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# TIBSO- A PROGRAM SYSTEM FOR THE CALCULATION OF THE PRODUCTION, TRANSFER, LIFE CYCLE AND RADIATION OF RADIONUCLIDES IN A COMPOUND NUCLEAR REACTOR SYSTEM

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ABSTRACT

The goal of the program system TIBSO is the calculation of production, transfer, cumulation and filtration of radio isotopes in the cooling system of an atomic power plant. There is no restriction on the complexcity of the cooling system, only the time-independence of technological parameters is assumed.

The theoretical basis of the applied method and the description of the program system TIBSO are given in this report.

АННОТАЦИЯ

Система программ TIBSO используется для расчета возникновения, переноса, накопления и фильтрации радиоактивных изотопов в системе охлаждения АЭС. Система охлаждения может быть неограниченной сложности, только технологические параметры должны быть независимыми от времени.

В данном отчете обсуждается теоретическая основа использованного метода и описывается система программ TIBSO.

KIVONAT

A TIBSO programrendszer atomerőművekben keletkező és a hütőrendszerbe jutó rádióaktiv anyagok terjedésének, felhalmozódásának és szürésének számitására szolgál. A hütőkör és a szürőrendszer bonyolultsági foka nincs korlátozva, csupán a technologiai paraméterekről tesszük fel, hogy időben változatlanok.

A riport tartalmazza a használt módszer elméletét és a programrendszer leirását.

## 1. INTRODUCTION

It is known that there are many ways of producing radionuclides in a compound reactor system and it is also known that they can escape or disappear in many ways. Radionuclides may be borne in the fuel elements as fission products and by diffusing through cladding they may appear in the cooling system. They may arise through the activation of the structural materials and get into the coolant. Radionuclides are filtered in cooling loop by different filters whose purpose is to dimimish the concentration of certain nuclides.

In our institute, this very complicated problem has been solved first by the program TIBS [1] imposed significant restrictions on the complexity of reactor cooling loop. /e.g. only one filter could be treated in a loop/. Though the TIBS was successfully applied in many practical cases, it became clear that a more general treatment of the problem would be necessary.

The goal of the newly developed TIBSO program system is to eliminate any restriction on the complexity of the reactor cooling system. Only the linearity and the time independence of technological parameters are assumed.

In the next section the basic idea of the method to be used is described. In sections 3, 4, the set of linear equations of the method and its solution are outlined.

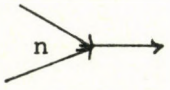
As TIBSO uses many nuclear and technological data, a system of internal library files has been developed. This is discussed in section 5.

In the sections 6-11 the components of the TIBSO program system are described.

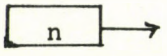
In a subsequent riport the application of TIBSO system to the calculation of corrosion activity will be presented.

## 2. A GENERAL METHOD FOR THE DESCRIPTION OF A COMPOUND NUCLEAR REACTOR SYSTEM

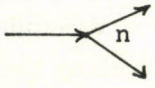
Even the most complicated reactor loop may be described as a composition of a number simple elements with definite properties:



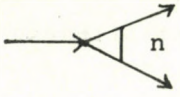

junction - the isotope concentration in the outgoing branch is the sum of both ingoing ones /n=001 ÷ 099/



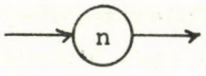

source - it gives certain isotopes to the loop /n=100 ÷ 199/




scalar branching - it divides the isotope stream into two parts with given proportions which are the same for all isotope /n=200 ÷ 299/




vector branching - it divides the isotope stream into two parts with different proportions for each isotope /n=300 ÷ 399/




filter - the concentration of the isotopes in the outgoing stream is proportional to the concentration inside the filter. Isotopes come from the ingoing stream. /n=400 ÷ 499/

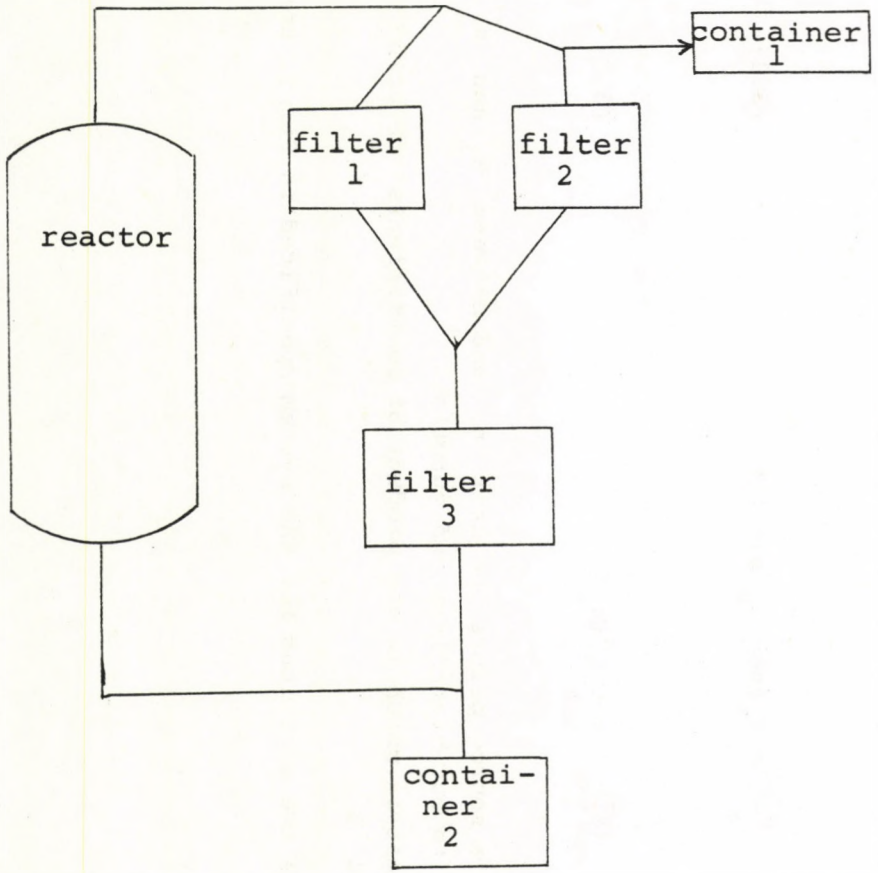

container - no outgiong isotopes. The concentration inside is determined by the ingoing stream /n=500 ÷ 599/

In Fig 1. an example of a real reactor loop and its corresponding description with the above elements is shown.

