AKTIV

A computer program for evaluating the activity, afterheat, and biological hazard potential of stainless steel structures in fusion reactor blankets

H.-J. Odenthal, W. Dänner, H. Gorenflo

IPP 4/154

May 1977



MAX-PLANCK-INSTITUT FÜR PLASMAPHYSIK

8046 GARCHING BEI MÜNCHEN

MAX-PLANCK-INSTITUT FÜR PLASMAPHYSIK GARCHING BEI MÜNCHEN

AKTIV

A computer program for evaluating the activity, afterheat, and biological hazard potential of stainless steel structures in fusion reactor blankets

H.-J. Odenthal, W. Dänner, H. Gorenflo

IPP 4/154

May 1977

This work was performed by INTERATOM GmbH under the terms of a special contract between MPI für Plasmaphysik, Garching, and INTERATOM, Bergisch-Gladbach.

Please address enquiries about this program to:

Dr. H.-J. Odenthal INTERATOM GmbH - 0213 Fusion -Postfach

5060 Bergisch-Gladbach 1

West-Germany

Die nachstehende Arbeit wurde im Rahmen des Vertrages zwischen dem Max-Planck-Institut für Plasmaphysik und der Europäischen Atomgemeinschaft über die Zusammenarbeit auf dem Gebiete der Plasmaphysik durchgeführt.

IPP 4/154

AKTIV

A computer program for evaluating the activity, afterheat, and biological hazard potential of stainless steel structures in fusion reactor blankets

H.-J. Odenthal W. Dänner H. Gorenflo

May 1977

Abstract

The computer program AKTIV was elaborated to calculate the activity, afterheat, and biological hazard potential of arbitrary materials in a fusion reactor blanket environment. This report describes the mathematical background of the program, the program structure, and the input requirements. A special section is devoted to a detailed description of the procedure for adapting the program to a certain material, in this first example stainless steel.

Additionally, two auxiliary programs called AKTOUT and AKTIN are described which were both elaborated to use the program AKTIV economically with respect to computer time.

CONTENTS

- 1. Introduction
- 2. The program AKTIV
 - 2.1 General remarks
 - 2.2 Mathematical background
 - 2.3 Program structure
 - 2.4 Description of subroutines
 - 2.4.1 The subroutine INPUT
 - 2.4.2 The subroutine PHI
 - 2.4.3 The subroutine NUK
 - 2.4.4 The subroutine MATCAL
 - 2.4.5 The subroutines OUTINT and OUTZON
 - 2.5 Application of AKTIV to a special material
 - 2.5.1 Data needs and arrangement
 - 2.5.2 Application to stainless steel
 - 2.6 Input description
- 3. The program AKTOUT
 - 3.1 General remarks
 - 3.2 Input description
- 4. The program AKTIN
 - 4.1 General remarks
 - 4.2 Input description

Acknowledgements

References

1. INTRODUCTION

Evaluation of the inventory of structural activity, nuclear afterheat, and biological hazard potential of fusion reactor blankets is necessary to answer questions about safety and environmental problems of future fusion power plants. In the past, quite a number of authors have published results [1 - 9] which in most cases, however, are restricted to a special blanket design and different structure materials. From these results it is hardly possible to determine reliably the effects of design and operational modifications on the activity or even the effects of completely different designs.

Although various results are available, little has been published about the computational methods and computer programs used by the different authors. There are a number of programs which have been developed for fission reactor application and it is most probable that such codes have been used, either in their original or a modified version, for the fusion reactor activity calculations. In general, the application of such a program always necessitates a critical review of the calculation procedure. This is due to the fact that the fusion reactor radiation environment with its characteristic hard neutron spectrum gives rise to a rather complicated buildup and decay behaviour of the various isotopes leading to a highly cross-linked activation chain structure.

Because of the importance of the activation problem for fusion development it was felt necessary to elaborate an activation program at IPP. Such a program should essentially meet the following conditions:

- It should readily fit into the already existing INDRA neutronics and photonics program system [10].
- It should be constructed in such a way as to be readily adaptable to either type of structure material.
- In its first version it should be applied to stainless steel, thus fitting into the present work of the IPP Systems Studies Project [11, 12].

This report describes the program AKTIV resulting from this work. It is to be regarded as a users' manual. Results obtained with this program will be published elsewhere.

2. THE PROGRAM A K T I V

2.1 General remarks

The program AKTIV is capable of providing all information about transmutation, activation, afterheat, and biological hazard potential for a given blanket. It is constructed in a very general form and can be used in any case where activating fluxes (neutrons, gammas, protons, etc.), corresponding cross-sections, and all initial conditions are known. The latter comprise primarily the initial concentrations of the chemical elements and their isotopic composition present in the blanket.

During irradiation these concentrations change with time because of radioactive decay processes and nuclear reactions, the numbers of which are defined as the products of fluxes and cross-sections. These "transmutations" give rise to changes in the isotopic and alloy composition.

The one result of these nuclear processes is that a number of unstable parent nuclides are produced which decay with a characteristic half-life (or decay constant) to either stable or again unstable daughter nuclides. The product of the number of radioisotopes and their decay constant is called "activity".

Each decay event is accompanied by an energy release the amount of which is characteristic of a certain radionuclide. The sum over the energies of all radionuclides produced is called "afterheat" or "decay power" if the time dependence is taken into account.

Finally, to each amount of activity of a certain radionuclide a "biological hazard potential" (BHP) can be assigned by relating the activity to the maximum permissible concentration of the radioisotope in air. The sum over the contributions of all radionuclides is commonly used as a measure of the hazard potential of any nuclear power plant.

All these data are calculated by AKTIV as a function of time for each space interval and each zone comprising a certain number of intervals which are specified by the program input. In doing this, the time dependence can be treated in three different modes corresponding to the operation sequence of the reactor:

- burn period: the reactor is operating, radionuclides are being produced and decay.
- shutdown period: the reactor is out of operation, all neutron fluxes are zero, the radionuclides decay.
- periodic operation: the reactor is periodically started and shut down, the periods being assumed to be constant.

A special program feature is that the shortest half-life involved should not be less than 0.1 second. Since the program was elaborated for running on an IBM 360 computer, a number of variables had to be defined in double precision. This assures a calculational accuracy of better than 1 % if the time variation of the activity is followed up to 10^{10} seconds.

2.2 Mathematical background

The essence of the program AKTIV is a procedure for calculating the change of the amounts of different nuclides depending on time. The change is caused by decay and by nuclear reactions. If there are $N_{i}(t)$ atoms from nuclide i at time t which decay with the decay constant λ_{i} , the following differential equation is valid:

$$\frac{d}{dt} N_i (t) = -\lambda_i \cdot N_i (t). \qquad (1)$$

In addition, it is possible that the nuclide i is enriched by the decay of nuclides j:

$$\frac{d}{dt} N_{i} (t) = \sum_{j \neq i} \lambda_{j}^{(j \to i)} \cdot N_{j} (t)$$
 (2)

under the condition that the nuclide j decays to nuclide i.

