI \begin{pmatrix} x \\ y \end{pmatrix}$ and $R \begin{pmatrix} Np \\ Dy \end{pmatrix}$, $R \begin{pmatrix} Ce \\ Dy \end{pmatrix}$ values are compared in Tables 4.5.34-37 for different position of the detectors in the macrocell. These results are discussed in detail in (Maiorov and Yudkevich, 1988, Szatmary, 1977, Becker, 1988, Bardos, 1978)). The main conclusions made in these reports are given below.

There is about 20% disagreement between measured and calculated with all design spectral codes and MCU disadvantage factors in the absorber cell in the macrocell D_7 (see Tables 4.5.35-36). Observed disagreements are so big that one can doubt in the reliability of experimental data or their treatment (correction for the foils etc.).

In the case of E_7 macrocell the results of calculations obtained with all the codes are in a good agreement with the measurements for all the detectors positions with the exception of central. The difference between calculated and measured values does not exceed 3%. The measured values for the central position are obviously erroneous.

The agreement of the most part of the microparameters measured in the fuel rods situated in different positions in the macrocells can be

estimated as satisfactory.

Table 4.5.34. Comparison of epithermal parameters $R_{\text{Dy}}^{\text{Np}}$, $R_{\text{Dy}}^{\text{Ce}}$.

Position	Code	$R_{\text{Dy}}^{\text{Np}}$		$R_{\text{Dy}}^{\text{Ce}}$	
		F-7	E-7B	F-7	E-7B
1	Measur.	4.288±0.087	3.810±0.067	1.079±0.025	1.107±0.018
	BETTY	4.430	3.850	1.184	1.151
	NESSEL4	4.286	3.767	1.184	1.156
2	Measur.	3.961±0.071	3.931±0.067	1.064±0.018	1.088±0.017
	BETTY	4.172	4.035	1.170	1.161
	NESSEL4	4.058	3.986	1.171	1.168
3	Measur.	3.999±0.074	4.035±0.068	1.096±0.021	1.146±0.017
	BETTY	4.092	4.098	1.166	1.165
	NESSEL4	3.984	3.997	1.167	1.169
Asymp.	Measur.	4.014±0.064	-	1.179±0.011	-
	BETTY	4.036	4.138	1.163	1.167
	NESSEL4	3.896	-	1.160	1.165

Table 4.5.35. Disadvantage factors for ^{235}U detector.

Lattice	Code	Position		
		0	1	2
D-7	Measurement	4.59±0.21	1.230±0.013	1.208±0.014
	BETTY	6.908	1.235	1.236
	NESSEL4	7.89	1.182	1.183
	MCU	7.71	1.21	1.20
	CASHE	6.38	1.189	1.190
	THERMOS	8.105	1.320	1.313
E-7	Measurement	1.210±0.012	1.236±0.014	1.197±0.016
	BETTY	0.847	1.239	1.237
	NESSEL4	0.929	1.190	1.186
	MCU	0.90	1.21	1.217
	CASHE	0.913	1.193	1.192
	THERMOS	0.900	1.303	1.306
F-7	Measurement	4.59±0.15	1.217±0.011	-
	BETTY	4.637	1.235	-
	NESSEL4	4.90		
	MCU	5.0		

Table 4.5.36. Disadvantage factors for ^{239}Pu detector.

Lattice	Code	Position		
		0	1	2
D-7	Measurement	4.55±0.18	1.176±0.01	1.160±0.011
	BETTY	8.462	1.156	1.151
	NESSEL4	9.60	1.140	1.143
	MCU	9.52	1.15	1.15
	CASHE	8.03	1.152	1.152
	THERMOS	10.09	1.158	1.158
E-7	Measurement	1.285±0.011	1.160±0.012	1.158±0.013
	BETTY	0.863	1.163	1.161
	NESSEL4	0.945	1.149	1.144
	MCU	0.91	1.16	1.168
	CASHE	0.930	1.154	1.153
	THERMOS	0.921	1.163	1.160
F-7	Measurement	5.91±0.19	1.175±0.008	-
	BETTY	5.820	1.157	-
	NESSEL4	6.22		
	MCU			

Table 4.5.37. Comparison of SI(Pu/U).

L a t t. t.	Code	Position of the cell / detectors			
		0		1	
		Absorber	H ₂ O	UO ₂	H ₂ O
D-7	Measur.	1.483±0.069	1.472±0.018	1.471±0.016	1.413±0.015
	BETTY	1.075	1.320	1.421	1.331
	CASMO-HEX	1.11	1.393	1.425	1.380
	NESSEL4	1.209	1.474	1.503	1.450
	MCU	1.15	1.43	1.48	1.41
	THERMOS	1.092		1.553	
E-7	Measur.	1.255±0.011	1.334±0.013	1.465±0.017	1.374±0.014
	BETTY	1.187	1.209	1.440	1.353
	CASMO-HEX	1.283	1.307	1.389	1.343
	NESSEL4	1.338	1.360	1.450	1.399
	MCU	1.29	1.31	1.42	1.39
	THERMOS	1.237		1.497	
F-7	Measur.	1.292±0.058	1.666±0.018	1.511±0.012	1.458±0.12
	BETTY	1.142	1.433	1.423	1.334
	CASMO-HEX				
	NESSEL4	1.179	1.496		
	MCU	1.20			
	THERMOS				

Table 4.5.37. (Continued)

L a t t i c e	Code	Position of the cell/detec.	
		2	
		UO ₂	H ₂ O
D-7	Measur.	1.487±0.015	1.422±0.014
	BETTY	1.428	1.339
	CASMO-HEX	1.421	1.375
	NESSEL4	1.488	1.434
	MCU	1.466	-
	THERMOS	1.553	-
E-7		1.487±0.019	1.438±0.01
	BETTY	1.436	1.347
	CASMO-HEX	1.409	1.363
	NESSEL4	1.480	1.428
	MCU	-	-
	THERMOS	1.521	-

4.5.6 Analysis of depletion experiments

Comparison of calculated and measured isotopic composition of spent fuel is the final stage in the validation efforts. Such a comparison gives information about code accuracy in reference to conditions of real power operation.

Data of isotopic compositions measurements, as a rule, are more difficult to interpret in comparison with data of criticals. There are many reasons for this: possible uncertainty of some parameters (The UO_2 temperature, for example), possible influence of operation history on isotopic composition, relatively low accuracy of some isotopes measurements and so on.

Two series of depletion experiments were treated within the framework of TIC activities - measurements performed with fuel of reactors of WWER-440 type (Zelenkov *et al*, 1981) and the YANKEE reactor (Nodvic, 1969). Destructive analysis of WWER-440 spent fuel were performed for fuel pellets removed from regions with both asymptotic and nonasymptotic neutron spectra. The last case requires the use of codes which allow the real geometry of the fuel assembly to be modelled taking into account its nearest environment.

The measurements described in (Nodvic, 1969) are characterized by choosing fuel pellets from regions with asymptotic spectrum, a great number of investigated samples, and the performing of independent measurements in a various laboratories. The detailed analysis of series of measurements were carried out with NESSEL-4 is described in (Heinrich, 1986).

Calculations of spent fuel isotopic composition are usually carried out for a fuel cell or fuel assembly configurations using the fuel lattice characteristics averaged over the time (T_{UO_2} , $\gamma_{\text{H}_2\text{O}}$, power density and so on) under the supposition that taking into account of their real time dependence practically does not influence the calculation results.

The validity of this approach was studied by Heinrich (KKAB Berlin). This question is also considered in (Becker, 1983) where problems of fuel temperature uncertainty and accuracy of neutron spectrum modelling in the investigated samples are investigated.

Similar investigations related to measurements with WWER-440 spent fuel were performed in the Kurchatov Institute (Moscow). The calculations were carried out with the use of the codes: UNIRASOS-2, BIPR-7 (3D

coarse-mesh simulator), PERMAK (2D fine-mesh simulator) (Novikov et al., 1989). BIPR-7 and PERMAK were used for imitation of investigated assembly real operation history and computation of power density, water density, fast to thermal flux ratio, moderator temperature at the positions of removed fuel rod samples. The obtained values of the above listed parameters as a function of time were then input into UNIRASOS-2 to calculate the isotopic composition of the samples.

Calculations have shown that a detailed modelling of operation history lead to a marked change of the results compared with those obtained by the simplest way (calculation of isolated fuel assembly with average parameters). For example, ^{235}U number density in the sample from asymptotic region was changed by 2-2.5%. This result agrees well with the conclusions in (Becker, 1983). The last allows one to infer that comparison of calculated and measured data for WWER-440 spent fuel should be performed under detailed modelling of real burnup conditions.

In this connection a procedure of interpretation of the measurements described in (Nodvik, 1969) seems more simple because it allows one to be limited by carrying out the uniform lattice calculations. An important advantage of these measurements is also the great number of investigated samples which provides a possibility of statistical treatment of the results.

Before discussing of calculated and measured data comparison it is worth noting that NESSEL-4 results are given in (Becker, 1983) mainly in graphic form that does not allow them to be directly included into the consideration. Therefore we limit ourselves by their qualitative description.

Figures 4.13-4.15 compare calculated values of uranium and plutonium isotopes number densities obtained with UNIRASOS-2, RAFORIN, BETTY-2 with the measured ones. Measurement data were treated by statistical methods and are presented in the form of expected value and confidence intervals. An algorithm of statistical treatment and its results are given in (Spoden and Moltzan, 1990).

It should be noted that in order to avoid uncertainties connected with experimental errors the others parameters are very often used instead of burnup as a characteristic of irradiation time.

For example, it is suggested that parameter τ determined as

$$\tau = \frac{\ln N^8}{\ln N^5} - \frac{\ln N_0^8}{\ln N_0^5}$$

be used in (Heinrich, 1986).

Here $N^{5,8}$, $N_0^{5,8}$ are ^{235}U , ^{238}U nuclear densities at the arbitrary and zero burnup points.

Calculations have shown that use of this parameter does not lead to essential change of discrepancies between calculated and measured number densities.

The number densities of ^{235}U and ^{236}U are compared in Fig.4.13. This figure demonstrates good agreement of *RAFORIN* and *BETTY-2* results with measured data. Both codes tend to slightly underprediction of ^{235}U density with burnup growth. The *UNIRASOS-2* slightly underpredicts number density of ^{235}U in a whole burnup interval. The difference between the *UNIRASOS-2* and *RAFORIN* results may be explained in two ways, viz.: different thermalization models used in these codes and some differences in approximations used for calculations in the resonance energy range.

$$\gamma = \frac{\ln N_0^{235}}{\ln N_0^{236}} \quad \text{UNIRASOS-2, BIPY-7 (3D)}$$

fig4-13

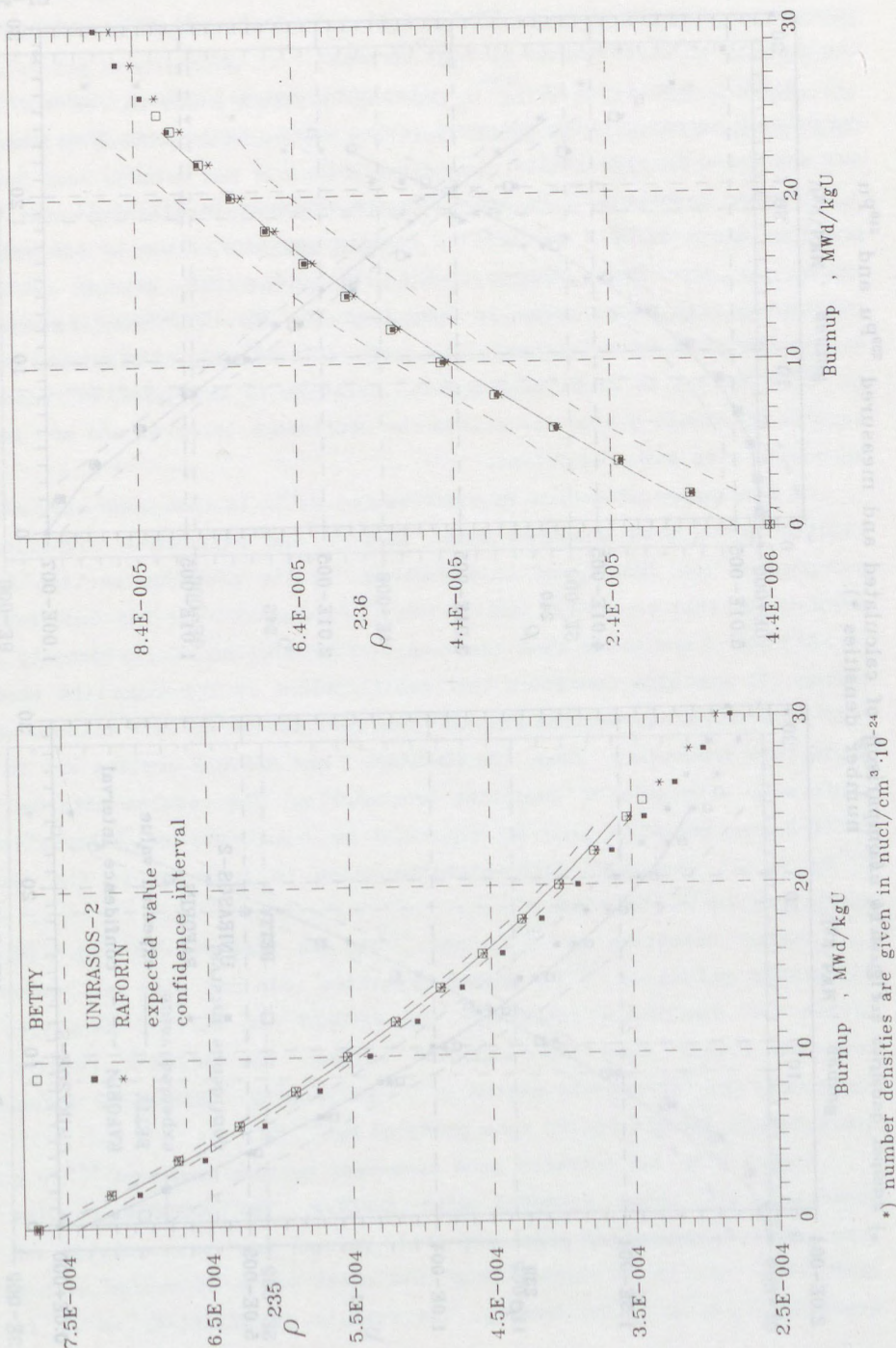
Fig. 4.13 Comparison of calculated and measured ^{235}U and ^{236}U number densities *).*) number densities are given in $\text{nucl}/\text{cm}^3 \cdot 10^{-24}$

fig4-14

Fig. 4.14 Comparison of calculated and measured ^{239}Pu and ^{240}Pu number densities *).

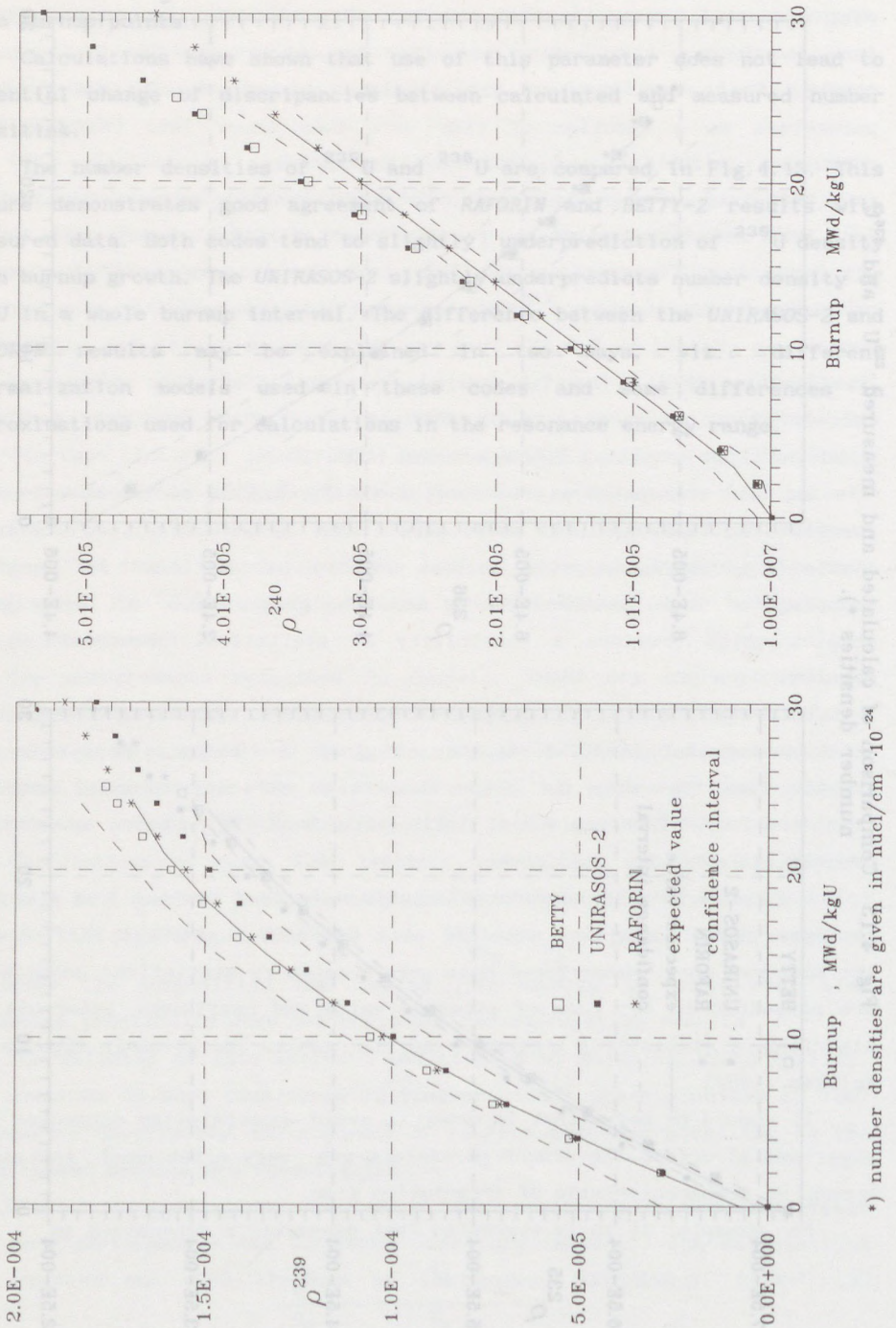
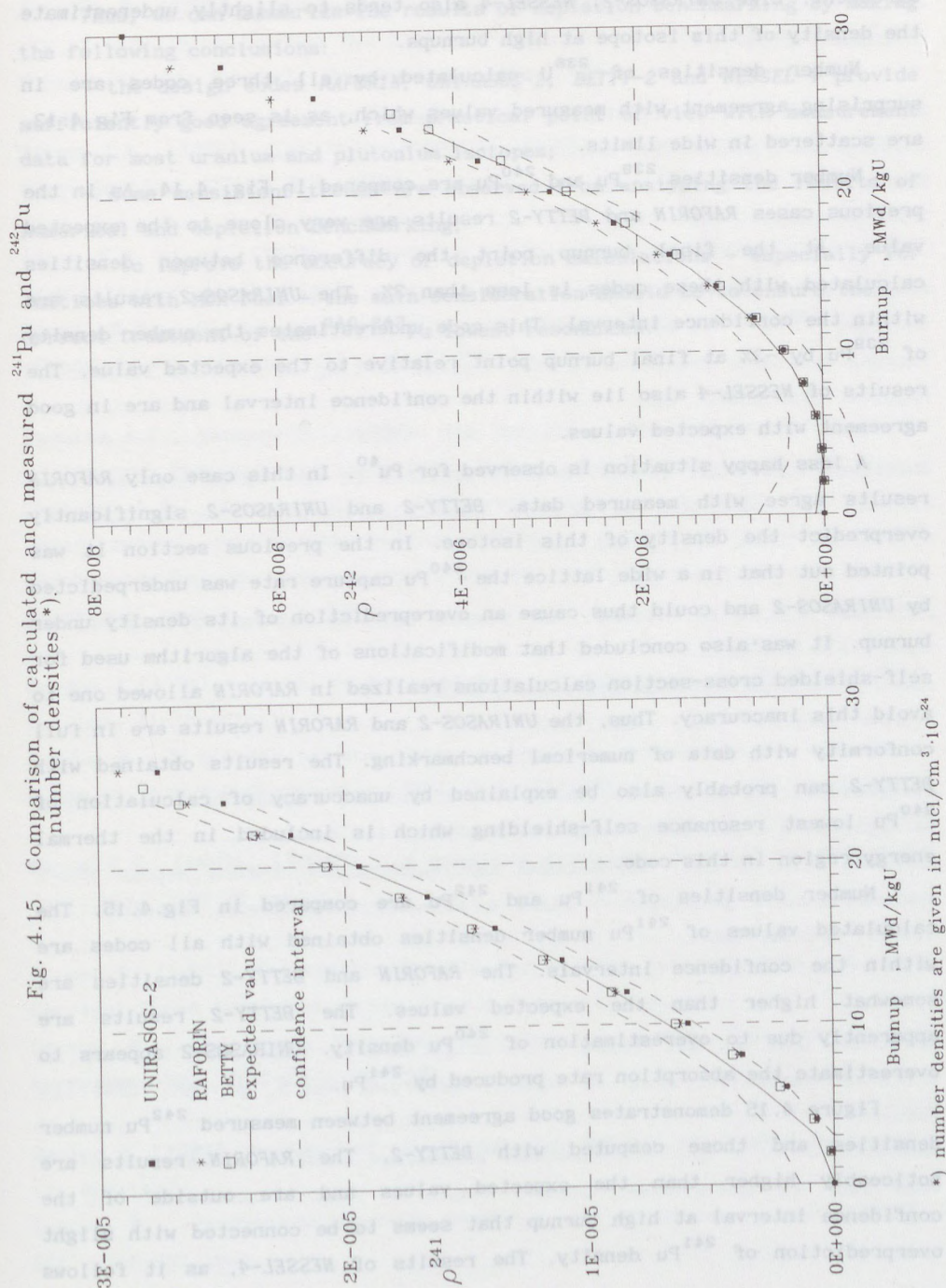


fig4-15



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Comparison of ^{235}U number densities at 24 Mwd/kgU burnup point obtained with *BETTY-2*, *RAFORIN* and *NESSEL-4* shows that they are in good agreement. Like *UNIRASOS-2*, *NESSEL-4* also tends to slightly underestimate the density of this isotope at high burnups.

Number densities of ^{238}U calculated by all three codes are in surprising agreement with measured values which, as is seen from Fig 4.13, are scattered in wide limits.

Number densities ^{239}Pu and ^{240}Pu are compared in Fig. 4.14. As in the previous cases *RAFORIN* and *BETTY-2* results are very close to the expected value. At the final burnup point the difference between densities calculated with these codes is less than 3%. The *UNIRASOS-2* results are within the confidence interval. This code underestimates the number density of ^{239}Pu by ~3% at final burnup point relative to the expected value. The results of *NESSEL-4* also lie within the confidence interval and are in good agreement with expected values.

A less happy situation is observed for Pu^{40} . In this case only *RAFORIN* results agree with measured data. *BETTY-2* and *UNIRASOS-2* significantly overpredict the density of this isotope. In the previous section it was pointed out that in a wide lattice the ^{240}Pu capture rate was underpredicted by *UNIRASOS-2* and could thus cause an overprediction of its density under burnup. It was also concluded that modifications of the algorithm used for self-shielded cross-section calculations realized in *RAFORIN* allowed one to avoid this inaccuracy. Thus, the *UNIRASOS-2* and *RAFORIN* results are in full conformity with data of numerical benchmarking. The results obtained with *BETTY-2* can probably also be explained by unaccuracy of calculation of ^{240}Pu lowest resonance self-shielding which is included in the thermal energy region in this code.

Number densities of ^{241}Pu and ^{242}Pu are compared in Fig. 4.15. The calculated values of ^{241}Pu number densities obtained with all codes are within the confidence intervals. The *RAFORIN* and *BETTY-2* densities are somewhat higher than the expected values. The *BETTY-2* results are apparently due to overestimation of ^{240}Pu density. *UNIRASOS-2* appears to overestimate the absorption rate produced by ^{241}Pu .

Figure 4.15 demonstrates good agreement between measured ^{242}Pu number densities and those computed with *BETTY-2*. The *RAFORIN* results are noticeably higher than the expected values and are outside of the confidence interval at high burnup that seems to be connected with slight overprediction of ^{241}Pu density. The results of *NESSEL-4*, as it follows

from (Becker, 1983), are in sufficient agreement with measurements for both isotopes.

Thus, we can summarize the results of depletion benchmarking by making the following conclusions:

- the design codes RAFORIN, UNIRASOS-2, BETTY-2 and NESSEL-4 provide sufficiently good agreement from practical point of view with measurement data for most uranium and plutonium isotopes;
- some consistent trends are observed from analysing the results of numerical and depletion benchmarking;
- to improve the accuracy of depletion calculations - especially for lattices with MOX fuel - the main consideration should be to ensure the correct treatment of the $^{240,242}\text{Pu}$ lowest resonances.

- Abagian L.P. et al. (1964).** Group Constants for Nuclear Reactor Calculations. (in Russian).
Абагян Л.П.: и др. Групповые константы для расчета ядерных реакторов. М., Атомиздат, 1964.
- Abagian L.P. et al. (1981).** Group Constants for Reactors and Shielding Calculations. Москва. (in Russian).
Абагян Л.П.: и др. Групповые константы для расчета реакторов и защиты. М., Энергоатомиздат, 1981.
- Abagian L.P., Gomin E.A., Yudkevich M.S. (1992).** Evaluation of constants of isotopes ^{239}Pu - ^{242}Pu and their Verification Conform to the Calculations of Thermal Reactors. Presented to 1992 Topical Meeting on Advances in Reactor Physics. Charleston, USA.
- Abdullaev X.S. et al. (1968).** Neutron spectrum in two-region graphite-water system. (In Russian). In Neutron Thermalization and Reactor Spectra. V.I. Vienna, IAEA, v.1, p.233, 1968.
- Abdullaev X.S. et al. (1969).** The thermal neutron relaxation lengths for water. (In Russian).
Длины релаксации тепловых нейтронов в воде.
Атомная энергия, т.26, с.538, 1969.
- Alekseev N.I. et al. (1991).** Validation of the MCU-1 Cross Sections Library as Applied to Light Water Moderated Reactors. (in Russian).
Алексеев Н.И., и др.: Верификация константного обеспечения версии MCU-1 применительно к реакторам с водой в качестве замедлителя. Препринт ИАЭ 5407/5, Москва. 1991.
- Andrianov G.I. et al. (1964).** Investigations of WWER Core Physics at Critical Assemblies. Proc. of Symp., Amsterdam, Vol.3, p. 355, 1964 (in Russian).
Андрианов Г.Я. и др.: Исследования физических свойств активной зоны ВВЭР на критических сборках. Proc. of Symp., Amsterdam,

Vol.3, p. 355, 1964.

Antilla M. (1989). Finish Results for a VMK Benchmark Problem Concerning Use of Gadolinium in Fuel Rod Lattices. Material of IAEA CRP on Safe Core Management with Burnable Absorbers in WWERS. 1989.

Askew J.R. (1966). The calculation of resonance captures in few-group approximation. AEEW-R 489, 1966.

Azova V.M. et al. (1984). Comparison of Calculated and Measured Data for ZR-6 Lattices. (in Russian).

Азова В.М.: Обсчет экспериментов на сборке ZR-6. Рабочий материал объединенного заседания III и IV ТГ ВМК, Варшава, 1984 г.

Badalov A.F., Kononov S.L. (1988). The Results of Monte-Carlo Calculations of Integral Parameters of Light Water Moderated Lattices. (in Russian).

Бадалов А.Ф., Кононов С.Л.: Результаты расчетов методом Монте-Карло характеристик легководных решеток ТВЭЛов с различным водо-топливным отношением. Вопросы атомной науки и техники, Сер. "Физика и техника ядерных реакторов", вып.3, с.24, 1988.

Bardos J (1978) Analysis of Measured Power Distributions in Perturbed ZR-6 Lattices (in Russian).

Бардош Й.: К вопросу анализа экспериментальных результатов по нейтронным полям на возмущенных решетках. KFKI-ZR-6-412/1978.

Barry R.F. (1963). LEOPARD - a spectrum dependent non-spatial depletion code. WCAP-3269-29 report.

Becker R. (1981). Calculation Results for Uniform Lattices obtained using Spectral Codes Available within TIC (in Russian).

Беккер Р.: Результаты расчетов невозмущенных решеток по спектральным программам ВМК. KFKI-ZR-6-533/1981

Becker R. (1983): Analysis of the Calculation Results for YANKEE Benchmark (in Russian).

Беккер Р.: Результаты анализа расчетов по модельной задаче YANKEE. KFKI-ZR-6-537/1983.

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Becker R., L. Almerot L. (1984). Comparison of Calculated and Measured Data for ZR-6 Unperturbed Lattices. (in Russian).

Беккер Р., Альмерот Л.: Результаты обчета невозмущенных решеток критсборок ZR-6. Материалы XIII-го симпозиума ВМК, Румыния, Куртя де Арджеш, 1984 г.

Becker R. (1987). Preliminary Analysis of Measured and Calculated Data for Regularily Perturbed ZR-6 Lattices of X-7 Type. (in Russian).

Беккер Р.: Первый анализ расчетов и экспериментов для регулярно-возмущенных решеток типа X-7 (Отчет рабочей группы М), Материалы XVI-го симпозиума ВМК, Москва, Том 1, с. 287, 1987.

Becker R. (1988). On the Activity of Working Group "M" During 1986-88 Years (in Russian).

Беккер Р.: О деятельности рабочей группы М в течение 1986-88 годов (Заключительный отчет рабочей группы М). Материалы XVII-го симпозиума ВМК, Варна.

Becker R. (1988). Results of Calculations of Uniform Lattices using Spectral, Diffusion and Transport Codes. Report KFKI-ZR-6-554/1988 (in Russian).

Р.Беккер: Обчет критических измерений для невозмущенных решеток со спектральными, диффузионными и кинетическими программами. KFKI-ZR-6-554/1988.

Becker R. (1988). Methods Used for Calculations of Wigner-Zeitz Cells in NESSEL-IV. KFKI-ZR-6-555/1988 (in Russian).

Р.Беккер: Описание метода расчета для ячеек типа Вигнера-Зейца по программе NESSEL-IV. KFKI-ZR-6-555/1988.

Becker R., Pshenin V.V., Lazarenko A.P. et al.(1988). Results of Spectral Codes Verification using Numerical and Experimental Benchmarks. Kernenergie Vol. 33, p.8, 1990.

Becker R. (1990). GDR Calculation Results of Gadolinium Fuel-Pin Lattices. Material of IAEA CRP on Safe Core Management with Burnable Absorbers in WWRs. 1990.

Bell J.I. (1959). Theory of effective cross sections. LA-2322, 1959.

Benoist P. (1964). Theorie du coefficient de diffusion des neutrons dans un reseau comportant des cavites. Report CEA R 2278.

Bernoceli E., Martinelly R. (1977). Light Water Lattice Data. Report NEACRP-U-190.

Bogachev G.A., Sidorenko V.D. (1975). Comparison of Different Thermalization Models. (in Russian).

Богачев Г.А., Сидоренко В.Д.: Сравнение некоторых моделей термализации нейтронов в ячейках реакторов. Материалы IV Симпозиума ВМК, Фрунзе с. 343, 1975.

Bohl H. and Hemphill A.P. (1961). MUFT-5 - A Fast Neutron Spectrum Program for Philco-2000. WAPD-TM-218.

Bohme R. et al. (1992). Improvements in the Prediction of LWHCR Lattice Parameters. IAEA-TECDOC-638, p. 205.

Bonalumi R. (1961). Neutron first collision probabilities in reactor physics. Energia Nucleare. 8,326.

Bondarenko J.J. Ed. (1964) Group constants for Nuclear reactor calculations. Consultants Bureau. New York.

Broeders C.H.M. (1992). Development of Calculational Procedures for the Neutron Physics Design of Advanced Reactor. IAEA-TECDOC-638, p. 163, 1992.

Cadilhac N. (1963). Methodes theoriques pour l'etude de la thermalization des neutrons dans les milieux absorbents infiniset homogènes. Rapport CEA R 2368, 1963.

Carlvic I. (1966). Nucleonik. 8,226.

Chawla R. et al. (1984). Reactivity and Reaction Rate Ratio Changes with Moderator Voidage in a Light Water High Converter Reactor Lattice. Nucl. Techn. V.67, p.360.

Consultants Report on Proposed Program for the Co-ordinated Research

Programme on Safe Core Management with Burnable Absorbers in WWERs. MJC/hp/8276, 1988.

Dancoff S.M., Ginsburg M. (1944). Surface resonance absorption in a close-packed lattice. CP-2157.

Deniz V.C. (1986). The theory of neutron leakage in reactor lattices. CRC -handbook of Nuclear Reactors Calculations. V.2, p.409. CRC Press Inc., 1986.

Devenyi A. (1978). The code ANICELL. 1985. KFKI-ZR-6-71/1978.

Edenius M., Ahlin A. (1987). CASMO-3: New Features, Benchmarking and Advanced Application. Proc. of Int. Conf., Paris.

Eremeev E.P. et al. (1968): Neutron Thermalization and Reactor Spectra. Vienna, IAEA, v.1, p.343. (in Russian).

Еремеев И.П. и др.: Neutron Thermalization and Reactor Spectra. V.I.Vienna, IAEA, p.343, 1968.

Fisher J.R. (1989). Evaluation of Assembly Cross Section Generator Code Discrepancies. IAEA-TECDOC-567, p. 293.

Fisher J.R. (1989). Evaluation of Cross Section Generator Code Differences Assembly Analysis. IAEA-TECDOC-567, p. 299.

Gado J., Szatmary.Z, Elwakil E. (1978) Report KFKI-ZR-6-48/1978.

Gado J. et al. (1977). The Interpretation of Measured Data for the Lattices Regularily Perturbed by Water Holes and Absorbers. (in Russian).

Гадо Я.и др.: Интерпретация экспериментов: решетки, регулярно возмущенные с ПЭЛами или водяными дырками. Материалы VI-го Симпозиума ВМК, Бухарест, с. 159, 1977.

Gado J. (1978). The pin cell burnup code BETTY. KFKI-ZR-6-35/1978.

Gado J. (1979). Simplified Model of Neutron Flux Distribution in the Lattices of Xn and K91 Type. (in Russian).

Гадо Я.: Упрощенная модель распределения нейтронного потока в решетках Xn и K91. Материалы VIII-го симпозиума ВМК, Зегжинек-Ядвизин, Том 1, 1979.

Gado J. (1980). Calculation of Neutron Thermalization in the Elementary Cell. (in Russian).

Гадо Я.: Расчет термализации в элементарной ячейке. Материалы IX Симпозиума ВМК, Нойбранденбург, Том 2, 1980.

Gado J. (1985). Comparison of Different Methods for Calculation of Neutron Transport Kernel. KFKI-ZR-6-542/1985 (in Russian).

Я.Гадо. Сопоставление результатов разных методов для расчета ядра переноса. KFKI-ZR-6-542/1985.

Gado J., Kerezturi A. (1986). Multigroup Transport Calculations of the Cells of Infinite Lattices. KFKI-ZR-6-544/1986 (in Russian).

Я. Гадо, А. Керестури. Многогрупповые кинетические расчеты для ячейки бесконечных топливных решеток. KFKI-ZR-6-544/1986.

Gado J., Alvarez K. (1986). Report of Working Group "B" on Elaboration of Benchmarks on a Basis of Results of Measurements at ZR-6. (in Russian).

Гадо Я., Альварез К.: Отчет рабочей группы "В" о переработке результатов измерений ZR-6 в тестовые задачи, Материалы 15-го Симпозиума ВМК, Росток, Том 1, с.28, 1986.

Gado J., Kerezturi A. I.Trostel (1990). TUC Program System KARATE. Report presented at Specialists Meeting on Advanced Calculation Methods for Power Reactors. Cadarache. France. September, 1990.

Gado J., Szatmari Z., Vidovszky I.: Editors. Alvarez et al. (1991). Experimental Investigations of the Physical Properties of WWER-type Uranium-Water Lattices. Final Report of TIC, Vol.3, Budapest.

Goldstein R. (1972) Doppler broadened intermediate resonances. TANS.15, p.291.

Gomin E.A., Majorov L.V.(1982). TERMAC - Code Package for Calculations of Group Cross Sections in the Thermalization Energy Range. (in Russian).

Гомин Е.А., Майоров Л.В.: Комплекс TERMAC для расчета групповых сечений нейтронов в области термализации. Физика и техника ядерных реакторов.

CHAPTER 4

Вып. 5(27), с. 70, 1982.

Gomin E.A., Majorov L.V. Yudkevich M.S. (1991). Some Aspects of Monte-Carlo Method Application to Nuclear Reactors Analysis. Prog. in Nucl. Ener. V 24, N 1-3, p. 211, 1991.

Hellstrand E. (1957). Measurements of the Effective Resonance Integral in Uranium Metal and Oxide in Different Geometries. J. Appl. Phys. Vol. 28, p. 1493, 1957.

Hellstrand E. (1966). Proc. of the National Topical Meeting of ANS. San Diego. V.2, 151.

Heinrich H. (1981) Das Programme NESSEL-4 zur Berechnung des lokalen Abbrands in H_2O - moderierten kernreactoren. Kernenergie, Vol. 24, p. 465.

Heinrich H. (1986) On the Possibility of Verification of Codes Assigned for Micro burnup Calculations Using the Data on Spent Fuel Isotopic Composition. (in Russian).

Хайнрих Х. О: возможностях проверки программ для расчетов микровыгорания на основании измерений концентрации нуклидов в выгоревшем топливе. Материалы XV Симпозиума специалистов ВМК по физике реакторов ВВЭР. Росток, Том 2, с. 610, 1986.

Hegyí Gy, Maraszy Cs. (1991). Hungarian Results of the Benchmark on the Use of Gd as Burnable Absorbers. Material of IAEA CRP on Safe Core Management with Burnable Absorbers in WWERs. 1991.

Honeck H.C. (1964). The calculation of the thermal utilisation and disadvantage factor in uranium water lattices. Nucl. Sci. Eng. 18, 49.

Jagannathan V. (1989) Indian Results of The Benchmark on The Use of Gd as Burnable Poison in WWERs. Material of IAEA CRP on Safe Core Management with Burnable Absorbers in WWERs.

Jonsson A. (1963). J. of Nucl. Energ. 17, 511, 1963.

Josefovich E. (1977) Rep. KFKI-ZR-6-527/1977 (in Russian).

Ishmaev S.N. et al. (1965). Experimental investigations of thermalization process in hydrogen containing moderators (in Russian).

In Pulsed Neutron Research. V.I.Vienna, IAEA, p.623.

С.Н. Ишмаев и др. Экспериментальное изучение процесса термализации в водородосодержащих замедлителях.

Ishmaev S.N. et al. (1966). The Anizotropy of Neutron Distribution in the Water Near Absorber. (In Russian).

Анизотропия спектра нейтронов в воде вблизи поглотителя. Препринт ИАЗ-1216, 1966. See also: In Neutron Thermalization and Reactor Spectra. Vienna, IAEA, v.II, p.193, 1968.

Ishmaev S.N. et al. (1968). (In Russian).

Neutron Thermalization and Reactor Spectra. V.I.Vienna,

a) Ibid, v.II, p.349.

b) Ibid, v.II, p.643.

Ishmaev S.N. et al. (1970) Neutron Thermalization in H_2O at $318^{\circ}K$ и $77^{\circ}K$. (In Russian). Препринт ИАЗ-1954.

Ishiguro Y., Takano H. (1971). PEACO - A Code for Calculation of Group Constants of Resonance Energy Region in the Heterogeneous Systems, JAERI Rep. 12191.

Ishiguro Y. et al (1986). Proposal of Benchmarks on Data and Methods to Calculate Reactor Characteristics in High Conversion Light Water Reactors. NEACRP-A-789.

Ishiguro Y. et al (1987). Resonance Absorption and Coolant Void Reactivity Coefficient in Tighter Pitch Lattices. Material of Advisory Group Meeting on Nuclear Data for Calculation of Thermal Reactor Reactivity Coefficients. Vienna.

Kavenoky A. (1969) Calcul et utilisation des probabilités de première collision des milieux hétérogènes à une dimension: les programmes ALCOLL et CORTINA, Note DEA-N-1077.

Kerezturi A. Analysis of Different Methods of Resonance Absorption

CHAPTER 4

Calculations. (in Russian).

Керестури А.: Анализ различных методов расчета резонансного поглощения. Материалы X Симпозиума специалистов ВМК по физике ВВЭР, Ереван, Том 1, с.159, 1981.

Kerezturi A. (1981) Numerical Methods for Thermalization Calculations. (in Russian).

Керестури А.: Нумерические методы, применяющиеся для расчета термализации. Материалы X Симпозиума специалистов ВМК, Ереван, Том 1, с. 139, 1981.

Kerezturi A. (1982) CERES- Design Code for Resonance Absorption Calculations. (in Russian).

Керестури А.: Инженерная программа CERES для расчета резонансного поглощения. Материалы XI Симпозиума ВМК, Варна, 1982.

Kerezturi A. (1982) Mutual Overlapping of the Resonances of Different Isotopes. (in Russian).

Керестури А.: Взаимная экранировка резонансов разных изотопов. Материалы XI Симпозиума специалистов ВМК, Варна, 1982.

Kerezturi A. (1987) Spatial Distribution of Resonance Absorption by U^{238} . (in Russian).

Керестури А.: Распределение резонансного захвата изотопа U^{238} . Материалы XVI Симпозиума ВМК, Москва, Том 1, с.140, 1987.

Kidman R.B.et al. (1972) Nucl.Sci.Eng. 48, 189.

Kowalska K. (1975). The S-WIMS code for CYBER-72. IBJ 1509/CYFRONET/PR/A Report.

Kulikowska T., Sadovska B. (1990). Polish Results for a Hexagonal Benchmark Problem. Material of IAEA CRP on Safe Core Management with Burnable Absorbers in WWERS. 1990.

Kurchatov I.V. (1956). Some Aspects of Developing Nuclear Energy in the USSR. (in Russian).

Курчатов И.В.: Некоторые вопросы развития атомной энергетики в СССР. М., 1956.

Levin M. (1963). Resonance Integral Calculations for U^{238} Lattices. Nucl. Sci. Eng., Vol. 16, p.271.

Laletin N.I. (1963). Differential Equation of Neutrons Thermalization for an Infinite Uniform Media. (in Russian).

Лалетин Н.И.: Дифференциальное уравнение термализации нейтронов в бесконечных однородных средах. Атомная энергия, т.14, с.458 1963.

Laletin N.I. (1967). Surface Pseudosources Method for Solving Neutron Transport Equation. (in Russian).

Лалетин Н.И.: Метод поверхностных псевдоисточников для решения уравнения переноса нейтронов. Препринт ИАЭ-1374, Москва, 1967.

Laletin N.I. et al (1990). Surface Harmonics and Surface Pseudosources Methods. Proc. of Int. Conf. on the Physics of Reactors, Marseille, 1990.

Laletin N.I. et al. (1990) Description of WIMS-SU. (in Russian).

Лалетин Н.И. и др.: Комплекс программ WIMS-SU. Вопросы атомной науки техники, сер. "физика и техника ядерных реакторов", вып.1, с. 26, 1990.

Liikala R.C., Uotinen V.O., Jenqu U.P. (1972) Nucl. Techn., Vol.15, p. 272.

Lehman M (1974). Report KFKI-ZR-6-505/1974 (in Russian).

Lehman M (1977). Evaluation of the Approaches Used in the Lattice Codes. (in Russian).

Оценка приближений, используемых в программах для расчета микроячеек. Рабочий материал ТГ ВМК, 1977.

Liman G.F., Maiorov L.V. (1981). NEWRAS, a Code for Calculating of Differential Scattering Cross Sections of Thermal Neutrons. (in Russian).

Лиман Г.Ф., Майоров Л.В.: Программа NEWRAS для расчета дифференциальных сечений рассеяния медленных нейтронов//Вопросы атомной науки и техники. Сер. "Физика и техника ядерных реакторов." Вып.8(21), с.32, 1981.

Liman G.F., Maiorov L.V., Yudkevich M.S. (1985). MCU Code Package for Solving Problems of Radiation Transport in the Reactors. (in Russian)

Лиман Г.Ф., Майоров Л.В., Юдкевич М.С.: Пакет программ MCU для решения

CHAPTER 4

методом Монте-Карло задач переноса излучений в реакторах. Вопросы атомной науки и техники. Сер. "Физика и техника ядерных реакторов." Вып.7. с.27, 1985.

Lutz D. (1990): Results for Sidorenko Benchmark. Material of IAEA CRP on Safe Core Management with Burnable Absorbers in VVERs.

Maierov L.V (1962) Asimptotic Distribution of Thermal Neutrons Far From a Planar Source. Proc. Brokhaven Conf. on Neutron Thermalization. BNL-719(C-32) v.4, p.1375.

See also: Журн.вычисл. мат. и мат. физ., т.2, с.635, 1962 (in Russian).

Maierov L.V, Turchin V.F. Yudkevich M.S. (1964). The chemical bond influence on neutron thermalization.

Proc. 3d UN Int. Conf. Report USSR. N364. UN New York. 1965.

Maierov L.V et al (1965) Thermalization of neutrons in graphite-water systems for large temperature gradients (In Russian).

Pulsed Neutron Research. Vienna. IAEA. p.657.

Maierov L.V (1965) Asymptotic of the scattering law for thermal neutrons. (in Russian).

Майоров Л.В. Асимптотика закона рассеяния тепловых нейтронов. Атомная энергия, т.19, вып.1, с.67.

Maierov L.V., Truchanov G.I. (1967). Certain methods for solving neutron thermalization problems. (In Russian). Neutron Thermalization and Reactor Spectra. Vienna, IAEA, v.1, p.145, 1968.

Майоров Л.В., Труханов Г.Я. Некоторые методы решения задач термализации.

Maierov L.V. Yudkevich M.S. (1988). Neutron Constants in the Thermal Reactors Calculations. Moscow. Energoatomizdat. (in Russian).

Майоров Л.В., Юдкевич М.С.: Нейтронно-физические константы в расчетах реакторов на тепловых нейтронах, М., Энергоатомиздат, 1988.

Marchuk G.I. (1961). Methods of Reactor Calculations. (in Russian).

Марчук Г.И.: Методы расчета ядерных реакторов. М., Госатомиздат, 1961.

- Marchuk G.I. et al (1962).** Methods of calculating Slow Neutron Spectra. Proc. Brokhaven Conf. on Neutron Thermalization. BNL-719(C-32) v.2, p.706.
- Marchuk G.I. et al (1964)** Methods for modelling neutron thermalization. Proc 3d UN Int. Conf. Report USSR. N365. UN New York. 1965.
- Mostovoi V.I. et al (1958)** Neutron spectrum measurements in uranium water lattices. Proc 2nd UN Int. Conf. PUAE 16, p.254.
- Mostovoi V.I. et al (1960)** Study of neutron spectra in systems with hydrogen-containing moderator. Conf. at Balaton-Eszed. Hungary.
- Mostovoi V.I. et al (1962).** Measurement of neutron spectra in uranium-water and uranium-mono isopropyl diphenyl lattices. Proc. Brokhaven Conf. on Neutron Thermalization. BNL-719(C-32) v.2, p.411.
- Mostovoi V.I. et al (1963)** Investigations of Thermalization Capabilities of the Water and some organic Compounds on the Basis of Inelastic Scattering Cross Sections Measurements. (in Russian).
Исследование термализующих свойств воды и некоторых органических соединений с помощью измерения сечений неупругого рассеяния медленных монохроматических нейтронов. Препринт ИАЭ-404. М., 1963.
- Mostovoi V.I. et al (1964).** Experimental investigations on neutron thermalization. Report USSR. N367. Proc. 3d UN Int. Conf. Report USSR. N365. UN New York. 1965.
- Mostovoi V.I. (1970)** Neutron Thermalization. (in Russian).
Мостовой В.И.: Термализация нейтронов. Препринт ИАЭ-2018. М., 1970.
- Mostovoi V.I. et al (1978)** Review on investigations of the neutron thermalization. (in Russian).
Мостовой В.И. Исследования по термализации нейтронов. Атомная энергия, т.44, вып.1, с.65, 1978.

CHAPTER 4

- Muller A, Linnatz E. (1963). Nucleonik. 5, 1963.
- Nikolaev M.N., Chochlov M.N. (1967). System of Subgroup Constants. (in Russian).
- Николаев М.Н., Хохлов М.Н.: Система подгрупповых констант. В кн. "Бюллетень информационного центра по ядерным данным", вып. 4, Атомиздат, с. 392, 1967.
- Nikolaev M.N. et al. (1984). Multigroup Approximation in the Theory of Neutron Transport. (in Russian).
- Николаев М.Н. и др.: Многогрупповое приближение в теории переноса нейтронов. М., Энергоатомиздат, 1984.
- Nodvik R.I. (1969). Supplementary Report on Evaluation of Mass Spectrometer and Radiochemical Analysis of YANKEE Core I Spent Fuel. WCAP 6086, 1969.
- Novikov A.N., Pshenin V.V., Lizorkin M.P. et al. (1990) Problems of VVER In-Core Fuel Management. IAEA-TECDOC-567, p.325, 1990.
- Osipov V.K., Tebin V.V. (1981) Calculation of Slowing Down Neutron Spectrum in the Cells of Thermal Heterogeneous Reactor (code SCOC-RT). (in Russian).
- Осипов В.К., Тебин В.В.: Расчет спектра замедляющихся нейтронов в ячейках теплового гетерогенного реактора (программа SCOC-RT). Материалы X Симпозиума ВМК, Ереван, Том 2, с. 721, 1981.
- Pshenin V.V. (1980) Adjustment of Cross Sections Library on a Basis of the Integral Experiments Data. (in Russian).
- Пшенин В.В.: Коррекция малогрупповой библиотеки микросечений по данным интегральных экспериментов на легководных решетках. Материалы IX Симпозиума ВМК, Нойбранденбург, Том 2, 1980.
- Pshenin V.V., Tebin V.V. (1982) Use of Equivalence Theorem for Calculation of ^{238}U Resonance Integrals. (in Russian).
- Пшенин В.В., Тебин В.В.: Использование теоремы эквивалентности для интерполяции резонансных интегралов ^{238}U . Материалы IX Симпозиума специалистов ВМК по физике ВВЭР, Варна, 1982.
- Pshenin V.V., Lazarenko A.P. (1988). Results of Solution of Benchmarks on Burnup of Tight Lattices with MOX Fuel. (in Russian).

Пшенин В.В., Лазаренко А.П.: Результаты решения тестовых модельных задач по выгоранию топлива в тесных решетках со смешанным уран-плутониевым топливом. Вопросы Атомной науки и техники, Сер. "Физика и техника ядерных реакторов", Вып.4, с.9, 1988.