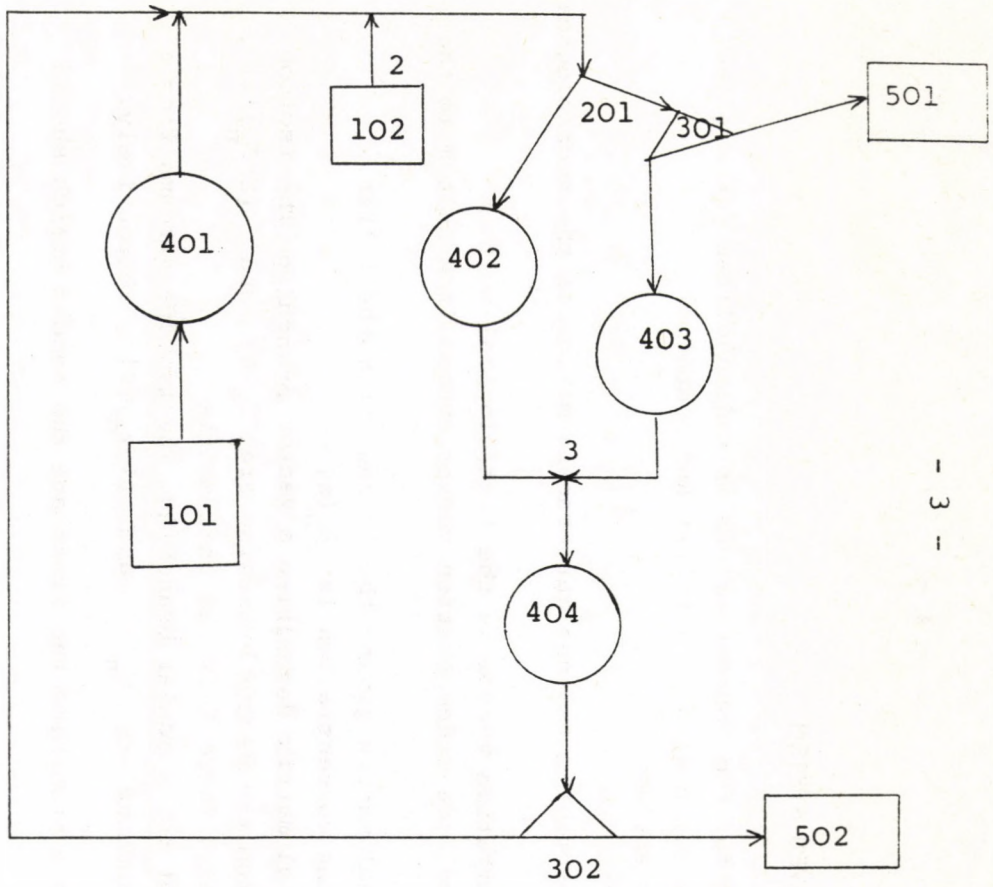
It should be pointed out that for the case of fission products a reactor core is generally represented by a source and a filter. The source gives the isotope production in the fuel elements while the filter describes the process of getting these isotopes into the coolant.

The branching before the third filter means that certain isotopes are instantly removed with a given efficiency from the coolant. Such a technological step can be represented with the elements vector branching and container.

The above listed simple elements are called technological units and the system composed of them is called a derived system.




a/ a reactor system




b/ Derived system

101 - source from fission products

102 - source from coolant activation

Fig.1

## 3. EQUATIONS FOR A DERIVED SYSTEM

We are looking for the concentrations of radionuclides /at a given point in time or in equilibrium/in each filter and container.
The following notations are used.

- $T_n$ - matrix, describing the nuclear transformation in the technological unit n
- $(n)$ - the concentration vector in the technological unit n
- $[\ell_{mn}]$ - $\ell_{mn}=1000m+n$ the concentration vector stream from unit m to the unit n
- $\Omega_n$ - the diagonal matrix giving the leakage from the filter The outgoing concentration is $\Omega_n(n)$
- $\Gamma_n$ - the diagonal matrix describing a vector branching The isotope streams from the vector branching are $\Gamma_n|\ell|$ and $(E-\Gamma_n)|\ell|$, respectively, where E is the unit matrix
- $\gamma_n$ - coefficient for a scalar branching. The isotope streams from a scalar branching are $\gamma_n|\ell|$ and $(1-\gamma_n)|\ell|$, respectively.

In the case of a branching the first and the second branch should be specified.

The basic equation for a technological unit is

$$\frac{d(n)}{dt} = T_n(n) - \Omega_n(n) + |\ell_{kn}| \qquad /3.1/$$

where

$$[\ell]_{kn} = \sum_i Q_i^k(k_i) \qquad /3.2/$$

$k_i$ - a filter or a source before the unit n, and between $k_i$ and n there are no other units but branchings and junctions,

$Q_i^k$ - a diagonal matrix which is the product of coefficients of branching between $k_i$ and n .