In the case of neutron activation one has similar equations:

$$\frac{d}{dt} N_i (t) = -\sum_{i \neq i} \sum_{n} G_n^{(i \rightarrow j)} \cdot \phi_n \cdot N_i (t)$$
 (3)

and

$$\frac{d}{dt} N_{i} (t) = \sum_{j \neq i} \sum_{n} G_{n}^{(j \rightarrow i)} \cdot \emptyset_{n} \cdot N_{j} (t), \qquad (4)$$

where n is the index for the energy interval of the neutron spectrum, $\mathfrak{S}_n^{(i \to j)}$ is the cross-section for a neutron reaction converting the nuclide i to the nuclide j within the energy interval n, and \emptyset_n is the corresponding neutron flux. Equation (3) expresses the decrease, and eq. (4) the increase of the nuclide i.

In general, there are both forms of nuclear processes so that the change of nuclide i as a function of time is described by the sum of eqs. (1), (2), (3) and (4):

$$\frac{d}{dt} N_{i} (t) = - \left(\lambda_{i} + \sum_{j \neq i} \sum_{n} \mathfrak{G}_{n}^{(i \rightarrow j)} \cdot \mathfrak{O}_{n} \right) \cdot N_{i} (t)$$

$$+ \sum_{i \neq i} \left(\lambda_{j}^{(j \rightarrow i)} + \sum_{n} \mathfrak{G}_{n}^{(j \rightarrow i)} \cdot \mathfrak{O}_{n} \cdot N_{j} (t) \right). \tag{5}$$

With the definitions

$$A_{ii} = - (\lambda_i + \sum_{j \neq i} \sum_{n} G_n^{(i \rightarrow j)} \cdot \emptyset_n)$$
 (6)

and

$$A_{ij} = \lambda_{j}^{(j \to i)} + \sum_{n} \sigma_{n}^{(j \to i)} \cdot \emptyset_{n}$$

$$i \neq j$$
(7)

equation (5) can be transformed to

$$\frac{d}{dt} N_{i}(t) = \sum_{j} A_{ij} \cdot N_{j}(t).$$
 (8)

It should be mentioned that the values λ_i , $\mathfrak{S}_n^{(i \to j)}$, \emptyset_n are all $\stackrel{>}{=} 0$, so that

$$A_{ii} \stackrel{<}{-} 0 \tag{9}$$

and
$$A_{ij} \stackrel{>}{=} 0$$
. (10)

By constructing the vector

$$\overrightarrow{N}(t) =
\begin{cases}
N_1(t) \\
\vdots \\
N_{NN}(t)
\end{cases}$$

where NN is the number of nuclides, and the matrix

$$\vec{\overline{A}} = (A_{ij})$$
 (12)

one can write for the system (8) of all differential equations

$$\frac{d}{dt} \vec{N}(t) = \bar{A} \circ \vec{N}(t) \tag{13}$$

where osymbolizes a maxtrix multiplication (here with a vector).

The matrix \bar{A} is called 'transition matrix'. The general solution of eq. (13) is given by

$$\vec{N}(t) = \vec{P}^{\bar{A} \cdot (t - t_0)_0} \vec{N}(t_0), \tag{14}$$

where \vec{N} (t_o) is the vector \vec{N} at the initial time t_o (t_o < t).

In our case all computations start at time t_0 = 0, so that eq. (14) transforms to the special form

$$\vec{N}(t) = e^{\vec{A} \cdot t} \cdot \vec{N}(0). \tag{15}$$

With the matrix definition

$$=$$
 $=$ $C(t) = e^{A \cdot t}$ (16)

the solution (15) becomes

$$\vec{N}(t) = \vec{C}(t) \cdot \vec{N}(0).$$
(17)

The matrix C (t) is called 'operator matrix' at time t.

The problem now consists in the evaluation of the operator matrix \bar{c} (t).

By using eq. (16) we get \bar{c} (t) in the form of a Taylor series [13]:

$$\bar{\bar{C}}(t) = \bar{T} + \sum_{\nu=1}^{\infty} \frac{1}{\nu!} \cdot (\bar{\bar{A}} \cdot t)^{\nu}, \qquad (18)$$

where T is the unit matrix.

Because this series has to converge rapidly, the value t has to meet the following condition:

$$|A_{MAX}| \cdot t < 1, \tag{19}$$

where $|\mathbf{A}_{\mbox{MAX}}|$ is the absolute value of the maximum element of the matrix $\bar{\mathbf{A}}.$

Usually this condition is not fulfilled, so that one has to use a different method to calculate the series.We choose a time value τ with τ < t, for which eq. (19) is valid:

$$\tau < \frac{1}{|A_{MAX}|}$$
 (20)

The matrix $\bar{\mathbb{C}}$ ($\bar{\tau}$) can then be evaluated by breaking off the Taylor series (18) so that the error is less than a given error P. Because of eq. (16) the operator matrix can now be computed for the time $2 \cdot \tau$ by a simple matrix multiplication

$$\overline{\overline{C}} (2 \cdot \tau) = \overline{\overline{C}} (\tau)^{0} \overline{\overline{C}} (\tau) = [\overline{\overline{C}} (\tau)]^{2}. \tag{21}$$

By this procedure the error P changes to 2 \cdot P. After sufficient successive applications of eq. (21) one has the matrix $\bar{\overline{C}}$ (t) for any time t.

In this program AKTIV we only compute $\vec{\mathbb{N}}$ (t) for values of t which are an integer number of seconds. For this reason it is necessary to evaluate first the operator matrix for 1 sec: $\bar{\bar{\mathbb{C}}}$ (1). An integer number m is choosen so that

$$\tau = \frac{1}{2^{m}} [sec] \tag{22}$$

and condition (20) are fulfilled. Equation (21) applied $^{\text{m}}$ times gives $\bar{\bar{\mathbb{C}}}$ (1).

Successive application of eq. (21) yields

$$\overline{C}$$
 (2), \overline{C} (4), \overline{C} (8), ..., \overline{C} (2 $^{\dot{q}}$), ...,

where q is an integer.

To get $\bar{\mathbb{C}}$ (t), the program computes the dual representation of t, which means that

$$t = \chi_0 \cdot 2^0 + \chi_1 \cdot 2^1 + \chi_2 \cdot 2^2 + \dots + \chi_{\nu} \cdot 2^{\nu} + \dots$$
 (23)

$$\bar{C} (t) = \bar{C} \left(\sum_{\nu} \gamma_{\nu} \cdot 2^{\nu} \right) = e^{-\bar{A} \cdot \sum_{\nu} \gamma_{\nu}} \cdot 2^{\nu}$$

$$= \prod_{\nu} \left(e^{\bar{A} \cdot 2^{\nu}} \right)^{\gamma_{\nu}} = \prod_{\nu} \left(\bar{C} (2^{\nu}) \right)^{\gamma_{\nu}}.$$
(24)

In our case all computations start at time t_0 = 0, so that eq. (14) transforms to the special form

$$\vec{N}(t) = e^{\vec{A} \cdot t} \cdot \vec{N}(0). \tag{15}$$

With the matrix definition

the solution (15) becomes

$$\vec{N}(t) = \vec{C}(t) \cdot \vec{N}(0). \tag{17}$$

The matrix C (t) is called 'operator matrix' at time t.

The problem now consists in the evaluation of the operator matrix \bar{C} (t).

By using eq. (16) we get \bar{C} (t) in the form of a Taylor series [13]:

$$\overline{\overline{C}} (t) = \overline{T} + \sum_{\nu=1}^{\infty} \frac{1}{\nu!} \cdot (\overline{A} \cdot t)^{\nu}, \qquad (18)$$

where T is the unit matrix.