Pshenin V.V. et al (1989). RAFORIN, Assignment, the Main Approaches and Preliminary Result of Verification. (in Russian).

Пшенин В.В. и др.: Программа РАФОРИН. Назначение, алгоритм и предварительные результаты тестирования. Материалы XVIII Симпозиума ВМК, Прахатице, с.803, 1989.

Pshenin V.V. et al (1989). UNIRASOS-2, Description of Methods and Results of Verification. (in Russian).

Пшенин В.В. и др.: УНИРАСОС-2: алгоритм и результаты тестирования. Материалы совещания ТГ-3 ВМК, с.172, Москва, 1989.

Pshenin V.V., Sidorenko V.D. et al (1989). Calculation Results for Gadolinium in Fuel Rod Lattices. Material of IAEA CRP on Safe Core Management with Burnable Absorbers in VVERs.

Pshenin V.V. et al (1992). Analysis of VVER Characteristics with Tight Lattice and MOX Fuel. IAEA 622-13-TC-700, p. 44.

Pshenin V.V. et al (1992). Comparison of Calculations for WVER-1000 Lattices Containing BA Rods with Gadolinium. Material of CRP on Safe Core Management with Burnable Absorbers in VVERs. 1992.

Rubin I.E. (1989) Results of Calculations of Self-shielded Cross Sections for Gadolinium Isotopes. (in Russian).

Рубин И.Е.: Некоторые результаты расчета резонансной блокировки сечений изотопов гадолиния. Материалы совещания ТГ-3 ВМК, с. 209, Москва, 1989.

Ramiro G. (1989) Calculations Results for the Lattices of X-3 and X-7 type obtained using WIMS-D4. (in Russian).

Рамиро Г.: Расчет параметров в решетках с неоднородностями X-3 и X-7 по программе WIMS-D4. Материалы XVIII-го симпозиума ВМК, Прахатице, с. 420, 1989.

Sauer A. (1963) Approximate escape probabilities. Nucl.Sci.Eng. Vol. 16, p.

Seifert E. (1976). Calculation of ZR-6 Lattices Using Monte-Carlo Method. KFKI-ZR-6-526/1976 (in Russian).

Э.Зайферт: Расчет решетки сборки ЗР-6 методом Монте-Карло. KFKI-ZR-6-526/1976.

Sergeev V.K., Karpov A.S. (1985). Calculations of Neutron Spectrum in the Resonance Energy Range (Code SLOGR). (in Russian).

Сергеев В.К., Карпов А.С.: Расчет спектров нейтронов в резонансной области (программа SLOGR). Вопросы атомной науки и техники, сер. "Физика и техника ядерных реакторов", вып. 4, с. 33, 1985.

Sidorenko V.D. (1976) On the Use of Four-Group Approach for Calculation of WWER Lattice. KFKI-ZR-6-524/1976 (in Russian).

В.Д. Сидоренко: Применение 4-х группового подхода к расчету нейтронно-физических характеристик решеток ВВЭР. KFKI-ZR-6-524/1976

Spoden E, Molcan K. (1990). Analysis of Measurements of Spent Fuel Isotopic Composition. Материалы XIX Симпозиума ВМК, Шиофок, с. 431, 1990 (in Russian).

Шподен Э., Мольцан К.: Анализ измерений выгорания топлива реактора АЭС. Материалы XIX Симпозиума ВМК, Шиофок, с. 431, 1990.

Strawbridge L.E., Barry R.F. (1965). Criticality Calculations for Uniform Water-Moderated Lattices. Nucl. Sci. Engng., Vol.23, N1, p.58.

Szatmary Z. et al. (1978) Adjustment of Cross Sections Libraries and Accuracy of Measurements at Critical Facility. (in Russian).

Сатмари З.и др.: Подгонка библиотек групповых констант и точность измерений на сборке. Материалы VII Симпозиума ВМК по вопросам физики ВВЭР. Прага, Том 2, с.26, 1978.

Szatmary Z. et al. (1977) Data evaluation problems in reactor physics. Theory of program RFIT. 1977. Rep. KFKI-ZR-6-43/1978.

Szatmary Z. Ed., Bardos J. et al. (1985). Experimental Investigations of the Physical Properties of WWER- Type Uranium-Water Lattices. Final Report

of TIC. Vol.1, Budapest.

Tebin V.V., Yudkevich M.S. (1980). On Taking into Account the Energy Dependence of the Collision Density Caused by Resonance Scattering when Computing Group Cross Sections. (in Russian).

Тебин В.В., Юдкевич М.С.: Учет энергетической зависимости плотности столкновений, обусловленной резонансным рассеянием, при расчете групповых сечений. Вопросы атомной науки и техники, Сер. "Ядерные константы", Вып.1 (36), с.16, 1980.

Tebin V.V., Yudkevich M.S. (1981). Subgroup Parameters in the Energy Range of Resolved Resonances. (in Russian).

Тебин В.В., Юдкевич М.С.: Подгрупповые параметры в области разрешенных резонансов. Препринт ИАЭ-3395/5, Москва, 1981.

Tebin V.V. et al (1985). A Project of SAPHIR Code Package. (in Russian).

Проект пакета программ САПФИР для решения задач расчета ячейки реактора. Вопросы атомной науки и техники, Сер. "Физика и техника ядерных реакторов" Вып.4, с.68, 1985.

Tebin V.V. (1991). A Generalized Subgroup Approach to Calculating Resonance Absorption of Neutrons in Nuclear Reactors. IAEA Tecdoc-491. 1991.

Thermal Benchmark Compilation, CSEWG Data Testing Subcommittee. June, 1974.

Thie J.A. (1961) Nucl. Sci. Eng. 9, 286.

Turchin V.F. (1963). The Slow Neutrons. (in Russian).

Турчин В.Ф.: Медленные нейтроны. М., Атомиздат, 1963.

Tverbakk O.P., Doderlein J.M. (1985) Kjeller report. KR-75.

Vidovski I., Krinig K. (1988). Temperature Dependence of Bucklings and Reflector Savings. KFKI-ZR-6-412/1988 (in Russian).

Weiss Z., Stammli R. (1964). Nucl.Sci.Eng. 19,374.

Wigner E.P., Wilkins J.E. (1944) AECD-2275.

Williams M.L. (1966). The slowing down and thermalization of neutrons. North-Holland Publ.Co. 1966.

Williams M.L. et al.(1985). Analysis of Thermal Reactor Benchmarks with Design Codes Based on ENDF-B/V data. Nucl. Techn., V.71, p. 386.

Yamamura Y., Sekija T. (1971) Wigner Continuous Slowing Down for the Fast Neutron Spectrum. Nucl. Sci. Eng., v.63, p. 213.

Zaleski K. Description of MICROBE Code. Материал для подготовки II тома сборника трудов BMK (in Russian).

Залески К.: Описание программы MICROBE. Рабочий материал для подготовки II тома сборника трудов BMK.

Zelenkov A.G. et al. (1981). Full Analysis of WWER-440 Spent Fuel. (in Russian).

Зеленков А.Г. и др.: Полный анализ выгоревшего топлива АЭС с ВВЭР-440. Атомная Энергия, т. 51(1981), вып. 1, с. 53.

5. FINE MESH DIFFUSION CODES

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5.1 INTRODUCTION

The so called fine mesh diffusion codes are employed for pin by pin power distribution calculations in WWERs. Usually every hexagonal cell with the size corresponding to a fuel rod lattice step is presented as one calculational point in such codes. In code packages for WWER core calculations the fine mesh codes are used together with 3D coarse mesh core simulator codes, which consider the fuel assembly as an elementary cell. When core design calculations are carried out, the fine mesh codes give information about the fuel pin power peaking factor and its dependence on core burnup and outer parameters variations. This information is needed for core safety analysis. Results of fine mesh calculations are also used for treating data of the in-core monitoring system and for verifying coarse mesh codes. The significance of the problems mentioned above requires high accuracy of fine mesh codes. Accuracy improvement and development of fine mesh codes was one of the main tasks solved by TIC experts. Experimental data obtained by TIC experts on the ZR-6 critical facility were a good basis for the verification of fine mesh codes.

Fine mesh codes are traditionally based on the following approaches:

- a) The cells of the real heterogeneous lattice previously should be homogenized;
- b) Few group neutron diffusion parameters of homogenized cells should be calculated for each cell type using one of the spectral codes described in Chapter 4;
- c) The flux distribution is assumed to be described by a few group diffusion equation in homogenized cells and in the whole core;
- d) The neutron spectrum is divided into energetic groups (usually from two up to four) and as a rule only one group of thermal neutrons is

selected;

e) Differential diffusion equations are usually solved using the simplest finite difference approximation in which one calculational point corresponds to one cell;

f) As a rule it is assumed that the WWER core may be described by a regular hexagonal lattice. Naturally the fuel pins form a regular lattice in WWER fuel assemblies. But the regular hexagonal mesh cannot be kept on the whole core exactly because of the gaps between assemblies are not described by hexagonal cells with the exactly same size. Therefore some corrections of equations or neutron diffusion parameters for such cells have been inserted in most of the fine mesh codes.

A short description of the main features of fine mesh codes developed by TIC experts will be given in Section 5.6.

In the described formulation the fine mesh problem is reduced to solving a system of linear equations which includes from several hundreds up to tens of thousands of equations (depending on core size). These equations represent the finite difference form of the diffusion equation for a set of adjacent hexagonal prisms with known few group neutron diffusion parameters. The computational methods of problems with a large number of equations were also developed and investigated by TIC experts.

For a general estimation of fine mesh codes accuracy there is a necessity to estimate the inaccuracy of all approximations which have been done during the fine mesh algorithm elaboration.

The least proved of the traditionally used fine mesh approximations is the approximation in which the method of cell homogenization and asymptotic neutron diffusion parameters are employed for nonuniform lattices calculations. Obviously that neutron spectrum in the given cell type depends on the properties of the surrounding cells and non-diffusional effects can be significant on cell boundaries. Up to the beginning of the TIC cooperation the method of homogenization was proved only for uniform lattices and small flux gradients. Its accuracy for nonuniform lattices needed additional verification. Therefore one of the main TIC tasks was to check the approximations a), b), c) and to elaborate algorithms taking into account the more accurate definition of these hypotheses.

The second main task was the mutual verification of codes based on the simplest finite difference equations with one point per cell. A set of WWER type numerical benchmarks was elaborated and solved for such

verification.

The following problems are mathematical problems. The simplest finite difference equations provide high calculational accuracy for a fine mesh size step that is significantly less than the neutron diffusion length. In the opposite case the problem was to fix the limits of the simplest finite difference equation applicability and to elaborate more complicated neutron balance equations. Acceleration of the iterative procedures was also significant problem.

Mutual validation was the next main development stage of fine mesh codes. The global criterion concerning quality of fine mesh codes is the agreement of calculational results with those from precision code calculations and experimental data. Comparisons with experimental data are less convenient because the uncertainty of nuclear data may tend to inaccuracy which is inconsistent with the used mathematical approximations. Nevertheless, validation based on experimental data was mainly used by TIC experts. From the point of view of validating global fine mesh codes, measurements on the ZR-6 critical facility have given significant and qualitative data because the critical conditions, the fuel pin activation and reaction rates for some types of detectors were measured in a great number of core configurations.

This chapter surveys the main fine mesh methods and codes which were developed and are used in those institutions working together as part of the TIC. As an example some calculational results obtained with different codes are compared with the experimental data. Modifications of homogenization theory based on the finite difference method for taking into account the spectrum deformation in nonuniform lattice are described.

5.2 SIMPLEST FINITE DIFFERENCE PRESENTATION OF THE DIFFUSION EQUATION

In a few group diffusion approximation the neutron flux distribution in any region with given boundary conditions is described as follows:

$$-\text{div} D^{(k)}(r) \text{grad} \Phi^{(k)}(r) + \left[\Sigma_s^{(k)}(r) - \Sigma_a^{(k)}(r) \right] \Phi^{(k)}(r) = S^{(k)}(r) \quad (5.2.1)$$

In equation (5.2.1), k is the energetic group number, S^k is the neutron source for group k :

$$S^k = \frac{\chi_k}{K_{eff}} \sum_{j=1}^{N_g} \nu \Sigma_f^j \Phi + \sum_{j=1}^{N_g} \Sigma_s^{j \rightarrow k} \Phi, \quad (5.2.2)$$

where N_g is the number of energetic groups, χ_k is the share of fission neutrons ejected in the energetic group k , $\nu \Sigma_f^j$ is the neutron production cross section, $\Sigma_s^{j \rightarrow k}$ is the neutron removal cross section from group j into group k , K_{eff} is the eigenvalue.

On boundaries of subregions or cells with different neutron diffusion parameters, to equations (5.2.1) should be added the neutron flux Φ and current $D \nabla \Phi$ continuity conditions. On the outer region surface some kind of boundary condition should be satisfied. For example

$$\nabla_n \Phi + \beta \Phi = 0,$$

where $\nabla_n \Phi$ means the normal gradient of the neutron flux. By means of a hexagonal net the calculational region is divided into hexagonal cells in such a way that for each of them, the diffusion properties should be constant in the inner cell space (homogeneous or homogenized cells) and the size of cells should be significantly less than one neutron diffusion length. Taking into account continuity conditions, equation (5.2.1) may be rewritten for a two dimensional case as a system of algebraic equations

$$\frac{4}{3h^2} \sum_{i=1}^6 \frac{D_0^k D_1^k}{D_0^k + D_1^k} (\Phi_0^k - \Phi_1^k) + (\Sigma_{a0}^k + \Sigma_{s0}^k + D_{z0}^k B_z^2) \Phi_0^k = S_0^k \quad (5.2.3)$$

Index 0 means given cell, index 1 means surrounding cells, h is the cell size, D_0^k is the radial diffusion coefficient, Σ_{a0}^k is the absorption cross section, Σ_{s0}^k is the removal cross section into other groups, D_{z0}^k is the axial diffusion coefficient, B_z^2 is the axial buckling. The term $D_{z0}^k B_z^2$ is included in the neutron balance to take the axial leakage into account.

For calculations of axially uniform cores similar to ZR-6, it is enough to solve two dimensional problems by taking into account the axial leakage by using a known axial buckling. In the other cases the three dimensional fine mesh codes should be employed or axial buckling of core subregions should be taken from 3D coarse mesh calculations.

Usually a radial reflector is included in the fine mesh calculational region. In view of this, the boundary conditions on the outer reflector

surface have no great importance. As a rule, the condition of zero flux ($\beta=\infty$) on the outer reflector boundary is assumed.

In calculations of WWER type core and of ZR-6 critical facility, it is convenient to take into account the core symmetry. There are some types of rotation or reflecting symmetries for which the azimuthal sector of the core with angles 30, 60 or 180 degrees is repeated 12, 6 or 2 times, accordingly. In these cases it is enough to calculate only one of the symmetry sectors. The condition of neutron reflection on symmetry axes should be used for reflecting symmetry. For rotation symmetry the corresponding cells which are positioned on different axes should be considered as joined cells.

Borresen scheme. In some of fine mesh codes, which were developed in TIC, the so called Borresen scheme was employed for simplifying the numerical solution. The Borresen scheme (Borresen, 1973) involves the simplification of expression (5.2.3) using the approximate equality

$$\frac{D_0^k D_1^k}{D_0^k + D_1^k} \approx \frac{1}{2} \sqrt{D_0^k D_1^k} \quad (5.2.4)$$

Substitution of (5.2.4) in (5.2.2) with the following replacement of unknowns by

$$\phi_1^k = \frac{\psi_1^k}{\sqrt{D_1^k}} \quad (5.2.5)$$

gives an equation system for which only one element from each line of matrix should be stored in the memory (for the (5.2.3) system, six elements should be stored). Thus, this scheme has a less computer memory requirement. The number of mathematical operations per cell in iterations is also less than for the (5.2.3) scheme. It should be mentioned that approximation (5.2.4) is sufficiently correct only if D_0^k and D_1^k do not differ significantly.

Features of neutron balance equation for irregular lattices in gaps between fuel assemblies are described in reports [556, 561, 562] and in Section 5.3.

The simplest method for taking into account lattice irregularity is the use of the so called compression factor. In this method the real irregular cells between assemblies are replaced by hexagonal cells

corresponding to a regular hexagonal inner assembly lattice. Neutron cross sections of such cells are multiplied by the compression factor which is equal to the ratio of volumes of irregular and regular cells. In this case for the same flux level the reaction rates are preserved in irregular cells and their contributions to core neutron balance are approximately kept.

It should be mentioned that all ZR-6 configurations can be described by a regular hexagonal net.

The simplest method for taking into account irregularities in the lattice is the use of so called compression factors. In this method the irregular cells between assemblies are replaced by hexagonal cells of the same volume. The reaction rates are then calculated for these regular cells and multiplied by the compression factor which is equal to the ratio of volumes of irregular and regular cells. In this case for the same flux level the reaction rates are preserved in irregular cells and their contributions to core neutron balance are approximately kept.

It should be mentioned that all ZR-6 configurations can be described by a regular hexagonal net.

5.3 FINITE DIFFERENCE EQUATION FOR IRREGULAR MESH [561]

Equation (5.2.3) is derived on the assumption that the core is presented as a set of regular hexagonal homogeneous cells. However in the WWER core the regularity of cells is violated for cells positioned in gaps between fuel assemblies. To take into account the influence of this on the accuracy of the model, the following neutron balance equation form can be used.

Let us consider the group diffusion equation:

$$-\text{div} \nabla \phi + \Sigma \phi = F \quad (5.3.1)$$

where F is the right side of (5.2.1) and the group index is omitted.

Integrating (5.3.1) on elementary cell R_0 and using Green's theorem one can obtain:

$$-\int_{\Gamma(R_0)} D_0 \frac{\partial \phi}{\partial n} d\Gamma + \iint_{R_0} \Sigma(x, y) \phi(x, y) dx dy = \iint_{R_0} F(x, y) dx dy \quad (5.3.2)$$

Let us present double integrals as:

$$\iint_{R_0} \Sigma(x, y) \phi(x, y) dx dy \approx \Sigma_0 \iint_{R_0} \phi(x, y) dx dy = \quad (5.3.3)$$

$$= \Sigma_0 \mu(R_0) \left[\frac{1}{\mu(R_0)} \iint_{R_0} \phi(x, y) dx dy \right] = \Sigma_0 \mu(R_0) \phi_0$$

where

Σ_0 - average value of $\Sigma(x, y)$;

ϕ_0 - average value of $\phi(x, y)$;

$\mu(R_0)$ - area of R_0 .

Let us approximate the diffusion member of (5.3.2) using average values:

$$D_0 \frac{\partial \phi}{\partial n} = \alpha_0 \phi_0 + \alpha_1 \phi_1 \quad (5.3.4)$$

and let us define α_0 and α_1 in such a manner that (5.3.4) will be true for

some special choice of $\phi(x,y)$ satisfying continuity conditions. Let us write the continuity condition for $x=a$ as:

$$\phi(x,y) = \begin{cases} \delta_1 + \delta_2 \frac{x-a}{D_0} & \text{for } x \leq a \\ \delta_1 + \delta_2 \frac{x-a}{D_1} & \text{for } x \geq a \end{cases} \quad (5.3.5)$$

where a is the distance from the origin of the coordinate system to the centre of border R_{01} between cells R_0 and R_1 .

Taking into account that (5.3.4) should be satisfied for arbitrary δ_1 and δ_2 one can obtain for α :

$$\alpha_0 + \alpha_1 = 0$$

$$\alpha_1 = \frac{1}{\frac{\beta_{01}}{D_0} + \frac{\beta_{10}}{D_1}} \quad (5.3.6)$$

where:

$$\beta_{01} = -\frac{1}{\mu(R_0)} \iint (x-a) dx dy \quad (5.3.7)$$

$$\beta_{10} = \frac{1}{\mu(R_0)} \iint (x-a) dx dy$$

Taking into account (5.3.4) and (5.3.6) one can write the balance equation as:

$$\sum_{i=1}^I l_{oi} \frac{1}{\frac{\beta_{oi}}{D_0} + \frac{\beta_{io}}{D_i}} (\phi_o - \phi_i) + \mu(R_0) \Sigma_o \phi_o = \mu(R_0) F_o \quad (5.3.8)$$

where: I - number of neighbouring cells;

R_0 - the cell under consideration;

$R_1, \dots, R_i$ - neighbouring cells;

l_{oi} - length of border between R_0 and R_i ;

β_{oi} - is defined by (5.3.7);

$$F = \frac{1}{\mu(R_0)} \iint_{R_0} F(x, y) dx dy - \text{source.}$$

For a regular mesh, balance equation (5.3.8) transforms to its traditional form (5.2.3).

For example, values of μ , β and l are presented below for the case corresponding to Figure 5.1

$$\begin{aligned} l_{32} &= l_{12} = h_s; & l_{43} &= l_{24} = l_{40} = \frac{R_0}{\sqrt{3}}; & l_{ij} &= R_{ji}; \\ \beta_{24} &= [2h_o + h_h]/4; & \beta_{34} &= [3h_o + 2h_h]/6; & \beta_{32} &= [3h_o + h_h]/6; \\ \mu_{04} &= h_o/2; & \mu_o &= \mu_4 = h_o^2 \frac{\sqrt{3}}{2}; & \mu_1 &= \mu_2 = h_o^2 \frac{2\sqrt{3}}{2} + h_o \left[h_3 \frac{h_o}{\sqrt{3}} \right]; \\ \mu_3 &= \left[h_s^2 + 4h_s - \frac{h_o}{\sqrt{3}} + \frac{h_o^2}{3} \right] \frac{\sqrt{3}}{4} \end{aligned}$$

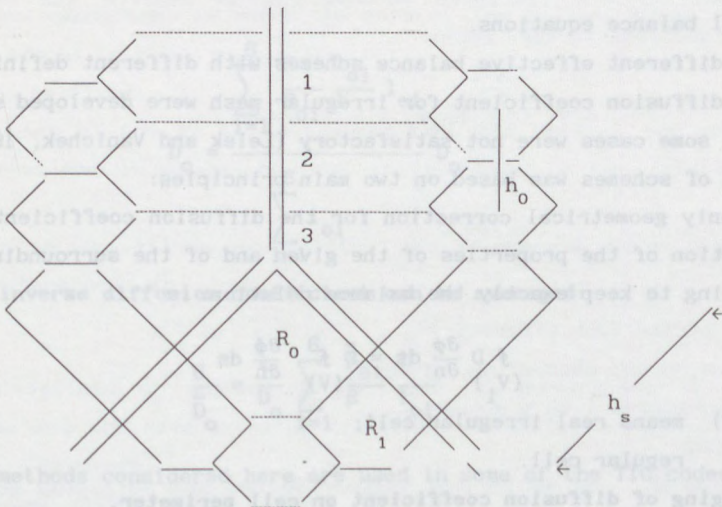


Figure 5.1 Irregular mesh for assembly gap

h_o - regular mesh step;

h_s - assembly shift compared to regular mesh.

Using (5.3.8) one can write the balance equation similar to (5.2.1) in the final form:

$$\sum_{i=1}^I \frac{l_{oi}}{\frac{\beta_{oi}}{D_{o,g}} + \frac{\beta_{io}}{D_{i,g}}} \left[\phi_{o,g} - \phi_{i,g} \right] + \mu_o \Sigma_{o,g} \phi_{o,g} = \quad (5.3.10)$$

$$= \mu_o \sum_{k=1}^{g-1} \Sigma_{o,k \rightarrow g} \phi_{o,k} + \frac{\mu_o}{K_{eff}} \chi_{o,g} \sum_{k=1}^N \left[\nu \Sigma_f \right]_{o,k} \phi_{o,k}$$

where: $g=1,2,\dots,N$ is the group index.

The simplified form of the equation taking into account mesh irregularity can be obtained using a compression factor, i. e.:

$$\tilde{\Sigma}_i = \Sigma_i \frac{V_i}{V}; \quad \tilde{D}_i = D_i \frac{V}{V_i} \quad (5.3.11)$$

where: V_i is an irregular cell area;

V is a regular cell area.

Parameters with the tilde are used as effective parameters in traditional balance equations.

Some different effective balance schemes with different definitions of effective diffusion coefficient for irregular mesh were developed since the results in some cases were not satisfactory (Lelek and Vanichesk, 1980). The derivation of schemes was based on two main principles:

- a) using only geometrical correction for the diffusion coefficient without a modification of the properties of the given and of the surrounding cells;
- b) attempting to keep exactly the balance relation:

$$\oint_{(V_i)} D \frac{\partial \phi}{\partial n} ds = \tilde{D} \oint_{(V)} \frac{\partial \phi}{\partial n} ds$$

where: (V_i) means real irregular cell;

(V) regular cell.

Averaging of diffusion coefficient on cell perimeter.

Keeping currents continuous one can obtain:

$$\tilde{D} = D \frac{P}{P_i} \quad (5.3.12)$$

where: P_i - perimeter of irregular cell;

P - perimeter of regular cell.

Only a small improvement in the calculational results was obtained using (5.3.12).

Geometrical weighting factor for the diffusion coefficient.

In (5.3.10) approximation of differential operator can be rewritten as:

$$\frac{l_{oi}}{\beta_{oi} + \frac{l_{oi}}{D_o}} \left(\phi_o - \phi_i \right) = \frac{l}{\beta \frac{l_{oi}}{D_o} + \frac{l_{oi}}{D_i} \frac{l}{\beta}} \left(\phi_o - \phi_i \right), \quad (5.3.13)$$

where β and l without indexes are the corresponding parameters of the regular cell. The following expressions are suggested for effective diffusion coefficient:

$$\tilde{D}_o = \frac{1}{6} \sum_{i=1}^6 \frac{\beta}{\beta_{oi}} \frac{l_{oi}}{l} D_o \quad (5.3.14)$$

or

$$\tilde{D}_o = \frac{\sum_{i=1}^6 \frac{\beta}{\beta_{oi}} \frac{l_{oi}}{l} l_{oi}}{\sum_{i=1}^6 l_{oi}} D_o \quad (5.3.15)$$

The inverse diffusion coefficient can be averaged:

$$\frac{6}{\tilde{D}_o} = \frac{1}{D_o} \sum_{i=1}^6 \frac{\beta_{oi}}{\beta} \frac{l}{l_{oi}} \quad (5.3.16)$$

The methods considered here are used in some of the TIC codes.

5.4. ITERATIVE METHODS

In codes for solving the system of equations (5.2.2)-(5.2.3), developed in TIC-countries, mostly a 2-cyclic iterative method, generally consisted of an inner iteration for determining neutron fluxes in groups and an outer iteration for calculating the fission source and k_{eff} is used. For the described type of problems, where the number of equations may reach thousands or even tens of thousands, the most important task is to achieve rapid convergence of the iterative process because of the otherwise huge computation time requirement. For this reason, in addition to the need to improve the physical model utilized in the codes, the convergence acceleration methods are of great importance.

The over-relaxation method is used in TIC-codes to accelerate convergence of inner iterations. Additionally the methods of factorization AGA and EVA (Woznitski, 1973), Chebyshev's methods, Lyusternik's methods and Sheldon's methods with Chebyshev's parameters are used.

Different modifications of Chebyshev's method (Marchuk, Lebedev 1981), (Zikova and Lelek 1983) are used in practice to accelerate outer iterations.

To describe the iterative methods let us rewrite the system of diffusion equations in the form:

$$A_g \phi_g = \sum_{l=1}^{g-1} B_{lg} \phi_l + \frac{1}{k_{eff}} S_g(\phi) \quad (5.4.1)$$

where

$$S_g(\phi) = \sum_{l=1}^N C_{gl} \phi_l \quad (5.4.2)$$

$g=1, 2, \dots, N$.

Matrices describe such effects:

A_g - diffusion and absorption, group g ;

B_{lg} - removing from l to g group;

C_{gl} - fission.

Let us choose $\phi^{(0)}$ as an initial vector. We use the following scheme for the outer iterations:

$$A_g \phi_g^{n+1/2} = \sum_{l=1}^{g-1} B_{lg} \phi_l^{n+1/2} + S_g(\phi^n) \quad (5.4.3)$$

$$\phi_g^{n+1} = \gamma_{n+1} \left[\phi_g^{n+1/2} - \beta_{n+1} \phi_g^n \right] \quad (5.4.4)$$

or

$$S_g \left[\phi_g^{n+1} \right] = \gamma_{n+1} \left[S_g \left[\phi_g^{n+1/2} \right] - \beta_{n+1} S_g \left[\phi_g^n \right] \right] \quad (5.4.5)$$

$$g=1,2,\dots,N; n=0,1,\dots,$$

where β_{n+1} are parameters for accelerating convergence;

γ_{n+1} are some normalizing multipliers.

To realize the method (5.4.3)-(5.4.5) in each group we need to find the solution of equations

$$A_g \phi_g = b_g, \quad g=1,2,\dots,N, \quad (5.4.6)$$

with known right-hand sides b_g .

Let us refer to iterations (5.4.3)-(5.4.5) as outer, and the iterations for resolving of the equations (5.4.6) as inner.

We describe in detail only the methods that are used in the codes of TIC-countries. The relationships between the outer iterations and the approximate solution of the system (5.4.6) obtained from inner iterations is set by the accuracy condition. For each outer iteration the number of inner iterations may be defined by:

- a) the given accuracy of the solution of equations;
- b) the condition, in which the norm of the initial error is reduced to given proportion;
- c) to be fixed.

In cases b) and c) it is assumed that the initial approximation in inner iterations is chosen so that it converges to the solution of the task.

Based on suggestions (Lelek, 1975) the accuracy of outer iterations is usually determined by

$$\varepsilon_g^{(n)} = \alpha_g \left\| S_g \left[\phi_g^{n+1} - \phi_g^n \right] \right\|,$$

where multipliers α_g depend on the rate of convergence of the outer iterations and are calculated on the basis of analytic evaluations or of numerical experiment.

a) Inner iterations.

The number of equations in system (5.4.6) can be up to several tens of thousands. For this reason only iteration methods of resolving were realized in practice. With regard to the particular problem (varying coefficients, hexagonal grids, nonstandard regions) iterative methods

convenient for realization were applied. The method of over relaxation (SOR) is the basic method of such kind.

$$\phi^{k+1} = \phi^k + \omega \left[D^{-1} \left[L\phi^{k+1} + U\phi^k + b \right] - \phi^k \right] \quad (5.4.7)$$

where for the given order of grid's nodes

$$A = D - U - L$$

L - lower triangular matrix;

U - upper triangular matrix;

D - diagonal matrix;

ω - relaxation parameter.

We use the index of group g and the index of outer iterations k in formula (5.4.7). Matrix $R(\omega) = (D - \omega L)^{-1} \left[(1 - \omega)D + \omega U \right]$ is the transition operator in method (5.4.7).

The choice of relaxation parameter ω depends on matrix A . For square and cubic grids A is a 2-cyclic matrix and the optimal ω is determined exactly

$$\omega_{\text{opt}} = 2 / \left[1 + \sqrt{1 - \rho[R(1)]} \right] \quad (5.4.8)$$

where $\rho[R(1)]$ - spectral radius of the matrix $R(1)$.

For a hexagonal grid and a 7-point scheme matrix A is not a 2-cyclic matrix. In this case the ω calculated by formula (5.4.8) is not the optimal one, however iterative process is accelerated with that value of ω . The value ω from (5.4.8) is usually used. Alternatively the certain parameter characterizing the convergence rate is introduced, and the ω value is changed in outer and inner iterations to achieve the optimal rate.

For example, $\rho[R(1)]$ may be evaluated in the first outer iteration. If one wishes to carry out the first inner iteration in each group by the Gauss-Seidel's method (formula (5.4.7) with $\omega=1$), then

$$\rho[R(1)] = \lim_{k \rightarrow \infty} \frac{\|\phi^k - \phi^{k-1}\|}{\|\phi^{k-1} - \phi^{k-2}\|} \quad (5.4.9)$$

The accuracy of calculation ρ by (5.4.9) is small but sufficient for determining of ω .

There are more complex algorithms such as the methods of factorization AGA and EVA (Woznitski, 1973), (Woznicki, 1979), (Woznicki, 1983), line-relaxation method SLOR, Chebyshev's methods (Marchuk, Lebedev 1981),

alternating-direction methods with alternating parameters (Marchuk, Lebedev 1981), (Shishkov, 1976), Sheldon's method with Chebyshev's acceleration (SSOR + Chebyshev's acceleration) (Lebedev, 1985).

Let us discuss the last method in detail because:

- a) for equations with very large number of unknowns this method has better asymptotic convergence rate than that of the SOR-method if the optimal values of parameters are utilised.
- b) the codes in which SOR is realized with utilising simple reordering of unknowns can easily be transformed into corresponding codes employing the method discussed.

Thus, let us write the modification of Sheldon's method with Chebyshev's parameters in the following form. Approximation ϕ^{k+1} is defined by the scheme

$$\phi^{k+1/3} = \phi^k + \omega \left[D^{-1} \left[L\phi^{k+1/3} + U\phi^k + b \right] - \phi^k \right] \quad (5.4.10)$$

$$\phi^{k+2/3} = \phi^{k+1/3} + \omega \left[D^{-1} \left[L\phi^{k+1/3} + U\phi^{k+2/3} + b \right] - \phi^{k+1/3} \right] \quad (5.4.11)$$

$$\phi^{k+1} = \phi^k + \alpha_{k+1} \left[\phi^{k+2/3} - \phi^k \right] \quad (5.4.12)$$

$$\alpha_{k+1} = 1 / \left[1 - q \sin^2 \frac{\omega_k \pi}{2} \right] \quad (5.4.13)$$

$$k=0, 1, 2, \dots$$

Here ω ($1 < \omega < 2$) and q ($0 \leq q \leq 1$) are the fixed parameters, and $\omega_k \in [0, 1]$ are members of infinite T-sequence (Marchuk, Lebedev 1981).

The members of that sequence are such that the values $\cos \omega_i$, $i=1, 2, \dots, 3^r$, $r=0, 1, \dots$, are the roots of Chebyshev's polynomials of the first kind $T_{3^r}(x)$, which are taken in some special order to provide the stability of iterations.

Equations (5.4.10) correspond to the formulae of the SOR-method, when the unknowns are taken in the normal order. Equation (5.4.11) corresponds to the formulas of the SOR-method, when the unknowns are taken in reverse order, that is easy to realize in a code. Equations (5.4.12) and (5.4.13) are usual equations for correction with Chebyshev's parameters.

The method requires storage of two arrays of unknowns in the memory. The cost of one iteration for method (5.4.10) - (5.4.13) is approximately

twice as much as the one in the SOR-method. The optimal values of parameters ω and q in each group are determined by a numerical experiment for resolving special model problems.

It should be noted another important property of method (5.4.10)-(5.4.13): the transition matrix of method (5.4.10)-(5.4.11) is symmetric and positive. It has a good influence on the convergence of outer iterations.

In PERMAK-Y code the ω_k set is taken as the first 36 members of the T-sequence corresponding to the roots of $T_{36}(x)$ for ω_k . The $\cos \omega_k \pi$ are values of the periodically continued array of 36 numbers:

0.; 0.866025404; -0.866025404; 0.6427876097; -0.6427876097;
 0.342020143; -0.342020143; 0.9848077530; 0.4487991802;
 -0.448799180; 0.802123192; -0.802123192; 0.9579895123;
 -0.957989512; 0.549508978; -0.549508978; 0.1160929141;
 -0.116092914; 0.918216106; -0.918216106; 0.7273736415;
 -0.727373641; 0.230615870; -0.230615870; 0.9983081582;
 -0.998308158; -0.999048221; 0.5372996083; -0.5372996083;
 0.843391445; -0.843391445; 0.4617486132; -0.4617486132;
 0.887010833; -0.887010833

For further acceleration of iterations the idea of the KP-method (Marchuk, Lebedev 1981) may be used.

Let ϕ be the exact, $\tilde{\phi}$ an approximate solution (5.4.6). Let $w = \phi - \tilde{\phi}$ denote the error of the approximate solution. Then this error satisfies the system of equations:

$$A_g w = r \quad (5.4.14)$$

where $r = A_g \tilde{\phi} - b_g$ is the residual. Let us replace the equation for the error by the simpler equation:

$$B \eta = r \quad (5.4.15)$$

in which matrix B is "close" to matrix A , but is much simpler. Then $\eta \approx w$ and, consequently, for the new approximation we may take function determined by the formula:

$$\phi \approx \tilde{\phi} + \gamma \eta \quad (5.4.16)$$

where parameter γ either equals 1, or changes from iteration to iteration.

As simple model problems it is usually considered ones which may be solved with using well converging iterative methods. For example, it may be

the problem of solving the grid equations for the coarse grid or for more uniform reactor, than real one (on the condition that the number of grid points is conserved).

The last approach was used in PERMAK-Y code (Lizorkin, Kourchenkova, Lebedev, 1988) in which equations (5.4.15) are solved by the method (5.4.10)-(5.4.13). As it turned out, in method (5.4.10)-(5.4.13) the optimal parameters ω and q obtained from solving the model problem (5.4.15) provided a good convergence of iterations for all variants of WWER problems, because the simple problem was a well chosen.

In PERMAK-Y code the optimal values of parameters ω and q for each group are as follows:

$q^{(1)}$	$q^{(2)}$	$q^{(3)}$	$q^{(4)}$	$\omega^{(1)}$	$\omega^{(2)}$	$\omega^{(3)}$	$\omega^{(4)}$
0.82	0.73	0.61	0.39	1.78	1.70	1.61	1.51

Here upper indexes are the group numbers.

b) Outer iterations.

Let us rewrite the equation (5.4.1) in the form :

$$P\phi = k_{\text{eff}}\phi \quad (5.4.17)$$

where $P=(A-B)^{-1}S$. Equation (5.4.17) is the equation for the largest eigenvalue of operator P . Let us assume that the spectrum of operator P (with the exception of $\lambda_1=k_{\text{eff}}$) lies in an ellipse with the foci at the points of the real axes m , M , and the point k_{eff} not belonging to that ellipse. To determine an eigenfunction of equation (5.4.17) the two algorithms using Chebyshev's polynomials can be considered.

1) The method using only one previous approximation (Marchuk, Lebedev 1981). This is determined by Eqs. (5.4.3)-(5.4.5), and it may be written in the form:

$$\phi^{n+1} = \gamma_{n+1} \left[P\phi^n - \beta_{n+1}\phi^n \right] \quad (5.4.18)$$

where β_{n+1} represents some iterative sequence.

The operator S and, therefore, operator P usually have a multidimensional kernel (e.g. a set of eigenvectors corresponding to the zero eigenvalue). Thus point $\lambda=0$ is the P operator eigenvalue of a large multiplicity. Moreover, the difference approximation to P (or corresponding

to operator realized by the inner iterations: $P\phi^n$) may have a small in modulus complex eigenvalues. That is why it is appropriate for an iterative process to be supplemented periodically by iterations (5.4.18) with $\beta_{n+1}=0$.

As is usually assumed, the spectrum of P is real and nonnegative, so

$$K_{\text{eff}} = \lambda_1 > \lambda_2 \geq \lambda_3 \geq \dots \geq \lambda_n \geq \dots \geq 0 \quad (5.4.19)$$

Let the eigenfunctions $\varphi_1, \varphi_2, \dots, \varphi_n$ correspond to eigenvalues $\lambda_1, \lambda_2, \dots, \lambda_n$.

In order to accelerate the iterations let us construct a polynomial $P_1(\lambda)$ of degree 1, that satisfies the following conditions:

$$P_1(0)=0, P_1(\lambda_1)=1.$$

Let $T_1(x)$ be a degree 1 Chebyshev's polynomial of the first kind; its roots are the numbers:

$$t_k = \cos \frac{2k-1}{2l} \pi, \quad k=1, 2, \dots, l.$$

Then the polynomials are defined as follows

$$P_1(\lambda) = \frac{T_1(x)}{T_1(\theta)},$$

where

$$x = \frac{1}{M-m}(t_1 M + m - \lambda(1+t_1)), \quad \theta = \frac{1}{M-m}(t_1 M + m - \lambda_1(1+t_1));$$

and their roots are:

$$\bar{\beta}_1 = 0, \quad \bar{\beta}_k = (t_1 M + m - (M-m)t_k) / (1+t_1). \quad (5.4.20)$$

Let $l=27$, and $\bar{\beta}_{28} = \bar{\beta}_{29} = 0$. Utilising the sequence of $\bar{\beta}_k$ (5.4.20), $k=1, \dots, 29$, and method (5.4.18) we construct a cycle with period 29. Under that we assume, that $\bar{\beta}_1 = 0, \bar{\beta}_{10} = 0, \bar{\beta}_{20} = 0$, and the next $\bar{\beta}_k$ is taken from the sequence $\bar{\beta}_k, k=2, \dots, 27$ in order to provide stability of calculation.

For discussed iterative method it is taken into account possible situating the spectrum in the neighbourhood of 0. Thus the errors corresponding both to the kernel of operator P and to the eigenfunctions associated with the eigenvalues belonging to $[-\lambda_2 \text{tg}^2 \frac{\pi}{10^8}, \lambda_2]$ are diminished regularly (every 9-10 iterations).

Let $\lambda_1=1$, then the method will be convergent, if the spectrum of P (with the exception of λ_1) lies on an ellipse with the foci at the points $m = -\lambda_2 \text{tg}^2 \frac{\pi}{10^8}$, $M = \lambda_2$, and if the point $(\lambda_1, 0)$ lies on that ellipse.

In the PERMAK code the following array of parameters $t_k, k=1, \dots, 30$, is used:

1., 0., 0.866025404, -0.866025404,
 0.6427876097, -0.6427876097, 0.342020143, -0.342020143,
 0.9848077530, -0.9848077530, 1., -0.11609291412,
 0.4487991802, -0.4487991802, 0.802123192, -0.80212319276,
 0.9579895123, -0.9579895123, 0.549508978, -0.54950897808,
 1., 0.1160929141, 0.918216106, -0.91821610688,
 0.7273736415, -0.727373641, 0.230615807, -0.2306158074,
 -0.9983081582, 0.99830815828

The values of $\bar{\beta}_k$ are calculated by formula (5.4.20) with utilising the t_k parameter array. Here $\bar{\beta}_k=0$ corresponds to $t_k=1$, and other t_k values are taken in the corresponding order.

2) The method using two previous iterations.

We consider it when assumptions (5.4.19) holds. Then let:

$$\phi^{n+1} = \alpha_{n+1} P \phi^n - \beta_{n+1} [\phi^n - \phi^{n-1}] \quad (5.4.21)$$

where $\beta_1=0$, $\alpha_1 = \frac{2}{(2-\sigma)}$, and $\sigma = \lambda_2/\lambda_1$ is so called "dominance ratio", and:

$$\alpha_k = \frac{4T_{k-1} \left[(2-\sigma)/\sigma \right]}{\sigma T_k \left[(2-\sigma)/\sigma \right]}, \quad \beta_k = \frac{T_{k-2} \left[(2-\sigma)/\sigma \right]}{T_k \left[(2-\sigma)/\sigma \right]},$$

Method (5.4.21) requires that vectors ϕ^n , ϕ^{n-1} be stored in the memory.

To use methods (5.4.18), (5.4.21) effectively we need good evaluations for λ_2 and λ_2/λ_1 . It is difficult to obtain these evaluations beforehand. Some simple and rough approaches are:

- to determine λ_1 and λ_2 from some geometric approach,
- to solve the problem corresponding to homogenized model in advance,
- to use Bauer's iterations to determine ϕ_1 , ϕ_2 and λ_1 , λ_2 from the solution of the corresponding problem with the rough grid (Apokorina, Knyazev, 1986).

Operator P is not a self-adjoint operator. To determine λ_1 and λ_2 we apply the method of moments, associated with using linear functionals. Let $l_k(\varphi)$, $k=1, m$ be a line-independent system of linear functionals and the eigenfunctions φ do not belong to their kernels. Then taking fixed value $\bar{\lambda}_2 < \lambda_2$ the first iterations are performed with using this value by means of

Eqs. (5.4.18) and (5.4.21) with $\lambda_2 = \bar{\lambda}_2$, and with calculating the values of $l_k(\phi^{n+1}), \dots, l_k(\phi^{n=m-1})$. Here $k=1, \dots, m$.

Approximating ϕ by the members containing functions $\varphi_1, \varphi_2, \dots, \varphi_m$, we obtain the system of the moment equations to determine an approximate values of λ_1, λ_2 :

$$\sum_{i=1}^m B_{ij}^n \lambda_1^k = C_{kj}^n, \quad (5.4.22)$$

where $j = 1, \dots, m$; $k=0, 1, \dots, m$.

In this system the coefficients $C_{kj}^n = l_k(\phi^{n+j})$ are known. They are calculated by utilising the linear functionals and the β_k parameters. As may be shown, the values ($\lambda_1, i=1, \dots, m$) are the roots of the certain algebraic equation of degree m . Thus, having determined exactly the value of λ_2 , we continue the iterative process with that value of λ_2 . The λ_1 value is also calculated from Eqs. (5.4.22).

PERMAK-Y code algorithm. In PERMAK-Y code $m=4$ was taken. The calculations show that for the individual iterations (5.4.18), (5.4.21) λ_1 (the solutions of system (5.4.22)) may be complex or negative. However it influences weakly determination of the main eigenvalue.

The grid points are reordered in the following way. From the set of the points we remove those in which the fission source S equals 0. The other points are renumbered, saving the same order of points.

Let us define the linear functionals in the form:

$$\begin{aligned} l_1(\phi) &= A(S) = \sum_{i=1}^{NT} S_i A_i, & l_2(\phi) &= d(S) = \sum_{i=1}^{NT} S_i D_i, \\ l_3(\phi) &= C(S) = \sum_{i=1}^{NT} S_i C_i, & l_4(\phi) &= f(S) = \sum_{i=1}^{NT} S_i F_i, \end{aligned}$$

where S_i is the fission source at point i for the outer iteration n , and NT is the total number of points.

Let $x = (1 - (i-1)/NT)$, $NT \geq i \geq 1$, where i -running index of the point.

Then we take:

$$\begin{aligned} A_1 &= 1, & D_1 &= 2x^2(4x^2 - 2), \\ C_1 &= 2x^2((4x^2 - 2)^2 - 2), & F_1 &= 2x^2(4x^2 - 2)((4x^2 - 2)^2 - 2). \end{aligned}$$

Now the system of nonlinear equations (5.4.22) may be obtained. For this purpose, let us represent the approximations ϕ^k obtained in the form:

$$\phi^k = \sum_{i=1}^4 a_i \phi_i \quad \text{and} \quad \alpha_i = l_1(\phi^{k+1/2}).$$

Then, after 4 iterations, we obtain:

$$\begin{aligned} \phi^{k+1/2} &= \sum_{i=1}^4 a_i \lambda_i \phi_i \\ \phi^{k+3/2} &= \sum_{i=1}^4 a_i \lambda_i \frac{(\lambda_i - \beta_1)}{(\alpha_i - \beta_1)} \phi_i \\ \phi^{k+5/2} &= \sum_{i=1}^4 a_i \lambda_i \frac{(\lambda_i - \beta_1)(\lambda_i - \beta_2)}{(\alpha_i - \beta_1)(\alpha_i - \beta_2)} \phi_i \\ \phi^{k+7/2} &= \sum_{i=1}^4 a_i \lambda_i \frac{(\lambda_i - \beta_1)(\lambda_i - \beta_2)(\lambda_i - \beta_3)}{(\alpha_i - \beta_1)(\alpha_i - \beta_2)(\alpha_i - \beta_3)} \phi_i, \end{aligned} \quad (5.4.23)$$

because we always require that the solutions ϕ^j should be normalized so that $l_1(\phi^j) = \text{const} = \gamma$. Calculating functionals $l_j(\phi)$, $j=1,2,3,4$, we obtain the general moment system:

$$\begin{aligned} \sum_{i=1}^4 B_{ij} &= h_{0j} \\ \sum_{i=1}^4 B_{ij} \lambda_i &= h_{1j} \\ \sum_{i=1}^4 B_{ij} (\lambda_i - \beta_1) \lambda_i &= h_{2j} \\ \sum_{i=1}^4 B_{ij} (\lambda_i - \beta_1)(\lambda_i - \beta_2) \lambda_i &= h_{3j} \\ \sum_{i=1}^4 B_{ij} (\lambda_i - \beta_1)(\lambda_i - \beta_2)(\lambda_i - \beta_3) \lambda_i &= h_{4j}, \end{aligned} \quad (5.4.24)$$

where $B_{ij} = a_i l_j(\phi^i)$, $h_{ij} = l_j(\phi^{k+1/2})$, $i=1,3,5,7$.

Transforming system (5.4.24) to the form (5.4.22) and taking into account $B_{ij}^n = B_{ij}$ we get:

$$C_{0j}^n = h_{0j}, \quad C_{1j}^n = h_{1j}, \quad C_{2j}^n = h_{2j} + \beta_1 h_{1j}, \quad C_{3j}^n = h_{3j} + (\beta_1 + \beta_2) h_{2j} + \beta_1^2 h_{1j},$$

$$C_{4j}^n = h_{4j} + (\beta_1 + \beta_2 + \beta_3) h_{3j} + (\beta_1^2 + \beta_2^2 + \beta_1 \beta_2) h_{2j} + \beta_1^3 h_{1j}.$$

For any j system (5.4.22) is the moment system with unknowns B_{1j} and λ_1 , $i=1,2,3,4$. Excluding B_{1j} , we obtain the system of linear equations with symmetric functions of the roots:

$$\sigma_1 = \sum \lambda_1, \quad \sigma_2 = \sum \lambda_1 \lambda_j, \quad \sigma_3 = \sum \lambda_1 \lambda_j \lambda_k, \quad \sigma_4 = \lambda_1 \lambda_2 \lambda_3 \lambda_4. \quad (5.4.23)$$

If $f_1 = (-1)^1 \sigma_1$, then:

$$C_{0j}^n f_4 + C_{1j}^n f_3 + C_{2j}^n f_2 + C_{3j}^n f_1 + C_{4j}^n = 0, \quad j=1,2,3,4 \quad (5.4.25)$$

Solving system (5.4.25), we determine the values λ_1^n as the roots of equation:

$$\lambda^4 + f_1 \lambda^3 + f_2 \lambda^2 + f_3 \lambda + f_4 = 0 \quad (5.4.26)$$

The system (5.4.26) for a poor choice of the functionals l_k may be an ill-conditioned system of linear equations (when $n \rightarrow \infty$). Therefore to find the solution we apply the following method of regularization consisting of two steps.

First, using the first equation of the system (5.4.25) (if $j=1$), we exclude the unknown f_1 from the other equations. The system of equations for $\tilde{f} = (f_1, f_2, f_3)$ may be rewritten in the form:

$$\tilde{C} \tilde{f} = \tilde{\delta} \quad (5.4.27)$$

It may be singular.