As an example the equations for the system specificed in Fig 1. are the following

$$\frac{d(401)}{dt} = T_{401}(401) - \Omega_{401}(401) + (101401)$$

$$\frac{d(402)}{dt} = T_{402}(402) - \Omega_{402}(402) + \gamma_{201}\left(\Omega_{401}(401) + \Gamma_{302}\Omega_{404}(404)\right)$$

$$\frac{d(403)}{dt} = T_{403}(403) - \Omega_{403}(403) + (1-\gamma_{201}) \cdot \Gamma_{301}\left(\Omega_{401}(401) + \Gamma_{302}\Omega_{404}(404)\right) \qquad /3.3/$$

$$\frac{d(404)}{dt} = T_{404}(404) - \Omega_{404}(404) + \Omega_{402}(402) + \Omega_{403}(403)$$

$$\frac{d(501)}{dt} = T_{501}(501) + (E-\Gamma_{301})(1-\gamma_{201}) \cdot \left(\Omega_{401}(401) + \Gamma_{302}\Omega_{404}(404)\right)$$

$$\frac{d(502)}{dt} = T_{502}(502) + (E-\Gamma_{302})\Omega_{404}(404)$$

## 4. SOLUTION OF THE SYSTEM OF EQUATIONS /3.1/

The system of equations /3.1/ will be solved in the following cases:

a/ Solutions with zero initial distributions:
   stationary solution /o/
   transient solution at stepwise neutron flux rise /1/

b/ Solutions with given non-zero initial distribution:
   stationary solution /3/
   transient solution for a stepwise neutron flux rise or fall /4/

The numbers in parenthesis are the key-numbers for the type of solution.

Many methods for the solution of the system of Eqs./3.1/ are known [1]. Each of them has advantages and disadvantages In our program the simplest methods are chosen.

In a stationary case, when the left hand sides of Eqs./3.1/ are equal with zero, iteration method is applied. By studying the example given in /3.3/ we can state that the success of iteration depends on the intensity of feedback, which in the given case is represented by the term containing $\Gamma_{302}\Omega_{404}(404)$

In order to solve Eqs./3.1/ in the time-dependent case, let us write them in the form.

$$\frac{dn_j^i}{dt} = -D_j^i n_j^i + \sum_{k=1}^{j-1} P_j^i n_k^j + \sum_{l=1}^{m} Q_j^{li} n_j^l + R\delta_{lj}\cdot\delta_{li} \qquad /3.1/$$

where

$$D_j^i = \chi_j^i + \omega_j^i$$

$n_j^i(t)$ - the concentration of isotope j in the unit i

$\chi_j^i$ - coefficient of dissappering through decay or/and absortion

$\omega_j$ - coefficient of disappearing through leakage

$Q_j^{li}$ - $\omega_j^l \Gamma_j^{li}$

$\Gamma_j^{li}$ - branching coefficient between the unit l and i for the isotope j

R - source strength /time independent/

The solution of /3.1'/ approximately Γ

$$n_j^i(\tau) = n_j^i(o)e^{-D_j^i\tau} + S_j^i / D_j^i (1-e^{-D_j^i\tau})$$

where

$$S_j^i = \sum_{k=1}^{j-1} P_{kj}^i \bar{n}_k^j + \sum_{l=1}^{m} Q_j^{li} \bar{n}_j^l + R\delta_{lj}\cdot\delta_{li}$$

$\bar{n}$ - means a medium concentration defined by

$$S/D + \frac{1}{D\tau}(n(o) - n(\tau)) \qquad \text{if} \quad n(o) \geq n(\tau)$$

$$\frac{n(o)+n(\tau)}{2} \qquad \text{if} \quad n(o) < n(\tau)$$

## 5. INTERNAL LIBRARY FILES OF THE TIBSO PROGRAM SYSTEM

As TIBSO is intended for use on computers of medium capacity, a system of internal library files has been developed. In the construction of internal library files the one-field representation of data set applied in the FEDGROUP system [2] is used. This means that the elements of a data set are written continuously in a field which are output to a backing store with adequate blocking. When writing a program one need not take this blocking into account because special subroutines provide for the required quantities. If an internal library files is small enough it is possible to avoid the use of backing store for this file without any change in the program. Some of the internal files contain labelled data sets, i.e. the first word of each data set contains a literal of four characters. This literal facilitates the retrieval of the data set. In the case of unlabelled files the simple structure facilitates the retrieval.

Besides the label there are some integers /up to four/ at the beginning of each data set, serving for identification.

In the Table 5.1 the labelled data set introduced up till the present are described.

There are three internal files with labelled sets. The first is called Nuclear File and contains sets with the labels DEFI, EVAF, SOFI. The second is the Technological File, contains sets labelled TEFI. The third is called the System Inventory File, and contains sets with the labels SYST, FLUX, ISDI, GENE.

There are two unlabelled files used as a backing store during the calculation. They are called first and second auxiliary file, respectively.

Any of the internal files may be a permanent or a temporary one in sequential or in direct access form. /Of course, the direct acces is preferable/.

Table 5.1 LABELLED DATA SETS ON INTERNAL LIBRARY FILES

| Label | Integers for ident | length of id. | Data | length of data |
|---|---|---|---|---|
| DEFI | NEVI | 1 | $\lambda,(\sigma_j, j=1,NG),M_\sigma,\ (NK_i,(\sigma_j^i\ j=1,NG),i=1,M_\sigma),$ $M_D,\ (NK_i,\lambda_i,\ i=1,M_D)$ | $3+(M_\sigma+1)*NG+2*M_D+M_\sigma$ |
| EVAF | NEVI | 1 | $M_e,(\lambda_i,K_i,M_i,(E_{ij},I_{ij},j=1,M_i),\ i=1,M_e),\bar{E}_\beta,\bar{E}_\gamma,\bar{E}_\alpha$ | $1+3*M_e+2*\sum_{i=1}^{M_e} M_i$ |
| SOFI | NEVI,NEVE,KS | 3 | $\lambda_a,(\sigma_j,j=1,NG),(y_j,j=1,NG)$ | $1+2*NG$ |
| TEFI | NEVE,KT,(NEVE,KS) KT=2 | 2 or 4 | $M_F,(NEVI_i,\omega_i,i=1,MF)$ or $\rho$ | $1+2*M_F$ or 1 |
| SYST | KDAT | 1 | $N_b,\ ([\ell_i],i=1,N_b)$ | $N_b+1$ |
| FLUX | KDAT,NTASK,KTP | 3 | $M_n,(NEVT_i,(\varphi_j^i\ j=1,NG),i=1,M_n)$ | $1+M_n*(NG+1)$ |
| ISDI | KDAT,NTASK,KTP,NT | 4 | $N_F,N_I,(NEVT_i,i=1,N_F),(NEVI,i=1,N_I),((\rho_{ij},i=1,N_I),$ $j=1,N_F)$ | $2+N_I+N_F+N_I*N_F$ |
| GENE | KDAT,NTASK,KTP | 3 | $NTAU,(T_i,i=1,NTAU)$ | $1+NTAU$ |