Because this series has to converge rapidly, the value t has to meet the following condition:

$$|A_{MAX}| \cdot t < 1, \tag{19}$$

where $|\mathbf{A}_{MAX}|$ is the absolute value of the maximum element of the matrix $\bar{\mathbf{A}}.$

Usually this condition is not fulfilled, so that one has to use a different method to calculate the series. We choose a time value τ with τ < t, for which eq. (19) is valid:

$$\tau < \frac{1}{|A_{MAX}|} . \tag{20}$$

The matrix $\bar{\mathbb{C}}$ ($\hat{\tau}$) can then be evaluated by breaking off the Taylor series (18) so that the error is less than a given error P. Because of eq. (16) the operator matrix can now be computed for the time 2 • τ by a simple matrix multiplication

$$\overline{\overline{C}} (2 \cdot \tau) = \overline{\overline{C}} (\tau)^{0} \overline{\overline{C}} (\tau) = [\overline{\overline{C}} (\tau)]^{2}. \tag{21}$$

By this procedure the error P changes to 2 \cdot P. After sufficient successive applications of eq. (21) one has the matrix \bar{C} (t) for any time t.

In this program AKTIV we only compute $\overline{\mathbb{N}}$ (t) for values of t which are an integer number of seconds. For this reason it is necessary to evaluate first the operator matrix for 1 sec: $\overline{\mathbb{C}}$ (1). An integer number m is choosen so that

$$\tau = \frac{1}{2^{m}} [sec] \tag{22}$$

and condition (20) are fulfilled. Equation (21) applied m $\,$ times gives $\bar{\bar{C}}$ (1).

Successive application of eq. (21) yields

$$\overline{\overline{C}}$$
 (2), $\overline{\overline{C}}$ (4), $\overline{\overline{C}}$ (8), ..., $\overline{\overline{C}}$ (2 $^{\overline{q}}$), ...,

where q is an integer.

To get $\bar{\mathbb{C}}$ (t), the program computes the dual representation of t, which means that

$$t = Y_0 \cdot 2^0 + Y_1 \cdot 2^1 + Y_2 \cdot 2^2 + \dots + Y_{\nu} \cdot 2^{\nu} + \dots$$
 (23)

$$\bar{C} (t) = \bar{C} \left(\sum_{\nu} \gamma_{\nu} \cdot 2^{\nu} \right) = e^{\bar{A} \cdot \sum_{\nu} \gamma_{\nu}} \cdot 2^{\nu}$$

$$= \prod_{\nu} \left(e^{\bar{A} \cdot 2^{\nu}} \right)^{\gamma_{\nu}} = \prod_{\nu} (\bar{C} (2^{\nu}))^{\gamma_{\nu}}.$$
(24)

Because all $\bar{\mathbb{C}}$ (2 $^{\vee}$) matrixes have already been calculated, $\bar{\mathbb{C}}$ (t) is thus determined

[for
$$\nabla_{v} = 0 : [\bar{C}(2^{v})]^{\nabla_{v}} = \bar{T}$$

$$\nabla_{v} = 1 : [\bar{C}(2^{v})]^{\nabla_{v}} = \bar{C}(2^{v})].$$

It should be mentioned that all elements of \bar{c} (t) (for any t) are greater than or equal 0, so that matrix multiplications of \bar{c} consist in the addition of positive values. This means that computer errors are negligible.

The error P is chosen such that after a time t of 10^3 years the error is less than 1 %. For this reason it is sufficient to use

$$P = 10^{-17}. (25)$$

The vector \overrightarrow{N} (t) made up to the numbers of the different atoms can now be calculated from eq. (17).

- The activity in Ci is given by

$$A_{i}(t) = \frac{1}{3.7 \cdot 10^{10}} \cdot N_{i}(t) \cdot \lambda_{i}.$$
 (26)

 The change in the alloy composition can be derived from the weight of the isotopes in kg given by

$$W_{i}(t) = N_{i}(t) \cdot \frac{G_{i}}{N_{L}}, \qquad (27)$$

 $\mathbf{G_{i}}$ being the atomic mass of isotope i and $\mathbf{N_{L}}$ the Loschmidt number.

The nuclear afterheat in kW is calculated from

$$P_{i}(t) = 5.9274 \cdot 10^{-6} \cdot A_{i}(t) \cdot E_{i}$$
 (28)

 ${\rm E}_{f i}$ being the decay energy of isotope i in MeV

- The biological hazard potential in km³ is obtained from

$$BHP_{i}(t) = A_{i}(t) \cdot \frac{10^{-9}}{MPC_{i}}$$
 (29)

Here MPC $_i$ is the maximum permissible concentration of isotope i in air which has to be introduced in units of Ci/m 3 .

In a single program run all these results are calculated for a specified interval and a single period of the operation sequence, i.e. either the burn or the shutdown period. If more than one interval or more than one time period are to be evaluated, the entire procedure is repeated accordingly.

A minor change in the procedure described above is applied in the case that the activation behaviour during pulsed operation of the reactor is to be followed. The total time of one operating cycle separated into a burn period TBURN and a down period TOFF is used to define the first time step. The operator matrix is then obtained by

$$C(1) = C' (TOFF) \cdot C'' (TBURN), \qquad (30)$$

C' being the matrix for the shutdown period and C" being that for the burn period.

2.3 Program structure

The program AKTIV is subdivided into a MAIN program and seven subroutines:

INPUT

PHI

NUK

MATCAL

OUTMAT

OUTINT

OUTZON

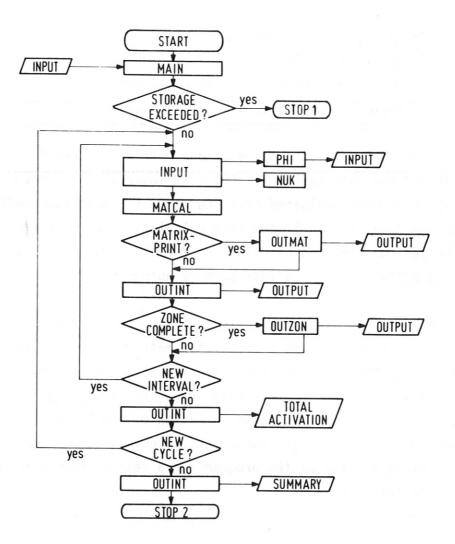
Additionally a BLOCK DATA subprogram is provided for the purpose of storing all information which makes the program applicable to a certain material.

The program structure of AKTIV is shown in Figure 1. MAIN reads all dimension parameters and checks them against the available storage. If the storage turns out to be too small an error message is produced and the program stops. Otherwise the subroutine INPUT is called which reads the entire input data block and advises the appropriate storage locations. INPUT also activates the subroutine PHI, which reads the fluxes from tape, and the subroutine NUK, which calculates the numbers of nuclides from the initial nuclide densities specified by the input. Finally, the required cross-sections are read from a second tape. The remaining information necessary for the calculations is stored in a BLOCK DATA subprogram.

Having prepared all data the calculation starts with the subroutine MATCAL. This routine establishes the initial operator matrix C(1) and evaluates all further matrices C(t) for the time steps desired. By means of these matrices all numbers of nuclides are calculated. As mentioned above, these calculations are restricted to one interval and one time period. If a printout of either the transition or the operator matrix is requested, this task is performed by OUTMAT.