As a result we consider the following system regularized:

$$(\tilde{C}^* \tilde{C} + \alpha I) \tilde{f} = \tilde{C}^* \tilde{\delta} \quad (5.4.28)$$

where $\tilde{C}^*$ -matrix adjoined to $\tilde{C}$, and α is a small positive parameter (in the PERMAK code $\alpha=10^{-4}$).

Then we determine the unknown f_1 value from the first of (5.4.25) equations and solve Eq. (5.4.27) by Ferrari's method utilising the values of f_1, f_2, f_3, f_4 obtained. From the 4 roots we take the real root close to the value C_{41} (non-accelerated value of λ_1). This regularization method allows one to obtain the value $\lambda_1 = \lambda_1$, if the system of equations is singular ($\tilde{C}=0, \tilde{\delta}=0$) for $n \rightarrow \infty$.

Now the system of nonlinear equations (5.4.22) may be obtained. For this purpose, let us represent the approximations λ_1^n obtained in the form:

5.5 ON THE IMPROVEMENT OF TRADITIONAL FINITE DIFFERENCE EQUATIONS

As was mentioned in Section 5.1. there are a number of reasons for the inaccuracy of the simplest finite difference equations (5.2.3):

a) Application of the diffusion equation (5.2.1) and homogenization theory is not sufficiently grounded for calculation of nonuniform heterogeneous WWER type lattices (see Chapters 2, 6 and 7).

b) Obviously the simplest finite difference equation (5.2.3) which is based on (5.2.1) is not accurate enough when the cell size is of the same order as the neutron diffusion length. This problem can be solved mathematically and the required accuracy can be achieved by using a more complicated balance equation than simplest finite difference equation. But the balance equation improvement will be largely useless until the initial equation (5.2.1) is not improved.

c) Obviously the neutron spectrum in the cell depends on the environment. The question is whether or not this effect will be taken into account using the four group finite difference approximation (5.2.3) of equation (5.2.1). This problem is discussed below.

As mentioned in Chapter 3, in Bonalumi's homogenization theory the neutron spectrum was proposed to be approximated in each group for the same cells in different environments by superposition of two spectra: asymptotic and transient.

$$\Phi(r, E) = \varphi_{\infty}(r, E) + a\varphi_t(r, E)$$

where a is an unknown factor.

Let us consider this approximation only for thermal neutron group for which spectral deformation is most important. This approximation gives the following correlation between average group neutron flux and two spectrum components averaged with regard to energy and volume.

$$\bar{\Phi} = \bar{\varphi}_{\infty} + a\bar{\varphi}_t$$

where

$$\bar{\varphi}_{\infty} = q / \bar{\Sigma}_{\infty},$$

q and $\bar{\Sigma}_{\infty}$ are neutron source and asymptotic absorption cross section.

The average cross section of each reaction can be expressed as:

$$\bar{\Sigma}^{(x)} = \bar{\Sigma}_{\infty}^{(x)} R_x (\bar{\varphi}_{\infty} / \bar{\Phi}) \quad (5.5.1)$$

where

$$R_x (\bar{\varphi}_{\infty} / \bar{\Phi}) = \frac{\bar{\varphi}_{\infty}}{\bar{\Phi}} + (\bar{\Sigma}_t^{(x)} / \bar{\Sigma}_{\infty}^{(x)}) (1 - \frac{\bar{\varphi}_{\infty}}{\bar{\Phi}}) \quad (5.5.2)$$

Thus the variation of neutron spectrum causes changing of cross section by factor R_x which has a linear dependence on the relation $\bar{\varphi}_{\infty} / \bar{\Phi}$.

Following (Lehman, 1977) let us denote value $\bar{\varphi}_{\infty} / \bar{\Phi}$ as the spectral index. For determining the dependence of factor R_x on the spectral index the space spectral problem for cell with some environment should be solved in addition to the asymptotic problem. After that the linear coefficient $(\bar{\Sigma}_t^{(x)} / \bar{\Sigma}_{\infty}^{(x)})$ of factor R_x is calculated in the obvious way using (5.5.1) and (5.5.2).

M. Lehman (Lehman, 1979) generalizes the application of the spectral index algorithm to employment for the case of nonlinear dependence of R_x on $\bar{\varphi}_{\infty} / \bar{\Phi}$. He proposes that the spectral index in traditional codes be used for taking into account the influence of cell environment. In equation (5.2.3) the cross sections are described as (5.5.1) and the balance equation transforms to a nonlinear equation. Cross sections and their dependence on spectral index are previously tabulated on the base of solving of model problems set.

The spectral index method is widely used in some of the codes developed by TIC experts. However this method does not solve all the problems concerning the accuracy of fine mesh equations (see Chapters 6 and 7).

5.6 THE MAIN FEATURES OF SOME DIFFUSION CODES

HEXAB [562] - this is a family of codes for 2D and 3D fine mesh neutron flux calculations for cores with a hexagonal lattice. Problems are solved for 30° sector of core symmetry. Irregularity of mesh on real

assemblies structure calculations is taken into account.

Flux logarithmic derivatives for each group are used on the outer core boundary.

The problem of effective multiplication factor K_{eff} and the corresponding eigenfunction determination is solved.

For inner iteration acceleration both the two sweep iterative technique AGA (Woznitski, 1973, Apostolov, Woznitski, 1975) and double successive over relaxation procedure AGA DSOR (Woznitski, 1983) are used.

FLEX [556] - is a 2D hexagonal fine mesh diffusion code for flux and adjoint function calculation in a core with 30° , 60° , 120° and 180° rotational symmetry. The use of an irregular mesh on assembly boundaries is possible.

On the outer core boundary for each neutron group and for each cell (or group of cells) the following boundary conditions are set:

$$\nabla_n \Phi + \beta \Phi = 0,$$

where $\nabla_n \Phi$ denotes the surface flux normal derivative.

Calculations using the "spectral index" method are possible.

HEXAGA (Woznitski, 1973, Apostolov, Woznitski, 1975, Woznitski Z. 1983) - 2D (**HEXAGA-III**) and 3D (**HEXAGA-III-120** and **30**) multi group diffusion codes. Regular triangular mesh in radial core cross section and arbitrary user given mesh step in axial direction are used. **HEXAGA-III** defines discrete real or adjoint solution of multi group stationary diffusion equations using the two sweep iterative method AGA combined with the successive over relaxation method. The calculational region is defined for **HEXAGA-III-120** as a 120° sector and for **HEXAGA-III-30** as a 30° sector of the core.

PERMAK (Lizorkin et. al. 1985, Lizorkin et. al. 1988) - 2D fine mesh few group hexagonal diffusion code for neutron flux and adjoint function calculation in the core with arbitrary symmetry. Calculation of pin by pin power distribution problems taking into account fuel burnup and feedback is possible. The "compression factor" is used to take into account mesh irregularity in the gaps between assemblies.

There are two ways to obtain higher accuracy calculations with **PERMAK**. In the first option three groups are used to describe the neutron trivialization region (full number of group equals to six) simultaneously

with a neutron balance scheme mathematical correction taking into account a small value of diffusion length to mesh step relation. The second way utilizes the nodal balance equation and presentation of thermal group by superposition of asymptotic and transient modes of flux (see section 6.2.3).

There are some code versions with different methods of iterative procedure acceleration (e. g. methods described in Section 5.4).

BRETISLAV [547] - 2D hexagonal code for neutron flux and adjoint function calculations taking into account mesh irregularity. Either effective multiplication factor or moderator critical level is calculated.

Problems with ten different core symmetry types can be solved.

Mesh irregularity can be taken into account using one of five different algorithms selected by the user. The modified Borresen scheme is used in two of the simplest algorithms. The algorithm described in section 5.3 is also available.

It is possible to solve problems using equation coefficients which are set parametrically.

The use of the following form of boundary conditions is available

$$\nabla_n \Phi^{(k)} + \sum_l \beta^{(k,l)} \Phi^{(l)} = 0,$$

where k and l - group numbers.

Convergence of iterative procedure is accelerated using the Gauss Seidel method combined with the over relaxation method for inner iterations and the Chebyshev method combined with Lusternik method for outer iterations. Four modifications of Chebyshev method are available and one of them should be selected by the user.

MOBY-DICK [551] - code package which includes the code **BORORO** (Krysl, Lehman, 1978) which is intended for few group fine mesh diffusion equations solving. Triangular, hexagonal or square mesh may be used.

The "compression factor" is used to take into account mesh irregularity without changing the diffusion coefficient.

Boundary conditions for the flux are set in the form

$$\nabla_n \Phi + \beta \Phi = 0$$

where β - is a nondiagonal matrix. Non-homogeneous boundary conditions

cannot be used.

Effective multiplication factor, critical moderator level, critical concentration of liquid boron acid or critical position of control rods can be defined using *MOBY-DICK*.

The Borresen approximation (Borresen, 1973) is used to represent the differential operator of diffusion equation.

Convergence of inner iterations is accelerated using SOR (successive over relaxation). For outer iterations some modifications of the Chebyshev method are used. The over relaxation factor is calculated on the first outer iteration.

The "Spectral index" method is available in the code for taking into account the influence of the environment on the thermal neutron spectrum in the cell. In this case, the nonlinear diffusion equation is solved. No correction of balance equation is connected with the mesh step size.

The *PERMAK* code is also included in the code package. This code is used for pin by pin power distribution analysis (on core burning and for some states or transient processes analysis).

SISSY (Koch, 1976) - 3D multi group code.

The calculated core is divided into axial layers. In the axial direction the properties of the substance are not changeable for a given layer. For each layer the two dimensional flux distribution is defined using finite difference diffusion code *MNATA* for 30^0 symmetry sector of core cross section.

On solving the synthesis equations system, the power method or Vilandt method is used. The eigenvalue is not estimated. For the Vilandt method it is required that the estimated eigenvalue should be set as an input parameter. For the iterative procedure the linear equations system should be solved. In that there are only a relatively small number of unknowns (some hundreds) it means that a direct algorithm can be used its solution using the Gauss method.

FEM-3D (Mai, 1980) - 3D multi group diffusion code based on finite element method. The core is divided into N prisms with triangle as its base. The sequence of calculations is as follows: input of initial data, definition of subregions and distribution of constants, preparing of matrix, iterative procedure, treatment of results.

Convergence of outer iterations is accelerated using Chebyshev polynomials. The linear equation system is solved using the method of adjoint gradients.

OSKAR (Gaertner, 1980) - hexagonal diffusion code with 9-point discretization of differential operator of diffusion equation. A triangular mesh is used. 60° , 120° , 180° or 360° core symmetries may be calculated. Arbitrary boundary conditions (with some small limitation) can be set. For the outer iteration, combined Chebyshev and Lusternik acceleration is used. The special algorithm is used to solve the three dimensional one group equation.

5.7 COMPARISONS WITH EXPERIMENTAL DATA

5.7.1 The simplest finite difference calculations using traditional neutron cross sections

Some examples of comparison of calculational and experimental pin by pin power distributions are demonstrated in figures 5.2-5.7. Calculated values of effective multiplication factor are presented. The deviations of calculational and measured power distribution for 30° core symmetry of ZR-6 critical facility described in (Experimental Investigations ..., 1985) are presented either.

Calculations have been carried out by PERMAK using the traditional asymptotic four group neutron cross sections prepared by UNIRASOS code. The use of any other simple finite difference code with asymptotic cross sections (prepared by one of spectral codes mentioned in Chapter 4) gives similar results.

The figures show that inaccuracy of calculation of effective multiplication factor in some cases reaches and exceeds 1%. Errors of power distribution near absorbers and reflector reaches about 10%. In asymptotic regions the error as a rule is not greater than 2-3%. The explanation of the inaccuracy is given from different points of view along with the ways for its improvement in Chapters 3, 6, 7 and in section 5.5 of this book.

fig 5-2

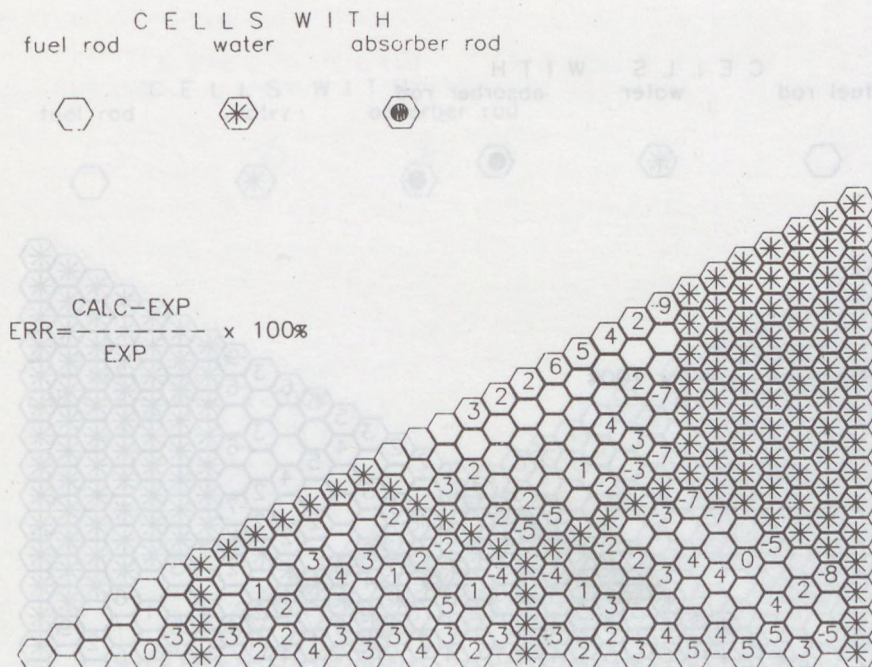


Fig. 5.2 ZR-6 critical facility. Configuration 101/100.
 An accuracy of PERMAK calculation using traditional balance equation.
 Calculated $K_{eff} = 0.9980$.

fig 5-3

C E L L S W I T H
fuel rod water absorber rod



$$ERR = \frac{CALC - EXP}{EXP} \times 100\%$$

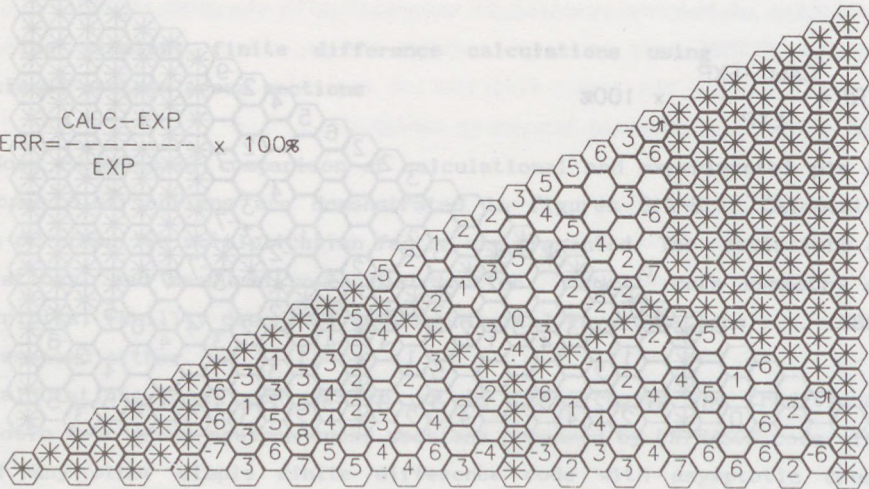


Fig. 5.3 ZR-6 critical facility. Configuration 102/102.
An accuracy of PERMAK calculation using traditional balance equation.
Calculated Keff=0.9998.

fig 5-4

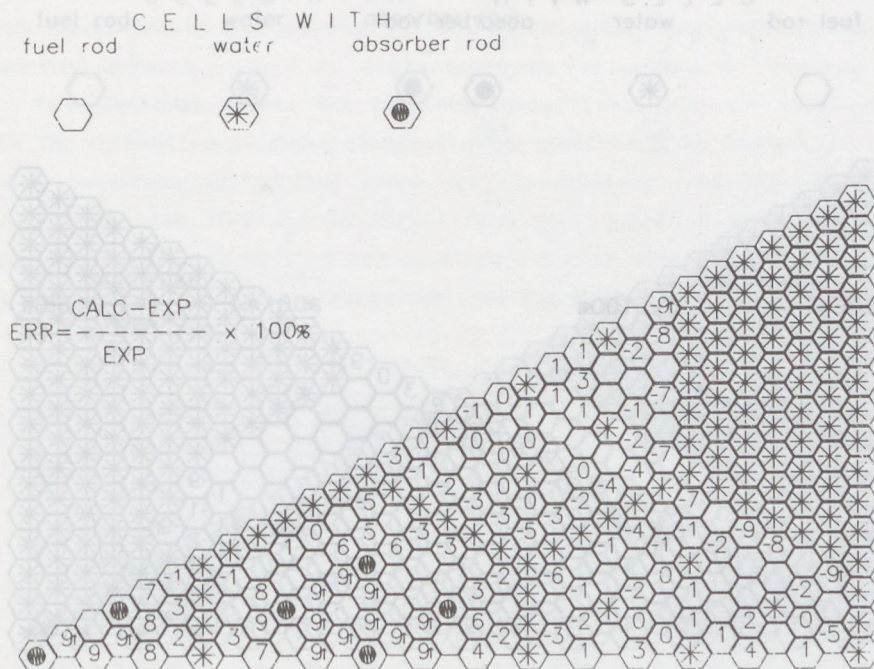


Fig. 5.4 ZR-6 critical facility. Configuration 103/103.
 An accuracy of PERMAK calculation using traditional balance equation.
 Calculated $K_{\text{eff}} = 0.9988$.

fig 5-5

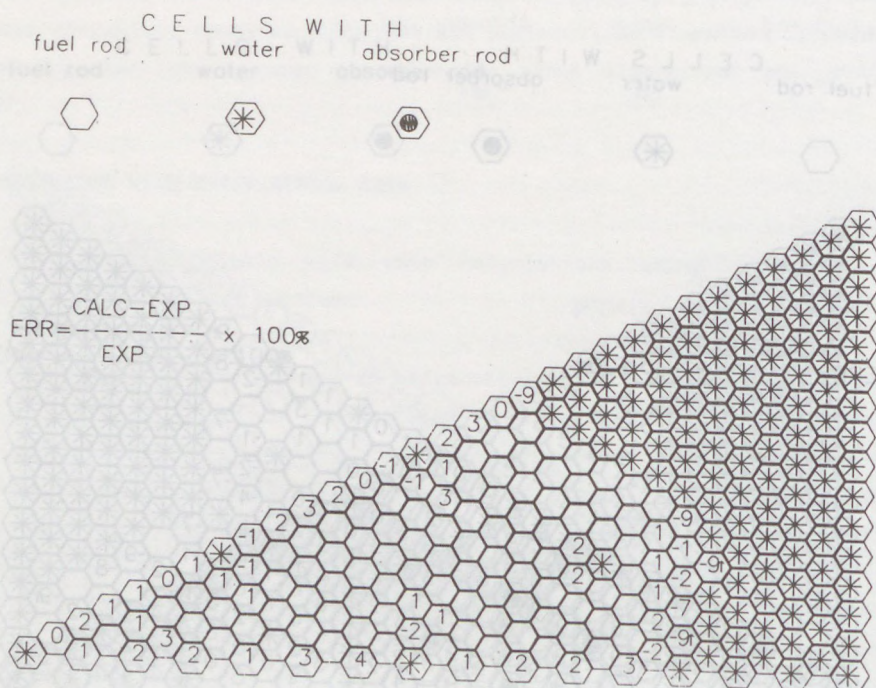


Fig. 5.5 ZR-6 critical facility. Configuration 57/57.
 An accuracy of PERMAK calculation using traditional balance equation.
 Calculated $K_{\text{eff}} = 1.0054$.

fig 5-6

CELLS WITH
fuel rod water absorber rod

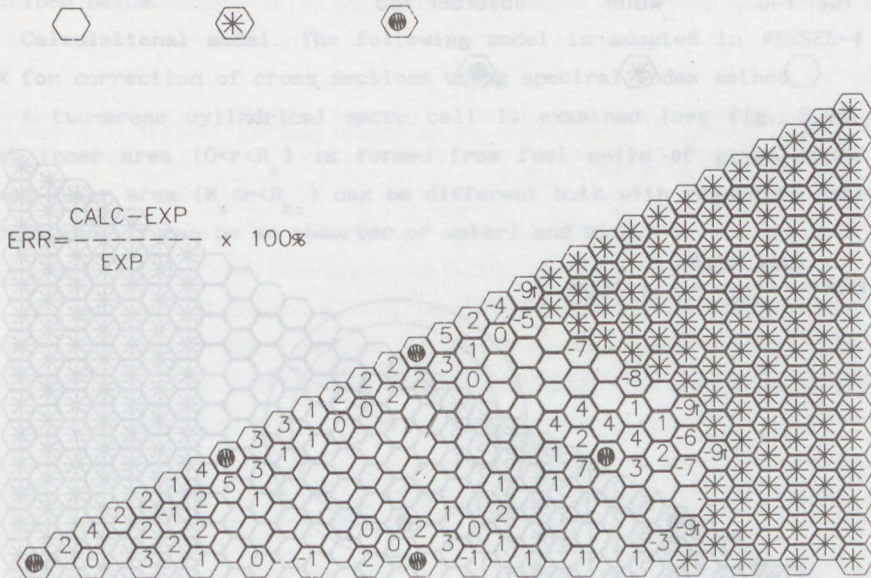


Fig. 5.6 ZR-6 critical facility. Configuration 58/57.

An accuracy of PERMAK calculation using traditional balance equation. Calculated K_{eff} = 1.0125.

fig 5-7

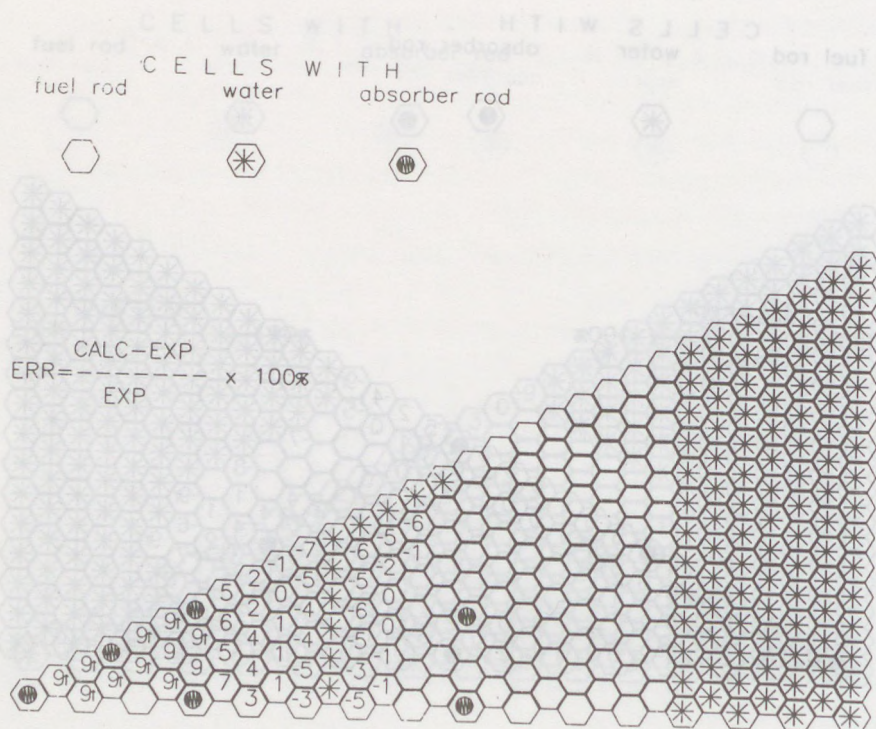


Fig. 5.7 ZR-6 critical facility. Configuration 90/87.
 An accuracy of PERMAK calculation using traditional balance equation.
 Calculated $K_{eff} = 1.0073$.

5.7.2 Spectral index method in FLEX

An example of using of spectral index method (see section 5.5 and references [557, 565]) in *FLEX* code is presented in this section. Spectral index method allows one to carry out more accurate calculations by means of the traditional finite difference approximation. In Chapter 3 it was shown that the same effect should be expected in the case of non asymptotic cross sections in regions near absorbers, reflector and water holes.

There are different realizations of spectral index method in different codes developed by TIC experts in some cases with fewer limitations than described below.

Computational model. The following model is adopted in *NESSEL-4* and *FLEX* for correction of cross sections using spectral index method.

A two-areas cylindrical macro cell is examined (see fig. 5.8). The first inner area ($0 < r < R_z$) is formed from fuel cells of given type. The second outer area ($R_z < r < R_{Mz}$) can be different both with regard to material composition (it can be an absorber or water) and size.

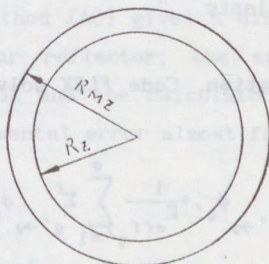


Fig.5.8 Macrocell structure.

Macro cell parameter determination is realized in two homogenization steps.

The first step. Multi group spectral spatial problem is solved for heterogeneous fuel cell with boundary condition $\left. \frac{\partial \phi}{\partial n} \right|_{z=R} = 0$, the cell is homogenized and multi group constants are obtained.

The second step. Macro cell with radius R_{Mz} is calculated. Multi group calculation is carried out using the multi group homogenized constants previously defined for the inner region in the first step. Reflective

boundary condition is set on the outer macro cell boundary. Thus the changing of multi group spectrum in inner region is taken into account as a function of environment selection.

Few group homogenized constants for selected subregions of macro cell are obtained using a multi group spectrum calculated in the second step. Few group constants of inner region depend on multi group spectrum perturbation caused by the outer region.

Different sets of few group constants of inner region can be obtained by varying the size of the outer region. Let us approximate the dependence of constant on environment as a function of spectral index χ defined as the relation of epithermal to thermal neutron flux in the inner region.

$$\chi = \frac{\phi_{ep1}}{\phi_{therm}} \quad (5.7.1)$$

A polynomial function is selected as an approximating function to describe the cross section dependence on χ .

$$\sum_g^x = \sum_g^x (\chi) = \sum_{n=0}^3 a_n \chi^n \quad (5.7.2)$$

where a_n are polynomial coefficients.

Model of fine mesh calculation. Code FLEX solves fine mesh diffusion equation

$$\nabla D_g \nabla \phi_g - \left(\Sigma_g^r + B_z^2 D_g \right) \phi_g + \sum_{g'=1}^{g-1} \Sigma_{g' \rightarrow g}^s \phi_{g'} + \frac{1}{K_{eff}} \sum_{g'=1}^g \Sigma_{g' \rightarrow g}^f \phi_{g'} + Q_g^a = 0 \quad (5.7.3)$$

Axial leakage is described using axial buckling B_z^2 .

In each cell position $\vec{L}$ the spectral index $\chi^F(\vec{L})$ is defined.

$$\chi^F(\vec{L}) = \frac{\sum_{g=1}^3 \phi_g(\vec{L})}{\phi_{th}(\vec{L})} \quad (5.7.4)$$

Local cross sections $\Sigma_g(\vec{L})$ are obtained using definition (5.7.2) for $\Sigma_g(\chi)$ and definition (5.7.4) for local value of $\chi^F(\vec{L})$. Thus for each cell in the core the few group cross sections are defined corresponding to local value of spectral index.

Results. Values of effective multiplication factors for some of core configurations of ZR-6 with different pin steps (11.0, 12.7, 19.05 mm) are presented in table 5.5.1. Calculations have been carried out using both the traditional method with asymptotic cross sections and the spectral index method. Corresponding results of traditional PERMAK calculations are given above for some of these core configurations.

Results show that correction on spectral index method improves the accuracy up to 0.1 - 0.2% in value of effective multiplication factor. Improvement of accuracy depends on core size and variations of spectrum hardness in fuel cells. The more cells represent perturbation or the smaller is the core, the larger is the spectral index correction in K_{eff} because the share of spectral perturbed cells is larger.

The influence of spectral index method correction on power distribution for three different core configurations is presented in figs. 5.9-5.11. The relative accuracies of corrected and traditional calculations are compared. Comparison for uniform core 154/154 with reflector is given in fig. 5.9. In figures 5.10 and 5.11 there are presented results for configurations which imitate assemblies core structure.

The traditional method (AC) gives a difference of up to 10% from the measured pin power near reflector; the spectral index method gives a difference of up to 2-3% and the calculated power distribution is within the range of the experimental error almost for all pins.

1200.1	0000.0	48.82	105\105	0.0-8.5-20.81
8000.1	8800.0	48.43	504\504	
0000.1	8000.1	48.34	808\808	
8888.0	8888.0	48.41	505\505	

Fig. 5.5 - ZR-6 critical factor calculations for 154/154 - 3A
An accuracy of 1% calculation
Upper figures - using of spectral index method
Lower figures - traditional asymptotic calculation

Table. 5.5.1 Values of K_{eff}

Lattice	Configuration	$B_z^2 10^4$	Method	
			SI	AC
12.7-3.6-0.0	154/154	18.21	0.9985	0.9937
R91/H ₂ O	101/100	64.62	0.9998	0.9927
	102/102	45.18	1.0004	1.0032
11.0-3.6-0.0	191/191	12.63	1.0015	1.0022
	192/192	10.90	1.0010	1.0014
	193/193	9.77	1.0005	1.0011
	195/195	8.22	0.9997	1.0004
	196/196	7.40	0.9993	1.0001
19.05-3.6-0.0	201/201	59.64	0.9990	1.0051
	204/204	43.89	0.9988	1.0038
	205/205	35.34	1.0008	1.0030
	207/207	14.98	0.9995	0.9998

Notice: AC - asymptotic calculations

SI - spectral index calculations

fig 5-10

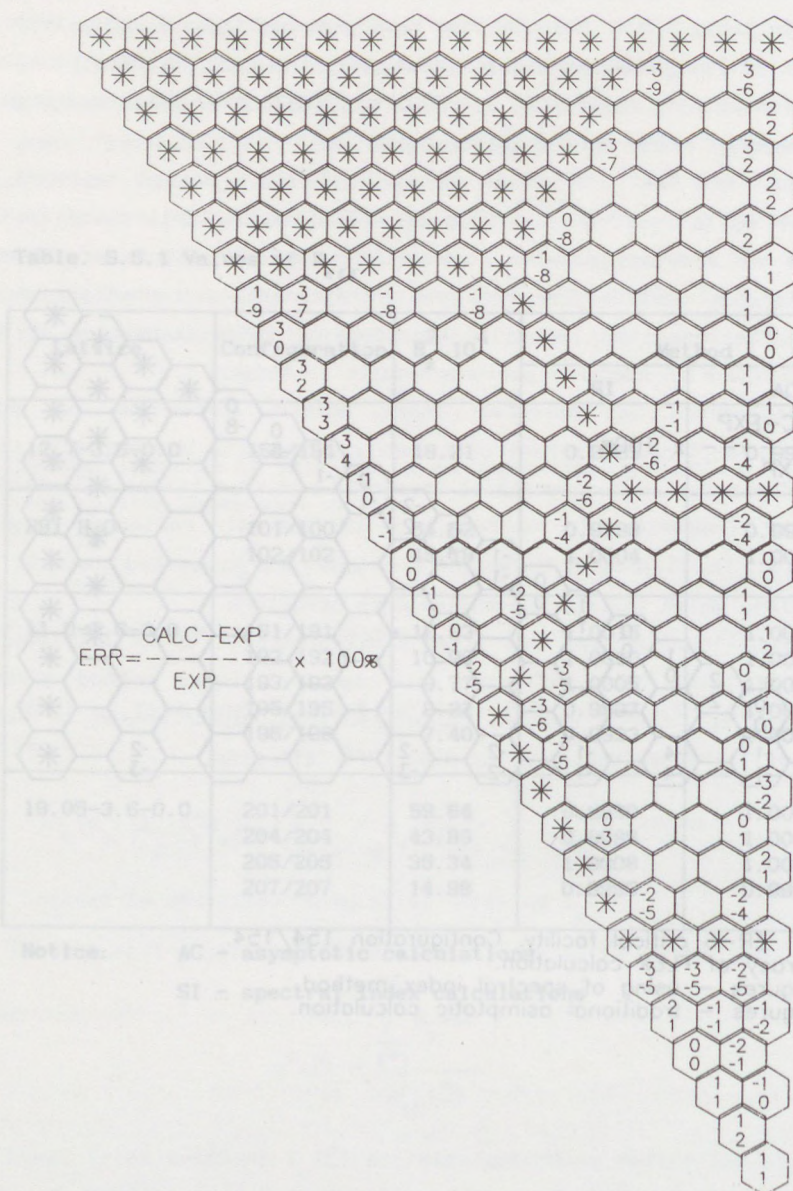


fig 5-11

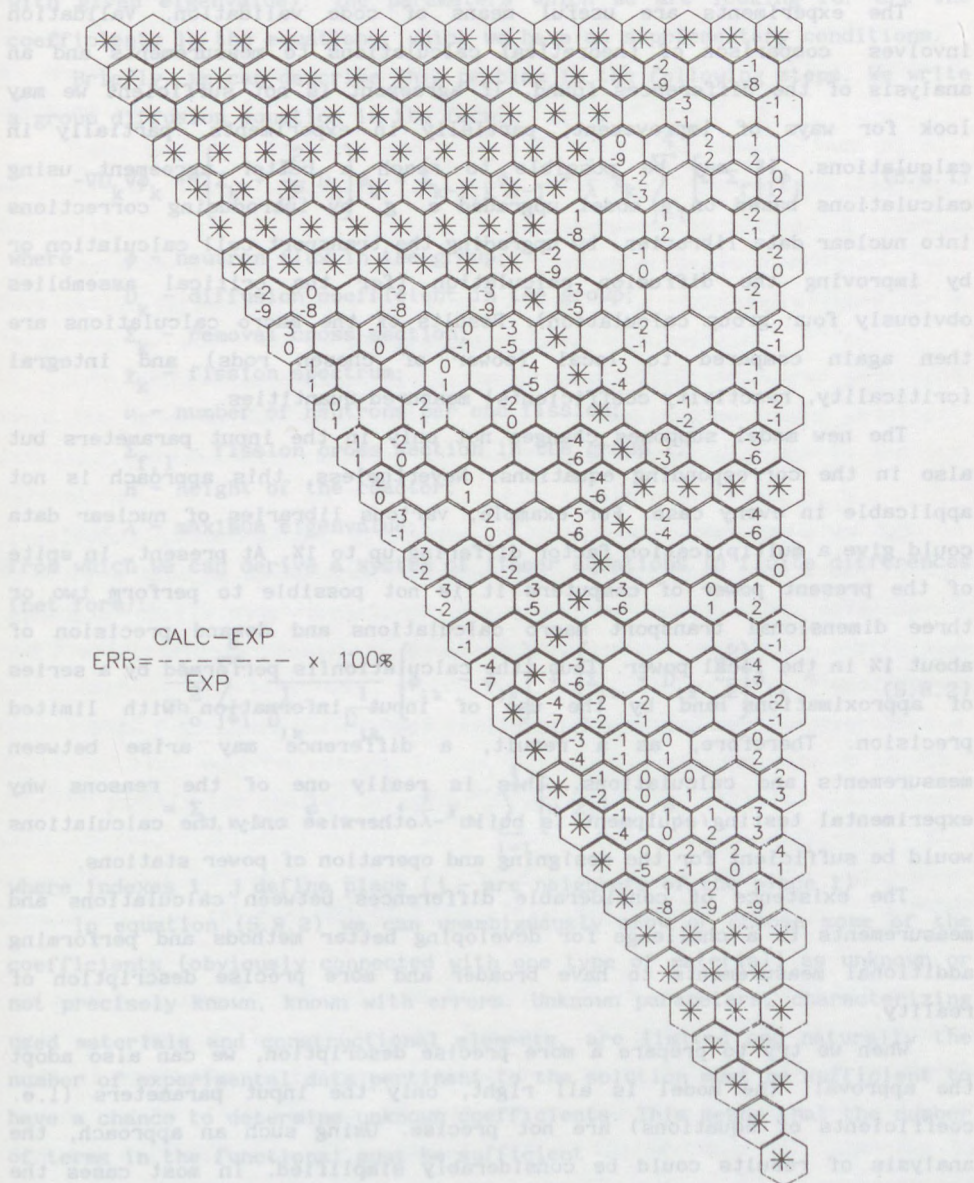


Fig. 5.11 ZR-6 critical facility. Configuration 102/102.
 An accuracy of FLEX calculation.
 Upper figures — calculation on spectral index method.
 Lower figures -- traditional asymptotic calculation.

5.8 CORRECTION OF EQUATION BASED ON EXPERIMENTS

The experiments are useful means of code validation. Validation involves comparison of theoretical calculations to measurements and an analysis of the differences found. If agreement is not sufficient we may look for ways of improvement, partially in experiments, partially in calculations. It may be possible to reach a better agreement using calculations based on a model upgraded e. g. by introducing corrections into nuclear data libraries, by upgrading the transport cell calculation or by improving the diffusion calculation (for the critical assemblies obviously four group calculation). Results of the macro calculations are then again compared to local (power of chosen rods) and integral (criticality, reactivity coefficients) measured quantities.

The new model supposes changes not only in the input parameters but also in the corresponding equations. Nevertheless, this approach is not applicable in every case. For example, various libraries of nuclear data could give a multiplication factor differing up to 1%. At present, in spite of the present power of computers it is not possible to perform two or three dimensional transport macro calculations and demand precision of about 1% in the local power. Thus, the calculation is performed by a series of approximations and by the use of input information with limited precision. Therefore, as a result, a difference may arise between measurements and calculations. This is really one of the reasons why experimental testing equipment is built - otherwise only the calculations would be sufficient for the designing and operation of power stations.

The existence of considerable differences between calculations and measurements is a challenge for developing better methods and performing additional measurements to have broader and more precise description of reality.

When we try to prepare a more precise description, we can also adopt the approval: the model is all right, only the input parameters (i.e. coefficients of equations) are not precise. Using such an approach, the analysis of results could be considerably simplified. In most cases the calculation for critical assembly is performed in the four group diffusion equations. If we formulate the agreement between calculations and measurements as a functional we obtain a complicated but exactly defined

variational problem - to minimize the functional with supplementary conditions (fulfillment of the system of partial differential equations with given eigenvalue). The parameters which we are looking for are the coefficients in the equations, which we have as supplementary conditions.

Briefly, we can describe this problem in the following steps. We write a group diffusion equation in the form:

$$-\nabla D_k \nabla \phi_k + \left[\Sigma_k + \frac{\pi^2}{H^2} D_k \right] \phi_k = \Sigma_{k-1,k} \phi_{k-1} + \frac{1}{\lambda} \chi_k \sum_{l=1}^4 \left[\nu \Sigma_f \right]_{l1} \phi_l \quad (5.8.1)$$

where ϕ - neutron flux in the group;

D_k - diffusion coefficient in the group;

Σ_k - removal cross section;

χ_k - fission spectrum;

ν - number of neutrons per one fission;

$\Sigma_{f,l}$ - fission cross section in the group l ;

H - height of the reactor;

λ - maximum eigenvalue;

from which we can derive a system of linear equations in finite differences (net form):

$$\begin{aligned} \frac{4}{3h_0^2} \sum_{j=1}^6 \frac{1}{\frac{1}{D_{1k}} + \frac{1}{D_{jk}}} \left(\phi_{1k} - \phi_{jk} \right) + \left[\Sigma_{1k} + D_{1k} \frac{\pi^2}{H^2} \right] \phi_{1k} = \\ = \Sigma_{1,k-1,k} \phi_{1,k-1} + \frac{1}{\lambda} \chi_{1k} \sum_{l=1}^4 \left[\nu \Sigma_f \right]_{l,1} \phi_{l,1} \end{aligned} \quad (5.8.2)$$

where indexes i, j define place (j - are neighbors of the place i)

In equation (5.8.2) we can unambiguously show or choose some of the coefficients (obviously connected with one type of material) as unknown or not precisely known, known with errors. Unknown parameters, characterizing used materials and constructional elements, are limited and naturally the number of experimental data pertinent to the solution must be sufficient to have a chance to determine unknown coefficients. This means that the number of terms in the functional must be sufficient

$$I = \sum_{\{p\}} \left[A_p^{\text{exp}} - N \sum_{l=1}^4 \Sigma_{f,p,l} \phi_{p,l} \right]^2 / \chi_p^2 + \left[\frac{1}{\lambda} \right] / \chi_\lambda^2 +$$

$$+ \sum_{r,s=1}^k W_{rs} \frac{\begin{bmatrix} x_r - x_{r0} \\ x_{r0} \end{bmatrix} \begin{bmatrix} x_s - x_{s0} \\ x_{s0} \end{bmatrix}}{x_{r0} x_{s0}} \quad (5.8.3)$$

where p - number of measurements;

N - normalization factor;

λ - eigenvalue;

A_p^{exp} - experimental value in the place i ;

χ_λ - artificially chosen error of the eigenvalue;

κ_r - unknown parameters;

κ_0 - initial estimation of κ ,

w_{rs} - correlation matrix of κ_r .

If we also take into account reactivity measurements, functional (5.8.3) has a more complicated form and also includes an adjoint solution. To minimize (5.8.3) two methods were developed: generalized Lagrange multipliers and least squares method, based on direct calculation of flux derivatives.

The generalized Lagrange multipliers lead to the changing I by L

$$L = I + \int dV \psi^+ \left[R - \frac{1}{\lambda} S \right] \phi + q_\phi \int dV \Sigma_f \phi \quad (5.8.4)$$

where $\left[R - \frac{1}{\lambda} S \right] \phi$ is symbolically written equation (5.8.1).

Minimization L leads to the singular equation for Ψ^+ and so ϕ must be orthogonal to Ψ^+ . Having Ψ^+ , partial derivatives of L over κ_k give direction to the minimum of I . A considerable practical advantage is that we solve the equation only for one function Ψ^+ , independently of the number of unknowns. The disadvantage is that we have only one direction but not the distance to the minimum. This method has been proved also for the case when we do not know completely which coefficients should be changed.

Direct calculation of derivatives leads to the equations for $\partial \Phi / \partial \kappa$

$$R \frac{\partial \phi}{\partial x} - \frac{1}{\lambda} S \frac{\partial \phi}{\partial x} = \left[-\frac{\partial R}{\partial x} + \frac{1}{\lambda} \frac{\partial S}{\partial x} - \frac{1}{\lambda} \frac{\partial \lambda}{\partial x} S \right] \phi \quad (5.8.5)$$

which have formally the same structure and properties as those for Ψ^+ . Using (5.8.5) in the process of minimizing (5.8.3) we obtain equations for $\Delta\kappa$ which are often near singular equations due to correlations between unknowns and small influence of unknowns on the result.

These negative features and also time consuming calculations of all derivatives favour treatment by the method of generalized Lagrange multipliers.

Lagrange multipliers also treat very simply the tolerances of fuel fabrication parameters which can lead to remarkable changes in fluxes for a large reactor where the solution of equations is not stable.

Both methods are included in the program EQCOR which was developed from the program BRETISLAV [547]. In this new program newly developed iteration schemes were included for the singular equations for Ψ^+ and its derivatives.

Suitable experimental data were the collection of measurements done on ZR-6 (TIC, vol. I. 1985) critical facility.

Table 5.8.1 demonstrates the degree of improvement when using Czech and Russian four group data for uranium rods, 3.6% enrichment, water and boron carbide absorbing rods. Improvement is noticeable particularly for a complicated core like 90/87 where the mean errors decrease by more than a factor of six. Relative changes in the corrected parameters were up to 30%.

To justify the quality of corrected data, various cores of other types were chosen, including cores with boron acid in the moderator. The comprehensive information given in Table 5.8.2 shows that the calculated parameters give the best agreement with the experimental results.

Table 5.8.1 Comparison of experimental and calculated data

N	Measured values			Values calculated with:			initial Russian data corrected Russian data initial Czech data corrected Czech data							
	L	H _e	λ _e	H _c	λ _c	K _{eff} (H _e)	Δ	Δ _{max}	(***)					
									1%	2%	3%	5%	8%	
78	57.7	70.44	12.74	64.88	7.18	1.0238	3.07%	18.9%	48	31	26	13	7	
				71.37	13.67	0.9965	1.30%	6.8%	38	15	6	3	0	
				67.42	9.72	1.0124	2.50%	8.2%	57	39	23	11	2	
				72.45	14.75	0.9932	1.36%	7.6%	40	19	7	2	0	
60	31.4	44.33	12.93	43.52	12.12	1.0120	2.19%	10.7%	41	20	9	6	4	
				44.20	12.70	1.0020	1.30%	4.9%	32	13	3	0	0	
				44.57	13.17	0.9965	2.61%	7.4%	48	34	20	5	0	
				44.27	12.87	1.0009	1.16%	4.3%	31	9	5	0	0	
60	70.9	81.33	10.46	74.99	4.09	1.0172	6.19%	12.9%	54	50	46	40	25	
				85.93	15.03	0.9897	0.91%	2.3%	25	4	0	0	0	
				76.78	5.88	1.0122	5.45%	10.7%	55	49	45	33	15	
				84.67	13.77	0.9928	0.98%	2.5%	28	6	0	0	0	
10	25.8	39.08	13.24	38.39	12.55	1.0059	3.27%	10.3%	87	67	47	21	4	
				39.10	13.26	0.9996	1.03%	3.9%	42	13	5	0	0	
				39.32	13.48	0.9953	2.86%	7.8%	73	54	45	22	0	
				38.70	12.86	1.0075	0.91%	3.4%	40	10	2	0	0	
30	61.5	74.05	12.55	70.28	8.22	1.0127	1.46%	6.4%	18	7	3	1	0	
				72.84	11.34	1.0040	1.02%	3.8%	11	4	2	0	0	
				73.88	12.38	1.0005	1.71%	4.9%	20	10	4	0	0	
				75.03	13.53	0.9972	1.07%	3.1%	15	4	2	0	0	

Notice:

N - number of check points, λ - extrapolated length (cm),

L - critical moderator level (cm), Δ - average power deviation,

H - critical core height (cm), Δ_{max} - maximal power deviation,

(***) - number of points with deviations higher than ...

Table 5.8.2 Checking calculations

	Measured values			Values calculated with:			initial Russian data corrected Russian data initial Czech data corrected Czech data									
N	L	H _e	λ _e	H _c	λ _c	K _{eff} (H _e)	Δ	Δ _{max}	(***)							
									1%	2%	3%	5%	8%			
29	67.2	80	Configuraton 187	73.77	6.57	1.0182	7.51%	19.0%	26	26	24	21				
				81.11	13.91	0.9971	3.58%	13.0%	24	17	13	7				
				76.63	9.43	1.0094	5.98%	15.9%	28	25	23	16				
				84.06	16.86	0.9909	3.14%	12.1%	25	17	11	6				
127	67.25	81.15	13.9 Configuration 103/103	76.03	8.78	1.0133	8.25%	20.4%	124	118	108	9				
				86.15	18.9	0.9892	1.90%	6.7%	83	57	30	5				
				76.38	9.13	1.0127	5.16%	16.9%	111	99	85	61				
				82.15	14.9	0.9977	2.26%	6.7%	93	64	37	10				
65	40.1	53.37	13.2 Conf. 147/147			1.0006	2.61%	9.0%	54	33	25	7				
						1.0008	1.01%	3.2%	25	12	1	0				
131	51.38	63.44	12.8 Conf. 100/100	63.66	12.28	0.9989	3.04%	10.9%	103	72	57	27				
				63.61	12.23	0.9992	1.20%	4.5%	67	23	6	0				

Notice:

- only Czech data for configurations 147 and 100 are presented,
- the same notations are used as in Table 5.8.1.

Conclusion of editor.

Using calculations by Monte-Carlo method it was shown in Chapter 3 that even for simplest ZR-6 configurations the four groups cell constants depend on cell position. On the other hand, in Chapter 3 it was also shown that improvement of calculational results can be achieved by changing the definition of coefficients in the diffusion equation without changing the form of the finite difference equation. These new coefficients can have no such significant dependence on cell position as have traditional four group constants. Apparently the success of the above described correction is explained by the theoretical conclusion of Chapter 3. In this case the corrected constants cannot be considered as improved traditional four group constants of real cells as actually they are a new set of coefficients and have a new physical sense.

REFERENCES

- Apokorina V., Knyazev A. (1986).** Description of Program BIPR-5M, (in Russian)
- Апокорина В., Князев А.: Аннотация программы БИПР-5М. Вопросы атомной науки и техники, серия: Физика и техника ядерных реакторов, вып.5. М., 1986.
- Apostolov T., Woznicki Z. (1975).** HEXAGA-II-A 2D Diffusion Program for Many Group Calculation of Hexagonal Lattices, (in Russian)
- Апостолов Т., Вознишки З.: Диффузионная двумерная программа HEXAGA-П для многогрупповых расчетов гексагональных решеток. Атомная энергия, 6(38), стр. 372-374, 1975.
- Apostolov T., Petkov P. (1978).** Calculations by Program HEXAB-II-30 of TIC Model Problems for Diffusion Programs, (in Russian)
- Апостолов Т., Петков П.: Расчеты модельных задач ВМК для диффузионных программ с программой ХЕКСАБ-П-30. Материалы VII-ого Симпозиума ВМК, Прага, 1978.
- Apostolov T., Petkov P. (1979).** Calculations of TIC Model Problems with Real Assembly Structure, (in Russian)
- Апостолов Т., Петков П.: Расчет модельных задач ВМК для диффузионных программ с учетом реальной кассетной структуры. Материалы VII-ой сессии 4-ой тематической группы ВМК, Прага, 1979.
- Apostolov T., Manolova M., Petkov P. (1980).** 2D Few Group Diffusion Program HEXAB-II-30E for Hexagonal Geometry, (in Bulgarian)
- Апостолов Т., Манолова М., Петков П.: ХЕКСАБ-П-30Е малогрупова двумерна дифузиона програма за шестоугална геометрия. Ядрена енергия, 11, 1980.
- Apostolov T., Petkov P. (1981).** Calculations with Real WWER Assembly Structure by Program HEXAB-II-30K, (in Bulgarian)
- Апостолов Т., Петков П.: Отчитане на реалната касетна структура на реакторите от типа ВВЕР в програмата ХЕКСАБ-П-30К. Ядрена енергия, 14, 1981.

Babushka I., Vitasek E., Prager M. (1969). Numerical Procedures for Solving Differential Equations, (in Russian)

Бабушка И., Витасек Э., Прагер М.: Численные процессы решения дифференциальных уравнений. Мир, М., СССР, 1969.

Borresen S. (1973). Simplified, Coarse-Mesh, Three-Dimensional Diffusion Scheme, Nucl. Sci. Eng., Vol.44, No 1, 1973.

Buckel G., Kufner K. and Stehle B. (1977). Benchmark Calculations for a Sodium Cooled Breeder Reactor by Two- and Three- Dimensional Diffusion Methods, Nucl. Sci. Eng., p.75-89, 1977.

Diffusions parametr fur nerdellaufgaben. (1975) Материал заседания Научного Совета ВМК, 1975.