Explanation to the Table 5.1

NEVI - name of the isotope; it is composed of
10000×IZ+10×IA+IS where
IZ - atomic number
IA - atomic mass
IS - 0,1,2,.. corresponding to the ground state, first, second etc. excited state

NK - name of daughter isotope

$\lambda$ - total decay constant

$\lambda_i$ - partial decay constant

$\sigma_j$ - total non-elastic cross-section /group averaged/

$\sigma_j^i$ - cross-section for a partial reaction /group averaged/

NG - number of groups for the above cross-section

$M_\sigma, M_D$ - number of partial neutron reactions and decay modes, respectively

$K_i$ - decay mode: 1 - gamma decay, $\pm 2$ - beta $\pm$ decay, 3 - alfa decay, 4 - internal conversion

$M_i$ - number of energy group for the particle arising from the decay of NEVI

$M_e$ - number of decay modes

$E_{ij}, I_{ij}$ - energy and intensity of the decay, respectively

NEVE - name of the mother nucleus

KS - source type: 1 - independent yield, 2 - neutron activated isotope, 3-source, independent on flux

$\lambda_a$ - rate of emission for the source isotope

$y_j$ - independent yield for group j

NEVT - name of the technological unit

KT - 1 for filter or for branching
2 for a source

$M_F$ - number of isotopes to be filtered or branched
$M_F$=0 for scalar branching; in this case $NEVI_i$ are omitted

$\omega_i$ - elements of a diagonal matrix for a filter or for a branching

$\rho$ - density of the isotope NEVE

KDAT - system identification number

$N_b$ - number of connection in the system

$|\ell_i|$ - connections

NTASK - task identification number

KTP - key number for the type of solution

$M_n$ - number of technological units for which flux is specified

$\varphi_j^i$ - flux in the technological unit $NEVT_i$ for group j

$NT_i$ - number of point in time

NTAU - number of time points

$T_i$ - the time points

## 6. THE STRUCTURE OF THE TIBSO SYSTEM

The scheme of the TIBSO program system is shown in Fig.6.1.

The abbreviations are explained as follows.

LIB Library preparatory program for compiling the Nuclear File and the Technological File from
- any nuclear decay and group constant libraries at disposal
- any data given on punched cards

In general, there are as many LIB programs as there are data sources, since each source has its specific format. It is not a very hard task to write a LIB program for a given data file

ILUP — Internal Library Utility Programs serve for
- outprint of a library with commentary text in order to facitate the data checking
- transforming the internal libraries into card-image format /see App.1/ and vice versa
- selection of data sets from a library
- merging of libraries

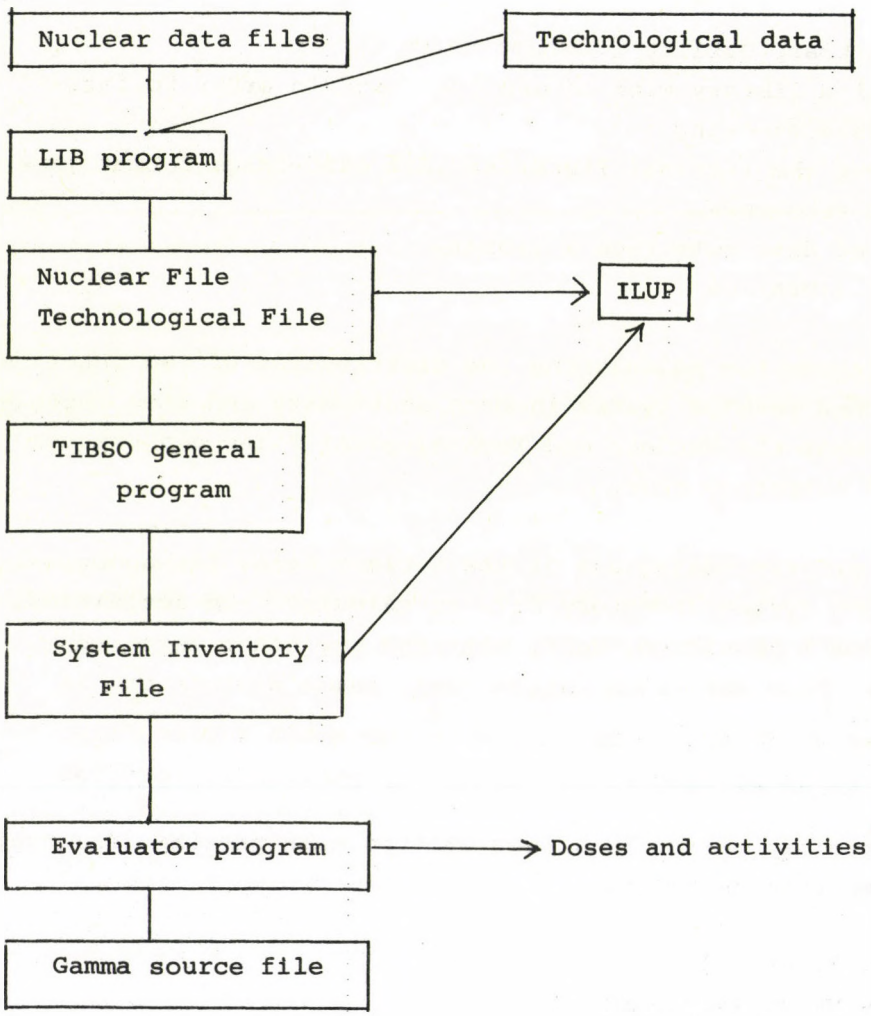
TIBSO — General program for calculating the distribution of radionuclides in a compound reactor system in both stationary and time dependent cases. It uses the Nuclear and Technological Files and creates the System Inventory File.