Subsequently, OUTINT is called, which calculates and prints on request the output information for a single interval. Optionally the following information can be edited as a function of time:

- number of nuclides
- activity of radioisotopes
- activity of elements
- total activity per unit volume
- weight of elements
- weight percentage of elements
- decay power of radioisotopes
- decay power of elements
- total decay power per unit volume
- biological hazard potential of radioisotopes
- biological hazard potential of elements



 $\underline{\text{Fig. 1}}$: Structure of the program AKTIV

Finally, OUTINT checks whether all intervals belonging to one zone have been treated. If not, control is transferred back to INPUT, otherwise OUTZON will be called, which prints, if desired, the following information about an entire zone:

- activity of radiosiotopes
- activity of elements
- decay power of radioisotopes
- decay power of elements
- biological hazard potential of radioisotopes
- biological hazard potential of elements

After completing these output operations control is transferred back to INPUT and the calculation for the next interval is started. If all intervals have been evaluated AKTIV turns to the next time period, e.g. to the decay period if the last calculation was performed for the burn period. When the calculations for all time periods are completed OUTINT provides a last summary output.

In the case of evaluating the activity during a periodic sequence of burn and shut down phases the operator matrices for both phases are established by MATCAL. After multiplication the operator matrix for one period is obtained. Now all time steps are divided by the duration of one cycle, this meaning a transformation of the "time units" from real seconds to periods. The subsequent calculations are performed as usual. Just at the end of the program run a retransformation has to be done for output reasons.

2.4 Description of subroutines

2.4.1 The subroutine INPUT

The subroutine INPUT prepares all data needed for the calculations in MATCAL and OUTINT. At first, all data specific to a certain material (except the cross-sections) are transferred from the BLOCK DATA subprogram (see section 2.5) by a COMMON statement:

COMMON /DATEN/ DAT1, DAT3, DAT4, IDAT8, IDAT12, IDAT14, IDAT9, DAT7, DAT5, DAT6, DAT2, IDAT10, IDAT11.

Next, all input data are read and all radii are checked for being arranged in increasing order. After having read in the fluxes from tape a first printout is provided by which, depending on the specification of NOGE(I), the fluxes, radii, volumes, and the initial densities may be edited. Afterwards, the nuclear data are transformed and then the cross-sections are read from a second tape.

When all data are read in the definition of the time variables for the first period to be treated is performed. The time steps between TZERO and TMAX (TZ(0) and TZ(NT), respectively) may be subdivided either linearly or logarithmically. In the latter case the single time instants TZ(I) are defined as

$$TZ(I) = A \cdot exp(B \cdot I) + C. \tag{31}$$

The three coefficients A, B, and C are chosen such that the following conditions are fulfilled:

$$TZ(0) = TZER0$$
 $TZ(NT) = TMAX$
 $TZ(I+10) = \checkmark \cdot TZ(I)$ $\checkmark = const.$

This means that for each decade the same number of time steps will be used. Subtracting TZERO from all TZ(I) always ensures that TZ(1) = 0.

At this stage of the calculation INPUT provides the possibility of storing on tape all parameters including the TZ(I) for later use in the program AKTOUT (see section 3).

To start the calculation for the first interval, the initial numbers of nuclides must be prepared. At the beginning this is done with the subroutine NUK. Later on the changed numbers appear in the data set RES in subroutine MATCAL. The transition matrix A is now constructed from the reaction rates and the decay constants $\lambda_{\bf j}$. The reaction rates are set zero in the case where the decay period is treated. The matrix construction is terminated by calling the subroutine MATCAL.

2.4.2 The subroutine PHI

The subroutine PHI is called by INPUT to read all fluxes from tape. It expects the fluxes to be written in a (6(I2, IX, F9.0)) format which is in accordance with the tape output of the transport programs of the INDRA system.

All flux data are read by the statement

READ (NTAPE, NFORM)((M(K), TEMP(K)), K = 1,6)

Here M(K) denotes a repetition number which specifies how often the corresponding value of TEMP(K) is to be successively stored in the working array.

The flux data which are input to PHI are arranged in a one-dimensional array. The first sub-array contains the fluxes in energy group 1, running from interval 1 to interval NIN, the second sub-array the fluxes of energy group 2, again running from interval 1 to interval NIN, and so on. For further calculation they have to be rearranged and stored in the two-dimensional working array FLUX (NI, NE), where NI denotes the index of the interval and NE that of the energy group. In the course of this procedure all fluxes are multiplied by a constant AFLUXM which can be specified by input. This quantity provides the possibility of adapting a given neutron flux spectrum to a different wall loading than that assumed for calculating the original fluxes.

2.4.3 The subroutine NUK

The subroutine NUK is used for calculating the initial numbers of nuclides from the element nuclide densities of a certain interval. It is called by INPUT separately for each interval.

NUK looks for the zone number in which the interval is located and selects the corresponding element nuclide density. To obtain the total number of nuclides for each isotope, it multiplies the element nuclide density by its natural isotopic fraction and by the volume

of the interval. Additionally, the result is multiplied by 10^{24} since usually the input densities are given in units of barn-at/cm 3 .

2.4.4 The subroutine MATCAL

The subroutine MATCAL represents that part of AKTIV which solves the set of differential equations. After searching for the maximum element A_{max} of the transition matrix $A_{i,j}$ a time increment τ is calculated from condition (20). As was outlined in section 2.2, this has to be done to achieve a rapid concergency of the Taylor series. Subsequently the operator matrix $C(\tau)$ is evaluated according to (18), taking into account as many terms of the Taylor series as are needed to restrict the inaccuracy to 10^{-17} . Since τ is, by definition (22), an inverse integer, the operator matrix C(1) for the first time step is found by squaring $C(\tau)$ m times:

$$C(1) = C(\tau)^{(2^m)}$$
 (32)

After this procedure is ended it is possible to call the subroutine OUTMAT for printing the matrices A and C(1).

As indicated by eq. (17) the solution of (13) reads as

$$N(t) = N(0) \cdot C(t).$$

To evaluate C(t), it is necessary to successively square the matrix previously evaluated, starting with C(1). At the same time, all time steps TZ(I) which correspond to t must be decomposed into the dual form. If this has been done the resulting numbers of nuclides N_i are calculated by means of eq. (24). The function of MATCAL is completed by calling the subroutine OUTINT and storing all N_i on tape.

2.4.5 The subroutines OUTINT and OUTZON

The subroutine OUTINT is called at three locations: once in subroutine MATCAL and twice in INPUT.

Its task if called by MATCAL is to print all results desired for a single interval. Which results are desired for which interval can be spcified by input (see section 2.6). The various possibilities have already been listed in section 2.3.

The first call of OUTINT by INPUT is done after complete evaluation of a time period. In this case a summary output is produced without splitting the results with regard to the single isotopes.

The second call of OUTINT by INPUT is done at the very end of the program run. At this place a table of contents is produced to assist rapid location of the required results.

OUTZON is called by MATCAL in the case that all intervals belonging to one zone have been evaluated. It prints, if desired, the summary results for the entire zone, which have also been specified in section 2.3.

2.5 Application of AKTIV to a special material

2.5.1 Data needs and arrangement

As mentioned initially in this report, AKTIV has been elaborated in such a way as to be able to treat any activation problem. To adapt the program to a certain problem the following information must be available:

- fluxes (for instance neutron fluxes) on tape
- cross-sections on tape
- further material and nuclear data in the BLOCK DATA subprogram.