Experimental Investigations of the Physical Properties of WWER-type Uranium-Water Lattices, Final Report of TIC, vol. 1, Akademiai Kiado, Budapest, 1985.

Gaertner K. (1980). First Experience with Solving 3D Diffusion Equation in Few Group Approximation and in Hexagonal Geometry with the help of Incomplete Block Factorization Method (in Russian)

Гержнер К.: Первый опыт при решении трехмерного диффузионного уравнения в малогрупповом приближении и гексагональной геометрии с помощью неполной блочной факторизации. Материалы IX-ого Симпозиума ВМК, Нейбранденбург, 1980.

Hageman, Kekkog (1968). Estimating Optimum Over relaxation Parameters, Math. of Comput., 22, 60-68, 1968.

Ionov V. (1974). NI-7000 Program (in Russian)

Ионов В.: Программа НИ-7000. Материалы ТГ-4 ВМК, Берлин, 1974.

Ionov V. (1975). Results for TIC Model Problems (in Russian)

Ионов В.: Расчет модельных задач ВМК для гексагональных программ. Материалы IV-ого Симпозиума ВМК, Фрунзе, 1975.

- Ivanov K., Manolova M., Apostolov T., Seregin A., Tsebeskov A., Tserniy V. (1988). Verification of Few Group Diffusion Program HEXAB-III-30 Against Fast Reactor Problems (in Russian)
- Иванов К., Манолова М., Апостолов Т., Серегин А., Чебесков А., Черный В.: Тестирование трехмерной малогрупповой диффузионной программы ХЕКСАБ-Ш-30 на модели быстрого энергетического реактора. Семинар специалистов стран-членов СЭВ, Варна, 1988.
- Koch R. (1976). Synthesis 3D Neutron Flux Distribution in Hexagonal Geometry (in Russian)
- Кох Р.: Разрывный синтез трехмерных функций распределения нейтронного потока для гексагональной геометрии, Материалы V-ого Симпозиума ВМК, Варна, 1976.
- Krysl V., Lehman M. (1978). BORORO-Novel Fast 2D Diffusion Code for Pinwise Core Calculation Using Borresen's Finite Difference Approximation (in Russian)
- Крысл В., Леман М.: BORORO - новый быстрый 2D диффузионный код для потвзльных расчетов активной зоны с модификацией конечно-разностной аппроксимации Борресена. Материалы VII-ого Симпозиума ВМК, Добриховеце, 1978.
- Lebedev V., Finogenov S. (1971). On the Application of Chebishev Parameters in Iterational Methods (in Russian)
- Лебедев В., Финогенов С.: Об использовании чебышевских параметров в итерационных методах. IBM, МФ, т.11, 2, стр.425, 1971.
- Lebedev V. (1985). Possibilities and Perspective of Irrational Methods' Application in Solving Reactor Problems on Multiprocessor Computers (in Russian)
- Лебедев В. И.: Возможности и перспективы использования итерационных методов для решения реакторных задач на многопроцессорных ЭВМ. ВАИТ, серия "Физика и техника ядерных реакторов", выпуск 5, 1985.
- Lehman M. (1977). New Features of THESEUS Program, (in Russian)
- Леман М.: Новые возможности программы THESEUS. Материалы VI симпозиума ВМК. Бухарест, 1977.

Lehman M. (1978). Calculation of Lattice Inhomogeneity's Effect on Diffusion Theory Cell Constants with the Help of Spectral Index Method, (in Russian)

Леман М.: Расчет влияния неоднородности решетки на диффузионные константы элементарных ячеек методом спектральных индексов. Материалы VII Симпозиума ВМК (1978), Прага, 1979.

Lelek V. (1975). Solution of Hexagonal Geometry Model Problems and Problems in Interpreting Measurements (in Russian)

Лелек В.: Решение модельных задач в гексагональной геометрии и вопросы интерпретации измерения. Материалы IV-ого Симпозиума ВМК, Фрунзе, 1975.

Lelek V., Nanicek I. (1980). Diffusion Coefficient in Lattice with Changing Pitch, (in Russian)

Лелек В., Ваничек И.: Коэффициент диффузии в решетках с неравномерным шагом, UJV 5442-R (1980). Материалы IX-ого Симпозиума ВМК, Нейбранденбург, 1980.

Lelek V. (1981). Cell and Assembly Homogenization with Diverse Surroundings, (in Russian)

Лелек В.: Гомогенизация ячеек и кассет при различных окружающих средах. Материалы X-ого Симпозиума ВМК, Ереван, 1981.

Lizorkin M., Kiryeeva I, Saprikin V. (1985). PERMAK Program. Description of the Algorithm and User's Guide, (in Russian)

Лизоркин М.П., Киреева И.Л., Сапрыкин В.В.: Программа ПЕРМАК. Описание алгоритма и инструкция по пользованию. Отчет библиотеки программ ВМК, София, 1985.

Lizorkin M., Kurchenkova G., Lebedev V. (1988). Description of Program PERMAK-U, (in Russian)

Лизоркин М.П., Курченкова Г.И., Лебедев В.И.: Аннотация программы ПЕРМАК-У. Вопросы атомной науки и техники, серия: Физика и техника ядерных реакторов, вып. 4, 1988.

Mai V. (1980). FEM-3D -A Program for Solving Multidimensional Diffusion

Equation by Finite Element Method (in Russian)

Май В.: Программа FEM-3D для решения многомерного уравнения диффузии методом конечных элементов. Материалы IX-ого Симпозиума специалистов ВМК, Нейбранденбург, 1980.

Manolova M., Apostolov T. (1982). HEXAB-III-30 -A Few Group, 3D Diffusion Program in Hexagonal Geometry (in Bulgarian)

Манолова М., Апостолов Т.: ХЕКСАБ-III-30 малогрупова тримерна дифузионна програма за хексаганална геометрия. Ядрена енергия, 17, 1982.

Marchuk G., Lebedev V. (1981). Numerical Methods in Neutron Transport (in Russian)

Марчук Г., Лебедев В.: Численные методы в теории переноса нейтронов. Атомиздат, М., 1981.

Numerical Methods in the Theory of Neutron Transport. (1986) Harwood Academic Publishers, Chur, Switzerland, 1986.

Seidel F. (1979). Results by Program FLEX for the Birtz Model Problem, (in Russian)

Зайдель Ф.: Результаты решения модельной задачи Бирца (2) по программе ФЛЕКС. Материалы VIII-ого Симпозиума ВМК, 1979.

Shishkov L. (1976). Methods for Solving 2D Reactor Core Diffusion Equation (in Russian)

Шишков Л.К.: Методы решения диффузионных уравнений двумерного ядерного реактора. Атомиздат, М., 1976.

Telbisz M. (1978). 3D Diffusion Program SNAP-3D, (in Russian)

Тельбис М.: Трехмерная программа диффузии SNAP-3D. Материалы VI-ой сессии IV-ой тематической группы ВМК, Прага, 1978.

Woznitski Z. (1973). Two-sweep Iterative Methods for Solving Large Linear Systems and Their Application to the Numerical Solution of Multi-group Multi-dimensional Neutron Diffusion Equations. Report 1447/CYF/PM/A, 1973.

Woznicki Z. (1979). HEXAGA-II-120, -60, -30 Two-dimensional Multi- group Neutron Diffusion Programs for a Uniform Triangular Mesh with Arbitrary Group Scattering. Report KFK-2789, 1979.

Woznicki Z. (1979). Integral Results of Calculations by HEXAGA for Model Problems (in Russian)

Вознишки З.: Интегральные результаты расчетов программы ХЕКСаГА для модельных задач. Информационное сообщение на VIII-ом Симпозиуме ВМК, 1979.

Woznicki Z. (1983). HEXAGA-III-120, -30 - Three Dimensional Multi - Group Neutron Diffusion Programs for a Uniform Triangular Mesh With Arbitrary Group Scattering. KFK - 3572, 1983.

Zikova H., Lelek V. (1983). Application of Chebyshev Polynomials to Refining the Dominance Ratio (in Russian)

Зикова Г., Лелек В.: Применение полиномов Чебышева с уточнением доминантного отношения. Материалы XII-ого Симпозиума ВМК, Татранска Ломница, 1983.

References to TIC reports (In Russian)

[545] Lelek V. Numerical method for adapting the core linear equations based on measurements. Report KFKI-ZR-6-545/1986.

Лелек. В.: Численный метод подгонки линейных уравнений реактора на основе измерений. KFKI-ZR-6-545/1986.

[547] Lelek V. The BRETISLAV mesh code for calculating the hexagonal geometry cores. Report KFKI-ZR-6-547/1986.

Лелек. В.: Сеточная программа BRETISLAV для расчета реактора гексагональной геометрии. KFKI-ZR-6-547/1987.

[550] Apostolov T. Factorization methods for solving the neutron diffusion problems. Report KFKI-ZR-6-550/1986.

Апостолов Т. и др.: Факторизационные методы решения задачи диффузии нейтронов. KFKI-ZR-6-550/1987.

[551] Krysl et al. Theoretical analysis of macrocode scheme. Report

KFKI-ZR-6-551/1987.

Крысл В., Леман М., Махачек Я.: Теоретические основы модульной макрокодовой системы MOBY-DICK. KFKI-ZR-6-551/1987.

[553] Lelek V., Pecka M. Using the critical assembly measurements for improving the group constants. Report KFKI-ZR-6-553/1988.

Лелек В., Пецка М.: Использование измерений на критической сборке для уточнения групповых констант ячеек с топливом и другими материалами. KFKI-ZR-6-553/1988.

[556] Aghte G., Becker R. Physical basis of the FLEX code. Report KFKI-ZR-6-556/1988.

Агте Г., Беккер Р.: Физические основы программы FLEX. KFKI-ZR-6-556/1988.

[557] Aghte G., Muller W. Report KFKI-ZR-6-557/1988.

Агте Г., Мюллер В.: Отчет KFKI-ZR-6-557/1988.

[561] Apostolov T., Lelek V. The problems of verification of diffusion codes. Report KFKI-ZR-6-561/1988.

Апостолов Т., Лелек В.: Проблемы состояния и проверки диффузионных программ. KFKI-ZR-6-561/1988.

[562] Apostolov T., Manolova M., Ivanov K. HEXAB code family. Report KFKI-ZR-6-562/1989.

Апостолов Т., Манолова М., Иванов К.: HEXAB - семейство диффузионных программ для гексагональной геометрии. KFKI-ZR-6-562/1989.

[565] Becker R. Report KFKI-ZR-6-565/1989.

Беккер Р.: Отчет KFKI-ZR-6-565/1989.

6. NEW METHODS FOR FINE MESH ANALYSIS OF WWER CORES

M. Lizorkin (sect. 6.2.3), M. Makai (sect. 6.3),

A. Novikov (sect. 6.2.1), V. Pshenin (sect. 6.2.2)

6.1 INTRODUCTION

As was mentioned in the Foreword, a considerable part of the theoretical investigations performed in the framework of TIC were devoted to developing new methods and improving the traditional methods of core analysis. Various aspects of these investigations are considered in Chaps. 3, 6, 7.

The present chapter describes a number of new approaches which are used for calculating rod by rod power distributions in WWER cores. Two sections summarize the results of investigations performed in KIAE (Russia) and KFKI (Hungary). Sections 6.2 and 6.3 contains descriptions of the approaches developed in KIAE and KFKI, respectively, and the results of their benchmarking.

It is necessary to note that the authors did not aim at a detailed survey of all works done in the framework of the TIC and known from the literature. The main aim was to give an account of the author's point of view and to describe some practical algorithms. To some extent the shortcoming of the personal view is compensated for by Chapters 3 and 7 as well as by the references there. It is again mentioned that the development of new approaches was carried out under continuous, often informal discussions of the obtained results and thus complement each other.

6.2 NODAL APPROACH FOR FINE MESH CALCULATIONS - ALGORITHM AND

RESULTS OF NUMERICAL BENCHMARKING

6.2.1 Effects of cells heterogeneity and transient solutions in fine-mesh calculations *

Bearing in mind that the effects of cell heterogeneity and transient solutions are the most important in the thermal energy region let us suppose, in developing the ideas stated in (Novikov, 1980, Novikov, 1982) that in each elementary cell of nonuniform lattice the thermal neutron flux can be represented as

$$F(\bar{r}, \bar{\Omega}, E) = F_{as} + F_{aa} + F_{ts} + F_{ta}. \quad (6.2.1)$$

where F_{as} and F_{aa} - asymptotic (a), symmetrical (as) and asymmetrical (aa) as regards the centre of the cell components of the neutron flux.

F_{ts} и F_{ta} - transient (t) components of the flux, symmetrical (ts) and asymmetrical (ta) as regards the centre of the cell.

It is supposed that

$$\begin{aligned} F_{as} &= a \Psi_{as} & F_{aa} &= \sum_m b_m \cos(m\varphi + \delta_{am}) \psi_{aam} \\ F_{ts} &= A \Psi_{ts} & F_{ta} &= \sum_m B_m \cos(m\varphi + \delta_{tm}) \psi_{tam} \end{aligned} \quad (6.2.2)$$

where φ - azimuthal angle measured the same way for all the cells, $\Psi = \Psi(r, E)$, δ_{am} and δ_{tm} - the initial phase shifts.

It is also supposed that functions ψ do not depend on φ and are stable characteristics of the cell of considered type (as for ψ_{as} , ψ_{aa} as ψ_{ts} , ψ_{ta}).

In the general case for computing of ψ functions multigroup transport calculations of heterogeneous nonuniform lattices containing all the types of considered cells are needed. Possible simplified ways of calculations of approximate values depending on Ψ functionals are discussed at the end of this section.

For simplification, later on it will be assumed that the considered lattices are in the critical state and are infinite over the height (in general, Ψ -functions depend on K_{eff} and B_z^2). Let us suppose also that asymmetrical parts of neutron flux can be represented by the first ($m=1$) azimuthal harmonics only (the influence of the members corresponding to $m>1$

* This section is based on (Novikov, 1983)

can be taken into account by the ways described in (Novikov 1982, Novikov, 1983, Novikov 1985).

Let us make further use of the continuity conditions at the boundary γ_1 common of cells "o" and "i" ($i=1\dots 6$):

$$\tilde{\Phi}_o^1 = \tilde{\Phi}_1^{1+3} \quad (6.2.3)$$

$$\tilde{J}_o^1 = \tilde{J}_1^{1+3}$$

Here $\tilde{H}$ - averaged over the side i value of H . In particular,

$$\tilde{\Phi}^i = \frac{\sqrt{3}}{h} \int F \, dE \, d\Omega^- d\gamma_1 = a\tilde{f}_{as} + b^i \tilde{f}_{aa} + A\tilde{f}_{ts} + B^i \tilde{f}_{ta} \quad (6.2.4)$$

$$\tilde{J}^i = \frac{\sqrt{3}}{h} \int (n_1^-, \Omega^-) F \, dE \, d\Omega^- d\gamma_1 = a\tilde{J}_{as} + b^i \tilde{J}_{aa} + A\tilde{J}_{ts} + B^i \tilde{J}_{ta},$$

where h is the lattice pitch.

In expressions (6.2.4) members corresponding to asymmetrical components of boundary flux are represented as a multiplication of coefficients b^i and B^i at boundary i and scalars - $\tilde{f}_{aa}$, $\tilde{J}_{aa}$, $\tilde{f}_{ta}$, $\tilde{J}_{ta}$. This results from the representation of $\cos(m\varphi + \delta_{am})$ (see correlation (6.2.2) for F_{ta} and F_{aa}) in the form $\cos\left[\frac{\pi}{3}(i-1)+\delta\right]\cos\Delta\varphi$ where variable $\Delta\varphi$ under integration of Φ and J over $d\gamma_1$ is changed from $-\frac{\pi}{6}$ to $\frac{\pi}{6}$. Therefore, the following expressions are valid for coefficients b^i and B^i

$$b^i = b \cos\left(\frac{\pi}{3}(i-1) + \delta_a\right) = -b^{1+3}$$

$$B^i = B \cos\left(\frac{\pi}{3}(i-1) + \delta_t\right) = -B^{1+3},$$

and the independence of $\tilde{f}_{aa} \dots \tilde{J}_{ta}$ from side superscript provides a possibility to introduce scalar diffusion coefficients D_a and D_t (see below).

It is necessary to pay attention to the fact that coefficients b^i can be determined using boundary currents in epithermal ($g=G-1$) group obtainable from a solution of a few group problem:

$$b^i = \frac{\tilde{J}_{(G-1)}^1 - \frac{1}{6} \sum_i \tilde{J}_{(G-1)}^1}{\tilde{J}_{aa(G-1)}} \quad (6.2.5)$$

Let us proceed further from formulae (6.2.3)-(6.2.5) and suppose that

$$\bar{\varphi}_a = \frac{\bar{S}}{\Sigma_a + \frac{4}{h} \frac{\tilde{j}_{as}}{\bar{f}_{as}}} \quad a = \frac{\bar{\varphi}_a}{\bar{f}_{as}} \quad (6.2.6)$$

$$\bar{\Phi} = \frac{1}{\omega} \int F \, dE \, d\bar{\Omega} \, d\bar{r} \quad A = \frac{\bar{\Phi} - \bar{\varphi}_a}{\bar{f}_{ts}}$$

Here S - thermal neutron source density,

$\omega = \frac{\sqrt{3}}{2} h^2$ - cell area,

$\bar{H}$ - averaged over cell value of functional H ,

Σ_a^a - is defined by correlation 6.2.11.

In this case it is possible - except for the unknown B^1 and B^{1+3} - to express average density of thermal neutron current across side $\tilde{J}_0^1$ in one of the following three ways (the conventions used are explained in 6.2.11)):

$$\begin{aligned} \tilde{J}_0^1 &= \frac{2}{h} \frac{D_{t0} D_{t1}}{D_{t0} + D_{t1}} \left[\bar{\Phi}_1 \bar{g}_1 - \bar{\Phi}_0 \bar{g}_0 + b_1^{1+3} \tilde{f}_{aa1} \left(1 - \frac{D_{a1}}{D_{t1}}\right) - b_0^1 \tilde{f}_{aa0} \left(1 - \frac{D_{a0}}{D_{t0}}\right) \right] = \\ &= \frac{2}{h} \frac{\tilde{D}_0^1 \tilde{D}_1^{1+3}}{\tilde{D}_0^1 + \tilde{D}_1^{1+3}} \left[\bar{\Phi}_1 \tilde{\epsilon}_1^{1+3} - \bar{\Phi}_0 \tilde{\epsilon}_0^1 \right] = \quad (6.2.7) \\ &= \frac{2}{h} \frac{D_{a0} D_{a1}}{D_{a0} + D_{a1}} \left[\bar{\Phi}_1 \bar{\epsilon}_1 - \bar{\Phi}_0 \bar{\epsilon}_0 + B_1^{1+3} \tilde{f}_{ta1} \left(1 - \frac{D_{t1}}{D_{a1}}\right) - B_0^1 \tilde{f}_{ta0} \left(1 - \frac{D_{t0}}{D_{a0}}\right) \right] \end{aligned}$$

It should be mentioned that coefficients B_0^1 and B_1^{1+3} needed for determining $\tilde{J}_0^1$ by the third way can be determined from the condition

$$\begin{aligned} \tilde{\Phi}_0^1 &= a_0 \tilde{f}_{as0} + b_0^1 \tilde{f}_{aa0} + A_0 \tilde{f}_{ts0} + B_0^1 \tilde{f}_{ta0} = \\ &= a_1 \tilde{f}_{as1} + b_1^{1+3} \tilde{f}_{aa1} + A_1 \tilde{f}_{ts1} + B_1^{1+3} \tilde{f}_{ta1} \end{aligned}$$

where $\tilde{\Phi}_0^1$ can, for example, be expressed by the correlation

$$\tilde{\Phi}_0^1 = \frac{1}{\tilde{D}_0^1 + \tilde{D}_1^{1+3}} \left[\tilde{D}_0^1 \bar{\Phi}_0 \tilde{\epsilon}_0^1 + \tilde{D}_1^{1+3} \bar{\Phi}_1 \tilde{\epsilon}_1^{1+3} \right] \quad (6.2.8)$$

Expressions (6.2.7) for $\tilde{J}_0^1$ allow one to write the balance equation for thermal neutrons in the following form

$$\frac{2}{3h} \sum_1 \tilde{J}_0^1 - \sum_{a0} \bar{\varphi}_{a0} - \sum_{t0} \left(\bar{\Phi}_0 - \bar{\varphi}_{a0} \right) + \bar{S}_0 = 0 \quad (6.2.9)$$

Reaction rates of type "β" averaged over a cell are determined by the formula

$$\bar{R}^\beta = \sum_a \bar{\beta}_a^\beta + \sum_t \bar{\beta}_t^\beta (\bar{\Phi} - \bar{\varphi}_a) \quad (6.2.10)$$

The conventions given below are used in the expressions (6.2.6)-(6.2.10) for scalars (the subscript of the cell is omitted):

$$\begin{aligned} D_a &= \frac{h}{2} \frac{\tilde{J}_{aa}}{\tilde{f}_{aa}} & D_t &= \frac{h}{2} \frac{\tilde{J}_{ta}}{\tilde{f}_{ta}} \\ \bar{g} &= g_a \frac{\bar{\varphi}_a}{\bar{\Phi}} + g_t \left(1 - \frac{\bar{\varphi}_a}{\bar{\Phi}} \right) & \bar{\epsilon} &= \epsilon_a \frac{\bar{\varphi}_a}{\bar{\Phi}} + \epsilon_t \left(1 - \frac{\bar{\varphi}_a}{\bar{\Phi}} \right) \\ g_a &= \frac{\tilde{f}_{as}}{\tilde{f}_{as}} \left(1 - \frac{\vartheta_a}{D_t} \right) & g_t &= \frac{\tilde{f}_{ts}}{\tilde{f}_{ts}} \left(1 - \frac{\vartheta_t}{D_t} \right) \\ \vartheta_a &= \frac{h}{2} \frac{\tilde{J}_{as}}{\tilde{f}_{as}} & \vartheta_t &= \frac{h}{2} \frac{\tilde{J}_{ts}}{\tilde{f}_{ts}} \\ \epsilon_a &= \frac{\tilde{f}_{as}}{\tilde{f}_{as}} \left(1 - \frac{\vartheta_a}{D_a} \right) & \epsilon_t &= \frac{\tilde{f}_{ts}}{\tilde{f}_{ts}} \left(1 - \frac{\vartheta_t}{D_t} \right) \\ \sum_a^\beta &= \frac{1}{\omega \tilde{f}_{as}} \int \sum^\beta \Psi_{as} dE d\bar{\Omega} d\bar{r} & \sum_t^\beta &= \frac{1}{\omega \tilde{f}_{ts}} \int \sum^\beta \Psi_{ts} dE d\bar{\Omega} d\bar{r} \end{aligned} \quad (6.2.11)$$

and for tensors depending on the side superscript

$$\begin{aligned} \frac{1}{\bar{D}^1} &= \frac{1}{D_a} \frac{\tilde{J}_{aa}^1}{\tilde{J}_{aa}^1 + \tilde{J}_{ta}^1} + \frac{1}{D_t} \frac{\tilde{J}_{ta}^1}{\tilde{J}_{aa}^1 + \tilde{J}_{ta}^1} \\ \tilde{\epsilon}^1 &= \tilde{\epsilon}_a^1 \frac{\bar{\varphi}_a}{\bar{\Phi}} + \tilde{\epsilon}_t^1 \left(1 - \frac{\bar{\varphi}_a}{\bar{\Phi}} \right) \\ \tilde{\epsilon}_a^1 &= \frac{\tilde{f}_{as}}{\tilde{f}_{as}} \left(1 - \frac{\vartheta_a}{\tilde{D}^1} \right) & \tilde{\epsilon}_t^1 &= \frac{\tilde{f}_{ts}}{\tilde{f}_{ts}} \left(1 - \frac{\vartheta_t}{\tilde{D}^1} \right) \end{aligned}$$

It is clear that when contributions of transient modes are negligible, equation (6.2.9) degenerates into the asymptotic form:

$$\frac{4}{3h} \sum_i \frac{D_{a0} D_{a1}}{D_{a0} + D_{a1}} \left(\bar{\Phi}_1 \in_{a1} - \bar{\Phi}_0 \in_{a0} \right) - \sum_{a0} \bar{\Phi}_0 + \bar{S}_0 = 0 \quad (6.2.12)$$

For the asymptotic region of a uniform lattice this equation is reduced to the form:

$$\frac{2}{3h} \sum_i \bar{D}_0 \left(\bar{\Phi}_1 - \bar{\Phi}_0 \right) - \sum_{a0} \bar{\Phi}_0 + \bar{S}_0 = 0 \quad (6.2.13)$$

where $\bar{D}_0 = D_{a0} \in_{a0}$

So far as equations of (6.2.13) type in the asymptotic region of a uniform lattice can be applied for all neutron groups it is worth using the following expressions for calculations of material buckling and migration area:

$$\bar{M}^2 = \frac{\sum_g D_{ag} \in_{ag} \bar{\Phi}_g}{\sum_g \sum_{a_g} \bar{\Phi}_g} \quad \bar{\kappa}^2 = \frac{\sum_g \left(\sum_{a_g} \bar{f}_{a_g} - \sum_{a_g} \bar{a}_{a_g} \right) \bar{\Phi}_g}{\sum_g D_{ag} \in_{ag} \bar{\Phi}_g} \quad (6.2.14)$$

In conclusion it should be admitted that the practical realization of the above described approach assigned for making more precise calculations in the thermal group can be made difficult by the absence of codes for generating the needed functionals and also by the necessity of significant modifications of codes used for fine mesh calculations.

It should be mentioned that several other approaches can be used to avoid these difficulties. The approximate values of all needed functionals can be calculated by standard cross sections generators. In this case most

of the asymptotic mode functionals (such as Σ , D , $\frac{\tilde{f}_s}{\bar{f}}$, $\frac{\tilde{j}_s}{\bar{f}}$, $\kappa^2 h^2$ and others) can be obtained without any modifications of standard codes by calculation of an isolated cell. It is useful to bear it in mind that one can write the following approximate correlation

$$\frac{\phi_a}{D_a} \approx - \frac{(\kappa h)^2}{8}$$

To obtain functionals of transient modes it is enough to provide the possibility calculating symmetrical distribution of thermal neutrons for a cell surrounded by a water buffer and an outer circular zone with a volume distributed thermal neutron source. When the functionals of the symmetrical transient mode are determined, D_t can be expressed approximately as

$$D_t \approx \frac{h^2 \sum_t \alpha}{16 \alpha - 1}$$

where $\alpha = \left(\frac{\tilde{f}_{ts}}{\bar{f}_{ts}} \right)^2$.

The solution of balance equation (6.2.9) in the already used fine-mesh codes can be realized in the simplest way when the neutron current is expressed by the second of three formulas contained in (6.2.7) when disregarding that D and ϵ are tensors. In this case a slight correction of D for nonfuel cells may be useful. It is also necessary to take it into account that the mentioned correction should be used in combination with a balance equation of (6.2.12) type for epithermal group when calculating a lattice containing strong absorbers.

6.2.2 Results of improved balance equation, numerical

benchmarking for slab geometry

A comparison of benchmark problems solutions obtained with a precise code and a code utilizing the approach described in the previous section provides detailed information about the accuracy of the given approach. In this case when the needed functionals of the trial functions are determined with the same precise code the resulting disagreements are interpreted practically unambiguously. Such procedure of verification for real hexagonal geometry can be carried out only with codes based on the Monte-Carlo method. The results of verifying some approaches obtained with the *MCU* code based on this method are discussed in detail in Chapter 3.

A simpler situation is slab geometry when the 1D transport code provides a possibility of realizing a fully consistent verification procedure. In this case it is possible to estimate the reliability of the most important assumptions made to obtain a balance equation in the form of (6.2.9). The results of calculations are briefly described below; they are discussed in detail in (Pshenin et al., 1984, Pshenin et al., 1988).

Reference solutions of benchmark problems and needed functionals of asymptotic and transient modes for elementary cells of slab lattice were obtained with the 1D 61-group (24 thermal group) transport code *CRAMS* (Averyanova et al., 1981) based on the characteristic method. Calculations based on the algorithm described in Sect. 6.2.1, on the standard finite-differences approach, and on the spectral index method (see Chapt. 5) were carried out with specially written code *MODISN*. They were performed using one and four group calculations with searching K_{eff} . In the one group

case, thermal fluxes and reaction rates were determined utilizing a source taken from transport calculation. A combination of one and four group calculations allows one to analyse the accuracy of algorithm (6.2.9) when calculating thermal neutron distributions and to estimate the effect of cell heterogeneity, the effect of spectrum deformation in epithermal groups and, therefore, to evaluate the expediency of using an algorithm of (6.2.9) type in the energy ranges of slowing down and fast neutrons.

Calculations have been performed for configurations formed by slab fuel cells with different isotopic contents, both homogeneous (with ^{235}U and ^{239}Pu as fissile isotopes) and heterogeneous. The main cells characteristics have been chosen close to the characteristics of the cells of real WWER fuel lattices. Asymptotic mode functionals for fuel cells were obtained from calculations of configurations formed by cells of considered type. The number of cells was varied to provide the condition $K_{\text{eff}} \approx 1.0$. Functionals of transient modes were obtained in accordance with the recommendations described in the previous section. Asymptotic mode functionals for water and absorber cells were determined by treating the results of calculations of configurations formed by some cells of considered type surrounded by fuel cells.

Calculations of configurations formed by homogeneous cells are a strict test for checking the reliability of suppositions about the universality of transient mode functionals. It is explained by the absence of the water buffer typical for heterogeneous cells which makes functionals more sensitive to features of neutron current energy distribution and consequently can lead to an increase in the calculation inaccuracy. Besides this, lattices formed by homogeneous cells are characterized by strong neutron spectrum deformations near water gaps, reflector, absorbers and so on. The last is illustrated by the data of Table 6.2.1. In this table asymptotic and transient modes functionals for homogeneous and heterogeneous fuel cells, water and absorber cells are presented. As can be seen from this Table the homogeneous fuel cell is characterized by a greater value of the ratio $\Sigma_t^{a,f} / \Sigma_a^{a,f}$, in comparison with the heterogeneous cell. It is clear that values of this ratio are directly connected with values of spectral deformation effects in nonuniform lattice. This table also shows that for a fuel cell with ^{239}Pu that mentioned ratio is much less than in the cell with ^{235}U . It is explained by the similarity of the net current spectrum to the Maxwell spectrum and by the energy dependence of resonance in ^{239}Pu cross sections at low neutron energy.

Table 6.2.1 Values of asymptotic and transient modes functionals for slab cells.

Function.	Cell type/fissile isotop			
	homog. / U^{235}	water cell	homog. / Pu^{239}	heter. / U^{235}
D_a	0.250	0.145	0.225	0.214
Σ_a^a	0.115	$1.95 \cdot 10^{-2}$	0.234	0.113
θ_a	$-8.57 \cdot 10^{-4}$	$1.69 \cdot 10^{-3}$	$-1.33 \cdot 10^{-3}$	$-3.48 \cdot 10^{-3}$
$\tilde{f}_{as} / \bar{f}_{as}$	0.999	1.002	0.998	1.190
Σ_a^f	0.0802	-	0.147	$7.76 \cdot 10^{-2}$
D_t	0.224	0.144	0.224	0.190
$\tilde{f}_{ts} / \bar{f}_{ts}$	1.082	1.012	1.120	1.408
Σ_t^a	0.146	$1.98 \cdot 10^{-2}$	0.237	0.127
θ_t	0.032	$4.03 \cdot 10^{-3}$	$4.55 \cdot 10^{-2}$	$7.17 \cdot 10^{-2}$
Σ_t^f	0.102	-	0.152	$8.65 \cdot 10^{-2}$

To estimate accuracy of calculations provided by using balance equation (6.2.9), some typical configurations - "water gap between fuel assemblies", "boundary between core and reflector", "supercell with absorber" - have been investigated.

Results of one-group calculations with thermal neutron source distribution taken from transport calculation, are presented for configurations formed by homogeneous fuel cells with ^{235}U and water cells in Figs.6.1-6.2. It is seen from these figures that the use of the standard finite difference approach leads to significant inaccuracy of absorption and fission reaction rates (26 and 8% respectively). Maximum deviations are observed near the boundary between regions with different properties.

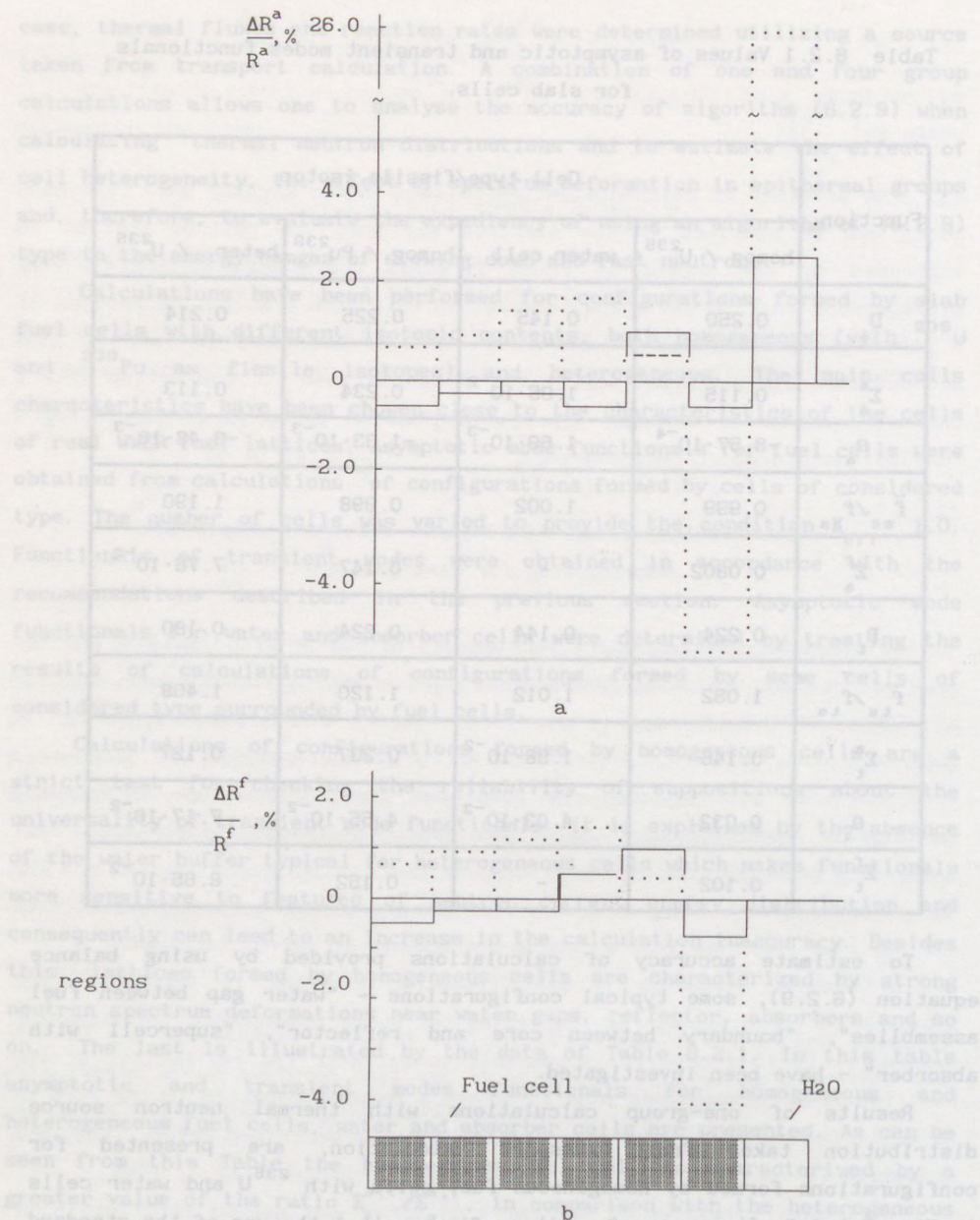


Fig.6.1 Comparison of absorption (a) and fission (b) reaction rates for configuration "gap between fuel assemblies" formed by homogenous cells (considered configuration is drawn in the bottom of the figure).

... - standard finite-difference balance equation.

— - equation (6.2.9) $\Delta R/R = (R - R_{tr})/R_{tr} \cdot 100$.

R_{tr} - result of transport calculation.

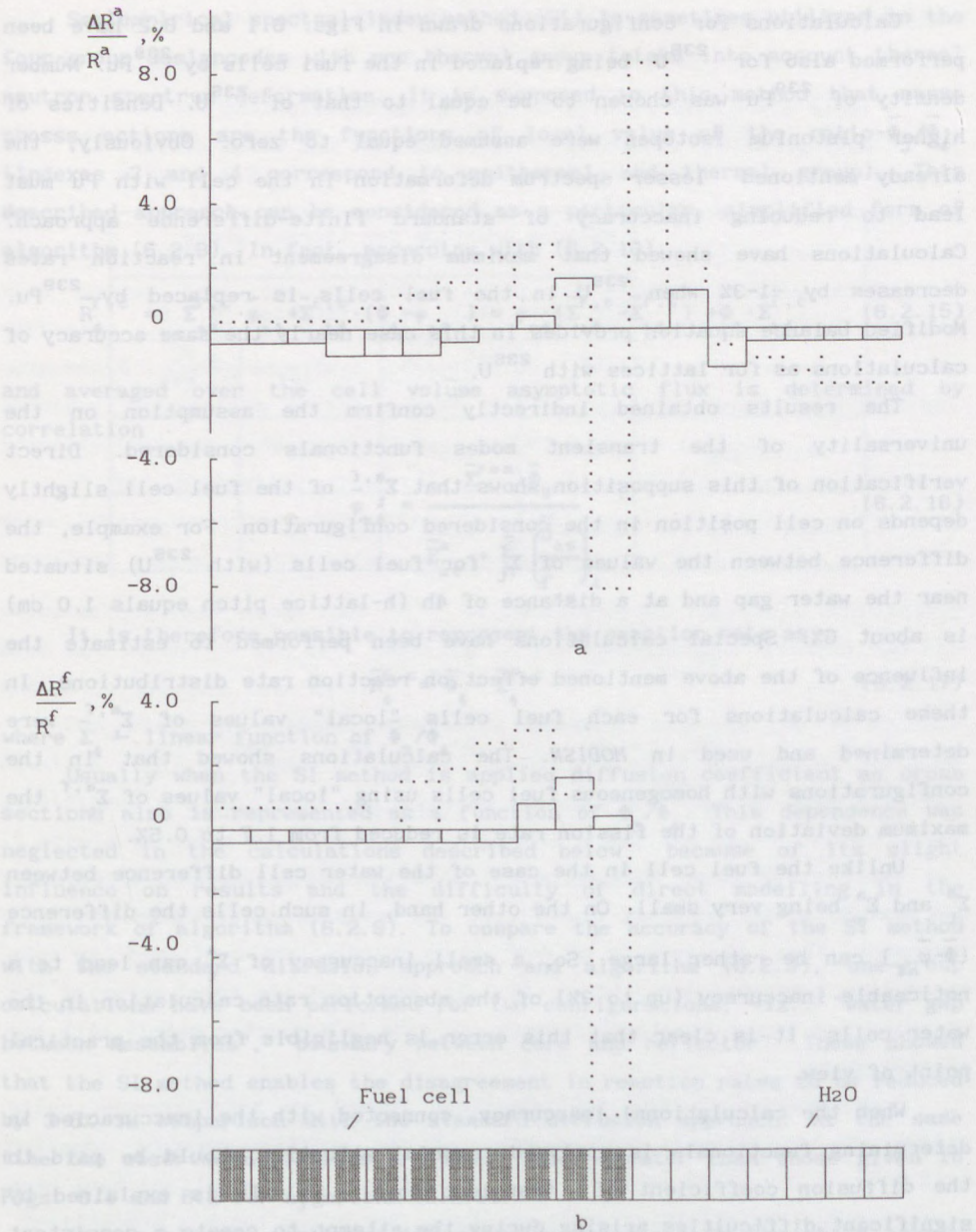


Fig.6.2 Comparison of absorption (a) and fission (b) reaction rates for configuration "boundary between core and reflector" formed by homogenous cells) Conventions as in Fig.6.1.

Use of balance equation (6.2.9) allows one to reduce disagreement in reaction rates up to 1.7%.

Calculations for configurations drawn in Figs. 6.1 and 6.2 have been performed also for ^{235}U being replaced in the fuel cells by ^{239}Pu . Number density of ^{239}Pu was chosen to be equal to that of ^{235}U . Densities of higher plutonium isotopes were assumed equal to zero. Obviously, the already mentioned lesser spectrum deformation in the cell with Pu must lead to reducing inaccuracy of standard finite-difference approach. Calculations have showed that maximum disagreement in reaction rates decreases by $\sim 1-3\%$ when ^{235}U in the fuel cells is replaced by ^{239}Pu . Modified balance equation provides in this case nearly the same accuracy of calculations as for lattices with ^{235}U .

The results obtained indirectly confirm the assumption on the universality of the transient modes functionals considered. Direct verification of this supposition shows that $\Sigma_t^{a,f}$ of the fuel cell slightly depends on cell position in the considered configuration. For example, the difference between the values of Σ_t^f for fuel cells (with ^{235}U) situated near the water gap and at a distance of $4h$ (h -lattice pitch equals 1.0 cm) is about 6% . Special calculations have been performed to estimate the influence of the above mentioned effect on reaction rate distributions. In these calculations for each fuel cells "local" values of $\Sigma_t^{a,f}$ were determined and used in MODISN. The calculations showed that in the configurations with homogeneous fuel cells using "local" values of $\Sigma_t^{a,f}$ the maximum deviation of the fission rate is reduced from 1.7 to 0.5% .

Unlike the fuel cell in the case of the water cell difference between Σ_t^a and Σ_a being very small. On the other hand, in such cells the difference $(\bar{\Phi} - \bar{\varphi}_{a4})$ can be rather large. So, a small inaccuracy of Σ_t^a can lead to a noticeable inaccuracy (up to 3%) of the absorption rate calculation in the water cells. It is clear that this error is negligible from the practical point of view.

When the calculational inaccuracy, connected with the inaccuracies in determining functionals is analysed, special attention should be paid to the diffusion coefficient of transient mode - D_t . It is explained by significant difficulties arising during the attempt to create a consistent algorithm for computing this functional. The calculations performed have shown that a variation D_t of the fuel cell by 11% leading to equality of D_t and D_a increases the deviation of average fluxes and reaction rates by not less than 0.3% . It can thus be concluded that D_t calculations can be based on the use of simplified approaches.

Semilempirical spectral index method (SI) is sometimes utilized in the four-group design codes with one thermal group to take into account thermal neutron spectrum deformation. It is supposed in this method that macro cross sections are the functions of local value of the ratio $\bar{\Phi}_3/\bar{\Phi}_4$. (indexes 3 and 4 correspond to epithermal and thermal group). This described approach can be considered as a particular, simplified form of algorithm (6.2.9). In fact, according with (6.2.10)

$$\bar{R}_4^{f,c} = \bar{\Sigma}_{a4}^{f,c} \cdot \bar{\varphi}_{a4} + \bar{\Sigma}_{t4}^{f,c} \cdot (\bar{\Phi}_4 - \bar{\varphi}_{a4}) = \bar{\varphi}_{a4} \cdot (\bar{\Sigma}_{a4}^{f,c} - \bar{\Sigma}_{t4}^{f,c}) + \bar{\Phi}_4 \cdot \bar{\Sigma}_{t4}^{f,c} \quad (6.2.15)$$

and averaged over the cell volume asymptotic flux is determined by correlation

$$\bar{\varphi}_{a4} = \frac{\bar{\Sigma}^{rem} \cdot \bar{\Phi}_3}{\bar{\Sigma}_{a4}^a + \frac{2}{h} \cdot \left(\frac{\tilde{j}_{as}}{\tilde{\tau}_f^{as}} \right)_4} \quad (6.2.16)$$

It is therefore possible to represent the reaction rate as

$$\bar{R}_4^{f,c} = \bar{\Phi}_4 \cdot \bar{\Sigma}_4^{f,c} \quad (6.2.17)$$

where $\bar{\Sigma}_4$ - linear function of $\bar{\Phi}_3/\bar{\Phi}_4$.

Usually when the SI method is applied diffusion coefficient as cross sections also is represented as a function of $\bar{\Phi}_3/\bar{\Phi}_4$. This dependence was neglected in the calculations described below because of its slight influence on results and the difficulty of direct modelling in the framework of algorithm (6.2.9). To compare the accuracy of the SI method with the standard diffusion approach and algorithm (6.2.9), one-group calculations have been performed for two configurations, viz.: "water gap between assemblies", "boundary between core and reflector". These showed that the SI method enables the disagreement in reaction rates to be reduced by 3-5% in comparison with the standard diffusion approach. At the same time the observed deviations are about twice greater than those given in Figs. 6.1 and 6.2 for algorithm (6.2.9).

As was already mentioned the above calculations in the whole energy range with searching of K_{eff} are the most interesting from the practical point of view. Results of such calculations for configurations with homogeneous fuel cells are presented in Table 6.2.2. It should be noted that upper group calculations with MODISN were carried out using the standard finite-difference diffusion approach. The cross sections of water cell in epithermal group used in these calculations were determined by

averaging with spectrum of water cell surrounded by the fuel cells.

Table 6.2.2. The results of four-group calculations for configurations formed by homogeneous fuel and water cells.

Configuration	Balance equation for thermal group			
	Fin.-diff. bal. eq.		Equation 6.2.9	
	ΔK_{eff}	$\delta R_{\text{max}}^f, \%$	ΔK_{eff}	$\delta R_{\text{max}}^f, \%$
"Water gap"	$1.0 \cdot 10^{-2}$	4.59	$3.2 \cdot 10^{-3}$	0.74
"Bound. with ref"	$2.7 \cdot 10^{-3}$	8.84	$9.0 \cdot 10^{-4}$	1.33

$$\Delta K_{\text{eff}} = \frac{\text{MODISN}}{K_{\text{eff}}} - \frac{\text{TRANS.}}{K_{\text{eff}}}$$

$$\delta R_{\text{max}} = \left(\frac{\text{MODISN}}{R} - \frac{\text{TRANS.}}{R} \right) / \frac{\text{TRANS.}}{R} \cdot 100$$

R - result of transport calculation.

Table 6.2.2 shows that on applying balance equation (6.2.9) only in the thermal group provides significant improving reaction rates and K_{eff} agreement. Thus, the results of four group calculations confirmed the main assumption made when deriving eq. (6.2.9), viz. that the total error of the standard four-group finite-difference approach is connected mainly with the thermal group.

Consideration of the configurations formed by heterogeneous cells allows one to estimate the accuracy of the modified balance equation (6.2.9) in a situation close to real. Corresponding calculations have been performed for the following configurations: "water gap between assemblies", "boundary between core and reflector", "supercell with absorber". The fuel and absorber cells studied consisted of UO_2 or B_4C layers of 0.61 cm thickness surrounded by water layers of the same size.

As it follows from Table 6.2.1 that the value of ratio $\tilde{f}_{\text{as}} / \bar{f}_{\text{as}}$, which is characteristic of cell heterogeneity, is equal to 1.19. For a real fuel cell of WWER-1000 with an enrichment value of 3.6%, this ratio does

not exceed 1.1. This means that the chosen cell parameters are representative of algorithm (6.2.9) validation results.

Reaction rate distributions in the thermal group computed with the use of fixed source distribution taken from transport calculation are compared in Figs. 6.3 and 6.4. It is seen from these figures that as in the previous cases the use of modified balance equation (6.2.9) provides a possibility to reduce errors of calculations up to ~2%. The calculations performed have also showed that the resulting error of standard finite difference diffusion approach is a result of the partial compensation of separate components. The predominant contribution in this error stems from the spectral deformation effect, which is not usually taken into account. Possibly this may be considered as a basis of the SI method.

It is interesting from the practical point of view to estimate directly the nonuniversality (dependence on a position in the lattice) of transient mode functionals of heterogeneous fuel cells. Special calculations have shown that $\bar{\Sigma}_t^{a,f}$ of heterogeneous fuel cell practically does not depend on the cell position in the configuration studied and the change is not more than by 1%.

Comparison of calculation results obtained with the use of balance equation (6.2.9) and SI method confirmed the conclusion on the significantly higher accuracy provided by algorithm (6.2.9) made earlier. It should be noted that for the studied configurations the SI method gives essentially better agreement with the transport calculation than the standard diffusion approach.

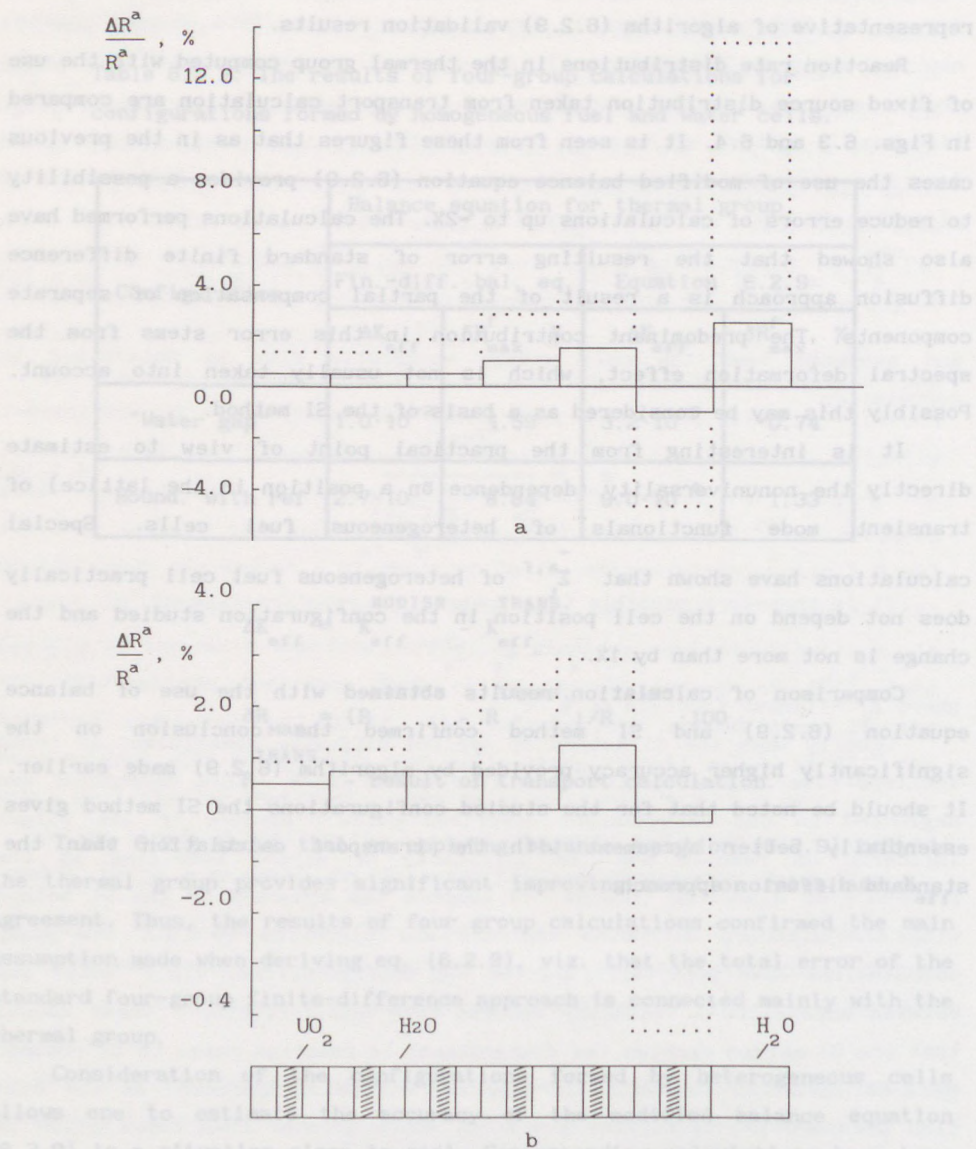


Fig. 6.3 Comparison of absorption (a) and fission (b) rates for configuration "water gap between assemblies" formed by heterogeneous slab cells. Conventions as in Fig. 6.1.