EVALU — These are program making use of the Nuclear File, Technological File and the System Inventory File to calculate the activities, doses, gamma intensities, decay heat and any other required quantities. From the gamma intensities, gamma sources can be constructed which are to be stored in the gamma source file. This file is to be used by the gamma ray penetration program

The TIBSO system may be run by a user written main program. The typical form of a main segment is as follows.

```
DIMENSION W(<n>),IW(<n>)
COMMON/TFIL/NB,MF,NE,NAUX,NSEG
COMMON/NPAR/NG,NN(3)
COMMON/FIL1/NPER(5)/FIL2/NBL(5), LCE(5)
EQUIVALENCE(W(1),IW 1))
DATA LFR/<n>/>
<assigment of values to the variables in COMMONs>
<opening the Internal Library Files>
<CALL leading segments of the library preparatory or/and selecting
 program>
CALL TIBSO(W,IW,LFR)
<closing the Internal Libraries>
<reopening the Internal Libraries>
<CALL leading segments of the evaluator programs>
STOP
END
```

Fig.6.1 TIBSO scheme




Explanation

<n> - length of the file of dynamical programing

NG - number of neutron groups

|NPER(k)| - where k=NB,NF,NE,NAUX,NSEG are the logical number of Nuclear, Technological, System Invertory and the two auxiliary files, respectively.

Convention:

NPER(K) { > 0, direct access file
< 0, sequential access file
>100, no backing store used (for small internal files)

NBL (k) - is the associated variable /in the case of direct access mode/ or the block position indicator /in the case of sequential access/ of the corresponding file

LCE (k) - is the buffer length for the corresponding file

The leading segment is the main segment for a part of the system. The leading segment of a library preparatory programme has the form

SUBROUTINE LIBxxx (W,IW,LFR,BF)

where

xx - up to three alphanumeric characters assigned to the actual data file to be processed to in an Internal Library File

W,IW - field for dynamical programming

BF - buffer field for the Internal Library File/s/ to be compiled

The leading segment of the general program
SUBROUTINE TIBSO (W,IW,LFR)
The leading segment for the Internal Library Utility Program
SUBROUTINE ILUP (W,IW,LFR,BF)
The leading segment of the evaluator program is
SUBROUTINE EVALU (W,IW,LFR,BF)

BF - buffer field for the Internal Library File/s/ to be used

## 7. THE NTDP SET, AND THE FIRST AND SECOND AUXILIARY FILES

For each source radionuclid /NRI/ in the TIBSO general program a set of constants, called Nuclear-Technological Decay and Production set /NTDP set/ is constructed. This set consists of the following subsets for each filter and container.

NEVT - name of the Technological unit /filter or container/

NEL - number of transitions in the decay chain initiated by NRI; an isotope occurs as many times as there are ways of producing it

$(NEV_i, NEVE_i, D_i, P_i, i=1,NEL)$

$NEV_i$ - name of the isotope i in the chain

$NEVE_i$ - its mother's name /0 for NRI/

$D_i$ - total rate of disappearing /including the technological leakage from the filter/

$P_i$ - rate of production from $NEVE_i$

R - rate of isotope NRI coming directly from source /=0, if there are filter/s/ in all branches leading from the source/

NET - number of filter/s/ connected directly with the unit in the backward direction /directly - means that there are no units other than branching and junctions between them/

$(NEVT_i, (\omega^i_j, j=1,NIZ), i=1,NET)$

$NEVT_i$ - name of the technological unit /filter/ emmitting the isotopes

NIZ - number of all possible isotopes which may come from NRI

$\omega^i_j$ - filtering coefficient in the filter i for the isotope j

Names of all possible isotopes are gathered in a separate set. j refers to the corresponding words of this set.

It is evident that the NTDP set is closely related to the coefficients of Eqs./3.1/.

To any NRI of each source unit an NTDP set and the list of daughter nuclides belong. When these quantities for all sources and NRI's are given then the specified derived reactor system is completely described. As they result in a relatively cumbersome calculation they can be stored on the second auxiliary file /NSEG/ together with the list of filters and containers.

The use of this second auxiliary file is inevitable in time dependent calculation, otherwise the whole system calculation needs to be repeated for each time point.

The system of Eqs./3.1/ is solved for each NRI of each source unit. The corresponding NTDP set provides the coefficients and the source term. The solution is stored on the first auxiliary file /NAUX/. After the cycles by NRI's and by sources have been performed the distributions of each isotope are summed up. The first auxiliary file, by contrast to the second one is always required.

It is possible to sum up the isotope distribution by means of the SYSTEM INVENTORY FILE, too, in which case one task can be performed in a number of successive runs; this is desirable if an individual run is too long.