As far as the fluxes are concerned they must be written on tape in a (6(I2, IX, F9.0)) format. They are read as ((M(K), TEMP(K)), K = 1,6), M being a repetition number and TEMP being the flux value in units of cm⁻² s⁻¹. They have to be arranged in a one-dimensional array, starting with group 1 (highest energy) for all intervals followed by group 2 for all intervals and so on.

The cross-section tape has to be prepared in the following way: At first NSNR integer numbers have to be placed indicating the number of non-zero cross-sections for each of the NSNR cross-section data sets. The format has to be (18I4). This line(s) has to be followed by the data sets of the non-zero cross-sections in barn (Format 6E12.6). Each data set starts with the cross-section for the highest energy group. Zero cross-sections which may appear at lower energies are supplied by the program.

The following information has to be prepared for the BLOCK DATA subprogram:

DAT1: Names of the isotopes to be listed as a set of hollerith constants, eight characters per name being allowed.

DAT2: Names of the output elements to be listed as a set of hollerith constants, four characters per name being allowed.

DAT3: Decay constants in sec⁻¹ of the radionuclides to be listed as double precision constants.

DAT4: MPC values in Ci/m³ of the radionuclides to be listed as real constants.

DAT5: Decay energies in MeV of the radionuclides to be listed as real constants.

DAT6: Atomic mass of all nuclides to be listed as real constants.

DAT7: Natural abundance in % of all stable isotopes to be listed as real constants.

IDAT8 : Number of stable isotopes per element to be listed as integer constants. The sequence must previously be defined.

IDAT9: Identification numbers of stable isotopes to be listed as integer constants. Sequence according to DAT7.

IDAT10: Total number of isotopes (stable and unstable) per output element to be listed as integer constants. The sequence must previously be defined.

IDAT11: Identification numbers of all isotopes to be listed as integer constants. The sequence of elements must agree with IDAT10. The sequence of the isotopes within the element groups may be arbitrary.

IDAT12: Description of nuclear reactions. For each of the NSIG reactions a four integer data set (I1, I2, I3, I4) is needed:

I1 = identification number of resulting nuclide

I2 = identification number reacting nuclide

I3 = identification number of cross-section data set

I4 = identification number of branching ratio

= 0 no branching exists

> 0 cross-section is multiplied by branching ratio
BR(I4)

< 0 cross-section is multiplied by (1-BR(I4))</pre>

IDAT13: Continuation of IDAT12 if storage for IDAT12 is exhausted.

IDAT14: Description of decay reactions. For each of the NLAMD reactions a three integer data set (J1, J2, J3) is needed:

J1 = identification number of daughter nuclide

J2 = identification number of parent nuclide

In constructing the BLOCK DATA information the following rules have to be observed:

- The nuclides have to be arranged in such a way that the stable nuclides are located behind the unstable ones.

- The sequence of elements in IDAT18 must agree with that in IDAT10 and DAT2
- The sequence of isotopes in DAT7 and IDAT9 must be compatible with that of IDAT8.

Finally, the DIMENSION statement in the subroutine INPUT has to be adapted to the amount of data available in the BLOCK DATA subprogram. Note that the size of the array IDAT12 in this statement also covers the contents of IDAT13.

2.5.2 Application to stainless steel

As a first example the program AKTIV has been prepared to treat the problem of stainless steel activation. The data definition described in this section is based upon the investigation of the relevant activation chains and of the amount of cross-section data available summarized in [14].

We restrict the problem to the four input elements which are the most frequent alloy constituents of stainless steel, i.e. iron, nickel, chromium, and manganese. Because of the reactions occurring during the activation process four further elements are produced at least within the scope of this necessarily restricted considerations, i.e. cobalt, vanadium, scandium, and titanium.

Table I shows the definition of the BLOCK DATA arrays DAT2, IDAT8, and IDAT10. Note that the non-natural elements Co, V, Sc, and Ti are preceded by the natural ones. IDAT8 lists the number of naturally occurring stable isotopes present in the initial alloy, and IDAT10 the total number of stable plus unstable isotopes present in the activated alloy.

The total of 14 stable isotopes defined by IDAT8 are listed in Table II together with their isotopic abundance (IDAT7) and their identification number (IDAT9). Note that the sequence of elements agrees with that in Table I.

Table I: Definition of DAT2, IDAT8, and IDAT10

	DAT2	IDAT8	IDAT10
Iron	'FE'	4	10
Nickel	'NI'	5	9
Chromium	'CR'	4	7
Manganese	'MN'	1	9
Cobalt	'CO'		11
Vanadium	1 1/1	2 E	5
Scandium	'SC'	, , , , , , , , , , , , , , , , , , ,	2
Titanium	'TI'	rggilege te	1

Table II: Definition of IDAT7 and IDAT9

		.DAT7		IDAT9
Iron	FE-54	5.84	55 g	46
	FE-56	91.86	11.6	47
1 10 00 075-608/8	FE-57	2.17		48
	FE-58	0.31		49
Nickel	NI-58	67.76	1.	50
	NI-60	26.16	5/10/	51
	NI-61	1.25		52
	NI-62	3.66		53
1 2 2	NI-64	1.16		54
Chromium	CR-50	4.31		41
as to the so	CR-52	83.76		42
	CR-53	9.55		43
	CR-54	2.38		44
Manganese	MN-55	100.00		45

The identification numbers follow from Table III which is set up separately and completely independently of the considerations performed so far. In the present case we have chosen a sequence in which the unstable isotopes preced the stable ones and are arranged in decreasing order of half-life. As can be seen from Table III, this sequence is valid for the BLOCK DATA arrays DAT1, DAT3, DAT4, DAT5, and DAT6. The values specified in this table are taken from the literature as far as the decay constants λ_i [15], the atomic masses G_i [16], and most of the values for the maximum permissible concentrations MPC $_i$ [17] are concerned. Some of the MPC values have been reevaluated [18]. The decay energies E_i were calculated according to [19].

The cross connection between the two independent sequences is provided by the array IDAT11. This array is constructed according to the contents of IDAT10 (see Table I). At first the identification numbers (see Table III) of the isotopes of the first element defined in IDAT10 are listed successively in increasing order such that the stable isotopes appear at the end. The subsequent elements are treated accordingly and the identification numbers of the relevant isotopes are directly attached to the previous ones. In this way the arrangement shown in Table IV results.

To define the array IDAT12 and its continuation IDAT13, it is necessary at first to check the availability of reaction cross--sections. In our case we took into account a total of 76 neutron reactions, which are summarized in Table V. The cross-section data of 74 of these reactions were taken from the DLC-33/MONTAGE-400 cross-section library [20]. Those for the 55 Mn(n, %) 56 Mn reaction were evaluated from ENDF/B-III using SUPERTOG [10]. The cross--section data for the 64 Ni(n, 65 Ni reaction were supplied by KFA Jülich [21] as point data. They were converted to a 100 group structure using the INDRA program GROUCO [10]. Using the identification numbers of the various isotopes defined in Table III and the reaction-type identification numbers defined in Table V, the arrays IDAT12 and IDAT13 can be filled by the four-integer combinations specified in Table V. The branching ratios necessary for some of the reaction specifications are supplied by the program input.

Table III: Definition of identification numbers and DAT1, DAT3, DAT4, DAT5, and DAT6.