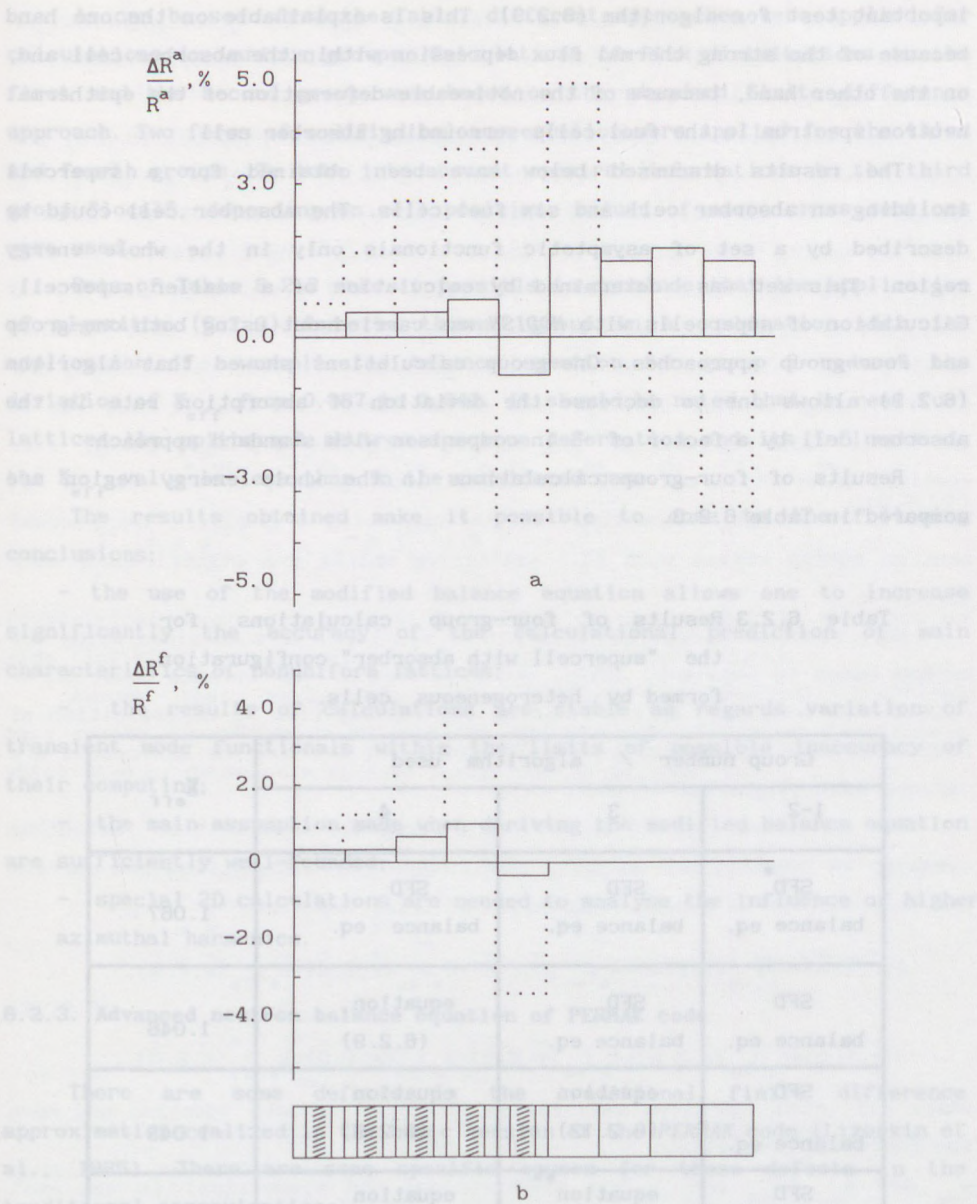


Fig.6.4 Comparison of absorption (a) and fission (b) rates for configuration "boundary between core and reflector" formed by heterogeneous slab cells.

Calculation of supercells with strong absorbers is a strict and

important test for algorithm (6.2.9). This is explainable on the one hand because of the strong thermal flux depression within the absorber cell and, on the other hand, because of the noticeable deformation of the epithermal neutron spectrum in the fuel cells surrounding absorber cell.

The results discussed below have been obtained for a supercell including an absorber cell and six fuel cells. The absorber cell could be described by a set of asymptotic functionals only in the whole energy region. This set was determined by calculation of a smaller supercell. Calculation of supercells with MODISN was carried out using both one-group and four-group approaches. One-group calculations showed that algorithm (6.2.9) allows one to decrease the deviation of absorption rate in the absorber cell by a factor of ~ 6 in comparison with standard approach.

Results of four-group calculations in the whole energy region are compared in Table 6.2.3.

Table 6.2.3 Results of four-group calculations for the "supercell with absorber" configuration formed by heterogeneous cells.

Group number / algorithm used			K_{eff}
1-2	3	4	
SFD* balance eq.	SFD balance eq.	SFD balance eq.	1.067
SFD balance eq.	SFD balance eq.	equation (6.2.9)	1.046
SFD balance eq.	equation (6.2.12)	equation (6.2.9)	1.048
SFD balance eq.	equation** (6.2.12)	equation (6.2.9)	1.042

* - standard finite-difference balance equation;

** - taking into account spectral deformation in the 3rd group

up $K_{eff}^{CRAMS} = 1.036$

As can be seen from the Table, different approaches were applied for calculations in various groups. Calculations of flux distributions in the first and the second group were based on the standard finite difference approach. Two forms of modified balance equation were applied for the third and fourth groups. To take into account spectral deformations in the third group "local", depending on cell position, values of macro cross sections were used.

Data of Table 6.2.3 make it possible to conclude that the application of algorithm (6.2.9) for the thermal group in a combination with the application of a complicated balance equation for group 3 reduces the deviation of K_{eff} from 0.067 to 0.042. It should be noted that in real fuel lattices the epithermal neutron spectrum deformation and its influence on the K_{eff} value is less than in the considered case.

The results obtained make it possible to come to the following conclusions:

- the use of the modified balance equation allows one to increase significantly the accuracy of the calculational prediction of main characteristics of nonuniform lattices;
- the results of calculations are stable as regards variation of transient mode functionals within the limits of possible inaccuracy of their computing;
- the main assumption made when deriving the modified balance equation are sufficiently well-founded;
- special 2D calculations are needed to analyse the influence of higher azimuthal harmonics.

6.2.3. Advanced neutron balance equation of PERMAK code

There are some defects in the traditional finite difference approximation realized in the basic version of the PERMAK code (Lizorkin et al., 1985). There are some specific causes for these defects in the traditional approximation:

- mutual influence of adjacent cells with different properties on few group effective neutron cross sections (mainly in thermal group) since the spectrum becomes nonasymptotic;
- lack of accuracy of finite difference in case of small diffusion length compared with the mesh step size;
- strong heterogeneity of cells.

From the practical point of view, the following items are insufficient.

These defects do not allow one to obtain high accuracy of calculations of pin power distribution in regions of nonuniform lattice. Underestimation of control rod efficiency is also caused by these defects.

Some attempts were undertaken to improve balance equation (5.3.2) for PERMAK. Satisfactory results were obtained by using 6 neutron groups with 3 groups in the thermal neutron region with modification of the balance equation taking into account the small diffusion length relative to mesh step. This improvement based on (Novikov, 1980) gives high accuracy of calculations (Lizorkin, 1980) in comparison with experimental data obtained on ZR-6. But this method is not widely used in practical calculations for the following reasons: firstly, this method takes into account only two of the three main reasons for the lacking accuracy mentioned above, viz. spectral interaction and mesh coarseness (heterogeneity of the cell is not taken into account); secondly, calculations using 3 group in the thermal neutron energy region with full scattering matrix are significantly more expensive.

More successful results (Lizorkin et al, 1990) were obtained using the method based on (Novikov, 1982). Modifications of the balance equation of PERMAK have been made by representing the thermal flux as superposition of four components (analogously with Section 6.2.1 but now the components are defined with slight difference).

Let us assume that in an arbitrary hexagonal cell with 30° azimuthal symmetry on geometry and material composition the thermal flux and current can be presented as linear combination of trial functions:

$$\Phi(\bar{r}, E, \bar{\Omega}) = A_a \varphi_{\omega a}(\bar{r}, E, \bar{\Omega}) + A_s \varphi_{\omega s}(\bar{r}, E, \bar{\Omega}) + B_a \varphi_{\tau a}(\bar{r}, E, \bar{\Omega}) + B_s \varphi_{\tau s}(\bar{r}, E, \bar{\Omega}), \quad (6.2.18)$$

$$J(\bar{r}, E, \bar{\Omega}) = A_a j_{\omega a}(\bar{r}, E, \bar{\Omega}) + A_s j_{\omega s}(\bar{r}, E, \bar{\Omega}) + B_a j_{\tau a}(\bar{r}, E, \bar{\Omega}) + B_s j_{\tau s}(\bar{r}, E, \bar{\Omega}),$$

where all trial functions satisfy the neutron transport equation and have the following properties:

$\varphi_{\omega a}$ and $\varphi_{\omega s}$ ($j_{\omega a}$ and $j_{\omega s}$) - assymmetrical and symmetrical in the cell "infinite" trial functions which are thermal flux (current) distributions in a cell placed in a physically infinite (from point of view of spectral perturbations) lattice of the same cells. Symmetrical trial function is determined by symmetrical inner source from upper neutron groups without neutron leakage in thermal group. Assymmetrical trial function is determined by assymmetrical source and satisfies condition that the cell boundary integral of current should be equal to zero;

$\varphi_{\tau a}$ and $\varphi_{\tau s}$ ($j_{\tau a}$ and $j_{\tau s}$) - asymmetrical and symmetrical in the cell transient trial functions which are solutions of neutron transport equations in the presence of non-vanishing net current or incoming current (without inner source);

A_a , A_s , B_a , and B_s - weighting factors.

The main difference between such a trial function definition from the definition in Section 6.2.1 is the taking into account of asymptotic symmetrical current as a part of the transient symmetrical function.

Averaging (6.2.18) over energy and over the cell side one can obtain an expression for the average flux and current on side i as

$$\tilde{\Phi}^{(i)} = A_a \tilde{\varphi}_{\omega a}^{(i)} + A_s \tilde{\varphi}_{\omega s}^{(i)} + B_a \tilde{\varphi}_{\tau a}^{(i)} + B_s \tilde{\varphi}_{\tau s}^{(i)} = \tilde{\varphi}_{\omega a}^{(i)} + \tilde{\varphi}_{\omega s}^{(i)} + \tilde{\varphi}_{\tau a}^{(i)} + \tilde{\varphi}_{\tau s}^{(i)} \quad (6.2.19)$$

$$\tilde{J}^{(i)} = A_a \tilde{j}_{\omega a}^{(i)} + A_s \tilde{j}_{\omega s}^{(i)} + B_a \tilde{j}_{\tau a}^{(i)} + B_s \tilde{j}_{\tau s}^{(i)} = \tilde{j}_{\omega a}^{(i)} + \tilde{j}_{\tau a}^{(i)} + \tilde{j}_{\tau s}^{(i)}$$

(symmetrical components have no dependence on side number i , averaged on side "infinite" symmetrical current component equals to zero).

Assume that analogously with (6.2.2) asymmetrical functions have cosine dependence on azimuth. In this case the following functionals which have no dependence on side number can be defined:

$$D_{\infty} = \frac{h \tilde{j}_{\omega a}}{2 \tilde{\varphi}_{\omega a}}, \quad D_{\tau} = \frac{h \tilde{j}_{\tau a}}{2 \tilde{\varphi}_{\tau a}}, \quad \theta = \frac{h \tilde{j}_{\tau s}}{2 \tilde{\varphi}_{\tau s}}, \quad (6.2.20)$$

$$\varepsilon_{\infty} = \frac{\tilde{\varphi}_{\omega s}}{\bar{\varphi}_{\omega s}}, \quad \varepsilon_{\tau} = \frac{\tilde{\varphi}_{\tau s}}{\bar{\varphi}_{\tau s}},$$

where h is the mesh step size, $\bar{\varphi}_{\omega s}$ and $\bar{\varphi}_{\tau s}$ are volume averaged values of symmetrical trial functions.

Taking it into account that

$$\bar{\Phi}_{\omega s} = A_s \bar{\varphi}_{\omega s}, \quad \bar{\Phi}_{\tau s} = B_s \bar{\varphi}_{\tau s}, \quad (6.2.21)$$

and using (6.2.19) one can write an expression which connects boundary flux and current with cell averaged flux

$$\tilde{\Phi}^{(1)} - \frac{h}{2} \tilde{J}^{(1)} \left[\frac{\tilde{J}_{\omega a}^{(1)}}{\tilde{J}^{(1)} D_{\omega}} \frac{1}{\tilde{J}^{(1)} D_{\omega}} + \frac{\tilde{J}_{\tau a}^{(1)}}{\tilde{J}^{(1)} D_{\tau}} \frac{1}{\tilde{J}^{(1)} D_{\tau}} \right] = \bar{\Phi}_{\omega s} \varepsilon_{\omega} + \bar{\Phi}_{\tau s} \varepsilon_{\tau} \quad (6.2.22)$$

Taking into account the conclusion of (Pshenin et al, 1988) about the small difference of D_{ω} and D_{τ} and the slight influence of this difference on calculational results, it was chosen for PERMAK:

$$D = D_{\tau} \quad (6.2.23)$$

Rewrite (6.2.22) as

$$\tilde{\Phi}^{(1)} - \frac{h}{2D} \tilde{J}^{(1)} = \bar{\Phi} \varepsilon, \quad (6.2.24)$$

$$\text{where } \bar{\Phi} = \bar{\Phi}_{\omega s} + \bar{\Phi}_{\tau s} \quad \text{and} \quad \varepsilon = \frac{\bar{\Phi}_{\omega s}}{\bar{\Phi}} \varepsilon_{\omega} + \frac{\bar{\Phi}_{\tau s}}{\bar{\Phi}} (\varepsilon_{\tau} - \theta/D).$$

Analogously expression (6.2.24) can be written for cell i which is adjacent to the given cell on boundary i . Taking into account continuity conditions for flux and current at the common boundary of cells one can express boundary flux and current as:

$$\tilde{\Phi}^{(i)} = \frac{D \bar{\Phi} \varepsilon + D^i \bar{\Phi}^i \varepsilon^i}{D \varepsilon + D^i \varepsilon^i} \quad (6.2.25)$$

$$\tilde{J}^{(i)} = \frac{2}{h} \frac{D}{D + D^i} \left[\bar{\Phi} \varepsilon - \bar{\Phi}^i \varepsilon^i \right]$$

Using continuity conditions for all of the cell sides one can write the thermal neutron group balance equation:

$$\frac{4}{3h^2} \sum_{i=1}^6 \frac{D}{D + D^i} \left[\bar{\Phi} \varepsilon - \bar{\Phi}^i \varepsilon^i \right] + \Sigma^a \bar{\Phi} = \bar{S}, \quad (6.2.26)$$

where Σ^a and all other neutron cross sections are linear combinations of Σ_{ω} and Σ_{τ} weighted with the corresponding share of $\bar{\Phi}_{\omega s}$ and $\bar{\Phi}_{\tau s}$ components in the total thermal neutron flux:

$$\Sigma = \frac{\bar{\Phi}_{\omega s}}{\bar{\Phi}} \Sigma_{\omega} + \frac{\bar{\Phi}_{\tau s}}{\bar{\Phi}} \Sigma_{\tau} \quad (6.2.27)$$

$$\bar{\Phi}_{\omega s} = \frac{S}{\Sigma^a} \quad \text{and} \quad \bar{\Phi}_{\tau s} = \bar{\Phi} - \bar{\Phi}_{\omega s} \quad (\bar{S} \text{ is the cell averaged source for the})$$

thermal group).

Equation (6.2.26) is a nonlinear equation since its coefficients (ϵ and Σ) depend on the solution. They should be corrected during the iterative process. Experience in utilizing of the new version of PERMAK shows that the rate of convergence of iterations is almost the same because spectral perturbations have a short distance influence in spite of the significant local values.

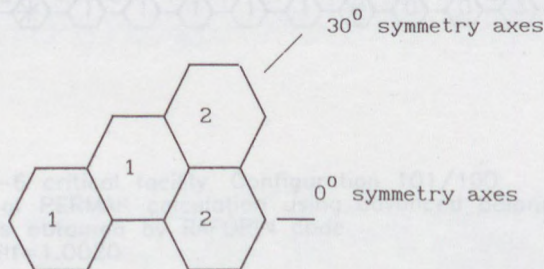
This algorithm differs from that described in section 6.2.1. Firstly, in 6.2.1 asymptotic and transient components of the symmetrical current are considered separately. In PERMAK the total symmetrical current is taken into account. Secondly, approximation (6.2.23) which is based on the conclusion of (Pshenin et al, 1988) allows one to neglect that one of the cell parameters is a tensor (either D or ϵ) which occurs in the algorithm of Section 6.2.1 if the difference of D_∞ and D_τ is taken into account. Both of these items simplified the realization of the algorithm.

In the epithermal energy group a more accurate definition of the equation is achieved by taking into account the cell heterogeneity using

$$\epsilon = \frac{\tilde{\varphi}_s}{\varphi_s} - \frac{h}{2} \frac{\nabla \tilde{\varphi}_s}{\varphi_s}.$$

The balance equation has the same form as (6.2.26) but it is linear (i.e. none of the coefficients have any dependence on the solution).

The necessary thermal cross sections for the algorithm, for example, can be obtained from precise multigroup calculations of the flux in the following supercell:



Cells of type 2 should differ from type 1 cells and their properties should provide a neutron current through the boundary between 1 and 2 type cells. On the basis of definitions (6.2.24-6.2.27) all the necessary functionals of type 1 cells can be obtained using cell averaged flux and reaction rates and boundary averaged flux and current.

The necessary functionals can also be obtained by considering other

supercells in such conditions that every trial function (6.2.18) should occur in them. For example, in *RAFORIN* (Pshenin et al, 1989) that is achieved by using the corresponding set of boundary conditions.

Some results of calculations using the described algorithm (*RAFORIN-PERMAK*) for the ZR-6 critical facility (Final Report of TIC, 1985) are presented in Figs. 6.5-6.10. These figures show that in comparison with traditional calculations (see Figs. 5.2-5.7) the criticality and power distribution are described significantly better. Calculations of effective multiplication factor have an accuracy of about 0.1-0.2% including the results for configurations with strong absorber rods. The power distribution is described within the accuracy of the measurements.

The balance equation has the same form as (6.2.5) but it is linear (1.6). The necessary thermal cross sections for the algorithm, for example, can be obtained from precise multigroup calculations of the flux in the following way: solve the balance equation for the flux in the multigroup approximation. The necessary thermal cross sections for the algorithm, for example, can be obtained from precise multigroup calculations of the flux in the following way: solve the balance equation for the flux in the multigroup approximation. The necessary thermal cross sections for the algorithm, for example, can be obtained from precise multigroup calculations of the flux in the following way: solve the balance equation for the flux in the multigroup approximation.

$$\frac{1}{4} \sum_{i=1}^4 \frac{D_i}{D_i + D} \left[\frac{1}{D_i} \frac{d\phi_i}{dx} - \frac{1}{D} \frac{d\phi}{dx} \right] = \frac{1}{D} \frac{d\phi}{dx} \quad (6.2.6)$$



Cells of type 2 should differ from type 1 cells and their properties should provide a neutron current through the boundary between 1 and 2 type cells. On the basis of definition (6.2.5-6.2.7) all the necessary functionals of type 1 cells can be obtained using cell averaged flux and reaction rates and reaction rates can also be obtained by considering other

fig 6-5

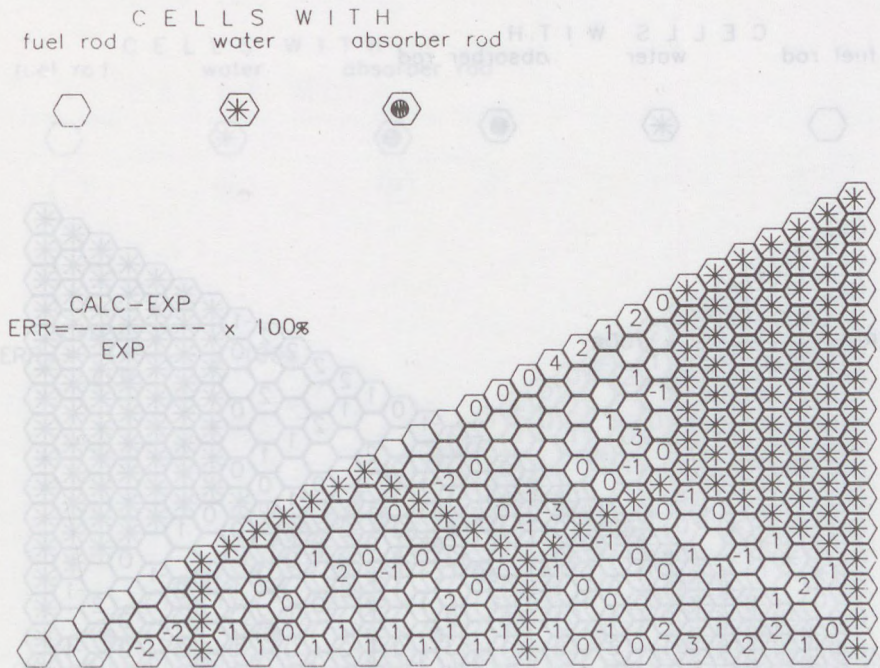


Fig. 6.5 ZR-6 critical facility. Configuration 101/100.
 An accuracy of PERMAK calculation using advanced balance equation
 with constants obtained by RAFORIN code.
 Calculated $K_{\text{eff}} = 1.0020$.

fig 6-6

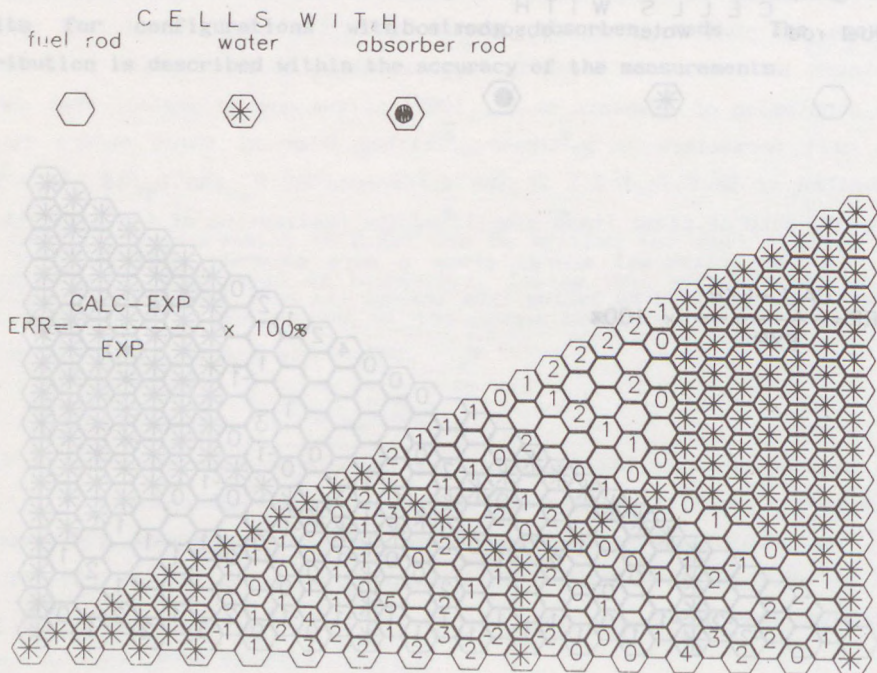


Fig. 6.6 ZR-6 critical facility. Configuration 102/102.
An accuracy of PERMAK calculation using advanced balance equation
with constants obtained by RAFORIN code.
Calculated Keff=0.9998.

fig 6-7

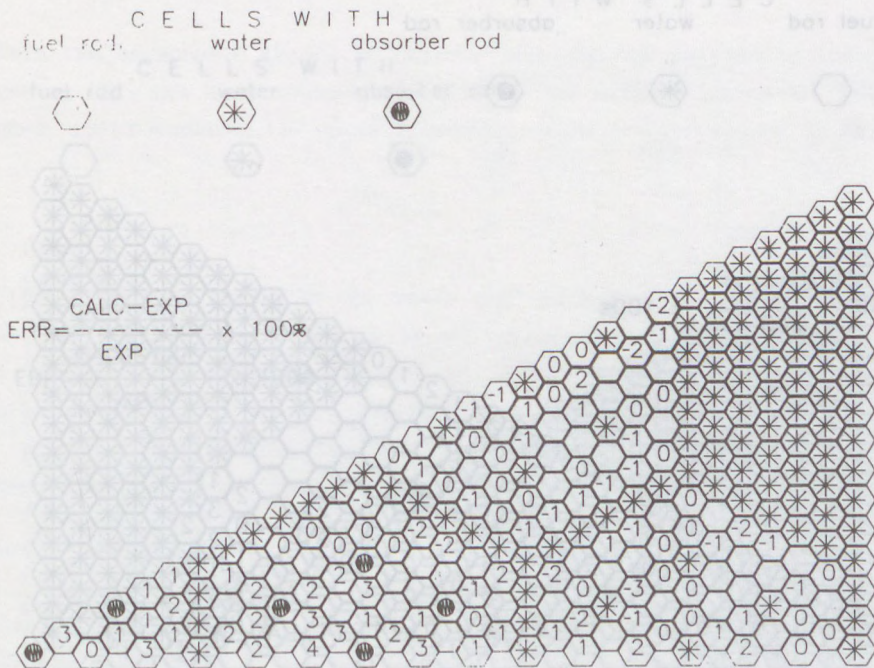


Fig. 6.7 ZR-6 critical facility. Configuration 103/103.
 An accuracy of PERMAK calculation using advanced balance equation
 with constants obtained by RAFORIN code.
 Calculated $K_{\text{eff}} = 0.9983$.

fig 6-8

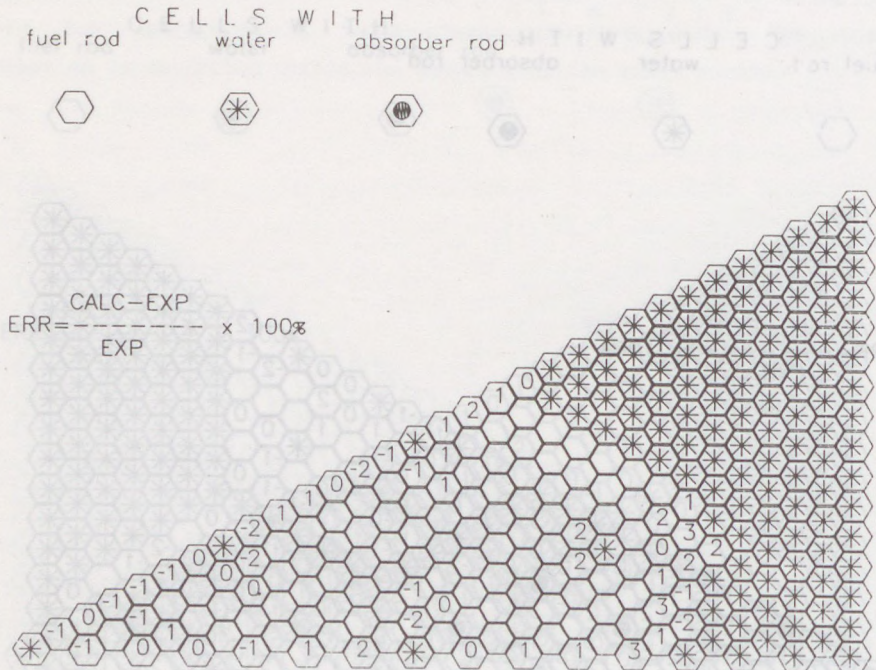


Fig. 6.8 ZR-6 critical facility. Configuration 57/57.

An accuracy of PERMAK calculation using advanced balance equation with constants obtained by RAFORIN code.

Calculated $K_{\text{eff}} = 0.9979$.

fig 6-10

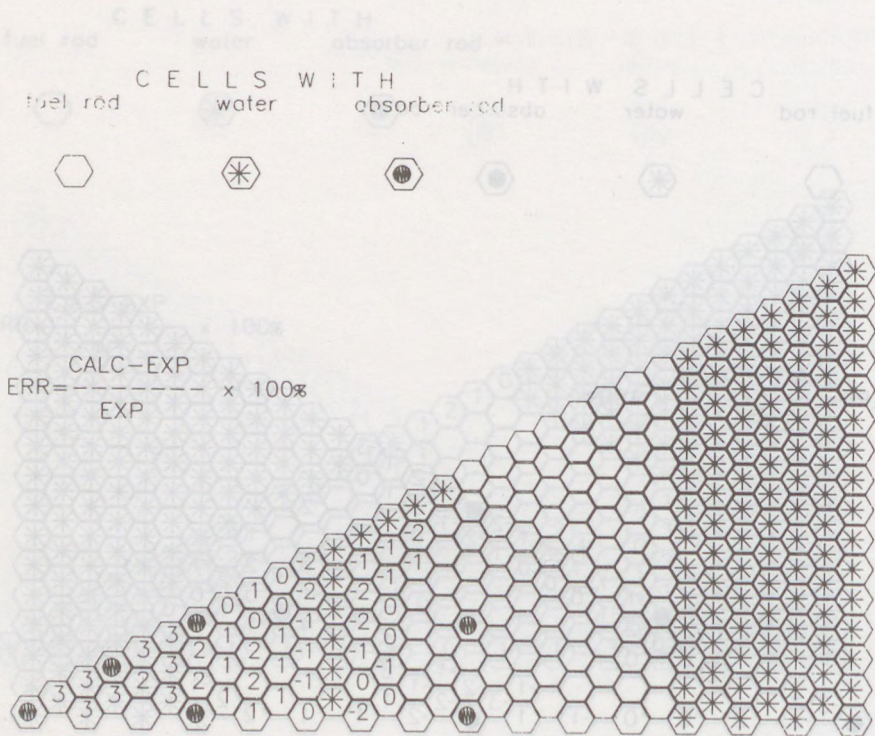


Fig. 6.10 ZR-6 critical facility. Configuration 90/87.
An accuracy of PERMAK calculation using advanced balance equation
with constants obtained by RAFORIN code.
Calculated K_{eff} =0.9977.

6.3 NON-LINEAR BALANCE EQUATION AND ITS SOLUTION

An upgraded mathematical model of non-uniform lattices is considered in the present Section. The model is based upon solving a nonlinear equation expressing neutron balance. The detailed derivation of the balance is deferred, first a generalization of the asymptotic lattices and the role of the cell's symmetries in the derivation are assessed.

6.3.1 Corrections for Asymptotic Lattice Theory

Within the asymptotic theory of uniform lattices the multigroup transport equation (TE) has been discussed by a number of authors (Benoist, 1964 and Hughes, 1978) assuming the space dependence of the neutron source to be

$$e^{i\mathbf{Br}} u(\rho),$$

in the considered energy group, where $u(\rho)$ is a periodic function. It is easy to see that this assumption is not correct and is superfluous as well and Rumyantsev's analysis (Rumyantsev 1962, 1963, Sidorenko, 1981) is applicable to the multigroup transport equation. The below given discourse is based on considerations utilized in quantum mechanics, and it generalizes Rumyantsev's result (Rumyantsev 1962, 1963). The TE is written as

$$\begin{aligned} \left(-\nabla^2 + \Sigma_g(\rho) \right) \Psi_g(\rho, \Omega) = & \sum_{g'=1}^G \int_{4\pi} d\Omega' \Sigma_{g',g}(\Omega', \Omega) \Psi_{g'}(\rho, \Omega') + \\ & + \frac{\chi_g}{K_{eff}} \sum_{g'=1}^G \nu \Sigma_{fg'} \int_{4\pi} \Psi_{g'}(\rho, \Omega) d\Omega \end{aligned} \quad (6.3.1)$$

in an infinite lattice, and the solution Ψ_g is invariant under translation by lattice vector $\mathbf{d}$, which connects the centers of two cells. Thus there is a point in expressing a particular solution of Eq.(6.3.1) with the help of eigenfunctions of the translation.

That particular solution has the form

$$\Psi_B(\rho, \Omega) = e^{i\mathbf{Br}} u_B(\rho, \Omega). \quad (6.3.2)$$

Function Ψ_B is called the Bloch function and is a generalization of

functions F_s and F_{as} defined in (Rumyantzev, 1962). Here B is a real vector. The TE is invariant under the symmetry transformations of the lattice. Therefore we may get new partial solutions, i.e. new Bloch functions, by applying these symmetry transformations to a given Bloch function. With a given k_{eff} , the flux in any energy group can be expressed as a linear combination of Bloch functions:

$$\Psi_g(\rho, \Omega) = \sum_B W(B) e^{iBr} u_{gB}(r, \Omega) . \quad (6.3.3)$$

In expression (6.3.3), the summation goes over all the vectors that belong to a given value of k_{eff} . An equation for function u_B is obtained by substituting expression (6.3.3) into the TE (6.3.1). A matrix notation is used below for the sake of simplicity, all the cross-sections in Eq. (6.3.1) are comprised into matrix Σ . Functions u_{gB} are suppressed in vector u_B that satisfies the equation

$$\left[\Omega \nabla + \Sigma(K_{eff}(B)) \right] u_B(r, \Omega) = -i(\Omega B) u_B(r, \Omega) . \quad (6.3.4)$$

The boundary condition prescribed for u_B fixes that u_B is periodic. When $B=0$, the solution of Eq. (6.3.4) has a physical meaning, it gives the flux in the infinite lattice, where there is no leakage. Function u_B can be assumed to depend weakly on parameter B and it can be approximated by the first few terms in its Taylor series:

$$u_B(r, \Omega) = u_0(r, \Omega) + iBu_1(r, \Omega) + (iB^2) u_2(r, \Omega) . \quad (6.3.5)$$

Function u_1 has as many components as vector B . Each component depends on the neutron energy. Function u_2 is a matrix, though here its off-diagonal elements are neglected. The set of vectors, admissible in expression (6.3.3), is also invariant under the symmetry transformations of the lattice (Binnebeck, 1974), (Makai 1979). Hence, if the cell is symmetrical then the Taylor series of function $k_{eff}(B)$ may not contain certain terms and it has the form:

$$k_{eff}(B) = K_\infty + \sum_1 K_{21} B_1^2 \quad (6.3.6)$$

Substituting Eqs. (6.3.5) and (6.3.6) into (6.3.4) and comparing the

coefficients of terms with given powers of the components of vector B, we get:

$$\left[\underline{\Omega \nabla} + \Sigma(K_\infty) \right] u_0(\rho, \Omega) = 0 \quad (6.3.7a)$$

$$\left[\underline{\Omega \nabla} + \Sigma(K_\infty) \right] u_{-1}(\rho, \Omega) = -\Omega u_0(\rho, \Omega) \quad (6.3.7b)$$

$$\left[\underline{\Omega \nabla} + \Sigma(K_\infty) \right] u_{211}(\rho, \Omega) = -\Omega_{11} u_{11}(\rho, \Omega) + K_{21} u_0(\rho, \Omega) \quad (6.3.7c)$$

Function u_B and its components in Eqs.(6.3.7) are called microfluxes. The boundary conditions for Eqs.(6.3.7) are derived from the periodicity of the solution at the cell's boundary on the one hand, and from the symmetries of the cell on the other:

$$\int_{4\pi} d\Omega_n u_0(\xi, \Omega) = 0 \quad (6.3.8a)$$

$$\int_{4\pi} d\Omega_n u_{11}(\xi, \Omega) = 0 \quad (6.3.8b)$$

$$\int_{4\pi} d\Omega_n u_{211}(\xi, \Omega) = 0 \quad , \quad (6.3.8c)$$

where ξ denotes a point on the boundary, Ω_n is the normal component of Ω at the boundary. In practical calculations the cell is often taken as symmetrical. The above formulae (6.3.8) are applicable to cylindrical cells, too. The following expression is obtained for the flux by means of Eqs.(6.3.3)and (6.3.5):

$$\Psi_g(\rho, \Omega) = \Phi(r) u_{0g}(r, \Omega) + \nabla \Phi(r) u_{1g}(r, \Omega) + \dots, \quad (6.3.9)$$

where the macroflux Φ is given by

$$\Phi(r) = \left[\sum_{B \in R} W(B) e^{iBr} \right] \quad (6.3.10)$$

The asymptotic theory has led to the following results. We can express the flux with the help of Bloch's functions having a free parameter B.

This parameter determines the leakage of the cell. Only the magnitude of the buckling vector can be determined from the criticality condition $k_{eff}=1$. The flux of a critical lattice is given by an expression in which Bloch's functions with such a parameter B may occur that corresponds to the $k_{eff}=1$ condition. The periodic component of the flux is obtained from Eqs. (6.3.5) and (6.3.7). The amplitude of vector B and the weight function $W(B)$ should be selected such that flux (6.3.9) should meet the known boundary condition at the boundary of the finite lattice. The macroflux satisfies a one group diffusion equation.

Equation (6.3.9) has been widely utilized for expressing the neutron flux at a given point ρ . The first term in this expression is the microflux multiplied by the macroflux. The second term accounts for the cross flow and equals the gradient of macroflux multiplied by the microflux u_1 . It is often assumed that the macroflux is composed with the help of a constant weight for every Bloch's function with $B=|B|$. In this case the macroflux in a two dimensional lattice is given by $J_0(B\rho)$.

The necessity to cope with diverse lattice inhomogeneities has led to major difficulties in uranium-water lattices. The above obtained expression describes well the flux when the neutron spectrum is asymptotic. However, in cells located close to an inhomogeneity, some correction is needed.

Above we have assumed all the cells to be identical. Below some methods for characterizing 'disturbed' lattices will be considered. A 'disturbed' lattice comprises fuel cells and inhomogeneities (e.g. absorber rod, assembly wall, water hole). The discussion is confined to cases where the cells are symmetrical and their geometry is the same: regular hexagon or square.

Let us point out two important features of the flux distribution in a periodic lattice without perturbation for those features can be exploited in the case of disturbed lattices as well:

- the macroflux satisfies the two energy group diffusion equation;
- the microfluxes can be obtained by solving the TE with prefixed boundary conditions that are related to the symmetry properties of the solution to the TE.

The effect of an inhomogeneity appears in the non-asymptotic neutron spectrum at the cell boundary. The few group constants (cross-sections) will depend on the surroundings in the vicinity of an inhomogeneity. The method given below helps overcome that inconvenience by calculating iteratively the constants of the diffusion equation that turns out to be a modified finite difference scheme.

Following (Makai 1982, 1984), let us investigate the structure of set R that contains the vectors B that correspond to a given k_{eff} in Eq. (6.3.10). From (Makai, 1983) it is known that set R consists of two subsets: R_{as} and R_{tr} . The first subset contains those B vectors with $B = \mu$, the second one with $B = \nu$, where $\nu > |\mu|$.

By virtue of the properties of these subsets, the macroflux can be shown to have two important properties of the two group flux. The boundary conditions, to be forced on microfluxes u_0 and u_1 are irreducible components of the general boundary conditions decomposed according to the cell'symmetries. By decomposing the entering currents at the cell boundary into irreducible components, it can be shown that the corresponding irreducible components (or shortly irreps) of the microflux u_B are the generalizations of u_0 and u_1 and the amplitudes of the irreducible components are obtained from a finite difference scheme. Taking into account the continuity of flux and current at the cell boundaries, the non-symmetrical components can be eliminated from the earlier mentioned difference scheme (Gado et al. 1983). The symmetrical component turns out to satisfy a finite difference equation. Here the constants in the difference equation are calculated not as in the traditional finite difference equation. An iterative procedure can be constructed in the frame of which all the necessary quantities are derived (Gado et al., 1983, 1984). For simplicity's sake let us consider a one dimensional lattice. Let us retain the second order in B^2 terms in the expansion

$$K_{eff}(B^2) = K_{\infty} + K_1 B^2 + K_2 B^4. \quad (6.3.11)$$

In Eq. (6.3.10), set R consists of those vectors B that correspond to the given k_{eff} value. With k_{eff} given, Eq. (6.3.11) has two roots $B^2 = \mu$ and $B^2 = \nu$. These roots are always real. Symbol μ will denote the positive root, the other root is not necessarily positive. Accordingly, the set R is decomposed as

$$R = R_{as} + R_{tr} \quad (6.3.12)$$

so that

$$B \in R_{as} \quad \text{if} \quad |B| = \mu. \quad (6.3.13)$$

$$B \in R_{tr}, \quad \text{if} \quad |B| = \nu. \quad (6.3.14)$$

The neutron flux can be written as

$$\Psi_g(r, \Omega) = \Phi_{as}(r) u_B^{as}(r, \Omega) + \Phi_{tr}(r) u_B^{tr}(r, \Omega) \quad (6.3.15)$$

$$\nabla^2 \Phi_{as}(r) = \mu^2 \Phi_{as}(r) \quad (6.3.16a)$$

$$\nabla^2 \Phi_{tr}(r) = \nu^2 \Phi_{tr}(r) \quad (6.3.16b)$$

Hence the macroflux has an important property, viz. it is composed of two terms each being an eigenfunction of the Laplace operator. In (Makai 1982, 1983), set R has been extended to the complex plane and the macroflux has been shown to be obtained from a two group diffusion equation.

6.3.2 Generalization of u_0 and u_1

Let us mention certain properties of functions u_0 and u_1 . Microflux u_0 is symmetrical with respect to inversion through the cell's center. Function u_{1x} and u_{1y} transform under rotations and reflections as do coordinates x and y of a vector, respectively. In other words they transform as given irreducible components of function u_B . We would only remark here that the irreducible representation (irrep) is a handy generalization of the even-odd notion, and leads to the following generalization: any function or vector can be decomposed into irreps. Let us decompose the boundary conditions into irreps (Makai, 1979, 1982) shown in Figs. 6.11 and 6.12 for hexagonal and square lattices, respectively. It is easy to show that the irreps have the following properties:

- a) A given irrep describes how the given component transforms under the symmetry transformations of the region.
- b) Irreps form a complete system, i.e. any function or vector can be decomposed into irreducible components.
- c) With the help of the irreps, vectors of specific transformation properties can be formed. Such vectors are, for example, the values of the function in question at symmetrically located points, its average values at the faces of the region. Such vectors are displayed in Figs. 6.11 and 6.12.
- d) Linear operators of reactor physics preserve the symmetry properties of the flux, i.e. Ψ belongs to the same irrep as does scalar flux, or as does the normal component of the neutron current, or as do the partial currents.

e) If the function given as boundary condition belongs to any irrep then the solution of the TE belongs to the same irrep, i.e. their symmetry properties are the same.

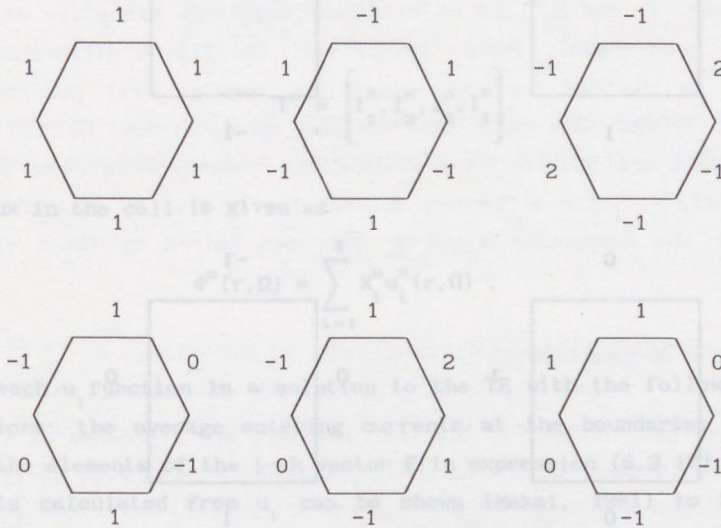


Fig.6.11. Irreducible boundary condition patterns for a hexagonal cell

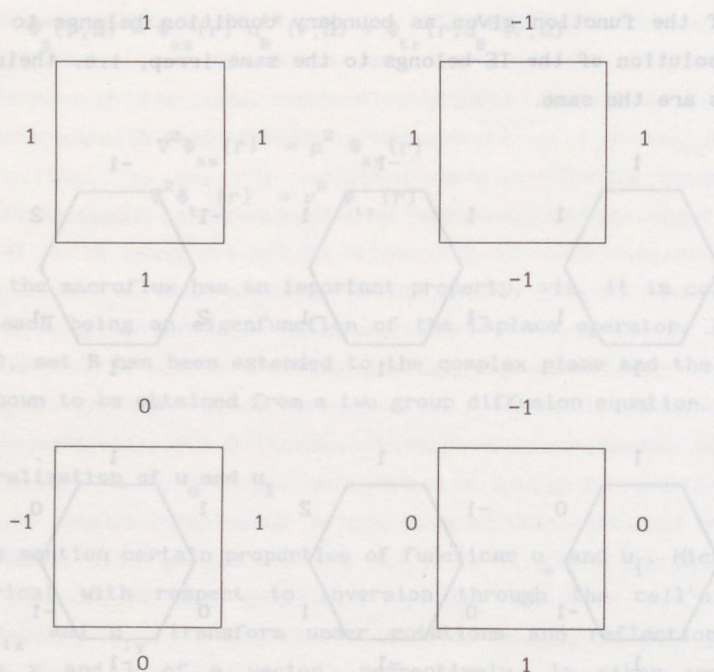


FIG. 6.12. Irreducible boundary condition patterns for

square cells

f) Some irreps are two-dimensional. In this case two linearly independent functions, the so called components, belong to the same irrep and a matrix describes the effect of a symmetry transformation.

g) The same matrix transforms the two components of a two-dimensional irrep.

h) The vectors describing the irreps in a square and in a regular hexagon are as follows:

$$\epsilon_1 = (1, 1, 1, 1); \quad \epsilon_2 = (1, -1, 1, -1);$$

$$\epsilon_3 = (0, 1, 0, -1); \quad \epsilon_4 = (1, 0, -1, 0);$$

$$\epsilon_1 = (1, 1, 1, 1, 1, 1); \quad \epsilon_2 = (1, -1, 1, -1, 1, -1);$$

$$\epsilon_3 = (2, -1, -1, 2, -1, -1); \quad \epsilon_4 = (0, 1, -1, 0, 1, -1);$$

$$\epsilon_5 = (2, 1, -1, -2, 1, -1); \quad \epsilon_6 = (0, 1, 1, 0, -1, -1).$$

Let us decompose the given entering currents at the boundary of the n -th square shaped cell according to the above given ξ vectors:

$$I^n = X_1^n \epsilon_1 + X_2^n \epsilon_2 + X_3^n \epsilon_3 + X_4^n \epsilon_4, \quad (6.3.17)$$

where

$$I^n = \begin{bmatrix} I_1^n, I_2^n, I_3^n, I_4^n \end{bmatrix}.$$

The flux in the cell is given as

$$\Psi^n(r, \Omega) = \sum_{i=1}^4 X_i^n u_i^n(r, \Omega), \quad (6.3.18)$$

where each u_i function is a solution to the TE with the following boundary conditions: the average entering currents at the boundaries of the cell equal the elements of the i -th vector ξ in expression (6.3.17). The partial currents calculated from u_i can be shown (Makai, 1981) to have average values at the cell faces proportional to the i -th vector ξ . Therefore the exiting currents are written as

$$J^n = X_1^n r_1^n \epsilon_1 + X_2^n r_2^n \epsilon_2 + X_3^n r_3^n \epsilon_3 + X_4^n r_4^n \epsilon_4. \quad (6.3.19)$$

The irreps X fix the entering currents at the boundaries:

$$X_k^n = I^n e_k \quad k=1, \dots, 4. \quad (6.3.20)$$

Let us introduce the following notation. Superscript 0 refers to the "central" cell, whereas superscripts 1, ..., 4 to its neighbors. The exiting current of the central cell is the entering current of one of the neighbours so making use of Eqs. (6.3.18) and (6.3.20) we get the following expression for X :

$$X_k^0 - \frac{1}{4} \sum_{i=1}^4 X_k^i r_k^i = Q_k^0 \quad (6.3.21)$$

The explicit source term has been derived in (Makai, 1981, Makai, 1982), here only the Q_1^0 term is given explicitly:

$$Q_1^0 = X_2^3 r_2^3 - X_2^1 r_2^1 + X_3^4 r_3^4 - X_3^2 r_3^2 + X_4^1 r_4^1 - X_4^2 r_4^2 + X_4^3 r_4^3 - X_4^4 r_4^4 \quad (6.3.22)$$

The terms X_2 and X_3 can be eliminated from Eq. (6.3.21) and the remaining components, viz. X_1 and X_4 , are of different magnitude since for any n $X_1^n \gg X_4^n$. Let us note (Makai, 1982a, 1982b) that the finite difference form (6.3.22) can be derived for any symmetrical regular cell provided the corresponding irreps have been used in the decomposition (6.3.17). The obtained results are general: the irreducible components of the partial currents satisfy a finite difference scheme. The problem of decoupling the equations for the components X_1 and X_4 has been solved by (Gado et al., 1983, 1984).