## 8. THE TIBSO GENERAL PROGRAM

The input of the TIBSO general programme is given in Table 8.1
The related output file is the SYSTEM INVENTORY FILE which contains the following data sets.

| label | Multiplicity of the output |
|---|---|
| SYST | for each technological scheme |
| FLUX | for each task of each technological scheme |
| GENE | for each non-stationary task of each technological scheme |
| ISDI | for each time point of each task of each technological scheme |

Table 8.1 Input for the TIBSO general program

| Card. | FORMAT | I/O list | Description |
|---|---|---|---|
| 1 | 2I4 | KDAT,NBRCH | KDAT - system identifier /KDAT=0 RETURN// NBRCH - number of connections |
| 2 | 9I8 | $L_i$,i=1,NBRCH | $L_i$ - name of connection /see 2./ |
| 3 | 4I4 | NTASK,KTP, NTAU,IFLAG | NTASK - task number* KTP - key number for the type of solution NTAU - number of time points IFLAG - { <0 no calculation of NTDP sets is required. NT=IFLAG,otherwise |
| 4** | 6E12.5 | $T_i$,i=1,NTAU | time points |
| 5*** | 3I4 | NTASKE,KTPE, NTE | They are NTASK, KTP and time point for the initial isotope distribution |
| 6 | I4 | MFN | number of technological units for which flux is given />0/ |
| 7 | I4 | NEVT | name of the technological unit |
| 8 | 6E12.5 | $FLUX_i$,i=1,NG | flux in NEVT. NG=number of group, to be specified in the COMMON/NPAR/ |

*Besides the identification of a run the NTASK has a key-number function, too, as shown in the following.

**Card 4 required only if KTP≠0, or KTP≠3

***Card 5 required only if KTP>2

| NTASK | function |
|---|---|
| <0 | RETURN |
| 0 | new technological scheme will be specified |
| 1÷999 | convergence required for the total isotope distribution |
| 1000÷1999 | convergence required for the total isotope distribution in each technological unit |
| 2000÷2999 | convergence required for total concentration of each isotope in the whole system |
| 3000÷3999 | convergence required for the concentration of each isotope in each technological unit |

Of course, the last four functions have a meaning only in stationary cases.

## 9. SEGMENTS FOR INTERNAL LIBRARY COMPILATION

Nuclear data /decay and cross-section data/ are available on magnetic tapes. These files have specially fitted segments to convert the data into internal library sets.

### The ORIGEN library [3]

The library belonging to the ORIGEN program contains decay data and three group constants for isotopes of structural materials, for fission products and for actinides. There are yield data for fission products, too. Data sets labelled DEFI and SOFI are prepared by the following leading segments:

LIBORI - for structural materials

LIBDRF - for fission products

LIBACT - for actinides

The data are processed sequentially. Selective processing can be achieved by introducing the appropriate selection rules into the segment in an ad hoc way.

The DLC-19 library [4]

This library contains decay and gamma production data for isotopes. Data sets with the label EVAF are prepared by LIBDLC.

The ENDF/B-IV fission product library

This library contains decay data and point-wise cross-sections for 825 fission product nuclei. It cannot be used directly for the construction of DEFI sets because few-group cross-sections must be calculated first from the point-wise data. This is a task for the FEDGROUP program system [2].

Data sets with the label EVAF are prepared by LIBEF.

No data sets labelled SOFI can be prepared because of the lack of yield data in the ENDF/B-IV file.

The DEFI sets are prepared by LIBED. The few-group constants calculated by FEDGROUP are input from a separate file.

Very often it is necessary to introduce data in the TIBSO system through punched card input. In this case the possibility of simple and error-free punching is the main requirement. The segment LIBRSR compiles any of the labelled internal library sets from data given on punched card. The card input of LIBRSR is organized on the basis of NAMELIST statement offered by the FORTRAN specification of IBM/360.

| NAMELIST name | list |
|---|---|
| IDPAR | IDE(4),IS,M1,M2,RTOT |
| SIGMA | NK(20),SG(30) |

Input for each internal library set begins with IDPAR. The numbers for IDE should be the quantity in the second column of Table 5.1. $1 \leq IS \leq 8$, corresponding to the data sets DEFI,EVAF,SOFI,TEFI,SYST, FLUX,ISDI, GENE, respectively. The input obviously depends on the actual data set and is fully described in Table 9.1.

RETURN from LIBRSR occurs when IS=0.

Table 9.1 Input for LIBRSR

| TYPE | NAMELIST | INPUT | Multiplicity |
|---|---|---|---|
| DEFI | IDPAR | IS=1,IDE(1)=NEVI,M1=$M_\sigma$,M2=$M_D$,RTOT=$\lambda$ | 1 |
| | SIGMA | SG=($\sigma_j$,j=1,NG) | (NG-1)/30+1 |
| | SIGMA | NK=($NK_i$,i=1,M1),SG=(($SG^i_j$,j=1,NG),i=M1) | MAXO((M1-1)/20, (NG*M1-1)/30)+1 |
| | SIGMA | NK=($NK_i$,i=1,M2),SG=($\lambda_i$,i=1,M2) | (M2-1)/20+1 |
| EVAF | IDPAR | M1=$M_D$,IS=2,IDE(1)=NEVI, RTOT=$\lambda_i$,M1=$K_i$,M2=$M_i$ | |
| | SIGMA | SG=($E_{ij}$,$I_{ij}$,j=1,M2) | (2*M2-1)/30+1 } $M_D$ |
| SOFI | IDPAR | IS=3,RTOT=$\lambda_a$,IDE=NEVI,NEVE,KS | |
| | SIGMA | SG=($\sigma_j$,j=1,NG),($y_j$,j=1,NG) | (2*NG-1)/30+1 |
| TEFI | IDPAR | M1=$M_F$,RTOT=$\rho$,IS=4,IDE=NEVI,KT,NEVE,KS | |
| | SIGMA | NK=($NEVI_i$,i=1,M1),SG=($\omega_i$,i=1,M1) | ($M_F$-1)/20+1 |
| SYST | IDPAR | M1=$N_b$,IDE(1)=KDAT,IS=5 | |
| | SIGMA | NK=($\ell_i$,i=1,$N_b$) | ($N_b$-1)/20+1 |
| FLUX | IDPAR | M1=$M_n$,IS=6,IDE=KDAT,NTASK,KTP | |
| | SIGMA | NK=($NEVT_i$,i=1,M1), SG=(($\varphi_j$,j=1,NG),i=1,M1) | MAXO((M1-1)/20, (M1*NG-1)/30)+1 |
| ISDI | IDPAR | M1=$N_F$,M2=$N_I$,IS=7,IDE=KDAT,NTASK,KTP,NT | |
| | SIGMA | NK=($NEVT_i$,i=1,$N_F$),($NEVI_i$,i=1,$N_I$) | MAXO(($N_F$+$N_I$-1)/20, |
| | | SG=($\varphi_{ij}$,i=1,$N_I$),j=1,$N_F$) | ($N_F$*$N_I$-1)/30)+1 |
| GENE | IDPAR | M1=NTAU,IS=8,IDE=KDAT,NTASK,KTP | |
| | SIGMA | SG=($T_i$,i=i,NTAU) | (NTAU-1)/30+1 |