ID- No.	Name (DAT1)	^λ i (DAT3)	MPC _i (DAT4)	E _i (DAT5)	G _i (DAT6)
1	Mn-53	5.94D-15	9.5E-8	0.052	52.942
2	Fe-60	2.20D-13	9.5E-9	0.349	59.934
3	Ni-59	2.93D-13	2. E-8	0.067	58.934
4	Ni-63	2.20D-10	2. E-9	0.119	62.930
5	Co-60	4.17D-9	3. E-10	15.448	59.934
6	Fe-55	8.14D-8	3. E-8	0.057	54.938
7	V-49	2.43D-8	1.4E-7	0.043	48.949
8	Mn-54	2.57D-8	1. E-9	4.950	53.940
9	Co-57	2.97D-8	6. Ę-9	0.870	56.936
10	Sc-46	9.55D-8	8. E-10	12.806	45.955
11	Co-56	1.04D-7	1.7E-9	21.716	55.940
12	Co-58	1.13D-7	2. E-9	6.141	57.936
13	Fe-59	1.80D-7	2. E-9	7.706	58.935
14	Cr-51	2.90D-7	8. E-8	0.172	50.945
15	V-48	5.02D-7	2. E-9	18.246	47.952
16	Mn-52	1.41D-6	5. E-9	21.309	51.946
17	Ni-57	5.35D-6	1.3E-8	12.444	56.940
18	Co-58m	2.15D-5	3. E-7	0.148	57.936
19	Mn-56	7.46D-5	2. E-8	14.997	55.939
20	Ni-65	7.64D-5	2. E-8	7.216	64.930
21	Co-61	1.20D-4	1. E-10	3.248	60.932
22	Cr-49	2.75D-4	1. E-10	8.992	48.951
- 23	Mn-52+	5.50D-4	1. E-10	20.736	51.946
24	Co-62	8.25D-4	1. E-10	15.549	61.934
25	Co-60m	1.10D-3	1. E-10	0.498	59.934
26	Fe-53	1.36D-3	1. E-10	13.444	52.946
27	Fe-61	1.93D÷3	1. E-10	14.084	60.937
28	Ti-51	1.99D-3	1. E-10	7.321	50.947
29	V-52	3.08D-3	1. E-10	14.825	51.945
30	Cr-55	3.20D-3	1. E-10	6.313	54.941
31	Fe-53m	3.46D-3	1. E-10	0.0	52.946
32	Mn-57	6.80D-3	1. ६−10	7.115	56.938
33	V-53	7.22D-3	1. E- 10	12.152	52.944

Table III: Continued

ID-No.	Name (DAT1)	λ _i (DAT3)	MPC _i (DAT4)	E _i (DAT5)	G _i (DAT6)
34	Co-62+	7.70D-3	1. E-10	21.041	61.952
35	Mn-58	1.07D-2	1. E-10	16.598	57.940
36	V-54	1.61D-2	1. E-10	32.046	53.947
37	Co-63	2.52D-2	1. E-10	9.431	62.934
38	Sc-46m	3.71D-2	1. E-10	0.842	45.955
39	Mn-58+	2.31D-1	1. E-10	0.0	57.940
40	Co-64	1.73D 0	1. E-10	0.563	63.393
41	Cr-50				49.946
42	Cr-52				51.941
43	Cr-53				52.941
44	Cr-54				53.939
45	Mn-55				54.938
46	Fe-54				53.940
47	Fe-56				55.935
48	Fe-57				56.935
49	Fe-58				57.933
50	Ni-58				57.935
51	Ni-60				59.931
52	Ni-61				60.931
53	Ni-62				61.928
54	Ni-64				63.928

Table IV: Definition of IDAT 11

		IDAT11									
Iron	2	6	13	26	27	31	46	47	48	49	
Nickel	3	4	17	20	50	51	52	53	54		
Chromium	14	22	30	41	42	43	44				
Manganese	1	8	16	19	23	32	35	39	45		
Cobalt	5	9	11	12	18	21	24	25	34	37	40
Vanadium	7	15	29	33	36						
Scandium	10	38									
Titanium	28										

Table V: Definition of IDAT12 and IDAT13

No	Reaction	IDA	T12 / 1	DAT 1	.3	Comment
No.	Reaction	I1	12	13	14	48.1 %
1	V-49(n,2n) V-48	15	7	1	0	1)
	7 1 2 7	7	7	-1	0	1)
7 9	200		_	0	7	1 " " " " " " " " " " " " " " " " " " "
2	V-49(n, α) Sc-46m	38	7	2	7	1)
	V-49(n,α) Sc-46	10	7	2	-7	1)
		7	7	-2	0	1)
3	Cr-50(n,2n) Cr-49	22	41	3	0	
4	Cr-50(n, √) Cr-51	14	41	4	0	
5	Cr-50(n,d+np)V-49	7	41	5	0	,
6	Cr-50(n,t) V-48	15	41	6	0	
7	Cr-52(n,2n) Cr-51	14	42	7	0	· · · · · · · · · · · · · · · · · · ·
8	Cr-52(n,p) V-52	29	42	8	0	
9	Cr-53(n,p) V-53	33	43	9	0	~
10	Cr-53(n,d+np)V-52	29	43	10	0	
11	Cr-54(n,p) V-54	36	44	11	0	*
12	Cr-54(n,α) Ti-51	28	44	12	0	
13	Cr-54(n,d+np)V-53	33	44	13	0	
14	Cr-54(n,t) V-52	29	44	14	0	
15	Mn-53(n,2n)Mn-52m	23	1	15	2	2)
	Mn-53(n,2n)Mn-52	16	1	15	0	2)
		1	1	-15	0	2)
16	Mn_52/n_n=\ V=40	7	1	16	0	1)
10	Mn-53(n,n α) V-49	1	1	-16	0	1)
1	1	1	1	1	1	/

Table V: Continued

1		IDAT	12 /	IDAT13	3	Comment
No.	Reaction	I1	12	13	14	- Comment
17	Mn-54(n,2n)Mn-53	1	8	17	0	1)
	$\chi 1 - \chi = 1$	8	8	-17	0	1)
18	Mn-55(n,2n)Mn-54	8	45	18	0	1
19	Mn-55(n,∜)Mn-56	19	45	19	0	
20	Mn-55(n,p) Cr-55	30	45	20	0	1
21	Mn-55(n,α) V-52	29	45	21	0	
22	Fe-54(n,2n)Fe-53m	31	46	22	4	
	Fe-54(n,2n)Fe-53	26	46	22	-4	
23	Fe-54(n, ∛)Fe-55	6	46	23	0	e are-e l
24	Fe-54(n,p)Mn-54	8	46	24	0	
25	Fe-54(n,α)Cr-51	14	46	25	0	
26	Fe-54(n,d+np)Mn-53	1	46	26	0	
27	Fe-54(n,t)Mn-52m	23	46	27	2 .	
	Fe-54(n,t),Mn-52	16	46	27	-2	. John et al. 18 miles
28	Fe-55(n,d+np)Mn-54	8	6	28 - 28	0	1)
29	Fo F.F./n n. \Cv F1	14	6	29	0	1)
29	Fe-55(n,nα)Cr-51	6	6	-29	0	1)
30	Fe-56(n,2n)Fe-55	6	47	30	0	
31	Fe-56(n,p)Mn-56	19	47	31	0	
32	Fe-56(n,t)Mn-54	8	47	32	0	
33	Fe-57(n,p)Mn-57	32	48	33	0	
34	Fe-57(n,d+np)Mn-56	19	48	34	0	7 - 7 - 1 - 2 - 0
35	Fe-58(n ,%)Fe-59	13	49	35	0	
36	Fe-58(n,p)Mn-58m	39	49	36	6	10 00000000 100 1
1	Fe-58(n,p)Mn-58	35	49	36	-6	
37	Fe-58(n,α)Cr-55	30	49	37	0	
38	Fe-58(n,d+np)Mn-57	32	49	38	0	