6.3.3 Synthesis Method (KFKI)

The fluxes and currents at the cell boundary are expressed as the sum of a symmetrical (subscript 0) and a non-symmetrical (subscript 1) term:

$$\Phi_{ki}^g = B_{ko}^g + B_{ki}^g, \quad (6.3.23)$$

$$J_{ki}^{rg} = A_{ko}^{rg} + A_{ki}^{rg}. \quad (6.3.24)$$

Because of the continuity of fluxes and currents at the i -th boundary of the k -th cell, the following relation holds:

$$B_{ko}^g + B_{ki}^g = B_{k'o}^g + B_{k'i}^g, \quad (6.3.25)$$

$$A_{ko}^g + A_{ki}^g = -A_{k'o}^g - A_{k'i}^g. \quad (6.3.26)$$

Let us introduce new quantities α_{k1}^g and ϵ_{k1}^g as

$$\alpha_{k1}^g = \frac{h}{2} \frac{A_{k1}^g}{B_{k1}^g}, \quad (6.3.27)$$

$$\epsilon_{k1}^g = \frac{\left(B_{ko}^g - \frac{h}{2\alpha_{k1}^g} A_{ko}^g \right)}{\bar{\Phi}_k^g}, \quad (6.3.28)$$

where h is the lattice pitch, $\bar{\Phi}_k^g$ - volume averaged flux in group g . Now, the leakage of the k -th cell is given by

$$L_k^g = \frac{2}{h} \sum_{i=k}^6 \frac{\alpha_{ki}^g \alpha_{k,i}^g}{\alpha_{k1}^g + \alpha_{k,i}^g} \left[\epsilon_{k,i}^g, \bar{\Phi}_k^g, - \epsilon_{k1}^g, \bar{\Phi}_k^g \right] \quad (6.3.29)$$

because of the continuity of fluxes and currents. The average flux $\bar{\Phi}_k^g$ is a function of symmetrical flux components at the boundaries of the cell:

$$\bar{\Phi}_k^g = \sum_{g'=1}^G \Gamma_{(0)k}^{g',g} B_{k0}^g \quad (6.3.30)$$

Matrix $\Gamma_{(0)k}^{g',g}$ is considered to describe a given property of the cell. That consideration is based on the following considerations.

Let us describe the cell in first collision probability (FCP) approximation and let us expand the flux into irreps (index m). We get in few group approximation, neglecting the anisotropy of the scattering:

$$\begin{aligned} \Sigma_{t1}^g \Psi_1^{mg} = & \sum_{j=1}^N P_{ij00}^{mg} \left[\Sigma_{sj}^{gg} \Psi_j^{mg} + \sum_{g' \neq g}^{Gm} \Sigma_{sj}^{g',g} \Psi_j^{mg} + \frac{\zeta^m}{k_{eff}} \chi^g H_j^m \right] + \\ & + \Phi_m^g / 4 P_{s100}^{mg} + J_m^{rg} / 2 P_{s1r0}^{mg} + J_m^{\alpha g} / 2 P_{s1\alpha 0}^{mg} \end{aligned} \quad (6.3.31)$$

where $m=1,3,5$; $g=1, \dots, G$ and N is the number of space points; H_j^m - a priori known, normalized function of fission source distribution within the cell and

$$\zeta^m = \sum_1 \sum_g \nu \Sigma_{f1}^g \Psi_1^{mg} V_1 \quad (6.3.32)$$

The formulae for the P probabilities are not cited here, they are available in (Gado et al, 1984). They reproduce the usual FCPs when $m=0$ and for $m=1$ the program ANICELL (Devenyi, 1984) is capable of deriving them.

The solution of Eq.(6.3.31) explicitly depends upon k_{eff} . This dependence has the form

$$\Psi_i^{mg} = \sum_{g'=1}^G \left[\Psi_i^{m g g'} + \frac{R^{mg} \Psi_i^{m g f}}{K_{eff} - R^m} \right] \quad (6.3.33)$$

as was shown in (Gado et al. 1983, 1984). Here $F_m^{g'}$ is the m -th Fourier component of the scalar flux at the cell boundary. The first term gives the contribution due to a unit current (in group g') at the boundary to the intra cell flux (in group g). The second term is the contribution of the fission source.

Matrices of type Γ describe the reaction rate R_{xg} for any specific reaction in the cell and the ratio

$$\Sigma_{xg} = \frac{R_{xg}}{\Phi} \quad (6.3.34)$$

determines an effective cross-section for the cell and with them, the neutron balance in the cell is easily written down:

$$-\frac{2}{h} L_k^g - \Sigma_{ak}^g \bar{\Phi}_k^g + \frac{1}{K_{eff}} X^g \sum_{g'} \nu \Sigma_{fk}^{g'} \bar{\Phi}_k^{g'} + \sum_{g'} \Sigma_{sk}^{g'} \bar{\Phi}_k^{g'} = 0. \quad (6.3.35)$$

We wish to emphasize that the unknowns in Eq.(6.3.35) are the average fluxes of cell k . Clearly, if the leakage had the traditional form, we would have had the traditional finite difference form. Apparently, in a non-uniform lattice the average flux can be obtained from Eq.(6.3.35) with a good accuracy if reasonable assumptions can be accepted.

The cell is described by Γ_x matrices, which give the reaction rates type x for the symmetrical ($m=0$) modes, and by Γ_{jm} matrices, which give the current for every mode m at the cell boundary. It follows from Eq. (6.3.34) that retaining solely the mode subscript m , all the Γ -matrices depend on k_{eff} as

$$\Gamma_m = \left[\Gamma_{m1} + \frac{1}{k_{eff} - R^{mf}} \Gamma_{m2} \right] \quad (6.3.36)$$

The following iteration was proposed in (Gado et al., 1984) as a means of deriving every cell property and determining the neutron field.

1. First, before the iteration itself, the Γ_{1x} and Γ_{2x} matrices are calculated beforehand for every reaction type and for every cell type.
 2. Boundary fluxes and currents are obtained from cell averaged fluxes in accordance with (Gado et al. 1984). The flux is decomposed into irreps at the cell boundary, and the parameters Σ , α and ϵ are calculated.
 3. The cell average fluxes are calculated by solving Eq.(6.3.35) in a given cell.
 4. Step 3, is repeated for every cell. This completes one sweep.
 5. After the last sweep, k_{eff} is estimated from the overall balance.
 6. Steps 2-5, are repeated until a convergent solution is obtained.
- The approximations applied in the above described procedure are as follows.

- TE (6.3.31) is solved in cylindrical geometry;
- the angular dependence of the angle dependent flux is restricted to the terms P_0 and P_1 ;
- in the Fourier expansion of the flux at the boundary solely the first 6 components are retained.
- the cell is assumed symmetrical;
- the fission source is a priori known in the cell.

In accordance with the above proposed procedure the calculation of a non-homogeneous lattice is performed in two steps.

a.Cell calculation. The TE (6.3.31) is solved in a cell for $\Psi_1^{mgg'}$ with prefixed boundary conditions at the cell boundary, see Fig. 6.13. The number of groups is approximately 70. Another problem is solved to find Ψ_1^{mgf} , where the fission source is given and the flux at the cell boundary is zero. As a result, with the help of Eqs.(6.3.33)-(6.3.36) Γ matrices are obtained. Here the number of groups is 2-4.

b,Global calculation. As follows from Eq.(6.3.33), the reaction rates are calculated by means of Γ matrices and cell boundary fluxes. In one iteration the cell parameters α , ϵ and Σ are calculated whereas the cell average fluxes are calculated from Eq.(6.3.35). Hence the parameters α , ϵ and Σ can account for the local spectral phenomena at the boundary of the cell, in spite of the fact that at the stage where Γ matrices themselves have been calculated, the material properties of the cell had been fixed.

6.3.4 Correction for Lattice Pitch

It will be shown below how the method explained in Section 6.3.3 is capable of describing the neutron distribution in a uniform lattice, furthermore, parameters α and ϵ in a uniform lattice tend to the traditional diffusion coefficient (D) and to unity, respectively.

Expression (6.3.27) determines α as the ratio of the non-symmetrical components of the neutron current on the i -th cell boundary to the non-symmetrical components of fluxes on the same boundary. Both of these quantities are expressible by means of Γ matrices. Firstly, the boundary flux and its Fourier components are related as

$$\phi_{ki}^g = \sum_{m=1}^6 \epsilon_{m1} F_{km}^g, \quad (6.3.37)$$

where $\epsilon_m = [\epsilon_{m1}, \dots, \epsilon_{m6}]$ - irreps given by (6.3.17); and F_{km}^g - m -th Fourier component of the boundary flux; k -cell index; i -boundary index. Secondly, by virtue of Eq.(6.3.17), the Fourier components of the boundary current are

$$G_{km}^g = \sum_{g'=1}^G \Gamma_{Jkm}^{g'g} F_{km}^{g'},$$

where subscript J of the Γ matrix refers to its type, viz. the one determining the net boundary current. Thus we have

$$\alpha_{k1}^g = \frac{h}{2} \frac{\sum_{m>1} \sum_{g'=1}^G \Gamma_{Jkm}^{g'g} F_{km}^{g'} \epsilon_{m1}}{\sum_{m>1} F_{km}^g c_{m1}}$$

and

$$\epsilon_{k1}^g = \frac{\left(F_{k0}^g - \frac{h}{2\alpha_{k1}^g} \sum_{g'=1}^G \Gamma_{Jk1}^{g'g} F_{k1}^{g'} \right)}{\sum_{g'=1}^G \Gamma_{\phi k}^{g'g} F_{k0}^{g'}}.$$

In a finite uniform lattice a buckling is introduced and there

$$F_{k2}^g = F_{k5}^g = F_{k6}^g = 0, \quad k=1, \dots; \quad g=1, \dots, G.$$

As to the ratio of components F_{k3} to F_{k4} : the former is the amplitude of Fourier component $\cos\phi$, the latter of $\sin\phi$, and their ratio can be taken as constant. Therefore

$$\alpha_{k1}^g = \frac{h}{2} \frac{\sum_{g'=1}^G \Gamma_{jk4}^{g'g} F_{k4}^{g'}}{F_{k4}^g} = \frac{h}{2} \frac{G_{k4}^g}{F_{k4}^g}.$$

Thus α depends neither on the boundary index i and, in a uniform lattice, nor on the cell index k . The α parameter is the relation of a linear combination of cell surface fluxes to a linear combination of boundary currents:

$$\alpha_k^g = \frac{h}{2} \frac{\begin{bmatrix} J_{k2}^g + J_{k3}^g \\ \phi_{k2}^g + \phi_{k3}^g \end{bmatrix} - \begin{bmatrix} J_{k5}^g + J_{k6}^g \\ \phi_{k5}^g + \phi_{k6}^g \end{bmatrix}}{\begin{bmatrix} J_{k2}^g + J_{k3}^g \\ \phi_{k2}^g + \phi_{k3}^g \end{bmatrix} - \begin{bmatrix} J_{k5}^g + J_{k6}^g \\ \phi_{k5}^g + \phi_{k6}^g \end{bmatrix}}. \quad (6.3.38)$$

As can be seen from Fig. 6.12, (6.3.38) is a generalization of the expression

$$\frac{\text{current gradient}}{\text{flux gradient}}.$$

In slab geometry (6.3.38) is

$$\alpha_k^g = \frac{h}{2} \frac{J_{k1}^g + J_{kr}^g}{\phi_{k1}^g - \phi_{kr}^g} \quad (6.3.39)$$

and when h tends to zero then α tends to D , to the traditional diffusion coefficient.

Now let us consider ϵ . In an asymptotic uniform lattice ϵ does not depend on the boundary index i and has the form

$$\epsilon_k^g = \frac{F_{k1}^g - \frac{h}{2\alpha_k^g} J_{k1}^g}{\bar{\phi}_{kg}} \quad (6.3.40)$$

and tends to unity, since F_{kg} tends to the average flux when h tends to zero.

It follows from Eq. (6.3.40) that the cell average flux is given by

$$\bar{\phi}_{kg} = \frac{F_{k1}^g - J_{k1}^g h/2 \left(\alpha_k^g \right)^{-1}}{\epsilon_k^g}$$

this clearly indicates that in the non-linear iteration the cell averaged fluxes are expressed by means of boundary fluxes and currents. Similar improvements have been applied either in the coarse mesh method to account for the large mesh size (Borresen, 1981), (Marakazov, 1977), or in the investigation of the obtained new schemes (Takeda 1979). (Lukas and Wehman 1981) have introduced auxiliary mesh points (e.g. cell edge centers). No auxiliary points are needed in the theory expounded above, the correction is introduced by the Γ matrices which reflect the physical properties of the cell.

6.3.5 Effect of the Cell's Surroundings

In the non-linear iteration, every reaction rate or boundary current is expressed with the help of Γ matrices as

$$R_x^g = \sum_{g'} \Gamma_x^{g'g} \left[K_{eff} \right] F_0^{g'}$$

Obviously, the mode $m=0$ contributes only to the cell integrated reaction rates. The Γ matrices are precalculated, e.g. by the CYLAN program. However, during the iteration the Γ matrices may vary only together with K_{eff} . This is why the reliable determination of Γ matrices is significant.

They are calculated in the CYLAN program in the following manner. At the cell boundary a given neutron spectrum is assumed in a larger number (40-70) of energy groups and the leakage is condensed into few (2-4) groups only later. This is because the present capacity of the

computational means does not allow explicit calculations of large systems, and it is necessary to condense the energy spectrum in the second step of the calculation. Consequently, there is a contradiction between the two calculational steps since in the cell calculation step a many group spectrum should be considered. Specification of the entering current spectrum within each macro (or coarse) group is inevitable.

In principle, these spectra could be selected individually for each cell type and for each azimuthal harmonics although at present it is not clear how to determine them. When performing the below given calculations, the following approximation was accepted. A number of flux and current boundary spectra were obtained by means of the BETTY asymptotic spectral code for each cell type. The number of spectra was selected equal to the number of energy groups in the global calculational step. Afterwards, linear combinations of these spectra were formed so that the summed up flux should be unity in one of the macrogroups, and be zero in all the other macrogroups. According to the experience gained so far, the best results are achieved when the set of preselected spectra has included not only the asymptotic spectrum of the fuel cell typical for the given lattice, but also a softer and a harder spectra. Only the softer and harder spectra enter when performing two group calculation in the second step. We only remark here that the use of leakage spectra in calculating higher angular moments has improved the results. It is clear, however, that it would be premature to draw final conclusions regarding the best choice of spectra.

Usually the off-diagonal elements of the Γ matrices differ from zero, hence the same cell embedded into diverse surroundings represented by different neutron spectra at the cell boundary may acquire different cell parameters in the global calculation, see Eq. (6.3.35). This effect is nothing other than the "spectral correction", introduced by (Lehman, 1978). Thus the method described in Section 6.3.3 involves the spectral index method as a special case.

6.3.6 Off-diagonal Diffusion Coefficients

The non-linear iteration can also be expounded in another way, based on assuming matrix α to exist and to be independent of the cell boundary index. However, in this case it will not be a diagonal matrix with regard to the energy. On the i -th cell boundary the flux and current are continuous:

$$\phi_1 = \phi_1, \quad (6.3.41)$$

$$J_1 = J_1, \quad (6.3.42)$$

where i' denotes the neighbouring cell boundary. Let us express the boundary fluxes and currents as sums of one face averaged component (subscript 0) and the remainder (subscript i). We suppose matrix α to exist such that

$$G_1 = \frac{2}{h} \alpha F_1. \quad (6.3.43)$$

Now, Eqs. (6.3.41) and (6.3.42) become

$$\phi_1 = F_0 + F_1 \quad (6.3.44)$$

$$J_1 = G_0 + G_1. \quad (6.3.45)$$

From Eqs. (6.3.43)-(6.3.45) the following expressions are obtained for the boundary flux and current:

$$J_1 = \frac{2}{h} \left[\alpha^{-1} + \alpha'^{-1} \right]^{-1} \left\{ \left[F_0' - \frac{h}{2} \alpha'^{-1} G_0' \right] - \left[F_0 - \frac{h}{2} \alpha^{-1} G_0 \right] \right\}, \quad (6.3.46)$$

$$\phi_1 = \left[\alpha + \alpha' \right]^{-1} \left\{ \alpha' \left[F_0' - \frac{h}{2} \alpha'^{-1} G_0' \right] - \alpha \left[F_0 - \frac{h}{2} \alpha^{-1} G_0 \right] \right\}. \quad (6.3.47)$$

To simplify the above formula, matrix ϵ is introduced by the following definition:

$$\left[F_0 - \frac{h}{2} \alpha^{-1} G_0 \right] = \epsilon \bar{\phi} \quad (6.3.48)$$

and ϵ depends solely on symmetrical components that are expressible by means of Γ matrices:

$$G_0 = \Gamma_0 F_0, \quad (6.3.49)$$

$$\bar{\phi} = \Gamma_\phi F_0. \quad (6.3.50)$$

Therefore matrix ϵ can be written as

$$\underline{\epsilon} = \left[\underline{E} - \underline{\alpha}^{-1} \underline{\Gamma}_J \right] \underline{\Gamma}_0^{-1} \underline{\phi}, \quad (6.3.51)$$

where E is the identity matrix. The neutron balance now has the form

$$\frac{F}{V} \sum_{j=1}^6 L_j + R_a = R_f + R_s, \quad (6.3.52)$$

where F , V are the surface of one cell face and volume of the cell, respectively; R_a , R_f , R_s represent absorption, fission and slowing down rate, respectively. Reaction rates are expressed by Γ matrices as

$$R_x = \underline{\Gamma}_x \underline{F}_0. \quad (6.3.53)$$

In order to transform Eq.(6.3.52) to the required form, the reaction rates are written as

$$R_{xg} = \bar{\Sigma}_{xg} \bar{\phi}_g = \frac{\left[\underline{\Gamma}_x \underline{F}_0 \right]_g}{\left[\underline{\Gamma}_\phi \underline{F}_0 \right]_g} \bar{\phi}_g, \quad (6.3.54)$$

with the help of which the cell balance turns out to be an equation for the cell average fluxes:

$$\frac{4}{3h^2} \sum_{j=1}^6 \alpha' \left[\alpha' + \alpha \right]^{-1} \alpha \left[\underline{\epsilon}' \bar{\phi}' - \underline{\epsilon} \bar{\phi} \right] + \langle \bar{\Sigma}_a \rangle \bar{\phi} = \chi \frac{Q}{K_{eff}} + \bar{\Sigma}_a \bar{\phi}, \quad (6.3.55)$$

$$Q = \sum_{g'=1}^G \nu \bar{\Sigma}_{fg'} \bar{\phi}_{g'}. \quad (6.3.56)$$

Equations (6.3.55)-(6.3.56) are closed, the cell average fluxes can be determined from them. Thus we have shown the non-linear iteration to be capable of giving the average fluxes by equations analogous to the results obtained in (Laletin and Elshin, 1981), (Maiorov, 1983).

6.3.7 Higher Harmonics

Let us consider the Fourier components of the flux on the boundary and comprise quantities on the boundary into one vector:

$$\underline{\phi}_k^g = \left[\phi_{k1}^g, \dots, \phi_{k6}^g \right]$$

The m-th Fourier component is obtained as

$$\underline{\phi}_k^g = \sum_{m=1}^G \epsilon_m F_{km}^g$$

Because of the orthogonality of vectors ϵ_m , we have

$$F_{km}^g = \frac{1}{N_m} \underline{\phi}_k^g \epsilon_m$$

where $N_m = \epsilon_m \epsilon_m$. The boundary fluxes are positive and approximately equal. Thus the relation

$$F_{k1}^g \gg F_{km}^g, \quad m > 1$$

is fulfilled for any k and g. It is evident that the differences depend on the cell size and on the cell structure. Based on the numerical results obtained by the HEXAN code, in (Makai 1981; 1982) it was proposed to handle higher harmonics as perturbations. When the higher harmonics are neglected, the α and ϵ become cell characteristics that can be determined independently of the boundary conditions. It is easy to see that the same expansion in terms of vectors ϵ occurs in Eqs. (6.3.46) and (6.3.47) as it does in some expressions of (Laletin and Elshin, 1981).

6.3.8 Numerical Results

Calculations have been performed for the ZR-6 configurations (Final Report of TIC, 1985) given in Table 6.3.1. To perform 4 group calculations by the SNARE program, it was necessary to prepare Γ matrices for the following fuel types:

fuel (12.7/3.6/0.0);

water cell;

cell of absorber type D.

Γ matrices have been calculated by CYLAN in 70 energy groups.

Table 6.3.1. Calculated Configurations

Configuration	Description
47	Core + reflector
57	D7
58	E7
101	K91 no perturbation

The results given below have been obtained with the help of the same spectrum for all three fuel types determined as follows. The base ($m=0$) azimuthal harmonic has the weight 0.25. The higher harmonics are built up from the spectra of the following four cell types:

- standard fuel (12.7/3.6/0.0);
- standard fuel but the density of hydrogen doubled in the moderator and the density of ^{238}U is halved;
- standard fuel but the density of hydrogen halved in the moderator and the density of U238 is doubled;
- standard fuel but one quarter of ^{235}U density and adding auxiliary fissionable material.

For the non-symmetrical modes the corresponding leakage spectra at $k_{\text{eff}}=1.0$ was been used. Values of k_{eff} obtained by SNARE are given in Table 6.3.2. The calculated power distributions have been compared to measured distributions (Final Report of TIC, 1985) utilizing function No. 21 in program RFIT (Szatmary, 1977, 1979).

Table 6.3.2. k_{eff} values.

Configuration	k_{eff}
47	1.0000
57	0.9997
58	0.9993
101	1.0075

Figures 6.13-6.16 show the calculated and measured power distributions for each configuration. The obtained Student fractions are displayed as

- function of distance from the lattice centre, see Figs.6.17-6.20;
- function of distance from the center of macrocell X7 or K91,

involving the fuel pin in question, see Figs. 6.21-6.23 for configurations 57, 58 and 101.

The behaviour of the Student fractions shows the calculated results to describe well the power distribution in the investigated configurations. If one compares the distribution of Student fractions with results from the asymptotic approximations (Alvarez, 1987) a considerable improvement can be observed.

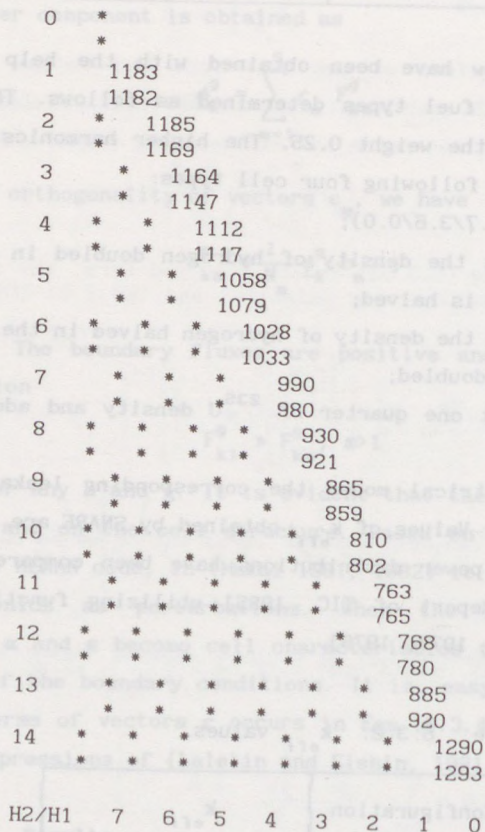


Fig. 6.13. Power distribution.

Configuration 47

$k_{\text{eff}} = 1.0000$ (upper number - measurement;
lower number - calculation).

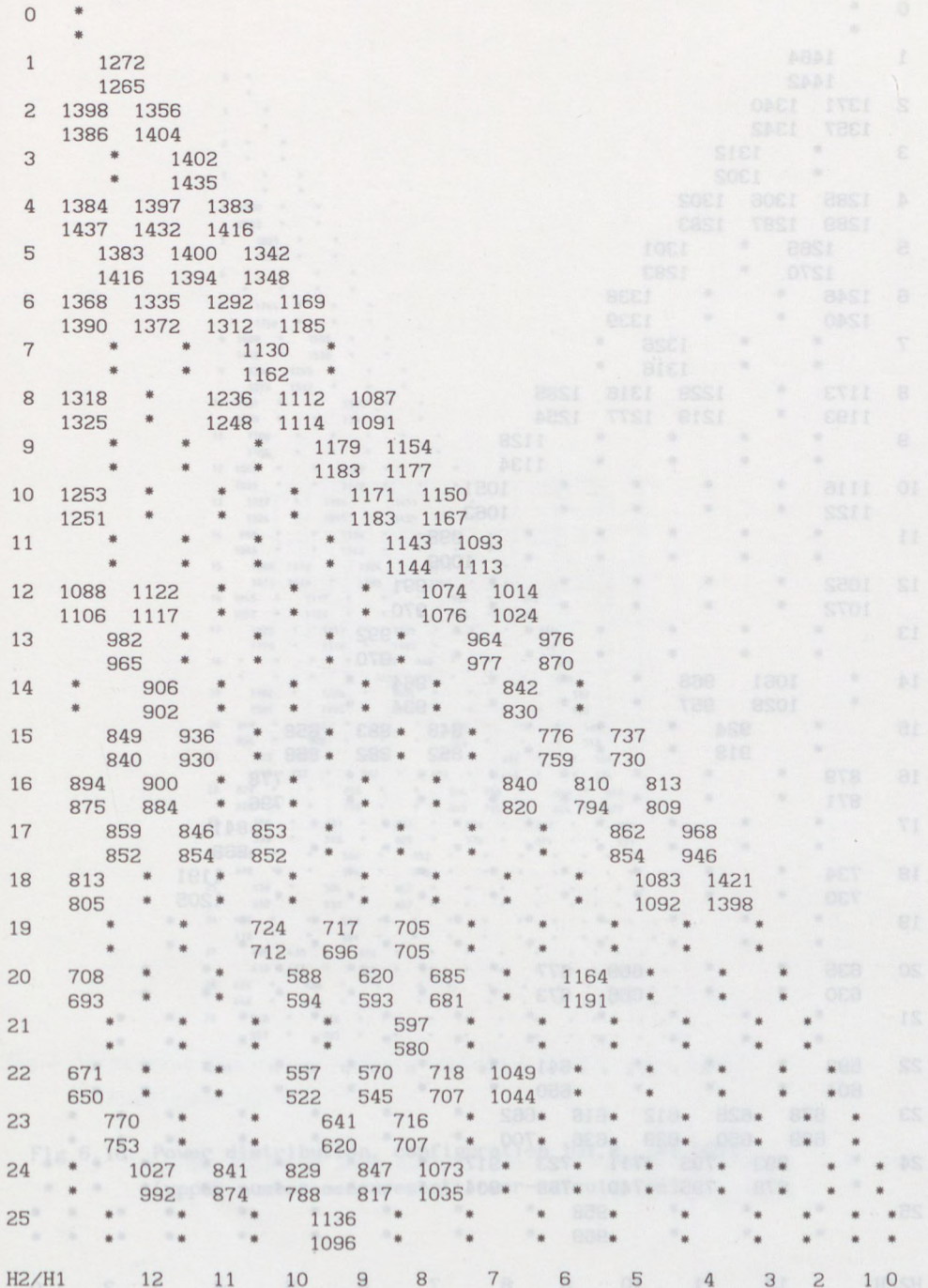


Fig.6.14. Power distribution (upper number-measurement; lower-calculation);

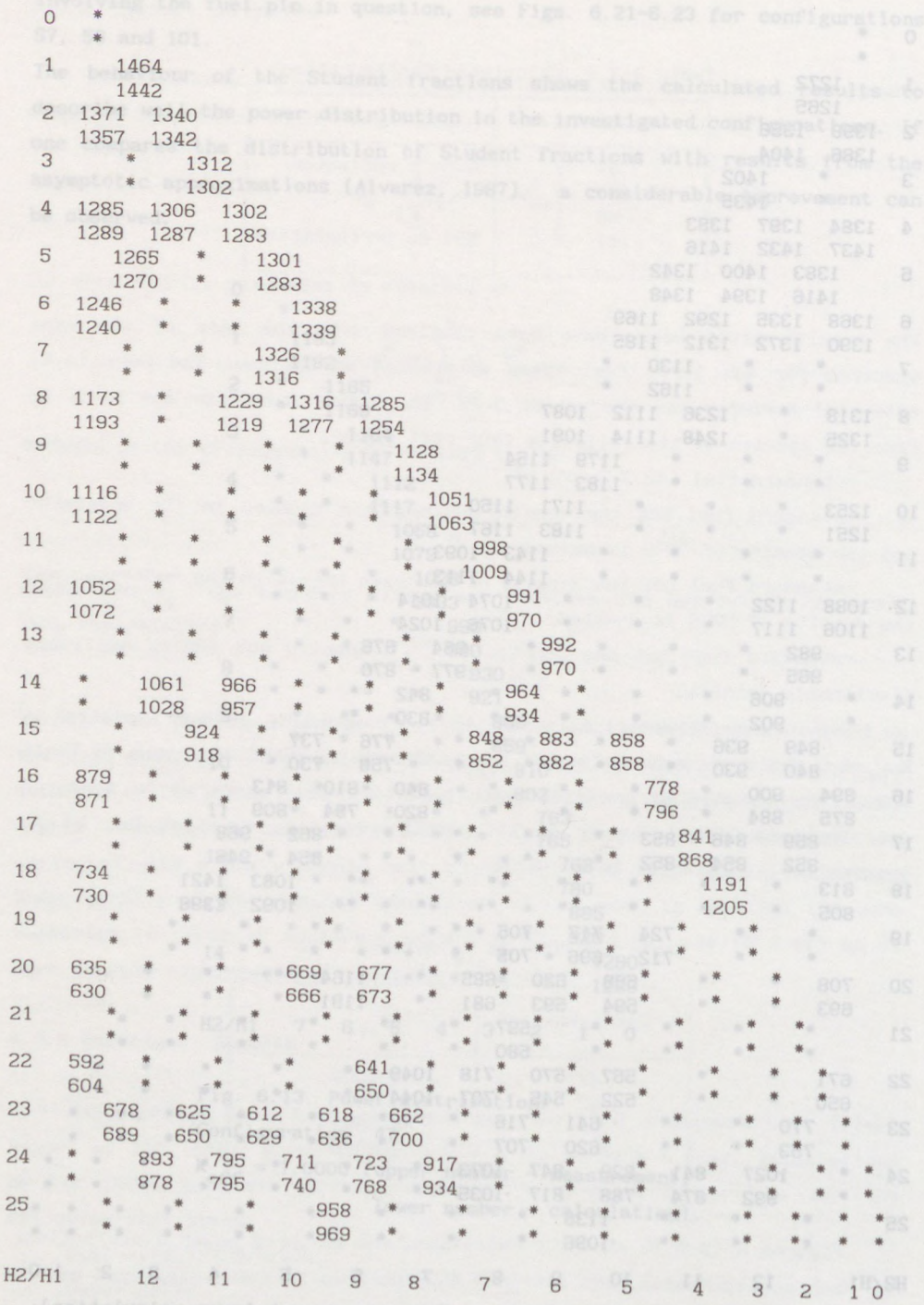


Fig. 6.15. Power distribution (measured and calculated)

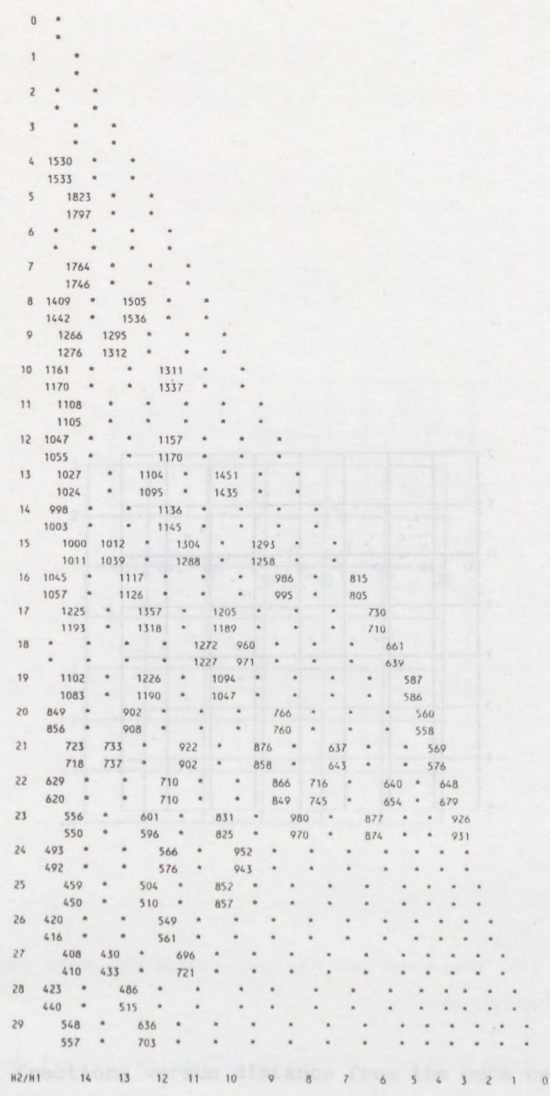


Fig 6.16. Power distribution, configuration 101, $k_{eff} = 1.0075$
(upper number-measurement; lower-calculation)

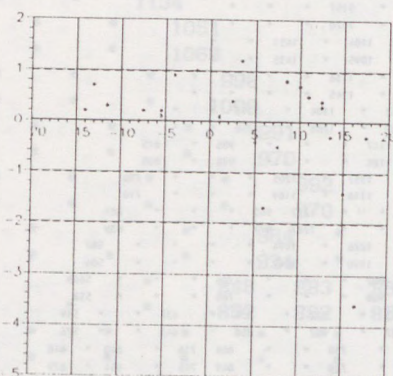


Fig. 6.17 Student fractions versus distance from the core centre
Configuration 47

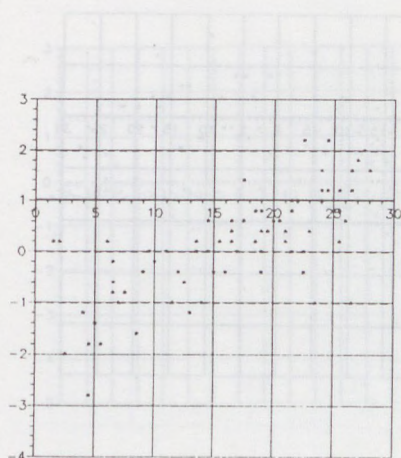


Fig.6.18 Student fractions versus distance from the core centre
Configuration 57

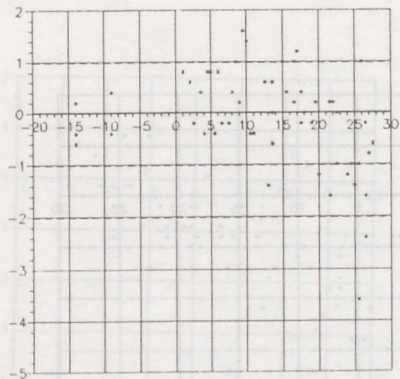


Fig. 6.19 Student fractions versus distance from the core centre
Configuration 58

Fig. 6.18 Student fractions versus distance from the core centre
Configuration 57

Fig. 6.17 Student fractions versus distance from the core centre
Configuration 47

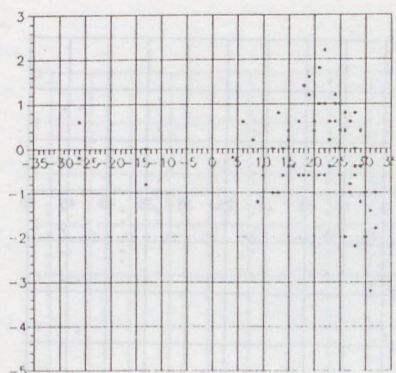


Fig. 6.20 Student fractions versus distance from the core centre
Configuration 101

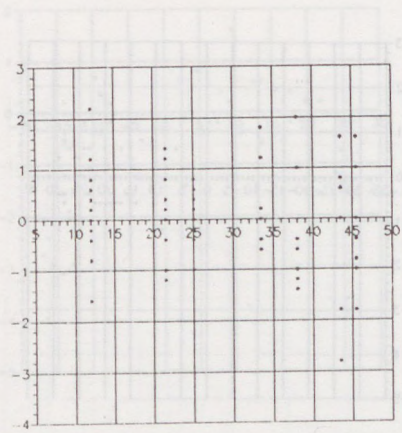


Fig. 6.10 Student fractions versus distance from the core centre
Configuration 58

Fig. 6.21 Student fractions versus distance from the macrocell
centre, configuration 57

REFERENCES

- Alvarez K. (1987). Comparison of experimental and calculational fields. Report KFKI-ZR-6-426/1987. In Russian.
- K. Árkai: Közvetlen mérési eredmények és számított mezők. KFKI-ZR-6-426/1987.
- Averyanova, S. P. et al. KRMS-A Many Energy Group Transport Program for Neutron Spectrum Calculation in Light Water Systems. In Russian.
- C.N.Árkai és az. KPMK - közvetlen mérési eredmények és számított mezők. KFKI-ZR-6-426/1987.
- Benard P. (1984). Theorie de Coefficients de Diffusion dans un Réseau Comportant des Cavités.
- van Ginnebeck J.J. (1977). Experimental Investigation of the Neutron Spectrum in a Heavy Water Reactor. Proc. Int. Topi. Mtg. of Nuclear Engineering.
- Devenyi A. (1984). AFIC. Report KFKI-1984-14.
- Final Report of TIC, Vol. 1. (1985). Experimental Investigations of The Physical Properties of MWCR-Type Uranium Water Lattices. Madenaki Kiado, Budapest, 1985.
- Gado J. (1977). The Neutron Spectrum Calculating Model of the program NETTY. Report KFKI-1977-14. Budapest.
- Gado, A. Devenyi, A. Kerecsen, M. Fekete (1980). A Novel Calculational Model for the Neutron Spectrum in a Heavy Water Reactor. Ann. nucl. Energy 11, 959.
- Gado J. et al. (1984). Ann. nucl. Energy 11, 959.

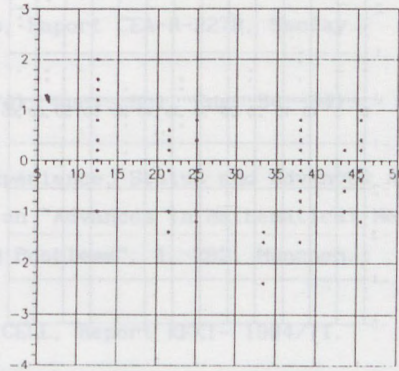


Fig. 6.22 Student fractions versus distance from the macrocell centre, configuration 58

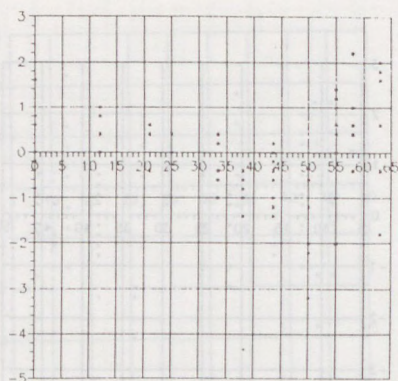


Fig. 6.23 Student fractions versus distance from the macrocell centre, configuration 101

Fig. 6.23 Student fractions versus distance from the macrocell centre, configuration 101

REFERENCES

- Alvarez K. (1987). Comparison of experimental and calculational fields. Report KFKI-ZR-6-426/1987. In Russian.
- К. Алварез: Сопоставление экспериментальных и расчетных полей. KFKI-ZR-6-426/1987
- Averyanova, S. P. et al. KRAMS-A Many Energy Group Transport Program for Neutron Spectrum Calculation in Light Water Systems. In Russian.
- С.П.Аверьянова и др. КРАМС - кинетическая многогрупповая программа для расчета спектра нейтронов в легководных системах.
- Benoist P. (1964). Theorie du Coefficient de Diffusion dans un Reseau Comportant des Cavites, Raport CEA-R-2278, Saclay.
- van Binnebeck J.J.(1974). Nucl. Sci. Eng. 54, 341.
- Borresen S. (1981). Experience, Status and Advances Applications of PRESTO, Proc. Int. Topl. Mtg. on "Advances in Mathematical Methods for the Solution of Nuclear Engineering Problems", 1, 283, Munchen.
- Devenyi A. (1984). ANICELL, Report KFKI- 1984/71.
- Final Report of TIC, Vol. 1. (1985). Experimental Investigations of The Physical Properties of WWER-Type Uranium Water Lattices, Akademiai Kiado, Budapest, 1985
- Gado J. (1977). The Neutron Spectrum Calculating Modul of the program BETTY, Report KFKI-1977-14, Budapest.
- Gado, A. Devenyi, A. Kereszturi, M. Makai (1983). A Novel Calculational Method for Non-Uniform Lattices, In Russian.
- Новый метод расчета неоднородных решеток, 2, 151, Материалы 12-ого Симпозиума ВМК, Татранска Ломница, 1983.
- Gado J. et al.(1984). Ann. nucl. Energy 11, 559.

Hughes R. P. (1978). Nucl. Sci. Eng. 67, 85.

REFERENCES

Laletin N. I. Elshin A. V. (1981). Derivation of Finite Difference Equation for Heterogeneous Reactor, In Russian.

Вывод конечно-разностных уравнений гетерогенного реактора, ИАЭ-3458/5, 1981

Lehman M. (1978). Calculation of Lattice Inhomogeneity's Effect on Diffusion Constants of Elementary Cells by Spectral Index Method, In Russian).

Расчет влияния неоднородности решетки на диффузионные константы элементарных ячеек методом спектральных индексов. Материалы 7-ого Симпозиума ВМК, 2, 300, Добржиловице, 1978.

Lizorkin M. (1980). Upgraded Calculation of Microdistributions in Program PERMAK, In Russian)

М.Лизоркин. Уточнение расчетного описания микрополей в программе ПЕРМАК. Материал ТГ-4 ВМК, ЧССР, 1980.

Lizorkin M., Pshenin V. (1980). Upgraded Diffusion Calculation of WWERs. in Russian.

М.Лизоркин, В.Пшенин. Уточнение диффузионных расчетов реакторов ВВЭР. Материал ТГ-2-4 ВМК, ПНР, 1984.

Lizorkin M., Kireyeva I., Saprikin V. (1985). Program PERMAK. Algorithm Description and User's Guide. In Russian.

М.П. Лизоркин, И.Л. Киреева, В.В. Сапрыкин. Программа ПЕРМАК. Описание алгоритма и инструкция по пользованию. Отчет библиотеки программ ВМК, НРБ, София, 1985.

Lizorkin M, Pshenin V., Novikov A., Lazarenko A. (1990). Nodal Methods for VVER Core Analysis, IAEA Meeting on Advanced Computational Methods, Cadarache, France, 1990

Lukas H., Wehmann U. (1981). A Fast Two - and Three-dimensional OneGroup Coarse-mesh Diffusion Program in Hexagonal Geometry, Proc. Int. Topl. Mtg. on "Advances in Mathematical Methods for the Solution of Nuclear Engineering Problems", 1, 299, Munchen, 1981.

Maierov, L. V. (1983). On Calculation of Finite Difference Equation

Constants for Heterogeneous Reactors, In Russian.

О расчете констант диффузионных конечно-разностных уравнений для гетерогенных реакторов, Вопросы атомной науки и техники, серия: Физика и техника ядерных реакторов, вып. 5(34), с.1, 1983.

Makai M. (1979). Calculation of Symmetric Cores, 1,215, Proc. VIII. Symposium of TIC, Jadvisin, (1979).

Makai M. (1981). Symmetry Considerations in Reactor Physics. In Russian. Соображения о симметриях в реакторной физике, 1, 193, Материалы 10-ого Симпозиума ВМК, Ереван.

Makai M. (1981). Symmetry Considerations in Reactor Physics. In Russian. Соображения о симметриях в реакторной физике, Доклад на совместном заседании тематических групп 2, 4 и 8, Пиештяны, 24-30 Мая 1981.

M. Makai (1982). Symmetries applied to Transport and Diffusion Equations, Proc. Int. Topl. Mtg. on "Advances in Reactor Physics and Core Thermal Hydraulics", 2, 684, Kiamesha Lake (NY), 1982.

Makai M (1982). Calculation of Large Symmetric Cores, Atomkernenergie, 41, 113.

Makai M. (1982). Symmetries Applied to Reactor Calculations, Nucl. Sci. Eng. 82.

Makai M (1982). Calculation of Large Symmetric Cores, Atomkernenergie, 41, 113.

Makai M. (1983). Considerations on Finite Lattice Homogenization. In Russian.

Соображения о гомогенизации конечной решетки, 2, 203, Материалы 12-ого Симпозиума ВМК, Татранска Ломница.

Makai M. (1984). Macro - and Microflux, I, Periodic Lattices, Nucl. Sci. Eng. 86, 319(1984).

CHAPTER 6

Marakazov A. A. (1977). Methodology for Calculating Assembly Powers for WWERs in 2 Group Approximation. In Russian.

Методика расчета мощностей кассет реакторов ВВЭР в двухгрупповом диффузионном приближении. Препринт ИАЭ-27816 М., 1977.

Novikov A. (1980). Improvements of Space-Energy Dependent Neutron Distribution Near Lattice Inhomogeneities. In Russian.

А.Н.Новиков. Уточнение пространственно-энергетического распределения нейтронов вблизи нарушений однородности решетки, Материал IX симпозиума ВМК (Нойбранденбург, ГДР, 1980).

Novikov A. (1982). Error Reduction in Fine Mesh Calculations. In Russian.

Новиков.А. Повышение точности мелкосеточных расчетов, Материал ТГ-4 ВМК (София, НРБ, 1982).

Novikov A. (1982). A Generalized Representation of Differential Operators in One Energy Group Equation. In Russian.

А.Н.Новиков. Обобщенное представление дифференциальных операторов одnogрупповых уравнений. Материал XI симпозиума ВМК (Варна, НРБ, 1982).

Novikov A. (1983). 2 Group Coarse-Mesh Problems Considering Cell Heterogeneity. In Russian.

А.Н.Новиков. Двухгрупповые редкосеточные задачи с учетом гетерогенности ячеек, Материал ТГ 2-4 ВМК (Берлин, ГДР, 1983).

Novikov A. (1983). Inclusion of Transient Solutions in Fine Mesh Calculations. In Russian.

А.Н.Новиков. Учет переходных решений в мелкосеточных расчетах. Материал XIV заседания Научного Совета ВМК, 1983.

Novikov A. (1985). Calculation of Functionals and Solution of Coarse Mesh Equations. In Russian.

А.Н.Новиков. Подготовка функционалов и решение редкосеточных уравнений, Материал ТГ 2-3-4 ВМК (ЧССР, 1985).

Pshenin V., Novikov A., Surnacheva I. (1984). Analysis of Possibilities of Low Error Fine Mesh Calculations. Slab Geometry Case Studies. In Russian.

В.В.Пшенин, А.Н.Новиков, И.И.Сурначева. Анализ возможностей повышения точности мелкосеточных расчетов на примере решения модельных задач в

плоской геометрии. Материал XIII симпозиума специалистов ВМК по физике ВВЭР, Бухарест, 1984.

Pshenin V., Novikov A., Surnacheva I. (1988). Analysis of Possibilities of Low Error Fine Mesh Calculations. Slab Geometry Case Studies. In Russian.
В.В.Пшенин, А.Н.Новиков, И.И.Сурначева. Анализ возможностей повышения точности мелкосеточных расчетов ВВЭР на примерах решения модельных задач в плоской геометрии. ВАНТ, Сер. Физика и техника ядерных реакторов, вып.4, 1988, с. 13.

Pshenin et al. (1989). Program RAFORIN. Requirements, Algorithm and Preliminary Test Results. In Russian.
В.В. Пшенин и др. Программа РАФОРИН. Назначение, алгоритм и предварительные результаты тестирования. Материал XVIII Симпозиума специалистов ВМК, 1989.

Rumyantzev G. Ya.(1962). Atomnaya energiya, 13, N6 (1962). In Russian.

Rumyantzev G. Ya.(1963). Atomnaya enegiya, 14, N4 (1963). In Russian.

Sidorenko V. D. (1981). Application of Asymptotic Approximation to Getting One Group Homogenised Assembly Constants and Boundary Conditions for Light Water Reactors. In Russian.

Использование асимптотического приближения для получения одnogрупповых гомогенизированных констант кассет и граничных условий в реакторе с легководным замедлителем, 2, 932, Материалы 10-ого Симпозиума ВМК, Ереван, 1981.

Slesarev I. S., Yaroslavtzeva, L. H. (1983). Calculational Scheme for Energetic Fast Reactors with Hexagonal Fuel Assemblies. In Russian.
Расчетная схема для исследования энергетических быстрых реакторов с гексагональными тепловыми сборками. Вопросы атомной науки и техники. Серия: Физика и техника ядерных реакторов, вып.4(33), 19(1983).

Szatmary Z. (1977). Data Evaluation Problems in Reactor Physics, Theory of Program RFIT, KFKI-1977-43, Budapest.

Szatmary Z. (1979). Systematic Comparison of Calculational Results and Macrodistribution Measurements. In Russian.

Систематическое сопоставление результатов расчетов и экспериментов макрораспределения, Материалы 8-ого Симпозиума ВМК, 1, ч. 4. Зегжинек-Ядвисин, 1979.

Takeda T. et al. (1979). Annals of Nuclear Energy, 6.

7. ADVANCED APPROACHES FOR NEUTRON-PHYSICAL CALCULATIONS OF NONUNIFORM REACTOR LATTICES

N. I. Laletin

7.1 INTRODUCTION

As a matter of fact the neutron flux $\phi(\omega)$ in a reactor is described with surplus accuracy by the following transport equation

$$L\phi(\omega) = \frac{1}{K_{eff}} K\phi(\omega) \quad (7.1)$$

$$L\phi(\omega) \equiv \Omega \nabla \phi(\omega) + \Sigma(r, E) \phi(\omega) - \int_0^\infty dE' \int_{4\pi} d\Omega' \left[\Sigma_s(r, E' \rightarrow E, \Omega \rightarrow \Omega') \phi(r, E', \Omega') \right] \quad (7.2)$$

$$K\phi(\omega) \equiv \int_0^\infty dE' \int_{4\pi} d\Omega' \left[\nu(E', E) \Sigma_f(r, E' \rightarrow E, \Omega \rightarrow \Omega') \phi(r, E', \Omega') \right] \cdot \frac{1}{4\pi}$$

where eigenvalue $1/K_{eff}$ is introduced formally to reduce the problem to the stationary case if the characteristics of the reactor under consideration differ from these of the critical reactor, $\omega = \{\vec{r}, E, \vec{\Omega}\}$.

The notations in Eqs. (7.1) and (7.2) are those used in the neutron transport theory (see e.g. (Davison, 1957)).

The simplest approximation of Eq. (7.1) in the form of either diffusion equation or P1-approximation is in most cases acceptable for homogeneous reactors. However, most of the existing reactors are heterogeneous: cross sections of interaction (especially absorption cross sections) of neutrons with different components of media vary considerably, and the sizes of the components expressed in the neutron free paths are usually of the order of unity. These conditions do not permit one to replace directly Eq. (7.1) by its simplest form to describe the heterogeneous reactor.