## 10. DETERMINATION OF PHYSICAL QUANTITIES FROM ISOTOPE DISTRIBUTION

The total activity in the technological unit i is calculated by the formula

$$A_i = \sum_{j=1}^{N_I} \lambda_j \rho_{ij} / 3.7 \times 10^{10} \quad \text{curie}$$

Evaluation of the total activity requires the corresponding DEFI sets. The gamma-sources are calculated from the following formula

$$I^i_{\gamma m} = \sum_{j=1}^{N_I} \rho_{ij} \lambda_{\gamma_j} \sum_{k=1}^{MM^\gamma_j} I^j_{\gamma k} / 100$$

$$E^i_{\lambda m} = \sum_{j=1}^{N_I} \rho_{ij} \lambda_{\gamma j} \sum_{k=1}^{MM^\gamma_j} E^j_{\gamma k} \times I^j_{\gamma k} / 100$$

It is assumed that

$$G_m > E^j_k > G_{m+1}$$

Where $G_m$ are the boundaries of the gamma-group system, specified by the punched card input of the evaluator program.

The Bremsstrahlung arising form a beta± decay electron/positron or from an electron of an internal conversion is calculated by means of the formula and data given in ref. 6. In the case of a beta-electron the total intensity is

$$I^j_\beta = 1.23 \times 10^{-4} \times (\bar{Z}+3) \times \sum_{k=1}^{MM^\beta_j} I^i_{\beta k} \times E^2_{\beta k j} / 100 \quad \text{MeV/decay}$$

In the case of internal conversion

$$I^j_c = 5.77 \times 10^{-4} \times \bar{Z} \times \sum_{k=1}^{MM^j_e} I^j_{ck} \times E^2_{ckj} / 100 \quad \text{MeV/decay}$$

where

$$Z = \frac{\sum_{i=1}^{n} \alpha_i Z_i^2}{\sum_{i=1}^{n} \alpha_i Z_i}$$

$Z_i$ - represents the atomic number of materials in the unit

$\alpha_i$ - represents their nuclear densities

In the case of positron a term

$$\sum_{k=1}^{MM} I_{\beta k}/100$$

should be added in order to take the annihilation into account.

The spectral distribution of Bremsstrahlung is calculated by means of Table 2.5 of ref. |6|.

The released decay heat is calculated by

$$Q \text{ watt} = c \times \sum_{j=1}^{N_I} \rho_{ij} \left(\lambda_\beta E_\beta^j + \lambda_\gamma^j E_\gamma^j + \lambda_\alpha^j E_\alpha^j\right)$$

where $c = 1.6 \times 10^{-19} \frac{\text{watt.sec}}{\text{eV}}$

The input of EVALU is controlled by the following NAMELIST list.

| NAMELIST name | list |
|---|---|
| SYSEV | IK=evaluation control number /see Table 9.1 |
| | KDAT = } identifies the ISDI set/s/ to be evaluated |
| | NTASK= } identifies the ISDI set/s/ to be evaluated |
| | KTP = } identifies the ISDI set/s/ to be evaluated |
| GAMGR* | MSYS=identifier of the gamma energy group system |
| | MG=number of energy groups |
| | SG(1÷10)= gamma-energy group boundaries |

*Required only when IK=-2 or -20. In the cases of IK=2 or IK=20 the gamma-group system of the previous evaluation is used.

In the time dependent case all time-points will be evaluated in one step. The evaluation is continued by the input of SYSEV unless KDAT=0. The latter will cause a RETURN to the main program.

Table 10.1 Values of the evaluation control number

| \|IK\| | type of eveluation |
|---|---|
| 0 | isotope inventory only |
| 1 | total activity only |
| 2 | gamma source only |
| 3 | decay heat only |
| 10 | inventory + total activity |
| 20 | inventory + gamma-source |
| 30 | inventory + decay heat |

## 11. THE INTERNAL LIBRARY UTILITY PROGRAMS

### Display and conversion of an internal library

The leading segment is

SUBROUTINE ILUP(W,IW,LFR,BF)

It facilitates

- the display of a labelled data set
- the conversion of a labelled data set from binary format into card image format and vice-versa

Its input controlled by

| NAMELIST name | list |
|---|---|
| UTIL | IS=type of data set /1÷8/<br>IDE(1÷4)=identifiers of the data set<br>IOP= service control number<br>NSET= number of subsequent sets to be serviced<br>LS= the number of words from which the scanning of the file begins |

The input is continued with UTIL unless IOP=0.

The service control number:

| IOP | control |
|---|---|
| 1 | display NSET number of data sets identified with IS and IDE |
| 2 | convert NSET number of data sets identified with IS and IDE into card image format |
| 3 | convert NSET number of data sets identified with IS and IDE from card-image format into binary format |
| 4 | 1 and 2 together |
| 5 | 1 and 3 together |

The card-image format of the internal libraries sets is described in Appendix 1.

Select the NUCLEAR FILE

The purpose of this utility is to reduce the dimensions of NUCLEAR FILE to be used in TIBSO calculation. The name of the leading segment is

SUBROUTINE SELECT(W,IW,LFR,BF1,BF2)

It facilitates the selection of

- DEFI sets of nuclei belonging to one decay scheme
- EVAF and SOFI sets for specified nuclei

The selected data sets will be stored on a new NUCLEAR FILE.