Table V: Continued

N		IDA	T12 ,	/ IDA	Г13	Comment
No.	Reaction	I1	12	13	14	Commenc
39	Fe-58(n,t)Mn-56	19	49	39	0	
40				1		1112 - 1111
40	Co-57(n,2n)Co-56	11	9	40	0	1)
4.1				-40	0	1)
41	Co-57(n,α)Mn-54	8	9	41	0	1)
		9	9	-41	0	1)
42	$Co-57(n,n\alpha)Mn-53$	1	9	42	0	1)
		9	9	-42	0	1)
43	Co-60(n,p)Fe-60	2	5	43	0	3)
		5	5	43	0	3)
	Co-60m(n,p)Fe-60	2	25	43	0	3)
		25	25	-48	.0	3)
44	$Co-60(n,\alpha)Mn-57$	32	5	44	0	3)
		5	5	-44	0	3)
	$Co-60m(n,\alpha)Mn-57$	32	25	44	0	3)
		25	25	-44	0	3)
45	Co-60(n,d+np)Fe-59	13	5	45	0	3)
		5	5	-45	0	3)
	Co-60m(n,d+np)Fe-59	13	25	45	0	3)
		25	25	-45	0	3)
46	$Co-60(n,n\alpha)Mn-57$	19	5	46	0	3)
		5	5	-46	0	3)
	Co-60m(n,nα)Mn-56	19	25	46	0	3)
		25	25	-46	0	3)
47	Ni-58(n,2n)Ni-57	17	50	47	0	
48	Ni-58(n ,∤)Ni-59	3	50	48	0	
49	Ni-58(n,p)Co-58m	18	50	49	1	
	Ni-58(n,p)Co-58	12	50	49	-1	7 - 37 7
50	Ni-58(n,α)Fe-55	6	50	50	0	786-97
51	Ni-58(n,d+np)Co-57	9	- 50	51	0	186-17
52	Ni-58(n,t)Co-56	11	50	52	0	

Table V: Continued

No.	Reaction	IDA	T12 /	IDAT1	3	Comment
NO.	Reaction	I1	12	13	14	Comment
53	Ni-59(n,d+np)Co-58m	18	3	53	1	2)
	Ni-59(n,d+np)Co-58	12	3	53	-1	2)
	11 35(11 , 4111) 30 30	3	3	-53	0	2)
54	Ni-59(n,rα)Fe-55	6	3	54	0	1)
	55 (,), 5 55	3	3	-54	0	1)
55	Ni-60(n,2n)Ni-59	3	51	55	0	
56	Ni-60(n,p)Co-60m	25	51	56	3	
	Ni-60(n,p)Co-60	5	51	56	-3	
57	Ni-60(n,t)Co-58m	18	51	57	1	
	Ni-60(n,t)Co-58	12	51	57	-1	
58	Ni-61(n,p)Co-61	21	52	58	0	
59	Ni-61(n,d+np)Co-60m	25	52	59	3	
	Ni-61(n,d+np)Co-60	5	52	59	-3	
60	Ni-62(n ,∜)Ni-63	4	53	60	0	
61	Ni-62(n,p)Co-62m	34	53	61	5	
	Ni-62(n,p)Co-62	24	53	61	- 5	9
62	Ni-62(n,α)Fe-59	13	53	62	0	
63	Ni-62(n,d+np)Co-61	21	53	63	0	
64	Ni-62(n,t)Co-60m	25	53	64	3	
	Ni-62(n,t)Co-60	5	53	.64	-3	
65	Ni-63(n,p)Co-63	37	4	65	0	1)
		4	4	-65	0	1)
66	Ni-63(n,α)Fe-60	2	4	66	0	1)
		4	4	-66	0	1)
67	Ni-63(n,d+np)Co-62m	34	4	67	5	2)
	Ni-63(n,d+np)Co-62	24	4	67	- 5	2)
		4	4	-67	0	2)
68	Ni-63(n,nα)Fe-59	13	4	68	0	2)
	7.5	4	4	-68	0 7	1)
69	Ni-63(n,t)Co-61	21	4	69	0	1)
		4	4	-69	0	1)

Table V: Continued

		ID	AT12	/ IDAT1	.3	Comment
No.	Reaction	I1	12	13	14	oommen o
70	Ni-64(n,2n)Ni-63	4	54	70	0	
71	Ni-64(n ,7)Ni-65	20	54	71	0	
72	Ni-64(n,p)Co-64	40	54	72	0	
73	Ni-64(n,α) Fe-61	27	54	73	0	
74	Ni-64(n,d+np)Co-63	37	54	74	0	
75	Ni-64(n,nα)Fe-60	2	54	75	0	
76	Ni-64(n,t)Co-62m	34	54	76	5	
	Ni-64(n,t)Co-62	24	54	76	-5	

A few comments are added to explain the contents of Table V.

1) The increase in the number of nuclides for an isotope resulting from a certain reaction is accompanied by a decrease in that for the target isotope. This negative contribution is automatically supplied by the program. It may, however, also be specified by the user, as was done in Table V for reactions starting from radioisotopes. In this case the following rules have to be observed:

where I1 and I2 specify the target isotope.

2) If the reaction product can exist in different states (ground and metastable states), the reaction must be specified twice applying the branching ratios. The decrease in the number of nuclides of the target isotope may be described as above. 3) If the target isotope can exist in different states, it is assumed that both have identical cross-sections. The decrease in the number of nuclides has to be specified for both states separately.

The last of the BLOCK DATA arrays, IDAT14, is filled by the three-integer combinations specified in Table VI, which describe the decay reactions involved. Only those resulting again in radio-isotopes have to be taken into account.

2.6 Input description

The input data for the program AKTIV are subdivided into five sections A to E. The values given in parentheses are those for the stainless steel problem.