At the same time, solution of the Boltzmann transport equation for the whole reactor takes too much effort and is not justified by the required precision. Taking into account the specific features of the reactor problems permits one to simplify the calculations significantly, i.e. to solve the transport equation in the limits of a number of comparatively small domains (specific reactor cells) only. The solution for the whole reactor volume is found by using suitable approximations. The procedure of the transition from Eq. (7.1) to simpler equations may be considered not as

the way to solve the transport equation but as the procedure for constructing the mathematical model to describe the neutron-physical processes in the reactor.

It means that we need not know exactly and in detail the neutron flux distribution $\phi(\omega)$. We are interested in getting an equation system for describing the neutron-physical processes in reactor which would allow us to obtain:

- a) limited number of the solution functionals for practical purposes with acceptable accuracy,
- b) results by computer calculation within an acceptable time.

Moreover, the mathematical model should be constructed in such a way that its parameters (e.g. group cross sections) might vary in certain limits neglecting their origin from micro cross sections of Eq. (7.1).

However, it is necessary to begin analysis of the whole procedure of constructing the mathematical model by considering the Boltzmann transport equation in order to understand the acceptability of different approximations and to estimate the errors which are accepted under their construction and to outline further improvements of the mathematical model if required.

In fact, the homogenization method, the method of "source-sink" and different variants of the albedo method are those widely used to describe a heterogeneous reactor.

7.1.1 Homogenization method

The homogenization method was initially suggested as a means of describing sufficiently large reactor (see, e.g. (Galanin, 1957); (Weinberg, Wigner, 1959)) consisting of identical cells. In this case the neutron flux distribution $\phi(\omega)$ was represented as

$$\phi(\omega) = \Psi(\omega) \varphi_s(\omega) \quad (7.3)$$

where $\Psi(\omega)$ is the function of smoothed distribution and $\varphi_s(\omega)$ is the -somehow- normalized neutron flux distribution in an infinite reactor consisting of identical cells.

For finding the function $\varphi_s(\omega)$ it is enough to solve the equation for a single cell using the condition of periodicity.

Let us propose that the function $\Psi(\omega)$ can be approximated by linear coordinate function inside a single cell, i. e.

$$\frac{1}{\Psi} \frac{d^2 \Psi}{dx^2} a^2 \ll 1 \quad (7.4)$$

where a is the lattice pitch.

Then for averaging the cross section over the cell volume it is enough to know $\varphi_s(\omega)$. In this case function $\Psi(\omega)$ satisfies the transport equation with averaged cross sections. However, since the neutron free paths are as a rule less than " a " or at least of the order of " a ", the satisfaction of the condition (7.4) means the satisfaction of condition

$$\frac{1}{\Psi} \cdot \frac{d^2 \Psi}{dx^2} \lambda^2 \ll 1$$

The last equation allows to replace the Boltzmann transport equation for $\Psi(\omega)$ by its diffusion or P1-approximation. Reasons discussed above satisfied researches while they took care about the correct averaging over the cell volume only of the most important cross sections, namely absorption cross section Σ_a , fission cross section Σ_f and group to group transition cross section Σ_{gg} .

When the problem of the correct calculation of the effective diffusion coefficient in the homogenization reactor arose it was realized that representation (7.3) is insufficient.

It was shown in number of publications of the 1950's and early 60's (Spinrad, 1955; Shevelev, 1957; Laletin, 1959; Smelov, 1959; Benoist, 1961; Leslie, 1962; Rumyanzev, 1962, 1963; Grigoriev and Novikov, 1968; Sidorenko, 1962) that besides function $\varphi_s(\omega)$ which is symmetrical relating the cell's centre and represents the flux's microstructure, the functions $\varphi_{as}(\omega)$ are required which are antisymmetrical along any coordinate and needed for getting the correct diffusion coefficient. The approach to the problem, the approximations used and the problem detalization in the mentioned publications were different, but their main idea was as follows.

- 1) The solution inside the single sell was represented as

$$\phi_1(\vec{r}) = \Psi_1 \varphi_1(\vec{r}) + \left(\frac{d\Psi}{dx} \right)_1 \varphi_{as}^x(\vec{r}) + \left(\frac{d\Psi}{dy} \right)_1 \varphi_{as}^y(\vec{r}) \quad (7.5)$$

(for simplicity the expression is written down only for one neutron group

and for the reactor which is infinite along the axis directed along the channel axis).

Here $\varphi_{as}^x(\vec{r})$ and $\varphi_{as}^y(\vec{r})$ are the functions which are antisymmetrical along coordinates "x" and "y" respectively ("x" and "y" are the Cartesian coordinates): Ψ_i , $(d\Psi/dx)_i$, $(d\Psi/dy)_i$ are constants with the meaning of cell average flux along the cell and average flux gradients respectively.

2) The finite-difference equations connecting the average fluxes in neighbouring cells were derived from balance conditions of the neutron balance in the cell "i" and of continuity of the neutron fluxes and currents on the faces of the neighbouring cells. The equation coefficients were expressed in terms of integrals of functions $\varphi_s(\vec{r})$ and $\varphi_{as}(\vec{r})$.

3) the finite-difference equations were substituted by the diffusion equations for homogeneous media. This stage was performed because differential equations are more convenient for analysis and getting solution in the "simple" cases and also because the computer calculations were not used widely.*)

Let us mention the following deficiencies of the approximations used:

- the results are valid only for describing the internal domains of long enough lattices, while condition (7.4) is satisfied. However the homogenization method stated here leads us to noticeable inaccuracy ($\approx 10-15\%$ in the average flux along the cell) in the points near the lattice non-uniformities (absorber cells in the core, boundary core-reflector, etc),
- detailed analysis of the derivation of the effective diffusion coefficients was performed only for one group diffusion equation.

*) During about forty years the computers are used in reactor calculations and the diffusion homogenized equations are widely used as before. Traditionally the homogenization approaches are based on replacing a heterogeneous cell by a diffusing homogeneous cell with utilising the various equivalence principles **without using the finite-difference equations on the first step** of deriving the diffusion equations (cf. (Shevelev, 1957), (Selengut, 1959), (Smelov, 1959), (Laletin, 1959), (Grigoriev and Novikov, 1968), (Bonalmi, 1973,1974), (Berna, 1971), (Deniz,1986), etc). It seems that above described interpretation of the homogenization theory reflects mostly the contemporary point of view presented in this book (cf. Chapters 3,6,7). (Editor's remark).

7.1.2 Other traditional approaches

The "source-sink method" equations were at first formulated (Feinberg, 1955; Galanin, 1955, 1971) by assuming that the reactor is a lattice of thread-like rods surrounded by the infinite moderator. It was considered that the neutron diffusion could be described everywhere in the moderator by P1-approximation of the spherical harmonic method (many-group diffusion or diffusion-neutron age scheme). The initial schemes were later refined.

In my opinion, the final neutron flux equations have practically no connection with the "source-sink" method which was mentioned in the latest publications (Kochurov, 1980; Gorodkov, 1988). In reality the connection in these equations exists between the neighbouring cells but not among all the reactor core rods. The equation coefficients look like functionals depended on the space-energy distributions inside the cells, and they are not the rod characteristics as it was for the "source-sink" method.

Concluding this section one can say a few words about a less known method for solving the problem under consideration, viz. the albedo method. This method as well as the homogenization method describes the neutron flux distribution in the cells by a few of trial functions. The distinction appears in the coupling equations for neighbouring cells which are derived from the continuity conditions of one-side currents instead of fluxes and total currents.

All the versions of this method published in references (Aoki, Shimizu, 1969; Pfeiffer, Shapiro, 1969; Maiorov *et al*, 1970; Barkov, 1977; Sanchez, McCormic, 1982) lose to homogenization method due to the larger number of unknowns (per cell) in the equations and because the trial functions used are not regulated in the order of their significance.

As a result, all trial functions for two-dimensional problems should be found by solving auxiliary two-dimensional problems in the albedo method while the most important symmetrical trial functions are (in most cases) found by solving appropriate one-dimensional problems in the homogenization method. The above mentioned disadvantages may probably be removed (for example, by regulating the trial functions in order of their importance, by fixing the representative combinations of the unknowns and excluding the rest of them from the equations).

The coupling among adjacent cells by using one-side currents is also implemented in the surface current method (Sanchez, McCormic, 1982). The corresponding coupling is written down for the "nodes" and in some "nodal

methods". In both cases the specific solution inside the cells and nodes does not, in my opinion, permit one to consider them simply as the version of the albedo method. A more detailed description of such approaches is out of the scope of this paper.

7.1.3 Final remarks

The results obtained by the above methods are still widely used. The most significant calculation errors of the values obtained by these methods should be expected near the break of cell lattice uniformity (near a reflector, control rods, etc). The corrections are introduced near the nonuniformity, however, as it follows from comparing calculations against the experimental results, in particular, ZR-6 experiments (Szatmary, 1985), the traditional methods including the usage of asymptotic theory describe the experimental distributions near non-homogeneous breaks or zone boundaries with an error of 10-15%.

The advanced accuracy methods for neutron flux distribution calculations, especially for investigating the nonuniform lattices are presented in this Chapter.

The incentive to develop advanced calculation methods is based on the following reasons:

- asymptotic models with a variety of corrections are widely used in the TIC countries, but the physical bases are often not clear;
- analysis of experiments has shown the weak features of the traditional method;
- contemporary WWER core designs require more accurate calculations.

A number of works have been devoted to improvements of the methods of assembly homogenization (Lelek, 1976; Ionov and Kireeva, 1976; Anrjeevsky, 1977; Chan din Chi and Makai, 1983) and of cell homogenization, as well as to refinement of the whole procedure of neutron flux distribution calculations (Laletin and Elshin, 1976; Laletin, 1977; Maiorov, 1977, 1978; Novikov, 1982, 1983, 1984; Gado *et al*, 1983). A number of results is widely published outside the TIC proceedings (Laletin, 1978, 1980, 1981, 1983; Elshin, Laletin, 1976; Laletin, Elshin, 1977, 1980, 1981, 1985; Laletin, 1983; Maiorov, 1983; Gado *et al*, 1984). In particular, publication (Szatmary and Gado, 1977) should be mentioned, its authors trying to define the diffusion constant for absorption rod from the finite-difference equation using spectrum and reaction rates from spectral calculations.

7.2 SURFACE HARMONIC METHOD

The approach to calculating stationary neutron flux distributions in nuclear reactors that allows the accuracy to be increased without significant complication of the traditional calculation procedure was developed by the author and by the author with his colleagues.

Starting from the precise neutron transport equation the whole neutron flux distribution calculation procedure is analyzed. The reasons for the assumed subdivision of the procedure into the stages are proved: cell calculation + whole reactor calculation + introducing feedback - all modification problems of cell coupling equations are under strict consideration including requirements which the modified equations put forward before the single cell characteristics calculations. Strictly speaking, the main significance of the work done is in this successive analysis although this approach, from the purely mathematical point of view, is a way of constructing the more accurate finite-difference equation to calculate neutron flux distribution in reactor.

The mentioned approach is known as the "Surface Harmonic Method (SHM)".

a) **Variational principle.** The solution is represented by the sum of functions which exactly satisfy the neutron transport equation describing the flux distribution inside the cell. Then the total error is concentrated on the outer boundary of the reactor volume and on the boundaries between the cells.

This statement requires explanation. Of course, in reality it is impossible for the results of the numerical calculations (the solutions inside the cells are just so determined) to satisfy exactly the transport equation. So the statement only means that we may neglect the errors of the solutions inside the cells during the derivation of the cell-coupling equations because, as a rule, these solutions are sought in the higher approximations to the transport equation, in more detailed group representations, etc, than equations used for solution sewing together at the cell boundaries. Therefore, representing the neutron flux distribution as follows

$$\phi^N(\omega) = \sum_{i=1}^I \sum_{k=0}^N a_{ik} \psi_{ik}(\omega) \quad (7.6)$$

where

ω is the combination of all variables on which the neutron flux depends, i.e. $\omega = \{\vec{r}, E, \vec{\Omega}\}$,

I is the number of cells into which the reactor volume is divided, i is the cell number,

$\psi_{ik}(\omega)$ are the trial functions describing the neutron flux distribution in cell " i ", k is the number of trial functions in cell " i ",

$N+1$ is the total number of trial functions in each cell in the considered approximation,

a_{ik} is the amplitude of corresponding trial functions.

Let us assume that $\psi_{ik}(\omega)$ precisely satisfies the equation in cell " i ", i.e. as we consider, $\psi_{ik}(\omega) = \phi_{ik}(\omega) \Theta(\vec{r})$, and

$$L\phi_{ik}(\omega) = K\phi_{ik}(\omega) \quad (7.7)$$

Here

$$\Theta(\vec{r}) = \begin{cases} 1, & \vec{r} \in V_i \\ 0, & \vec{r} \notin V_i \end{cases} \quad V_i \text{ is the volume of cell "i".}$$

where

$$L\phi = \vec{\Omega} \nabla \phi + \sum_t \phi - \int d\Omega' \int dE' \sum_s (\vec{r}, E', E, \vec{\Omega} \vec{\Omega}') \phi(\vec{r}, E', \vec{\Omega}') \quad (7.8)$$

$$K\phi = \frac{1}{4\pi} \int dE' \int d\Omega' \left[\nu(E', E) \Sigma_f(\vec{r}, E') \phi(\vec{r}, E, \vec{\Omega}') \right]$$

(the notations of these operators are common known).

The trial functions $\phi_{ik}(\omega)$ with different " k " differ due to conditions at the cell boundaries.

The statement that total approximation error under condition (7.6) is concentrated on boundary surfaces may be expressed mathematically in the following way:

$$\delta F_j = \left[\Psi_j^+, (\vec{\Omega}_n) \right] [\phi_+^N - \phi_-^N] \quad (7.9)$$

Here δF_j is variation of functional F_j stipulated by the condition that Eq. (7.6) satisfies the transport equation in the reactor volume only approximately;

$\Psi_j^+(\omega)$ is the importance function corresponding to the functional

F_j .

The parentheses denote a scalar product, that is in this case the following integral

$$(f, y) = \int_{\Gamma} d\vec{r}_s \int_{\{E\}} dE \int \frac{d\vec{\Omega}}{4\pi} f(\omega) y(\omega);$$

where n is the inward normal to the cell boundary;

$$\phi_{\pm}^N(\omega) = \lim_{\varepsilon \rightarrow 0} \phi^N(r_s \pm \varepsilon \vec{n}, E, \vec{\Omega}).$$

The exact value of the boundary solution $\phi(\vec{r}_s, E, \vec{\Omega})$ will appear in (7.9) instead of ϕ_-^N at the outer boundary of the volume under consideration.

If the importance function $\Psi_j^+(\omega)$ is expanded by the complete function system $f_{ik}(\omega)$, depending on variables $(i, \vec{r}_s, E, \vec{\Omega})$, expression (7.9) is transformed to the following:

$$\delta F_j = \sum_{i=1}^I \sum_{k=0}^{\infty} \Psi_{j,ik}^+ \left[f_{ik}(\vec{r}_s, \vec{\Omega}) [\phi_+^N - \phi_-^N] \right] \equiv \sum_{i=1}^I \sum_{k=0}^{\infty} \frac{\delta F_j}{\delta \Psi_{j,ik}^+} \Psi_{j,ik}^+ \quad (7.10)$$

The condition of vanishing the variational derivatives $\delta F_j / \delta \Psi_{j,ik}^+ = 0$ brings us to coupling equations solution in the neighbouring cells and provides exact values of these functionals (under the condition that all derivatives become zero), if their importance functions are expanded by system of functions $f_{ik}(\omega)$.

In reality, however, it is impossible to solve an infinite system of equations, and practical considerations make senseless any increasing of the calculation accuracy over a certain value.

Therefore, only several first, most important variational derivatives have to be equal to zero $\delta F_j / \delta \Psi_{j,ik}^+ = 0$. This should be done by appropriate choice of the parameters, (in our case these are amplitudes a_{ik}) the solution ϕ_N depending on them.

Besides equations for values linking a_{ik} for the neighbouring cells we also get boundary conditions for the cells belonging to the boundary layer.

In the above-mentioned works, viz. (see page 7-7) all possible productions of spherical functions $Y_n^m(\omega)$, characteristic functions of group intervals $\chi_g(E)$ and functions of coordinates of cell boundary points $W_k(\vec{r}_s)$ were taken as functions $f_{ik}(\omega)$. The reasons for such a choice and explicit expression of functions $W_k(\vec{r}_s)$ can be found in the same works.

Let us turn our attention to the following items.

ITEM 1. The obtained equations do not depend on the specific representation of the importance function of one or another type of functionals.

So, if the first $I(N+1)$ variational derivatives $\delta F_j / \delta \Psi_{j,ik}^+$ are equal to zero at a certain step of approximation, the exact values of all the functionals, the importance functions of which may be presented as

$$\Psi_j^+ = \sum_{i=1}^I \sum_{k=0}^N \Psi_{j,ik}^+ f_{ik}(\omega)$$

will be obtained.

The explicit form of a functional's importance function will be needed only if the functional itself can not be obtained by the approximation under consideration and it is desirable to estimate its error.

ITEM 2. The consideration of the approximation of angular dependence of $\Psi_j^+(\vec{r}, E, \vec{\Omega})$ was restricted (and, apparently, this is always sufficient) by spherical functions $Y_n^m(\vec{\Omega})$, where $n \leq 1$. In this case the equations

$$\left[f_{ik}(\omega), \vec{\Omega} \left[\phi_+^N - \phi_-^N \right] \right] = 0$$

appear to be linear combinations of conditions of continuity at the cell faces of group currents and neutron levels (the term "neutron level" is defined in the following section).

If the diffusion approximation on the cell boundary is valid, the neutron level is equal to the neutron flux and, therefore, all the equations may be derived from the conditions of continuity of currents and fluxes on the cell boundaries. It should be noted that any additional balance equations which sometimes being considered are not needed. The mentioned balance is automatically realized from representation of the solution in form (7.6).

ITEM 3. The choice of the function system $f_{ik}(\omega)$ puts certain limitations on the boundary conditions for the trial functions $\phi_{ik}(\omega)$ but does not define them completely. It is possible and at the same time obligatory to use such freedom to increase the accuracy of the solution obtained in the frames of chosen approximation. How to implement this is, to a considerable extent, a question of art of a researcher, however some common recommendations may be given. In any case, they should be discussed at the stage of considering how to calculate the cell characteristics.

To conclude the section, some notation of different approximations of SHM are given below:

$$(BG; (C_{\perp} + C_{\parallel})S),$$

where

B is the number of energy groups in the coupling equations of cell solutions (1G - one-group approach, 2G - two-group approach, etc),

$C_{\perp}$ and $C_{\parallel}$ are the numbers of boundary condition types related to one cell and one group ("Surface Harmonics") used for calculating the trial functions and respectively the number of trial functions for a cell and for a group. At the same time $C_{\perp}$ is a number of "azimuthal harmonics" and $C_{\parallel}$ is a number of "axial" harmonics.

The axis, the same as axis "z", is directed parallel to the fuel rod axes, the channel axes and the assembly axes, etc. The number related to the angular coordinates of the neutron flight is not included because, as was already noted, this approximation results from using the spherical harmonics, where $n \leq 1$.

The approximation (2G, 3S) is called the main approximation of SHM for two-dimensional problems and (2G, (3 + 2)S) - the main approximation of SHM for three-dimensional problems. Let us call these approximations simply the main approximations if it is clear from the context what method and what dimensionality problem are discussed.

b) About the next stages of equation deriving. Detailed descriptions of the procedure for deriving the final equations of SHM are discussed in the mentioned publications. Only the key items will be outlined here.

The following equations (Laletin, Elshin, 1980, 1981)

$$\phi_i^{nkg} = \sum_j \sum_{k'} C_{kk'}^{j(1)} \phi_j^{nk'g} \quad (7.11)$$

are obtained by setting the first variational derivatives to zero.

Here

$\phi_j^{nk'g}$ is the surface harmonic of order "k" for the angular moments of the equation ($0 \leq n \leq 1$) for the group "g" and the cell "j";

$C_{kk'}^j$, are the coupling coefficients of different harmonics in the neighbouring cells.

The sum over "j" is taken along the cells having the common boundary with cell "i". The explicit form of the coefficients $C_{kk'}^j$, is given in

(Laletin, Elshin, 1981).

It should be noted that

$$\phi_1^{0kg} = \int_{\Gamma_1} dr_s \int_{4\pi} d\Omega \int_{\{E_g\}} dE (\vec{\Omega} \cdot \vec{n}) W_k(r_s) \phi_1^N(E) = J_1^{kg} \quad (7.12)$$

are the surface harmonics of the group neutron currents in the cell "i", and

$$\phi_1^{1kg} = 3 \int_{\Gamma_1} dr_s \int_{4\pi} d\Omega \int_{\{E_g\}} dE (\vec{\Omega} \cdot \vec{n})^2 W_k(V_s) \phi_1^N(E) = l_1^{kg} \quad (7.13)$$

are the surface moments of the group neutron levels in the same cell.

$\{E_g\}$ in (7.12) and (7.13) denotes the energy group interval, Γ_1 is the boundary of cell "i". The coefficient 3 in (7.13) results from appropriate choice of normalization.

On the condition that the diffusion approximation on the boundary of the cell is true and taking into account that $3(\vec{\Omega} \cdot \vec{n})^2 = P_0(\vec{\Omega}) + 2P_2(\vec{\Omega})$, we get $l_1^{kg} \approx \phi_1^{kg}$, that is l_1^{kg} turns into the surface harmonics of neutron fluxes.

As far as $\phi_1^N(\omega)$ can be expressed as the sum of the trial functions, each of them being a solution of the transport equation in the cell, coupling equations exist and have the form

$$l_1^{kg} = \sum_{g'} S_{gg'}^{k1}, J_1^{kg'} \quad (7.14)$$

The surface harmonics with different "k" in equations (7.14) are separated owing to the symmetry of the cell and to utilising the trial functions corresponding the cell symmetry. Arranging corresponding variables J_1^{kg} and l_1^{kg} in energy vectors we come to the following equations

$$\vec{J}_1^k = \sum_j \sum_{k'} C_{kk'}^j, \vec{J}_j^{k'} \quad (7.15)$$

$$\hat{S}_k^1 \vec{J}_1^k = \sum_j \sum_{k'} C_{kk'}^j, \hat{S}_k^j, \vec{J}_j^{k'}$$

The individual notations were used for the matrix $\hat{S}$ with the lowest numbers "k" in our publications, namely:

$\hat{S}_0^1 = \hat{\varphi}_1$ is the matrix of the symmetrical trial functions,

$\hat{S}_0^1 = \hat{S}_2^1 = \hat{\psi}_1$ is the matrix of the antisymmetrical trial functions,

$\hat{S}_3^1 = \hat{S}_4^1 = \hat{\xi}_1$ is the matrix of the trial functions for symmetrical cells in the two-dimensional case.

The first moments $\vec{J}_1^k$ in this case are denoted as follows:

$\vec{J}_1^0 = \delta \vec{J}_1$ is the group neutron leakage (inflow) vector for the cell "i",
 $\vec{J}_1^1 = \vec{J}_1^x$ and $\vec{J}_1^2 = \vec{J}_1^y$ are the group vectors of the currents flowing along the axes "x" and "y" respectively, etc.

In our opinion, and proved by the pilot calculations, in most cases only matrix $\hat{\varphi}$ (which is responsible for the absorption and multiplication of neutrons in the cells) and matrix $\hat{\Psi}$ (which characterizes the diffusion resistance of the cells) should be calculated accurately enough with the help of the high precision codes.

As for matrices $\hat{S}_k$ with $k \geq 3$, they may be represented in the form $\hat{S}_k \cong s_k \hat{S}_1$, where s_k are the values which should be obtained from the simplified auxiliary problems (e.g., for homogenized cell supposing the diffusion approximation to be true in it).

In the particular case of a triangular lattices of rods, Eqs. (7.15) may be represented in the following form using five trial functions per a cell:

$$6\delta \vec{J}_1 = \sum_{j=1}^6 \vec{J}_j^1 \quad \hat{6\varphi}_1 \delta \vec{J}_1 = \sum_{j=1}^6 f_j^1 \quad (7.16)$$

$$3\vec{J}_1^x = \sum_{j=1}^6 \vec{J}_j^1 \cos \alpha_j \quad \hat{3\psi}_1 \vec{J}_1^x = \sum_{j=1}^6 f_j^1 \cos \alpha_j \quad (7.17)$$

$$3\vec{J}_1^y = \sum_{j=1}^6 \vec{J}_j^1 \sin \alpha_j \quad \hat{3\psi}_1 \vec{J}_1^y = \sum_{j=1}^6 f_j^1 \sin \alpha_j \quad (7.18)$$

$$3\vec{J}_1^3 = \sum_{j=1}^6 \vec{J}_j^1 \cos 2\alpha_j \quad \hat{3S}_3 \vec{J}_1^3 = \sum_{j=1}^6 f_j^1 \cos 2\alpha_j \quad (7.19)$$

$$3\vec{J}_1^4 = \sum_{j=1}^6 \vec{J}_1^j \sin 2\alpha_j, \quad 3\hat{S}_4 \vec{J}_1^4 = \sum_{j=1}^6 \hat{f}_j^1 \sin 2\alpha_j \quad (7.20)$$

where α_j is the angle between the radius-vector directed from the cell centre to the centre of the j -face of the cell, and the fixed direction,

$$\vec{J}_j^1 = -(\delta \vec{J}_1 - \vec{J}_1^x \cos \alpha_j - \vec{J}_1^y \sin \alpha_j + \vec{J}_1^3 \cos 2\alpha_j + \vec{J}_1^4 \sin 2\alpha_j) \quad (7.21)$$

$$\hat{f}_1^j = \hat{\varphi}_1 \delta J_1 - \hat{\psi}_1 (\vec{J}_1^x \cos \alpha_j + \vec{J}_1^y \sin 2\alpha_j) + \hat{\xi}_1 (\vec{J}_1^3 \cos 2\alpha_j + \hat{\xi} \vec{J}_1^4 \sin 2\alpha_j) \quad (7.22)$$

Here $\vec{J}_j^1$ is the vector of the neutron group currents through face " j " of the cell " i ", and $\hat{f}_j^1$ is the vector of the neutron group levels on face " j " of the cell " i ".

It is useful to write down the coupling between $\vec{J}_1^j$ and $\hat{f}_1^j$ excluding the amplitudes of $\vec{J}_1^x$ and $\vec{J}_1^y$ from Eqs. (7.21) and (7.22) and introducing values

$$\vec{\phi}_1 = (\hat{\varphi}_1 - \hat{\psi}_1) \delta \vec{J}_1.$$

As a result, we obtain a certain analog to the Fick's law

$$\vec{J}_j^1 = (\hat{\psi}_0 + \hat{\psi}_1)^{-1} \left[\vec{\phi}_1 - \vec{\phi}_0 - (X_j^x - X_0^x) \cos 2\alpha_j - (X_j^y - X_0^y) \sin 2\alpha_j \right] \quad (7.23)$$

where index "0" is the cell number adjacent to cell " i " and having common j face with it,

$$\vec{X}_1^x = (\psi_1 - S_3^1) \vec{J}_1^1; \quad X_1^y = (\psi_1 - S_4^1) \vec{J}_1^4.$$

Owing to the symmetry of the cell,

$$S_3 \equiv S_4 \equiv \xi.$$

Equations (7.16 - 20) are transformed to the following forms using Eq. (7.23)*):

$$\Lambda_D \vec{\phi}_0 - \hat{\Sigma}_{\Phi,0} \vec{\phi}_0 + \hat{S}_\Phi = 0 \quad (7.24)$$

$$\Lambda_D \vec{X}_0^x - \hat{\Sigma}_{x,0} \vec{X}_0^x + \hat{S}_x = 0 \quad (7.25)$$

*) It should be noted that in (Laletin and Elshin, 1980, 1981) Eqs. (7.24-26) are derived without utilising Eqs. (7.16-22) as one would think taking into account the above text. The system of equations (7.16-22) is apparently incompatible one (Shevelev, 1993). (Editor's remark).

$$\Lambda_D \vec{X}_{00}^y - \Sigma_{y,0} \vec{X}_0^y + \vec{S}_y = 0 \quad (7.26)$$

The following notation was used in Eqs. (7.24 - 26)

$$\Lambda_D \vec{A}_0 = \frac{2}{3a^2} \sum_{j=1}^6 \hat{\Delta}_{j0} (\vec{A}_j - \vec{A}_0); \quad (7.27)$$

$$\hat{S}_\phi = -\frac{2}{3a^2} \sum_{j=1}^6 \hat{\Delta}_{j0} \left[\left[\vec{X}_j^x - \vec{X}_0^x \right] \cos 2\alpha_j + \left[\vec{X}_j^y - \vec{X}_0^y \right] \sin 2\alpha_j \right] \quad (7.28)$$

$$\vec{S}_y = -\frac{2}{3a^2} \sum_{j=1}^6 \hat{\Delta}_{j0} \left[\left[\vec{\phi}_j - \vec{\phi}_0 \right] - \left[\vec{X}_j^x - \vec{X}_0^x \right] \sin 2\alpha_j \right] \quad (7.29)$$

$$\hat{S}_x = -\frac{2}{3a^2} \sum_{j=1}^6 \hat{\Delta}_{j0} \left[\left[\vec{\phi}_j - \vec{\phi}_0 \right] - \left[\vec{X}_j^y - \vec{X}_0^y \right] \cos 2\alpha_j \right] \quad (7.30)$$

$$\hat{\Delta}_{j0} = \frac{a}{2} \left[\hat{\psi}_j + \hat{\psi}_0 \right]^{-1} \quad (7.31)$$

$$\hat{\Sigma}_{\phi,1} = \frac{4}{a} \left[\hat{\varphi}_1 - \hat{\psi}_1 \right]^{-1}; \quad \hat{\Sigma}_{x,1} = \hat{\Sigma}_{y,1} = \frac{2}{a} \left[\hat{\psi}_1 - \hat{\xi}_1 \right]^{-1} \quad (7.32)$$

Only the amplitudes of the additional trial functions are presented in the equation for S_ϕ (7.28). If they are neglected (if one considers $\vec{X}_j^x = \vec{X}_j^y = 0$) the finite-difference equation with one unknown per a cell and a group is obtained:

$$\Lambda_D \vec{\phi}_0 - \hat{\Sigma}_{\phi,0} \vec{\phi}_0 = 0 \quad (7.33)$$

Though the form of this equation is such that the codes of the traditional homogenization method (in fact, this could be valid only under approximate diagonalization of matrices $\hat{\Delta}_{j0}$) may be suitable for solving it, the meaning of the vectors of the unknowns $\vec{\phi}_1$ and the finite-difference equation coefficients differs from usual one.

As a result, the values of the functionals are different (more accurate) from those obtained by the homogenization method. The meaning of the variables introduced will be discussed in the next section (the text follows (Laletin, 1981) to a significant degree).

c) **Neutron birth and absorption in the cell.** Let us consider the term $\hat{\Sigma}_{\phi, i} \phi_i$.

By definition,

$$\vec{\phi}_i = \left[\hat{\phi}_i - \hat{\psi}_i \right] \delta \vec{J}_i, \quad \hat{\Sigma}_i = \frac{4}{a} \hat{\psi}_i \left[\hat{\phi}_i - \hat{\psi}_i \right]^{-1}.$$

Consequently,

$$\hat{\Sigma}_{\phi, i} \vec{\phi}_i = \frac{4}{a} \delta \vec{J}_i = \frac{4a \delta \vec{J}_i}{a^2} = \frac{P \delta \vec{J}_i}{S} \quad (7.34)$$

The variables P and S are the perimeter and cross section of the cell respectively.

The perimeter of the square cell is $P = 4a$ ("a" is the lattice pitch) and the cross section is $S = a^2$ while for the hexagonal cell $P = 4a\sqrt{3}$ and $S = a^2\sqrt{3}$ ("a" is again the lattice pitch), and hence

$$P/S = 4/a.$$

Taking into account that $\delta \vec{J}_i$ is the symmetrical trial function amplitude vector, one may consider that $P \delta \vec{J}_{i, g}$ is equal to the total quantity of the g -group neutrons inflowing (or leaking if $J < 0$) into the cell. It is clear from the balance relationships that

$$P \delta \vec{J}_{i, g} / S = (\Pi_g^i - B_g^i) / V_i,$$

where Π_g^i is the total quantity of the neutrons of group "g" absorbed in or leaked off this group in the range of cell "i", and B_g^i is the number of neutrons of group "g" incoming into it from other groups and appearing due to the fission in this group inside the cell "i".

Thus it can be concluded that

$$\frac{P \delta \vec{J}_{i, g}}{S} = \frac{\Pi_g^i - B_g^i}{V_i} = \hat{\Sigma}_{\phi, i} \vec{\phi}_i$$

The variables $\hat{\Sigma}_{\phi, i}$ should be connected with the effective absorption cross sections $\Sigma_{a, g}^i$, fission cross sections $\Sigma_{f, g}^i$, and group to group transition cross sections $\Sigma_{g, g}^i$, for the cell under consideration. This connection, however, differs from the conventional one because $\vec{\phi}_i$ is not the vector of the cell average group neutron fluxes and because we do not suppose that the space-energy dependent neutron distribution is the same as in the infinite uniform lattice of such cells.

d) **Vector of the group unknowns.** The variable $\vec{\phi}_i = (\hat{\phi}_i - \hat{\psi}_i) \delta \vec{J}_i$ in Eqs. (7.24-26) is the vector of the group unknowns. The advantages of such a

choice will be discussed later. The structure of the variable $\vec{\phi}_1$ will now be considered.

Let us denote $\vec{\phi}_1 = \hat{\varphi}_1 \delta \vec{J}_1$. This variable is by definition equal to the vector of the neutron group levels averaged along the cell faces. This follows from the definition of matrix φ_1 consisting of the boundary group levels for the single symmetrically incoming currents, from the definition of the vector of the averaged along the cell boundary incoming currents $\delta \vec{J}_1$, and from the fact that the contribution of the rest trial functions, except $\hat{\varphi}_1$, will be equal to zero after averaging along the cell boundaries.

Let us present the variable $\vec{\phi}_1$ as

$$\vec{\phi}_1 = [1 - \hat{\psi}_1 \hat{\varphi}_1^{-1}] \hat{\varphi}_1 \delta \vec{J}_1 = [1 - \hat{\psi}_1 \hat{\varphi}_1^{-1}] \vec{\tilde{\phi}}_1$$

and the factor $\hat{\psi}_1 \hat{\varphi}_1^{-1}$ will be denoted as

$$\hat{\psi}_1 \hat{\varphi}_1^{-1} = -a^2 \hat{\kappa}_{01}^2 / 8.$$

Analysis of the variables $\hat{\varphi}_1^{-1}$ and $\hat{\psi}_1 = (2/a) \hat{D}_1^{-1}$ (the analysis itself will be given later) makes it clear that the value $\hat{\kappa}_0^2$ is the generalization of the value known as buckling of the flux. Therefore, the value of

$$\vec{\tilde{\phi}}_1 = [1 + a^2 \hat{\kappa}_{01}^2 / 8] \vec{\phi}_1$$

exceeds the value $\vec{\phi}_1$ if $\hat{\kappa}_{01}^2 > 0$ (convex distribution) and becomes less than $\vec{\phi}_1$ if $\hat{\kappa}_{01}^2 < 0$.

Let us emphasize that $\vec{\phi}_1$ always has nonnegative components. In fact $\vec{\phi}_1$ is by definition the vector with non-negative components. The value $a^2 \hat{\kappa}_{01}^2 / 8$ is positive for cells with multiplication coefficient $K_{\infty,1}$ (see later) larger than one.

Let us consider the initial equation

$$\vec{\phi}_1 = [\hat{\varphi}_1 - \hat{\psi}_1] \delta \vec{J}_1$$

with negative $a^2 \hat{\kappa}_{01}^2 / 8$ for the non-multiplicative cells.

The components of matrices $\hat{\varphi}_1$ and $\hat{\psi}_1$ under consideration are positive by definition and the inequalities $(\psi_1)_{gg} \leq (\varphi_1)_{gg}$, are always true. This is obvious as the written variables are the neutron levels on the boundaries of the same cell but under different conditions of incoming currents. The levels under the antisymmetrical boundary conditions $(\psi_1)_{gg}$, will approach (staying less all the time) the levels under symmetrical boundary conditions $(\varphi_1)_{gg}$, only under unlimited growing of "optical thickness" of

the cell.

e) Neutron exchange between the neighbouring cells. The complex $\Lambda_D \vec{\phi}_1 + S_\phi$ in Eq.(7.24) describes the neutron exchange intensity of the cell under consideration with the neighbouring cells.

The main term is $\Lambda_D \vec{\phi}_1$ which has the following unwrapped form

$$\Lambda_D \vec{\phi}_1 = \sum_{i=1}^M 2\hat{D}_i \left[\hat{D}_i + \hat{D}_0 \right]^{-1} \hat{D}_0 \frac{\vec{\phi}_1 - \vec{\phi}_0}{l^2} \quad (7.35)$$

where M is the number of cell faces, l is the length which may be expressed in terms of lattice spacing as $l = a$ for the square cell and $l = a\sqrt{3}/2$ for the hexagonal cell.

It is easy to prove that (7.35) is the simplest finite-difference analog to differential operator $\nabla \nabla \phi(r)$.

The term $\vec{S}_\phi$ describes the contribution of the additional trial functions for the neutron distribution in the cell in the neutron exchange.

The additional trial function amplitudes $\vec{X}_1$ may be excluded (expressed through $\vec{\phi}_1$), but this leads to more complicated finite-difference equations involving larger number of the cells. Thus (see [29]), exclusion of $\vec{X}_1$ leads to a nine-point equation instead of five-point equation (7.33) for the square cells under the additional condition of independence of $\hat{\psi}_1$ and $\hat{\xi}_1$ from cell numbers.

Equation (7.35) results from the fact that the Fick's law finite-difference analog is valid if the additional trial functions are neglected:

$$\hat{j}_1 = 2\hat{D}_1 (\hat{D}_1 + \hat{D}_0)^{-1} \hat{D}_0 (\vec{\phi}_1 - \vec{\phi}_0)/a \quad (7.36)$$

where $\hat{j}_1$ is the average neutron current through face "1" of the zero cell.

The fact of the proportionality of the face cell current to the difference $(\vec{\phi}_1 - \vec{\phi}_0)$ explains why it is preferable to use the cell variables $\vec{\phi}_1$ as the unknown group vectors in comparison with the other possible definitions such as the cell average fluxes $\hat{F}_1$ or the face averaged cell fluxes $\vec{\phi}_1$.

Using such variables would bring us to the currents proportional to the differences either $\hat{r}_1 \vec{F}_1 - \hat{r}_0 \vec{F}_0$ or $\hat{\beta}_1 \vec{\phi}_1 - \hat{\beta}_0 \vec{\phi}_0$, where r_1 are the coupling matrices $\vec{\phi}_1$ and $\vec{F}_1$, that is $\vec{\phi}_1 = \hat{r}_1 \vec{F}_1$ and β_1 are defined by equalities $\vec{\phi}_1 = \hat{\beta}_1 \vec{\phi}_1$. This makes the equations more complex without any benefit. In

particular, matrices $\hat{r}_i$ and $\hat{\beta}_i$ depend on the cell number even for the lattice where the diffusion coefficient can be considered as constant (D_i does not depend on "i") if matrix φ_i characterizing absorption and multiplication cell properties depends on the cell number. Taking into account these considerations, it is natural to call $\hat{\phi}_i$ a neutron group level vector in cell "i".

f) **Matrix $\hat{\psi}_i$.** Matrix $\hat{\psi}_i$ is composed of the boundary group levels resulting from the antisymmetrical incoming single group currents and is proportional to the diffusion cell resistance (see (Laletin, 1981)) because

$$\vec{f}_i - \vec{f}_{i+3} = 2\hat{\psi}_i \vec{j}_i^x, \quad (7.37)$$

where $\vec{f}_i$ and $\vec{f}_{i+3}$ are the group levels averaged along faces "3" and "1". It follows from Eq. (7.37) that the level difference corresponding to unit through passing current, i.e. the diffusion cell resistance, equals $2\hat{\psi}_i$, and the diffusion resistance related to the unit of length equals $2\hat{\psi}_i/a$. The latter variable can be naturally considered as the matrix reciprocal to the diffusion coefficient matrix $D_i^{-1} = 2\hat{\psi}_i/a$ and $D_i = a\hat{\psi}_i^{-1}/2$. To confirm this let us write down the inverse chain of transformations

$$\begin{aligned} \hat{D}_i \hat{D}_i^{-1} \vec{j}_i^x &= \vec{j}_i^x; \\ \vec{j}_i^x &= \hat{D}_i \frac{2\hat{\psi}_i}{a} \vec{j}_i^x = \hat{D}_i \frac{\vec{f}_i - \vec{f}_{i+3}}{a} = \hat{D}_i \frac{\vec{f}_i - \vec{f}_{i+3}}{a} \Rightarrow \vec{j}_i^x = \hat{D}_i \frac{\vec{f}_i - \vec{f}_{i+3}}{a} \end{aligned}$$

Consequently, the introduced notation converts the relationship between the through passing current and the level difference into the differential analog of the Fick's law.

g) **Matrix φ_i .** The matrix φ_i is composed of the boundary group levels corresponding to the unit currents symmetrically incoming the cell. The reciprocal matrix φ_i^{-1} is included in the equation (7.39). Let us derive the different expressions for it which will help us to understand the meaning of its components. First of all, note that φ_i^{-1} is a generalized concept of the logarithmic derivation of the flux over the cell boundary. In fact

$$\varphi_i^{-1} = \frac{1}{\varphi_i} = \frac{j_b}{\Phi_b} \cong \frac{D \frac{\partial \Phi}{\partial r} / b}{\Phi_b} = D \frac{\partial}{\partial r} (\ln \Phi)$$

in the one-group case and on the condition that diffusion approximation on the cell boundary is true.

Using the same approximations variable φ_1^{-1} can be expressed in terms of albedo

$$\varphi_1^{-1} = \frac{j_b}{\Phi_b} \cong \frac{j_1^+ - j_1^-}{(j_1^+ + j_1^-)2} = \frac{1 - \beta_1}{2(1 + \beta_1)}$$

where j_1^+ , j_1^- and β_1 are the incoming and emerging one-side currents and the cell albedo, respectively.

It is convenient to consider separately the cells with and without multiplication to better understand the correlation of variable φ_1^{-1} and the conventional characteristic such as the average along the cell group cross sections. The parallel consideration of the cells with and without multiplication will give a good basis for developing the profitable algorithms for calculating the components of φ_1^{-1} .

The cell without multiplication. In this case let us introduce special notation $\hat{\varphi}_1 = \hat{V}_1$ for the variable $\hat{\varphi}_1$.

The diagonal components of matrix $\hat{V}_1$ may be written using the balance considerations as follows

$$V_{gg} = \frac{P}{S} \frac{t_{gg}}{\Sigma_{agg}} \quad (7.38)$$

where t_{gg} is the ratio of the neutron level on the cell boundary to the cell averaged g-group neutron flux, Σ_{agg} is the cell averaged neutron absorption cross section (the sum of real absorption and removal to the other groups).

Equation (7.38) was obtained with the help of the following consideration: the total number of neutrons incoming to the cell is equal to P (the cell perimeter) because the unity current of the group "g" comes into the cell and nothing comes into the cell in the rest of the groups. All these neutrons are either absorbed in the same group "g" or leave into the other groups. Consequently, the number of such neutrons can be expressed as $\Sigma_{agg} \bar{\phi}_g S$, where $\bar{\phi}_g$ is the group "g" flux averaged over the cell. As $V_{gg} = \bar{\phi}_g$ is the boundary group "g" neutron level,

$$V_{gg} = \frac{\Gamma_g \bar{\phi}_g}{\bar{\phi}_g} / \bar{\phi}_g$$

The following equations

$$\bar{\phi}_g = P / (\Sigma_{agg})$$

and

$$V_{gg} = t_{gg} P / (\Sigma_{agg})$$

result from equality:

$$P = \sum_{agg} \bar{\phi}_g S.$$

The overdiagonal components of the matrix $V_{gg}, (g < g')$ in the cell without multiplication are equal to zero if the groups "g" are wide and all the thermal neutrons are united into one group, e.g. there is no scattering with the energy increase among the groups "g".

The subdiagonal components of the matrix $V_{gg}, (g > g')$ may be presented as follows

$$v_{gg'} = \frac{P p_{gg'} t_{gg'}}{\sum_{agg'}} \quad (7.39)$$

where $p_{gg'}$ is the probability of the neutron with the energy of group "g'" in the cell to avoid absorption while slowing down to group "g".

The other variables are defined in the same way as the diagonal components of the corresponding matrices. Equation (7.39) itself results from the balance relationship which is the same as for deriving (7.38).

The cell with multiplication. The simple use of the neutron balance relations in each group is not of much use because these relations connect the fluxes of different groups.

It is more interesting to split the matrix $\hat{\phi}_1$ into two components, one of them describing "own" neutrons of the cell and the other describing those incoming from the neighboring cells (see (Laletin, 1980, 1981)).

Such expansion has the form:

$$\hat{\phi}_1 = \frac{K_{\infty 1}}{K_{\infty 1} - 1} \left[\vec{\phi}_0^1 * \vec{P}^1 \right] + \hat{v}_1 \quad (7.40)$$

where

$\vec{\phi}_0^1$ is the neutron level vector in the conditionally-critical cell,

$K_{\infty 1}$ is the multiplication coefficient of the infinite uniform media composed of "1" type cells,

$\vec{P}^1$ is the vector with components chosen in such a way that the components of matrix $\hat{V}_1$ would not become infinite when $K_{\infty 1} = 1$, and

$[\vec{\phi}_0^1 * \vec{P}^1]$ is the matrix with components defined as follows:

$$\left[\vec{\phi}_0^1 * \vec{P}^1 \right]_{jk} = \phi_{0j}^1 P_k^1$$

It follows from (7.40) that $\hat{\phi}_1$ is not defined at $K_{\infty 1} = 1$ and it is natural as this means that when the outer neutron source is present in the critical media the "own" neutron flux becomes infinite. However, it is the

reciprocal matrix $\hat{\varphi}_i^{-1}$ that enters the finite-difference equation and it is definite under any value of $K_{\infty, i}$.

Inversion of matrix $\hat{\varphi}_i$ may be carried out analytically, and it results in the equation:

$$\hat{\varphi}_i^{-1} = \frac{S}{P} \frac{1}{c_i} \left[k_i \hat{\Sigma}_i - \rho_i \hat{\Sigma}_{ai} \right] \quad (7.41)$$

where $\rho_i = (K_{\infty, i} - 1)/K_{\infty, i}$ and $\hat{\Sigma}_{ai}$ is a matrix of the form $\hat{\Sigma}_{ai} = S\hat{V}^{-1}/P$.

The components of matrix $\hat{\Sigma}_i$ include the average cross sections and the flux cell-tilt factors computed for the conditionally-critical cell. Variables c_i and k_i depend on the ratios of corresponding cross sections and cell-tilt factors for the conditionally-critical cell, and components of the matrix $\hat{\Sigma}_{ai}$.

The equations for $\hat{\Sigma}_i$, $\hat{\Sigma}_{ai}$, k_i and c_i used in the two-group approach are given in (Laletin, 1980, 1981a).

Representation as

$$\hat{\varphi}_i = \left[\vec{\varphi}_\mu^i * \vec{\alpha}_i^1 \right] + \left[\vec{\varphi}_\nu^i * \vec{\beta}_i^1 \right] \quad (7.42)$$

may be more convenient than (7.41) when the flux inside the cell is described by the diffusion equation, e.g. during the calculation of the secondary homogenization for PWR type reactors. Here $\vec{\varphi}_\mu$ and $\vec{\varphi}_\nu$ are the vectors of the boundary fluxes in the two-group diffusion approach and correspond to the eigenfunctions connected with known two-group eigenvalues $\mu_i^2 \approx (K_{\infty, i} - 1)/M^2$ and $-\nu_i^2 \approx 1/L_i^2 + 1/\tau_i$. The vectors $\vec{\alpha}_i^1$ and $\vec{\beta}_i^1$ consist of the coefficients defined from the boundary conditions.

7.3 Analysis of relations of SHM with other approaches

In this section let us briefly repeat the main theses underlying SHM and then detail the main new aspects described by SHM equations which have not been included in the traditional homogenization equations. Let us establish the relations of SHM with some other approaches.

The main statements are:

1) The solution is sought as the sum of the trial functions which satisfy the transport equation in the individual cell and the definite conditions on the boundary of the cell. A set of the trial functions is determined for each cell in the form

$$\phi^N(\omega) = \sum_i \sum_k a_{ik} \phi_{ik}(\omega)$$

2) The residual appears when substituting the approximate expression for $\phi^N(\omega)$ into the transport equation (the approximation arises from restricting the summation along "k" by a certain number "N") and it is concentrated on the cell boundaries.

3) As a result the system of equations which connects the solution moments in adjacent cells appears in the following form

$$\phi_1^{nk} = \sum_j \sum_{k'} C_{kk'}^{ji} \phi_j^{nk'}$$

4) Since the trial functions satisfy the transport equation inside the cell, the connection between the separate energy-angle moments is reached on the cell boundaries. In the SHM the connection between the neutron levels (or approximately fluxes) and the currents has the form

$$\phi_1^n = \sum_n S_n^n \phi_1^{n'}$$

5) Then the transformation of the equations of items 3) and 4) to a form convenient for both their solution and their analysis is performed. The new variables are introduced: the neutron level in the cell and matrices of the effective cross sections of absorption, and the fission and neutron diffusion coefficients.

Let us discuss the new effects accounted for by SHM. For all these divisions the effects are - as always - conditional, since the contributions of these effects are not additive in the specific calculations. Along with it I shall point out the relationship of SHM equations with the equations, considered in publications as being devoted to the advanced calculation methods.

a) **The main mesh-size correction.** The main mesh-size correction in its pure form may be extracted in the approximation where the core consisting of the homogeneous cells is considered, the neutron transport inside the cells and coupling between the cells are taken in one-group approximation and the higher space harmonics are neglected. Then Eq. (7.24) takes the following form:

$$\frac{2}{3a^2} \sum \frac{2D_i D_k}{(D_i + D_k)} (\phi_i - \phi_k) - \sum \phi_k = 0 \quad (7.43)$$

Taking into account the definition of these variables and the above formulated approximations of the problem under consideration, the following equation is obtained:

$$\sum \phi_k = (\Sigma_a^k - \nu \Sigma_f^k / K_{eff}) F_k$$

where F_k is the neutron average flux in the cell, and

$$D_i = \bar{D}_i C_i,$$

where $D_i = 1/3\Sigma_{tr}^i$, $C_i = 1/K_j^i$, K_j^i is current-tilt coefficient, i.e. the ratio of the averaged by cell "i" neutron current in definite direction to the neutron current on the boundary of the same cell. In this case the value for r in the coupling relation $\phi_i = r_i F_i$ is obtained easily and has the form

$$r_i = 1/K_\phi^i (1 + \beta_1^2 a^2 / 8),$$

where $\beta_1^2 = (\Sigma_a^i - \nu \Sigma_f^i / K_{eff}) \bar{D}_i$, K_ϕ^i is the flux-tilt coefficient, i.e. the ratio of the averaged by cell "i" neutron flux to the averaged by cell boundary neutron flux.