The input of SELECT is controlled by

| NAMELIST name | list |
|---|---|
| PERIF | N1= peripheral number of the library underlying the selection |
| | N2= peripheral number of the selected library |
| SELCT | IS= type of data set /1÷3/ |
| | IDE= identification numbers |
| | IOP= service control number |
| | F= maximum flux factor* |
| | EPS= criterion number* |

*In the decay schemes only these nuclear transformations are to be accounted for where

$$F \cdot \sum_{j=1}^{NG} \sigma_j > EPS \qquad \text{or} \qquad \lambda_j > EPS$$

SELECT input /cont./

| | |
|---|---|
| IANY | MEXS=maximum length of a data set on the NUCLEAR FILE<br>LEXS=maximum /estimated/ number of daughter nuclei<br>NE=number of daughter nuclei which need not be retrieved<br>LE(1÷10)=name of the daughter nuclei which need not be retrieved |

Input is continued with SELCT till IOP=0

The service control number

| IOP | control |
|---|---|
| 1 | select the nuclei belonging to the decay chain originated by nucleus identified by IDE |
| 2 | previous selection + SOFI set for these nuclei |
| 3 | selection at IOP=1 + EVAF set for these nuclei |
| 4 | after selection at IOP=1, input is continued with PERIF |
| 5 | select a given seriey of daughter nuclei |
| 6 | select the data set for a given nucleus /no LANY needed/ |

## Sum up the nuclear density of the calculated radionuclides using the SYSTEM INVENTORY FILE

It may occur that the distribution of isotopes cannot be calculated for all NRI and source in one run. In this case the total numbers of isotopes in a unit can be obtained by summing up the distributions on the SYSTEM INVENTORY FILE. This job is performed by

SUBROUTINE SUMUP(W,IW,L,BF)

The input is controlled by

| NAMELIST name | list |
|---|---|
| ISET | ID1= the four identifier numbers of the ISDI sets to be summed up<br>ID2= the four identifier numbers of the output set<br>LS= the place on the SYSTEM INVENTORY FILE from which the ISDI sets to be retrieved begin /if LS≤0 then RETURN/ |

REFERENCES

[1] Z. Szatmari, to be published

[2] P. Vértes, FEDGROUP - a program system for producing group constats from evaluated nuclear data of files disseminated by IAEA,INDC/HUN/-13/L+Sp 1976

[3] ORIGEN - isotope generation and depletion code, ORNL code package

[4] RSIC Data Library collection, ORNL-TM-4095

APPENDIX 1.

The card-image format of the labelled Internal Library sets

| Card type | content 1 ÷ 72 | 73 ÷ 76 | 77 ÷ 80 |
|---|---|---|---|
| Head | empty | label | 0000 |
| Integer | integers in 9I8 format | label | number |
| Real | real numbers in 6E12.5 format | label | number |

A data set contains:

1 Head card

Integer cards: integers are placed contiguously in the same order as they are defined in Table 5.1

Real cards: the real numbers are placed contiguosly as they are defined in Table 5.1

APPENDIX 2.

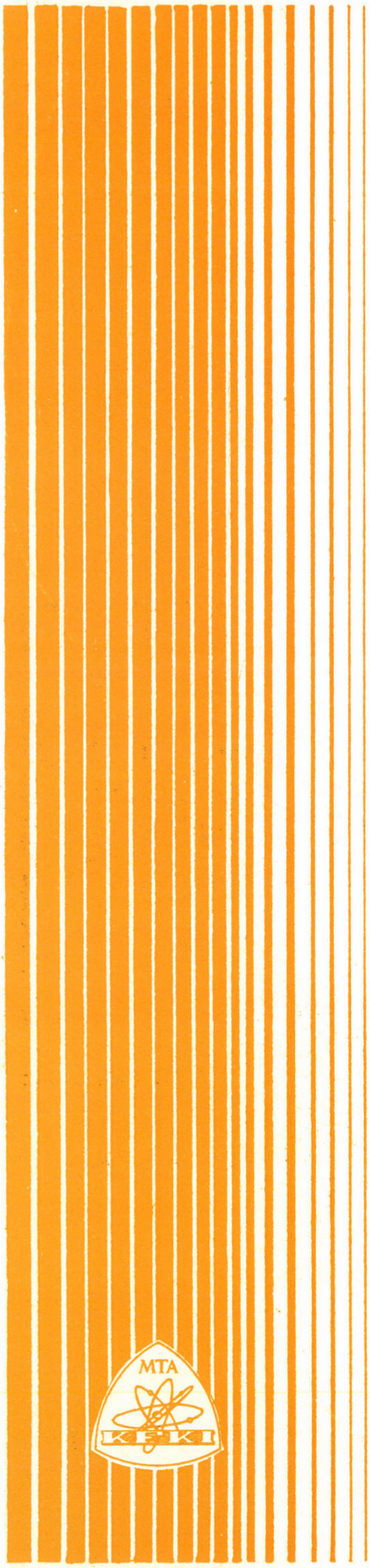
Output by request

Some outputs may be requested and omitted at will. This is controlled by the output control numbers given in

COMMON/COUT/NXOU,NYOU,NZOU,NWOU

Their effect is given in the Table below

| NAME | VALUE | segments /leading and related/ | Control effect |
|---|---|---|---|
| NXOU | ≠ 1 | LIBRSR/ADIN/ | print details of the compiled library sets |
| NYOU | = 1 | ILUP/REACAR/ | print the library sets given in card-image format |
| NZOU | ≤ 0 | TIBSO/SUMIZ,KONTIM/ | print the isotope distribution |
| | = 1 | | print the isotope distribution and supress the output to the SYSTEM INVENTORY FILE |
| NWOU | = 1 | TIBSO/KONTUR/ | print the NTDP set |

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Budapest, 1977. október hó