In this case variables C_i and r_i approximately, with the accuracy of the terms of order $\beta_1^2 a^2$, have the forms:

$$C_i \approx 1 - 0,069 \beta_1^2 a^2, \quad r_i \approx 1 + 0,103 \beta_1^2 a^2.$$

Note that Eq. (7.42), if expressed in terms of the newly defined variables F_i , has the form

$$\frac{2}{3a^2} \sum_{i=1}^6 \frac{2D_i C_i D_k C_k}{D_i C_i + D_k C_k} (r_i F_i - r_k F_k) - \sum \frac{\nu \Sigma_f^k}{K_{eff}} F_k = 0 \quad (7.44)$$

This equation actually coincides with the Askew-Takeda equation (Takeda et. al. 1979) for two-dimensional problems and in this case coefficients C_i and r_i are numerically very close to described above (Takeda brings (7.44) to the form of (7.43) by formal substitution and investigates numerically benefit of it).

Many publications (Lukas, Wehmann, 1981; Slesarev and Yaroslavtceva, 1983) are devoted to numerical investigations of (7.43) and its modifications).

In (Takeda et al, 1979):

$$C_1 \cong 1 - 2/27\beta_1^2 a^2 \cong 1 - 0,074\beta_1^2 a^2 \text{ and } r_1 = 1/(1 - 1/9\beta_1^2 a^2) \cong 1 + 0,11\beta_1^2 a^2.$$

Equation (7.43) in (Takeda et al, 1979) was obtained in the following way: the auxiliary mesh-points inside the cells were introduced, the equations coupling these auxiliary mesh-points with the main points of the mesh were written down, and then the auxiliary mesh-points were excluded analytically.

The same procedure was performed in (Marakazov, 1977) (implemented in codes BIPR-6 and BIPR-7) and the only distinction was that different auxiliary mesh-points were chosen. The resulting equation appeared to be more complicated, the coupling of the equation coefficients with the usual physically explicit variables was not so clear but the effect of the refinement ("the coarse-mesh effect" according to Askew) in practice has to be the same.

In essence the same effect is accounted for in Borresen's publications (Borresen, 1971, 1981) where the equations for joining the currents and fluxes on the cell faces were used to couple the adjacent cells under the assumption that the flux averaged by the cell (or "node") may be represented in the form

$$\bar{\phi}_1 = b\phi_1 + 2c\sum_j \phi_j^1$$

where $\bar{\phi}_1$ is the averaged node flux, ϕ_1 is the flux in the centre of the node, and ϕ_j^1 is the flux averaged by face "j" of the node "i".

Coefficients b and c were fitted numerically in the model problems, and this point is -in my opinion- the essentially weak point of this particular work.

Note that consideration of the one-group problem especially after the homogenization of the real cell does not give a full picture about the significance of the main mesh-size correction. The main corrections to the results received by the traditional equations of the homogenization method arise in nonuniform lattices and strongly depend on the number of groups used. In particular, in two-group approaches the variables a^2/L_g^2 appear beside the parameter $\beta_1^2 a^2$, where L_g is the diffusion length in group "g".

b) Accounting for the cell vicinity. Let us consider the cell average

absorption cross section as an example to make it clear how SHM accounts for different behavior of the same cells in different surrounding conditions. Let us take the case when the neutron exchange between the cells is considered in two-group approximation. In accordance with SHM the average thermal absorption cross section is represented in the form

$$\bar{\Sigma}_{a,2} = \frac{\bar{\Sigma}_a^{22} \bar{\varphi}_{22} \delta J_2 + \bar{\Sigma}_a^{21} \bar{\varphi}_{21} \delta J_1}{\bar{\varphi}_{22} \delta J_2 + \bar{\varphi}_{21} \delta J_1}$$

where $\bar{\Sigma}_a^{21}$ and $\bar{\varphi}_{21}$ are the energy-space averaged cross section and the thermal neutron flux respectively ($i = 1, 2$).

This averaging is performed using the distributions of the following problems:

- when $i=1$ the solution is defined under the boundary conditions of symmetrical incoming of the fast neutrons with zero current in the thermal group,
- when $i=2$ as above with incoming of the thermal neutrons with zero current in the fast group.

Since $\bar{\Sigma}_a^{22} \neq \bar{\Sigma}_a^{21}$, the cell average cross section $\bar{\Sigma}_{a2}$ changes depending on the ratio $\delta J_2 / \delta J_1$, i.e. it depends on the cell vicinity. This relationship may be represented in the form $\bar{\Sigma}_{a2} = f[\bar{F}_2 / \bar{F}_1]$. It is precisely the representation of the average thermal neutron cross section that is stated in (Leman, 1978) (the spectral index method). It is proposed to determine the relationship parameters by solving a set of problems for the identical cells having different surroundings and then to use them in the traditional mesh equations.

As was demonstrated, sufficiently good results for describing the thermal group near the boundary between the core and the reflector were obtained. Note that in (Leman, 1979) the "coarse-mesh" effect, which is important even in fine-mesh calculations in the vicinity of -say- the absorbing rods, is not accounted for.

The elements of the matrices φ_1 and ψ_1 are defined so that they explicitly provide the set of the problems for their determination. Let us call them "basic problems".*) However, one must underline that this does not at all mean that such problems should be adopted in real calculations.

*) These problems are connected with the boundary currents in the corresponding groups under zero currents in the other groups.

In reality it is more convenient to choose the problems which are the linear combinations of the basic problems.

For example a problem corresponding to the prescribed self-established uniform-lattice type spectrum (asymptotic spectrum) of the incoming (for $\hat{\varphi}$) or through passing (for $\hat{\psi}$) neutron currents on the cell boundary should be taken as a principle.

It is both convenient to represent the solution of such problems in the form of matrices $\hat{\varphi}$, $\hat{\psi}$, $\hat{\Sigma}_{\phi} = (\hat{\varphi} - \hat{\psi})^{-1}$, etc., and to try to rewrite these equations, expressing the coefficients directly using the variables Σ_{as}^a , Σ_s^a , etc., obtained for such problems. This approach is used in (Pshenin and Novikov, 1984, 1988).

In order to demonstrate the connection between these approaches let us write down the average thermal neutron absorption cross sections again. Using the form of (7.42) the following equation is obtained

$$\bar{\Sigma}_{a2} = \frac{\bar{\Sigma}_{a,2}^{\mu} \bar{\varphi}_{\mu}^{-2} K_{\mu} + \bar{\Sigma}_{a,2}^{\nu} \bar{\varphi}_{\nu}^{-2} K_{\nu}}{\bar{\varphi}_{\mu}^{-2} K_{\mu} + \bar{\varphi}_{\nu}^{-2} K_{\nu}}$$

where $\bar{\Sigma}_a^{\mu}$, $\bar{\varphi}_{\mu}^{-2}$ are the average cross sections and fluxes for the asymptotic solution, $\bar{\Sigma}_a^{\nu}$, $\bar{\varphi}_{\nu}^{-2}$ are analogous variables for the transient solution (they are denoted as $\Sigma_{a2}^{\mu} = \Sigma_a^a$, $\Sigma_{a2}^{\nu} = \Sigma_{f2}^a$ in (Pshenin, Novikov, 1988)). The coefficients K_{μ} and K_{ν} are expressed in the following way

$$K_{\mu} = j_{\nu}^1 \delta J_2 - j_{\nu}^2 \delta J_1, \quad K_{\nu} = j_{\mu}^1 \delta J_2 - j_{\mu}^2 \delta J_1$$

where j_{μ}^1 , j_{μ}^2 are the boundary currents for the asymptotic solutions of fast and thermal groups respectively and j_{ν}^1 , j_{ν}^2 are analogous expressions for the transient solution.

Both asymptotic and transient solutions may be acceptable for two-group representation of the neutron exchange between the cells. Switching over to the larger group numbers is, however, natural if the variables φ and Σ_{ϕ} are used. Moreover, even for two groups the equations using these variables are more convenient for solution than the equations with the coefficients expressed in terms of Σ_a^a , Σ_{tr}^a , etc.

As was mentioned, it is sometimes convenient, especially for heterogeneous cells, to distinguish cross sections for "own" neutrons and for "incoming" ones according to the representation of the matrix $\hat{\varphi}$ in the form (7.40). In this case matrix $\hat{\Sigma}_a$ has the form

$$\Sigma_{af} = k_1 \hat{\Sigma}_0 + \rho k_2 \hat{\Sigma}_a$$

where

$\hat{\Sigma}_0$ is the matrix of the cross sections averaged over the space-energy neutron distribution corresponding the zero currents on the cell surface, $\hat{\Sigma}_a$ is the analogous matrix for the incoming neutrons,

$$\rho = (K_\infty - K_{\text{eff}}) / K_\infty,$$

K_∞ is the multiplication coefficient in infinite media (consisting of the cells under consideration),

K_{eff} is the effective multiplication coefficient (unknown until the solution for whole reactor is obtained),

$\bar{k}_1$ and $\bar{k}_2$ are the functions of ratios of the average cross sections and the tilt coefficients of the "own" and "incoming" neutrons.

Equation (7.33) describes the case when the cells do not contain the outer volumetric sources. It is not difficult to write down the equations for the case with volumetric sources of the neutrons and it has already been done in the first publications about SHM (Elshin and Laletin, 1976; Laletin and Elshin, 1977; Maierov and Yudkevich, 1988).

c) **The nondiagonality of the diffusion coefficient matrix.** The neutron current through the face of adjacent cells in SHM is expressed (in the basic approximation) by

$$\vec{j}_1 = \hat{D}(\vec{\phi}_1 - \vec{\phi}_0)$$

For the sake of simplicity let us consider the lattice constructed of cells with identical diffusion coefficient matrices. In particular, let us write down the equation for the thermal neutron current of the two-group description of neutron exchange:

$$j_1^t = D_{tt}(\phi_1^t - \phi_0^t) + D_{tf}(\phi_1^f - \phi_0^f) \quad (7.45)$$

where the indices "t" and "f" refer to the thermal and fast neutrons respectively.

It is seen that the thermal neutron current also depends on the fast neutron level difference. It follows from analysis of equations for $D_{gg'}$ (Laletin, 1980, 1981a, 1981b) that nondiagonal components of the diffusion coefficients matrix are proportional (under condition $g > g'$) to the variables a^2/L^2 . In other words the effect under discussion, as in paragraph a), is connected with the finiteness of the lattice spacing "a". However, the distinctions of the space-energy in-cell distributions of the neutrons crossing the cell boundary in the different groups are significant as well.

After regrouping the terms the current in (7.45) may be represented in the form:

$$j_i^t = D_{as} \left[\phi_1^{as} - \phi_0^{as} \right] + D_{ts} \left[\phi_1^{tr} - \phi_0^{tr} \right]$$

where "as" and "tr" refer to asymptotic and transient spectra respectively.

The authors of (Pshenin et al, 1984, 1988) do the same thing but use different variables instead of the levels. However, apart from the equations to be solved becoming more complicated, some inconvenience arises during the parameter calculation due to $D_{as} = D_{tr}$, in contrast to SHM where values D_{tt} and D_{tf} almost always obey the following inequality:

$$D_{tf} \ll D_{tt}.$$

Let us also establish the connection between matrix D of SHM and the α_{ik}^g values playing the role of the diffusion coefficients in (Gado et al, 1984). Using (7.44) from (Laletin and Elshin, 1981), having identical variables in SHM and in (Gado et al, 1984) (with different notation), diverting from the difference of the averaged by faces neutron flux and corresponding local level and remaining in the limits of the main approximation, i.e. neglecting the higher surface harmonics, we obtain

$$\frac{1}{\alpha_{ki}^g} = \psi_{gg} + \frac{\Sigma \psi_{gg} (\delta J_g^g + J_1^g)}{\psi_{gg} (\delta J_g^g + J_1^g)}$$

We can see from this equation that α_{ik}^g even in this approximation is not a characteristic of the cell because it can be obtained only after the complete solution is available, because α_{ik}^g depend on the ratio

$$(\delta J_1^g + J_1^g) / (\delta J_g^g + J_1^g)$$

That is why the nonlinear iteration algorithm including recalculation of α_{ik}^g at each iteration is proposed in (Gado et al, 1984). Since there is the full set of equations in SHM it is possible to implement both the analogous nonlinear iteration process and all possible linear ones.

d) The higher surface harmonics. One more generalization of the Fick's law in SHM is connected with accounting for the higher surface harmonics in comparison with those included in the main approximation. The neutron current on the common face of two adjacent cells "j" and "o" accounting for the five surface harmonics, as mentioned above, has the form (see (7.23))

$$\vec{j}_j = \left[\hat{\psi}_0 + \hat{\psi}_j \right]^{-1} \left[\vec{\phi}_j - \vec{\phi}_0 - \left[\vec{X}_j^x - \vec{X}_0^x \right] \cos 2\alpha_j - \left[\vec{X}_j^y - \vec{X}_0^y \right] \sin 2\alpha_j \right]$$

Equation (7.24) is equivalent to

$$\sum_j \vec{J}_j - \hat{\Sigma}_\phi \vec{\phi}_0 = 0 \quad (7.46)$$

where the neutron balance in the cell is described.

Additional correlations for determining the amplitudes of the higher surface harmonics $\vec{X}_j^x$ and $\vec{X}_j^y$ are required to solve this equation. These correlations are written above (see (7.25) and (7.26)). However, it is possible to construct some nonlinear iteration procedure for solving (7.46), assuming that the neutron current and level (flux) on the cell face are connected in the following way (see (7.44) from (Laletin and Elshin, 1981))

$$\vec{f}_j^1 = \hat{\phi}_1 - \hat{\psi}_j^1 \left[\delta \vec{J}_1 + J_1^1 \right] - \left[\vec{X}_j^x \cos 2\alpha_j + \vec{X}_j^y \sin 2\alpha_j \right]$$

Hence,

$$\frac{-f_{jg}^1 + \tilde{\phi}_{1,g}}{\delta \vec{J}_1 + \vec{J}_1^1} = \psi_{gg} + \frac{\Sigma_{gg}, \psi_{gg}, (\delta J + j)_g}{(\delta J + j)_g} + \frac{\vec{X}_{j,g}^x \cos 2\alpha_j + \vec{X}_{j,g}^y \sin 2\alpha_j}{(\delta J + j)_g} \quad (7.47)$$

If we neglect the difference between the fluxes and levels on the cell faces and establish the correlations between different notations of the identical values, we shall see that the left part of (7.47) is equal to

$$\frac{\tilde{\phi}_{1g} - f_{jg}^1}{\delta J_{1,g} + J_{1,g}^1} = \frac{1}{D_p C_p^1} \equiv \frac{1}{\alpha_{1k}^g} \quad (7.48)$$

where the term $D_p C_p^1$ is from (Novikov, 1982, 1983) and the term α_{1k}^g is from (Gado *et al*, 1983; Gado *et al*, 1984).

The balance equations in the mentioned publications are analogous to (7.24) but the latter equation is not sufficient for complete solution of the problem (the terms $D_p C_p$ and α_{1k}^g are not the cell characteristics, since according to (7.48) they depend on a complete solution of the problem). Therefore the nonlinear iteration process was proposed in (Novikov, 1983) and implemented in (Lizorkin, 1983, 1985), (Jolkevich *et al*, 1984). The values C_{pi} and Σ_{pi} are recalculated in this iteration process.

Let us consider the fact that, in contrast to (Novikov, 1982a, Pshenin *et al*, 1984, 1988) devoted to "fine-mesh" equations in Novikov's terminology, in the "coarse-mesh" equations (Novikov, 1983, 1985) of the same authors the direct presence of nondiagonality in the diffusion coefficient matrix disappears.

This effect is taken into consideration along with accounting for the

effect of the higher surface harmonics in the nonlinear iteration process. The equations and the nonlinear iteration process proposed in (Gado et al, 1984) in reality coincide if the notations are in agreement with the notations of (Novikov, 1983, 1985). The equations in (Novikov, 1983, 1985) are given for two-group case and in (Gado et al, 1984) for arbitrary-group division, but it is not a matter of principle.

As was noted above, the other way of accounting for the higher surface harmonics is possible by excluding part of them from equations. This brings us to the equations connecting a larger number of cells among themselves.

Let us give an example of the equation for the square lattice obtained by using 8 trial functions per cell and per group. After excluding the higher surface harmonics and making some simplifications of the problem in which all the matrices S_n with $n \geq 1$ do not depend on the cell number, the following equation is obtained (Eq. (7.29) of (Laletin and Elshin, 1981))

$$\tilde{\Lambda} \tilde{\phi}_0 + \hat{\kappa}_0^2 \tilde{\phi}_0 = 0, \quad (7.49)$$

where

$$\tilde{\Lambda} \tilde{\phi}_0 = (1+k)^{-1} \left[(1-k) \Lambda_1 \tilde{\phi}_0 + 2k \Lambda_2 (1 - \hat{\kappa}_0^2 a^2) \tilde{\phi}_0 \right]$$

where

$\Lambda_1 \tilde{\phi}_0 = \frac{1}{a^2} \sum_{j=1}^4 (\tilde{\phi}_j - \tilde{\phi}_0)$ is the finite-difference analog of the Laplace operator on the "cross" pattern,

$\Lambda_2 \tilde{\phi}_0 = \frac{1}{2a^2} \sum_{j=5}^8 (\tilde{\phi}_j - \tilde{\phi}_0)$ - is the finite-difference analog of the Laplace operator on the "rotated cross" pattern,

$$\tilde{\phi}_1 = (\hat{\varphi}_1 - \hat{\psi}) \delta J_1, \quad \hat{\kappa}_1^2 = -\frac{8}{a} \hat{\psi} (\hat{\varphi}_1 - \hat{\psi})^{-1},$$

$$\hat{\psi} = (1-k)^{-1} (1+k) \hat{\psi}, \quad \alpha = \frac{1}{4} (1-k)^{-1} k$$

k is the expression (generally speaking, a matrix) depending on the ratio of $\hat{S}_n$, $n \geq 2$, to $\hat{S}_1 \equiv \hat{\psi}$.

The matrix k is transformed to the number under the approximations of (Laletin and Elshin, 1981). This number equals to $k=0.205$.

As a result,

$$\tilde{\Lambda} \tilde{\phi}_0 = 0,659 \Lambda_1 \tilde{\phi}_0 + 0,341 \Lambda_2 (1 - \hat{\kappa}_0^2 a^2) \tilde{\phi}_0$$

Now, if we neglect the term $\alpha \hat{\kappa}_0^2 a^2$ ($\alpha \approx 1/16$) this equation is about

equal to the best approximation of the Laplace operator of the nine-point pattern (see, e.g., (Tichonov and Samarsky, 1966)). The essential difference is that the neutron level is used as the variable instead of the solution value in the lattice node as in (Tichonov and Samarsky, 1966). It would be interesting to compare (7.49) with the finite-difference equation investigated by Gorodkov (Gorodkov, 1988). Primarily Gorodkov's (Gorodkov, 1973a, 1973b) finite-difference equations for the heterogeneous reactors were obtained by the transformation of the "source-sink" method (the same was done in (Kochurov and Malofeev, 1977)).

Later they were significantly modified and now the equations of (Gorodkov, 1988) no longer resemble the initial ones. They have the form

$$U_0 = (f+s)^{-1} (\Lambda_{00}^{-1} + f\Lambda_{1,0}^{-1}) \sum_{j=1}^2 \sum_{i=1}^4 d_{ij} (U_0 - U_{ij}) \quad (7.50)$$

Here matrices $\hat{\Lambda}_n$, which are proportional to the reciprocal matrices S_n in SHM, are used as the cell characteristics, the following equations being valid

$$\hat{\Lambda}_{01} = -4a\hat{\varphi}_1^{-1},$$

$$\hat{\Lambda}_{11}^{-1} = \frac{2}{a} \hat{\psi}_1$$

(The equality $\hat{\Lambda}_{1,0} = \hat{\Lambda}_{1,1}$ is accepted in (7.50) as it is supposed in the main version of the code HEM).

Unknown vector $U_i = (1 + f\hat{\Lambda}_1^{-1}\hat{\Lambda}_0)\tilde{\phi}_i$ is introduced, where $\tilde{\phi}_i$ is the neutron flux averaged by cell faces, f, s and d are the values calculated during a certain minimization procedure, which was used for solving series of model problems. Vector U_i is very close to the neutron level vector $\tilde{\phi}_i$ in (7.49) if the best values of f, s and d_j are chosen from a set given in (Gorodkov, 1988). Indeed,

$$U_i = (1 + f\hat{\Lambda}_{11}^{-1}\hat{\Lambda}_{0i})\tilde{\phi} = (1 - 0,20128 \ 8\hat{\psi}_i\hat{\varphi}_0^{-1})\tilde{\phi} = (1 - 1,610124 \ \hat{\psi}_i\hat{\varphi}_0^{-1})\tilde{\phi}$$

whereas

$$\tilde{\phi}_i \equiv \left[1 - \frac{1+k}{1-k}\hat{\psi}\hat{\varphi}^{-1}\right]\tilde{\phi} = \left[1 - 1,517\hat{\psi}_i\hat{\varphi}_0^{-1}\right]\tilde{\phi}.$$

The value $(1-k)/(1+k)=0.659$ should be compared with $d_1/(f+s)=0.6415$, and $k/(1+k)=0.1705$ with $2/(f+s)=0.1797$. The last pair of numbers may be compared only if component $\hat{\alpha}\hat{\kappa}_0^2 a^2$ of the term $\hat{\Lambda}_2(1+\hat{\alpha}\hat{\kappa}_0^2 a^2)\tilde{\phi}_0$ is neglected, which is possible at least in the problems considered in (Gorodkov, 1988) because $\hat{\alpha}\approx 0.0625$.

The author (Gorodkov, 1988) calculated one of the problems presented

in the last-cited work with the numerical coefficients, mentioned above as obtained from (7.49). The result obtained differs a little from the one calculated with optimal, in his opinion, set of the coefficients f , s , d . The SHM method also allows one to obtain nine-point finite-difference equations which are very close to the form recommended in (Gorodkov, 1988).

Finally, it is worth mentioning the publication (Kochurov and Malofeev, 1977). The equations are obtained and investigated at least for two-dimensional problems there and they should give results close to Gorodkov's.

e) The transport corrections on the cell boundaries. The neutron current and the neutron level are the two variables of SHM which take part in joining the solutions on the adjacent cell boundaries instead of the conventional neutron current and flux. Using the neutron level as one of the main variables is the consequence of the fact that the exact correlation is (Glasston and Edlund, 1952; Laletin and Boyarinov, 1985)

$$j_i = -\frac{1}{3\Sigma_{tr}} \nabla_j l_{ij} \quad (7.51)$$

and not Fick's law

$$j_i = -\frac{1}{3\Sigma_{tr}} \nabla_i \phi.$$

where j_i is the component "i" of the neutron current,

$$\Sigma_{tr} = \Sigma - \Sigma_{s1}^1; \quad \Sigma_{s1}^1 = \int (\vec{\Omega}\vec{\Omega}') \Sigma_s(\vec{\Omega}\vec{\Omega}') d\Omega,$$

$$l_{ij} = 3 \int \Omega_i \Omega_j \psi(\vec{\Omega}) d\vec{\Omega}.$$

The repeating indices in (7.51) suppose summation. It is not difficult to show that $l_{11} = \phi_0 + 2\phi_2$, i.e. it is the combination of the flux ϕ_0 and the second angle moment in the Legendre polynomial expansion

$$\phi_2 = \int P_2(\vec{\Omega}) \psi(\vec{\Omega}) d\vec{\Omega};$$

This combination has already appeared in the works devoted to more precise definition of the boundary conditions of the spheric harmonic method (Vladimirov, 1961), (Rumyanzev, 1961). Analogous changing the boundary conditions was investigated in the works on SHM and was realized in corresponding codes (Laletin and Sultanov, 1979). Since the neutron current value and direction are connected with the derivatives of the tensor components l_{ij} (it follows from (7.51)), the tensor was named the neutron level tensor (Laletin and Boyarinov, 1985) and its diagonal components - neutron levels.

There is a close connection between the neutron (local) level and the

cell neutron level and between nondiagonal tensor components and the higher surface harmonics in a cell.

The transport correction may be indirectly evaluated using the following consideration: if we use the finite-difference equations with the neutron currents and flux joints we shall obtain the diffusion equation for the neutron distribution in the uniform lattice in the limit of the fine-mesh lattice spacing whereas if in a similar situation we use the neutron currents and levels we shall obtain the equation in B-approximation. It is well known that increasing the accuracy of the multiplication coefficient in B_0 - (or in B_1 -) approximation for uranium-water WWR-type assembly may reach 0.5+1.0% in comparison with the diffusion approximation.

f) **The complementary remarks on SHM.** It should be mentioned several aspects of SHM which have already been discussed in some publications, but have not yet reached a degree of sufficient completeness.

The first aspect of SHM, which follows from the works close to it by their trend, refers to the special approach to defining the eigenvalue. Generally speaking, the multiplication coefficient is a kind of formal value and it is always possible to introduce another value easy to interpret but more suitable for the calculation algorithm of the SHM equations.

However, the problem of comparison of the calculations performed by SHM and by the other methods including the benchmark calculations, and the Monte Carlo method in particular, arises. It is then desirable to retain the consistent definition of the effective multiplication coefficient K_{eff} . In this case the multiplication coefficient enters the SHM equations not linearly and even not explicitly but through the dependence of the equation coefficients on it.

The different possibilities appear and they were investigated with a different degree of detailization. The first possibility is to introduce new iteration level, i.e. the K_{eff} iterations, in which the SHM equation coefficients, namely the elements of the matrices $\hat{\Sigma}_\phi$ and $\hat{D}$, are recalculated. The corresponding library of the cell characteristics is created beforehand for quick recalculation of the coefficients and they are approximated by polynomials of K_{eff} . Such calculations were performed by Laletin, Sultanov and Boyarinov as well as by Gorodkov. Similar iterations are present also in (Takeda, et al, 1979; Lukas, Wehmann, 1981; Slesarev and Yaroslavtceva, 1983).

The second possibility is that it is possible to transform the SHM equations so that K_{eff} enters in them linearly, provided the representation (7.40) of matrix ϕ (and $\hat{\Sigma}_\phi$ respectively) by a sum of two terms and neglecting the matrices $\hat{D}$ and $\hat{V}$ (and $\hat{\Sigma}_a$) dependence on K_{eff} and, as a result, additional iteration level is not required. This opportunity was tested in calculations performed by Laletin and Shahabasiyan and separately by Svadkovsky.

The third possibility is, may be, the most preferable but unfortunately it has not yet been implemented and tested; it also includes transformation of the cell characteristics to another form, however the resulting equations not only depend linearly on K_{eff} but the SHM equations hardly differ (in form) from those implemented in the codes based on traditional homogenization method. In this case the space-energy neutron importance functions (adjointed functions) in a cell are used to calculate the cell characteristics, though to a lesser degree.

A great deal of effort has been spent on finding the most rational current distributions on the cell boundaries. This problem arises from the need to diminish - as far as possible - the number of groups describing the neutron exchange between the cells.

In this connection it was suggested to account for the energy behavior of the neutron diffusion coefficient on the cell boundary (see (Laletin *et al*, 1987) during the calculation of the cell characteristics $\hat{\Sigma}_\phi$ and $\hat{D}$. The full satisfaction in this question is not yet reached.

Numerical results that are useful for understanding the significance of the new effects in SHM and in the related approaches can be found in literature (cf. Laletin *et al* papers, Novikov *et al*, Maiorov, Gorodkov).

All discussions above concerned the advanced reactor equations for two-dimensional problems. Analogous investigations are carried out for three-dimensional problems (Laletin and Elshin, 1985, 1986) and the ways of spreading SHM on the space-depending kinetic equations (Boyarinov, Sultanov) have also been considered. The three-dimensional equations in the SHM frames are obtained in (Laletin and Elshin, 1985, 1986), furthermore the corresponding code is written down (Elshin) - some numerical researches having been performed using it. The equations for finite-dimensional reactor with not depending on z-coordinate properties are obtained as the limit case of the three-dimensional SHM equations and they are used for the treatment of experiments (Laletin, Boyarinov). I should also like to mention Chepurnov's works in which the SHM equations are used in

(x,y)-plane but dependence on z-coordinate is represented by corresponding Fourier expansion.

The three-dimensional finite-difference equations with improved accuracy were also obtained in (Novikov, 1983). However, though A. Novikov's two-dimensional equations may be compared with SHM equations as was done above, this procedure appears to be more difficult for the three-dimensional case since the additional approximations (in particular, the assumption about the partial separation of variables for space coordinates) were introduced in (Novikov, 1982, 1983).

REFERENCES^{*)}

Anrjeevsky K. (1977). Diffusion coefficient calculation for non-uniform media. (In Russian).

Анджеевски К. К вопросу расчета коэффициента диффузии в неоднородных средах. Материалы 6-го симпозиума ВМК, Бухарест, 1977, с.363.

Aoki K., Shimizu A. (1969). Application of the Response Matrix Method to criticality calculations of the two-dimensional reactors. J.Nucl. Sci. Techn., v.2., p.149.

Barkov S.N. (1977) An Albedo method for calculating the heterogeneous reactor parameters. (In Russian).

Барков С.Н. Альбедный метод расчета характеристик гетерогенного реактора. Препринт ИАЭ-2930, М., 1977.

Benoist P. (1961). A General Formulation of the Diffusion Coefficient in a Heterogeneous Medium which may contain Cavities. J.Nucl. Energy, 1961, part A, v.13, p.97.

Berna Ph. (1973).^{*)} Comparison between Benoist and Selengut diffusion coefficients in one-velocity theory, when absorbing media are present in the cell. Jour. Nucl. Enrg. v.27, p.633.

Bonalumi R.A. (1971).^{*)} A unified theory of cell diffusion coefficient. Energia Nucleare. v.18, n.7/8, p.395.

Bonalumi R.A. (1973).^{*)} A rigorous diffusion model for cell homogenization. Energia Nucleare. v.20, n.1, p.39.

Borresen S. (1971) A Simplified Coarse-Mesh, three-dimensional diffusion scheme for calculating the cross power distribution in a Boiling Water Reactor. Nucl. Sci. Eng. v.44, p.37. 1971.

Borresen S. (1981) Experience, Status and Advance Applications of PRESTO, Proc. Int. Topl. Mtg. on Advances in Mathematical Methods for the Solution

^{*)} References supplemented by editor are marked be asterisk..

of Nuclear Engineering Problems, v.1, p.283, Munchen. 1981.

Chan Din Chi, Makai M. (1983) The SESHOM code for WWER assembly homogenization. (In Russian).

Чан Динь Чи, Макаи М. Seshom-программа гомогенизации кассеты ВВЭР, Материалы 12-го симпозиума ВМК, Татранска Ломница, 1983, т.2, с.218.

Deniz V.C. (1986).^{*)} The theory of neutron leakage in reactor lattices. CRC -handbook of Nuclear Reactors Calculations. V.2, p.409. CRC Press Inc., 1986.

Davison B. (1957) Neutron Transport Theory. Oxford University Press.

Feinberg S.M. (1955) (In Russian).

Фейнберг С.М. - В кн.: Материалы Межд. конф. по мирному использованию атомной энергии. Т. 5, Р.669, Женева, 1955.

Gado J., Devenyi A. Kereszturi A., Makai M. (1983). A Novel Computational Method for Non-Uniform Lattices, (in Russian).

Гадо Я., Девини А., Керестури А., Макаи М. Новый метод расчета неоднородных решеток, Материалы 12-го симпозиума ВМК, Татранска Ломница, т.2, с.151, 1983.

Gado J., Devenyi A., Kereszturi A., and Makai (1984). A new approach for calculating non-uniform lattices. Ann. nucl. Energy 11, p.559.

Galanin A.D. (1957). Theory of the thermal neutron reactors. (In Russian).

Галанин А.Д. Теория ядерных реакторов на тепловых нейтронах. М., Атомиздат, 1957.

Galanin A.D. (1971). Theory of the thermal neutron reactors. (In Russian).

Галанин А.Д. Теория гетерогенного реактора. М., Атомиздат, 1971.

Glasstone S. and Edlund M.C. (1952). The Elements of Nuclear Reactor Theory. D. van/Vostrand Company, Inc. New York.

Gorodkov S.S. (1973). A new method for calculating the heterogeneous reactors (In Russian).

Городков С.С. Новый метод расчета гетерогенных реакторов. Препринт ИАЭ-2251, М., 1973.

Gorodkov S.S. (1973). Quasi-albedo method for two-group calculating heterogeneous reactors (In Russian).

Городков С.С. Двухгрупповой расчет гетерогенного реактора квазиальбедным методом. Препринт ИАЭ-2293 М., 1973.

Gorodkov S.S. (1988). Comparison of mesh algorithms for calculating the neutron fields. In Russian.

Городков С.С. Сравнение сеточных алгоритмов расчета нейтронных полей в больших реакторах. Атомная энергия, т.65, с.184, 1988.

Grigoriev I., Novikov V.M. (1968). Neutron Diffusion in heterogeneous media (In Russian).

Григорьев И.С., Новиков В.М. Диффузия нейтронов в гетерогенных средах. М., Атомиздат, 1968.

Elshin A.V., Laletin N.I. (1976). Neutron Diffusion in the plane lattice. (In Russian).

Ельшин А.В., Лалетин Н.И. Поперечная диффузия нейтронов в плоской решетке. Препринт ИАЭ-2721, М., 1976.

Jolkevich et al (1984) Testing the coarse-mesh algorithms. (In Russian).

Жолкевич Е.А., Белява Е.Д., Киреева И.Л. Тестирование редкосеточных алгоритмов на примерах решения одnogрупповых модельных задач с гомогенными кассетами. Материал ВМК, 1984.

Ionov V., Kireeva I. (1976) The NII-7000 code. (In Russian).

Ионов В.С., Киреева И.Л. Блок гомогенизации кассет на основе программы НИ-7000. Материалы 5-го симпозиума ВМК, том 1. Варна.

Kochurov B.P., Malofeev V.M. (1977) A finite-difference approach for solving equations of the heterogeneous reactor (In Russian).

Кочуров Б.П., Малофеев В.М. Разностный подход к решению уравнений гетерогенного реактора. Атомная энергия, т.42, с.87, 1977.

Kochurov B.P. (1980) Numerical methods in theory of the heterogeneous reactor. In Russian.

Кочуров Б.П. Численные методы в теории гетерогенного реактора. М., Атомиздат, 1980.

- Laletin N.I. (1958) Neutron propagation in heterogenous media. The 2nd Geneva Conference. Report A/CONF/15/P2189. UN. NY.
- Лалетин Н.И. Труды Второй межд. конф. по мирному использованию атомной энергии. Женева, 1958. Докл. советских ученых. Т.2 М., Атомиздат, 1959, с.634.
- Laletin N.I., Elshin A.V. (1976). The finite-difference equations of heterogeneous reactor (In Russian).
- Лалетин Н.И., Ельшин А.В. Конечно-разностные уравнения гетерогенного реактора, Материалы 5-го симпозиума ВМК, Варна, 1976, том 1.
- Laletin N.I. (1976) The principles of elaborating the finite-difference equations of heterogeneous reactor. (In Russian).
- Лалетин Н.И. Принципы построения конечно-разностных уравнений гетерогенного реактора, Материалы 6-го симпозиума ВМК, Бухарест, 1977, с.616.
- Laletin N.I., Elshin A.V. (1977). Increasing the homogenization method accuracy. In Russian.
- Лалетин Н.И., Ельшин А.В. Уточнение метода гомогенизации гетерогенного реактора, Атомная энергия, 43(4), с.247, 1977.
- Laletin N.I. (1978) The principles of elaborating the neutron transport finite-difference equations. (In Russian).
- Лалетин Н.И. Принципы построения конечно-разностных аналогов уравнения переноса нейтронов для некоторого класса задач. В сб. Вариационно-разностные методы в математической физике. Под ред. Г.И.Марчука, Новосибирск. с.93, 1978.
- Laletin N.I., Sultanov N.V. (1979). Advanced pseudo-source method for calculating neutron flux in clusters. (In Russian).
- Лалетин Н.И., Султанов Н.В. Развитие метода поверхностных псевдоисточников для расчета нейтронных полей в ячейках с пучком стержневых твэлов. Атомная энергия. т.46, с.148, 1979.
- Laletin N.I. (1978) The heterogeneous reactor equations. Homogenization Methods in Reactor Physics, Lugano, Switzerland, 13-15 november 1978. IAEA. Vienna. 1980.

Лалетин Н.И. Уравнения гетерогенного реактора (Основные принципы построения). Докл. на совещание специалистов МАГАТЭ, 1978.

Laletin N.I., Elshin A.V. (1980). The Derivation of Finite-difference Equations for Heterogeneous Reactors. I. Kurchatov Institute IAE-3280/5. In Russian.

Лалетин Н.И., Ельшин А.В. Вывод конечно-разностных уравнений гетерогенного реактора, 1 Квадратная решетка блоков, Препринт ИАЭ-3280-5, М., 1980.

Laletin N.I., Elshin A.V. (1981) Derivation of Finite Difference Equation for Heterogeneous Reactor. II. (in Russian)

Лалетин Н.И., Ельшин А.В. Вывод конечно-разностных уравнений гетерогенного реактора II. Квадратная, треугольная и двойная решетки блоков, Препринт ИАЭ-3458-5, М., 1981.

Laletin N.I. (1981a) The heterogeneous reactor equations. (In Russian).

Лалетин Н.И. Об уравнениях гетерогенного реактора. Вопросы атомной науки и техники. Серия: Физика и техника ядерных реакторов, вып. 5(18), с.31, 1981a.

Laletin N.I. (1981b) The physical sense analysis of the advanced homogenization equations. (In Russian).

Лалетин Н.И. Анализ физического смысла величин, входящих в уравнения уточненного метода гомогенизации. Материал ВМК, СССР, 24-30 мая 1981b.

Laletin N.I. (1983) Basic principles for developing equations for heterogeneous reactor - a modification of the Homogenization Method. Nucl. Sci. Engn. 85. 133 (1983).

Laletin N.I., Boyarinov V.F. (1985). The efficient diffusion coefficient. In Russian.

Лалетин Н.И., Бояринов В.Ф. Эффективный однорупповой коэффициент диффузии нейтронов в решетках реакторов. Атомная энергия, т.59, с.91, 1985.

Laletin N.I., Elshin A.V. (1985). Derivation of finite-difference equations of heterogeneous reactor. (In Russian).

Лалетин Н.И., Ельшин А.В. Вывод конечно-разностных уравнений гетерогенного реактора. Трехмерный гетерогенный реактор. Препринт ИАЭ-40905, М.

- Laletin N.I., Elshin A.V. (1986). The Advanced Finite-difference Equations for Heterogeneous Reactors. (In Russian).
- Лалетин Н.И., Ельшин А.В. Система уточненных конечно-разностных уравнений для трехмерного гетерогенного реактора. Атомная энергия, т.60, с.96, 1986.
- Laletin N.I. et al (1987). Some effects and the accuracy improvement in SGM (In Russian).
- Лалетин Н.И., Султанов Н.В., Бояринов В.Ф. Исследование некоторых эффектов и уточнений в МПГ, Материал XVI Симпозиума ВМК. М., 1987.
- Leek V. (1976) The assembly homogenization with using the importance function. (In Russian).
- Лелек В. Гомогенизация кассет с применением сопряженных функций. Материалы 5-го симпозиума ВМК. Том П. Варна, 1976.
- Lehmann M. (1978). Calculation of Lattice Inhomogeneity's Effect on Diffusion Constants of Elementary Cells by Spectral Index Method, (in Russian).
- Леман М. Расчет влияния неоднородности решетки на диффузионные константы элементарных ячеек методом спектральных индексов. 7 симпозиум ВМК, Доброжиовице, 1978, т.2, с.300-322.
- Lizorkin M.P. (1983) Approximation of finite-difference operator by taking into account the azimuthal harmonics. (In Russian).
- Лизоркин М.П. Исследование точности явного учета азимутальных гармоник в аппроксимации дифференциального оператора (одна группа). Материал совещания ТГ2-4 ВМК, Берлин, 1983.
- Lizorkin M.P. (1985) The model problem solutions with using the PERMAC code. (In Russian).
- Лизоркин М.П. Результаты решения модельных задач по программе ПЕРМАК и тестирование алгоритмов с одной точкой на кассету. Материал двухсторонней консультации специалистов СССР и ГДР, Берлин, 1985.
- Leslie D.C. (1962) The weighting of diffusion coefficients in cell calculations. J.Nucl. Energy, 1962, v.16, p.1.
- Lukas H., Wehmann U. (1981) A fast two-and three-dimensional one group coarse-mesh diffusion program in hexagonal geometry. Proc, Int. Topl. Mfg.

on Advances in Mathematical Methods for the Solution of Nuclear Engineering Problems, Vol. 1, p.299, Munchen, 1981.

Maierov L.V., Frank-Kamenetsky A.D., Trukhanov G.Ya. (1970) The Application of Albedo Method for Calculating the Clusters. Kurchatov Institute IAE-4208/5. In Russian.

Майоров Л.В., Труханов Г.Я., Франк-Каменецкий А.Д. Применение альбедного метода к расчету пучка стержней. Препринт ИАЭ-1981, М., 1970. (См. 7 также в кн. "Методы расчета полей тепловых нейтронов в решетках реакторов". Под ред. Я.В.Шевелева. М., Атомиздат, 1974).

Maierov L.V. (1977) The neutron field calculations for complex heterogeneous assemblies. In Russian.

Майоров Л.В. Расчет полей нейтронов в сложных гетерогенных системах, Материалы 6-го симпозиума ВМК, Бухарест, 1977, с.626.

Maierov L.V. (1978) Some problems of WWER type reactor homogenization. In Russian.

Майоров Л.В. Некоторые вопросы теории гомогенизации реакторов ВВЭР, Материалы 7-го симпозиума ВМК, Добжиховице, 1978, т.1, с.141.

Maierov L.V. (1983) Calculation of parameters of the diffusion finite-difference equations. In Russian.

Майоров Л.В. О расчете констант диффузионных конечно-разностных уравнений для гетерогенных реакторов. Вопросы атомной науки и техники. Серия: Физика и техника ядерных реакторов, выпуск 5(34), с.1 (1983).

Maierov L.V., Yudkevich M.S. (1988) Neutron Physical Constants in Thermal Reactors Calculations. Energoatomizdat. Moscow. In Russian.

Майоров Л.В., Юдкевич М.С. Нейтронно-физические константы в расчетах реакторах на тепловых нейтронах. Энергоатомиздат. М., 1988.

Marokazov A.A. (1977). Methodology for Calculating Assembly Powers for WWERs in 2 Group Approximation, (in Russian),

Мараказов А.А. Методика расчета мощностей кассет реакторов ВВЭР в двухгрупповом диффузионном приближении. Препринт ИАЭ-2781, М., 1977.

Novikov A.N. (1982) A Generalized Representation of Differential Operators in One Energy Group Equation, (in Russian)

Новиков А.Н. Обобщенное представление дифференциальных операторов одnogрупповых уравнений, Материалы XI симпозиума ВМК, Варна, 1982.

Novikov A.N. (1982) About improving accuracy of the fine-mesh calculations. (In Russian).

Новиков.А. Повышение точности мелкосеточных расчетов, Материал ТГ-4 ВМК (София, НРБ, 1982).

Novikov A.N. (1982) Increasing accuracy of fine-mesh calculations. (In Russian).

Новиков А.Н. Повышение точности мелкосеточных расчетов. Рабочий материал ТГ-4 ВМК, София, 1982.

Novikov A.N. (1983) 2 Group Coarse-Mesh Problems Considering Cell Heterogeneity, (in Russian)

А.Н.Новиков. Двухгрупповые редкосеточные задачи с учетом гетерогенности ячеек, Материал ТГ 2-4 ВМК (Берлин, ГДР, 1983).

Novikov A.N. (1985) Calculation of Functionals and Solution of Coarse Mesh Equations, (in Russian)

А.Н.Новиков. Подготовка функционалов и решение редкосеточных уравнений, Материал ТГ 2-3-4 ВМК (ЧССР, 1985).

Pfeiffer W., Shapiro J.L. (1969) Reflection and Transmission Functions in Reactor Physics. Nucl. Sci. Eng., v.38, p.253.

Pshenin V.V., Novikov A.N., Surnacheva I.I. (1984). Analysis of Possibilities of Low Error Fine Mesh Calculations. Slab Geometry Case Studies, (in Russian)

Пшенин В.В., Новиков А.Н., Сурначева И.И. Анализ возможностей повышения точности мелкосеточных расчетов на примерах решения модельных задач в плоской геометрии. Материалы XIII симпозиума ВМК, Бухарест, 1984.

Lukas H., Mahajan U. (1981) A fast two-and three-dimensional one group coarse-mesh diffusion program in hexagonal geometry. Proc. Int. Topi. Mtg.

Pshenin V.V., Novikov A.N., Surnacheva I.I. (1985): Analysis of Possibilities of Low Error Fine Mesh Calculations. Slab Geometry Case Studies, (in Russian)

Пшенин В.В., Новиков А.Н., Сурначева И.И. Анализ возможностей повышения точности мелкосеточных расчетов ВВЭР на примерах решения модельных задач в плоской геометрии. Вопросы атомной науки и техники. Серия: Физика и техника ядерных реакторов, вып. 4, с.17, 1988.

Rumyantzev, G. Ya. (1961): The boundary conditions for the P_n -method. (In Russian).

Румянцев Г.Я. Граничные условия в методе сферических гармоник. Атомная энергия, т.10, вып. 1, с.26, 1961.

Rumyantzev, G. Ya. (1961): Neutron Diffusion in Periodical Lattices (In Russian).

Румянцев Г.Я. Расчет диффузии нейтронов в периодических решетках. Атомная энергия, т.13, с.556, 1962.

Rumyantzev, G. Ya. (1963): The boundary conditions for the Boltzmann equation describing neutron flux in periodical lattices. (In Russian).

Румянцев Г.Я. Граничные условия к решению уравнения Больцмана в периодических решетках. Атомная энергия, т.14, с.371, 1963.

Selegnut D.S. (1959).^{*)} Report HW 60220, p.65.

Szatmary Z., Gado J. (1977) Calculation of few-group parameters of non-uniform lattices. (In Russian).

Сатмари З., Гадо Я. Расчет малогрупповых констант топливных решеток, содержащих неоднородности. Материалы 6-го Симпозиума ВМК, Бухарест, 1977, с.154.

Sidorenko V.D. (1969) Many group calculation of criticality and depletion for the fuel uniform lattices. Kernenergia, v.12, p.5/6. (In Russian).

Сидоренко В.Д. Многогрупповой расчет критичности и выгорания однородных топливных решеток.

Shevelev Ya.V. (1957). (In Russian).

Шевелев Я.В. Диффузия нейтронов в плоской уран-водной решетке. Атомная энергия, 1957, т.2, с.234.

Shevelev Ya.V. (1993).^{*)} Private communication. In Russian.

Slesarev I. S., Yaroslavtzeva, L. N.: Calculational Scheme for Energetic Fast Reactors with Hexagonal Fuel Assemblies, (in Russian).

Расчетные схема для исследования энергетических быстрых реакторов с гексагональными тепловыми сборками. Вопросы атомной науки и техники. Серия: Физика и техника ядерных реакторов, вып.4(33), 19(1983).

Smelov V.V. (1959) The approximate method of the heterogeneous reactor homogenization. (In Russian).

Смелов В.В. О приближенном методе гомогенизации гетерогенного реактора. Атомная энергия, 1959, т.6, с.546.

Szatmary Z. (Editor), (1985).

Bardos I, R.Becker, C.Dabrowski, L.Gacsi, J.Gado, E.T.Jozefowicz, Iu.Ia. Kravchenko, K.Krinizc, A.Stanolov, Z.Szatmary, L.Turi, I.Vidovszky.

Final report of TIC, Volume 1, Experimental Investigations of the Physical Properties of WWER-type Uranium-Water Lattices, Akademia Kiado, Budapest.

Sanchez, N.J.McCormick. (1982) A Review of Neutron Transport Approximations. Nucl. Eng. v.80, p.481.

Spinrad B.I. (1955) Anisotropic Diffusion Lengths in Diffusion Theory. J.Appl. Phys., v.26, p.548.

Takeda T. et al. (1979) Effective one-group coarse-mesh method for calculating three-dimensional power distribution in fast reactors. J. of Nuclear Energy, v.6, p.65.

Tichonov A. and Samarsky A. (1956) The mathematical physic equations (In Russian).

Тихонов А.Н., Самарский А.А. Уравнения математической физики. М., Наука, 1966.

Vladimirov V.S. (1961) Mathematical problems of one-velocity transport theory. (In Russian).

Владимиров В.С. Математические задачи однокоростной теории переноса нейтронов. Тр. мат. ин-та им. В.А.Стеклова АН СССР, М.

Weinberg A.M. and Wigner E.P. (1959) The Physical Theory of Neutron Chain Reactor. The University of Chicago Press.

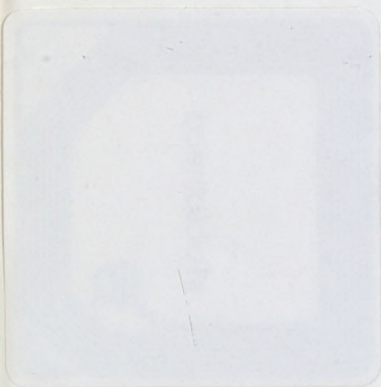
8. CONCLUSION

The present volume surveys the major achievements of TIC in the theoretical-calculational development of uranium-water lattices. The main results can be summarized as follows.

1. Data libraries have been elaborated and validated. The calculations, which are based on these libraries are accurate enough.
 2. Monte Carlo codes have been created utilizing the evaluated nuclear data. Applications of the Monte-Carlo codes have been elaborated in order to verify and validate the design codes.
 3. Advanced design methods have been developed for calculating heterogeneous reactors. These methods have made it possible to increase the accuracy of reaction rate calculation by a factor of 5-10. Advanced methods are used both for fine mesh and coarse mesh calculations. Generally accepted homogenization theories have been revised. The advanced methods may improve the design calculations of various reactor types.
 4. Advanced methods for both cell and assembly parameters have been elaborated.
 5. Design codes have been created to calculate cell parameters and to perform fine mesh calculations. These codes are verified and validated using the ZR-6 experimental results.
 6. Advanced methods and codes are incorporated in the WWER design code packages used for nuclear plant exploitation.
- It should be noted, however, that the rich experimental material provided by the ZR-6 facility has not yet been used fully. It is desirable to perform an exhaustive analysis of the ZR-6 experiments.



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