A: <u>Title and Control parameters</u>

Card 1: Format (18 A4)

TITLE Title card

Card 2: Format (10 I6)

Number of input elements (4)
Number of output elements (8)
Total number of isotopes (54)
Number of unstable isotopes (40)
Number of energy groups
Number of intervals
First interval to be calculated
Last interval to be calculated
Number of zones
Geometry
= 1/2 plane/cylindrical

Table VI: Definition of IDAT 14

No.	Decay		IDAT14	
		J1	J2	J3
1	Fe-53 → Mn-53	1	26	0
2	Co-63 → Ni-63	4	37	0
3	Co-60m → Co-60	5	25	0
4	Cr-49 → V-49	7	22	0
5	Ni-57 → Co-57	9	17	0
6	Sc-46m → Sc-46	10	38	0
7	Co-58m → Co-58	12	18	0
8	Mn-52m → Mn-52	16	23	8
9	Fe-61 → Co-61	21	27	0
10	Fe-60 → Co-60m	25	2	0
11	Fe-53m → Fe-53	26	31	0

Card 3: Format (9¹⁶)

NTC	Logical tape-no. for the flux origin (1)
NTC1	Logical tape-no. for cross-section origin (2)
NTC2	Logical tape-no. for stored output (3)
NSNR	Number of cross-section types (76)
NSIG	Actual number of reactions (119)
NLAMD	Number of decay reactions (11)
NBR	Number of branching ratios (8)
NTM	Number of time periods
NTMAX	Maximum number of time steps

Card 4: Format (E12.6)

AFLUXM Multiplication factor for fluxes

B: Geometry and branching ratios

Card 5: Format (18I4)

NIZ(I) Number of intervals per zone (NZ entries)

Card 6: Format (6E12.6)

R(I) Radii of interval boundaries (NIN+1 entries)

Card 7: Format (6E12.6)

BR(I) Branching ratios to metastable isotopes (NBR entries) (8)

C: Element description

Card 8: Format (18A4)

TITLE(I) Title card

Card 9: Format (6E12.6)

DEN(I) Initial element number density per zone (NZ entries)

Note: Repeat section C data for each element involved, that is NE times (maximum 18).

Note: For stainless steel the sequence is fixed:

Card 9.1 Iron

Card 9.2 Nickel

Card 9.3 Chromium

Card 9.4 Manganese

D: Output control parameters

Card 10: Format (1814)

General output options

NOGE(1) Store calculated results on tape

= 0/1 no/yes

NOGE(2) Print fluxes

= 0/1 no/yes

NOGE(3) Print radii and volumes

= 0/1 no/yes

NOGE(4) Print initial element densities

= 0/1 no/yes

NOGE(5) Print summary

= 0/1 no/yes

Card 11: Format (1814)

Output options for single intervals

NSTEU(1) Specification of interval

 $(JNIN1 \leq NSTEU(1) \leq JNIN2)$

NSTEU(2) Print options

= 1 transition matrix

= 2 operator matrix

= 3 number of nuclides

= 4 activity per isotope

= 5 activity per element

= 6 activity per unit volume

= 7 weight per element

= 8 weight percentage per element

= 9 decay power per isotope

= 10 decay power per element

= 11 decay power per unit volume

= 12 biological hazard potential per isotope

= 13 biological hazard potential per element

Note: Repeat NSTEU(1) and NSTEU(2) for each print required.

At last give "0".

Card 12: Format (1814)

Output options for single zones

NSTEU(1) Specification of zone

 $(NSTEU(1) \leq NZ)$

NSTEU(2) Print options

= 1 activity per isotope

= 2 activity per element

= 3 decay power per isotope

= 4 decay power per element

= 5 biological hazard potential per isotope

Note: Repeat NSTEU(1) and NSTEU(2) for each print required. At last give "0".

E: Parameters for time phases

Card 13: Format (416, E12.6)

NPER Character of time phase

= 1 Burn phase

= 2 Shutdown phase

= 3 Periodic sequence of burn and shutdown

phases

NCH Mode of time scale

= 1/2/3 linear /logarithmic/ optional

LINP Origin of initial numbers of nuclides

= 1 Take values of previous phase

= 2 Calculate from initial element densities

NT Number of time steps (minimum 3)

TMAX Maximum time to be considered

Card 14: Format (2E12.6); only needed if NPER = 3

TBURN Duration of burn phase

TOFF Duration of shutdown phase

Card 15: Format (6E12.6); only needed if NCH = 3

TZ(I) Time interval boundaries (NT entries)

Note: TZ(1) = 0., TZ(NT) = TMAX

Note: Repeat section E data for each time phase.

3. THE PROGRAM AKTOUT

3.1 General remarks

The program AKTIV combines two disadvantageous features if applied to large problems. It needs a significant computer time which is mainly dependent on the number of intervals and the number of time phases to be calculated. Additionally, it produces a bulky amount of print output unless it is restricted to some kind of summary information. In-depth information should, however, be the usual purpose of time consuming computer runs.

To avoid these disadvantages, a special version called AKTOUT was developed. This program starts from the primary results calculated by AKTIV (i.e. the time dependent numbers of nuclides) and stored on tape and calculates all secondary information in a very fast computer run. This procedure allows the program AKTIV to be run only once for a problem. The separate use of AKTOUT allows information about the final results to be extracted step by step. This information is obtained in the same shape as from AKTIV. Additionally, plot output can be produced.

The structure of AKTOUT is shown in Fig.2.

The main change as compared with AKTIV is that it dispenses with the subroutine MATCAL while receiving from tape the information which was prepared in a previous AKTIV run. The remaining structure is completely equivalent as are the main subroutines. The only extension is the incorporation of the subroutine PLOT, which provides the plot output.

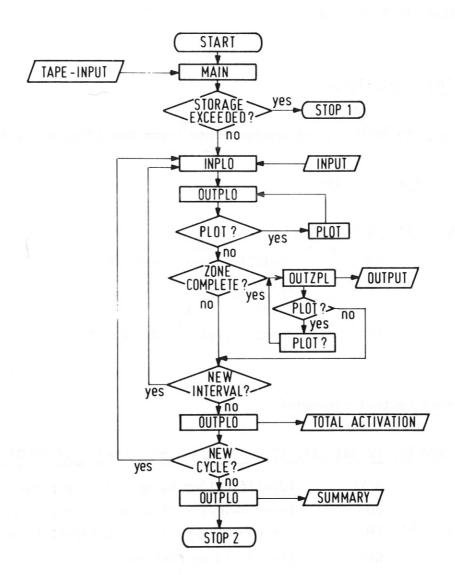


Fig. 2: Structure of the program AKTOUT

PLOT may be called in OUTPLO or OUTZPL, yielding a graphical display of results for an interval and zone, respectively. All results are plotted as functions of time and separately for the different time phases. Both axes may be chosen to be linearly or logarithmically subdivided. PLOT uses the IPP subroutine UNIPLT, which is a multi-purpose plotting routine and is not described here.

3.2 Input description

The input to AKTOUT is subdivided into three sections: A, B, and C.

A: General parameters

Card 1: Format (314)

NTC1 logical tape-no. for input

NOGE write summary

= 0/1 no/yes

NPLOT number of plots desired

B: Plot control parameters

Card 2: Format (I4, 2E12.6, 7I4); only needed if NPLOT \neq 0.

NCYC Identification number of time phase

To lower boundary of time interval to be plotted

TM upper boundary of time interval to be plotted

NPC plot is to be made for

= 1 interval

= 2 zone

NPCH results to be plotted

for NPC = 1

= 3 number of nuclides

= 4 activity per isotope

= 5 activity per element

= 6 activity per unit volume

= 7 weight per element

= 8 weight percentage per element

= 9 decay power per isotope

- = 10 decay power per element
- = 11 decay power per unit volume
- = 12 biological hazard potential per isotope
- = 13 biological hazard potential per element

for NPC = 2

- = 1 activity perisotope
- = 2 activity per element
- = 3 decay power per isotope
- = 4 decay power per element
- = 5 biological hazard potential per isotope
- = 6 total activity per zone
- = 7 total decay power per zone
- = 8 total biological hazard potential per zone

NR identification number of interval or zone

INTRN interpolation option

= 0/1/2/3 no/linear/quadratic/cubic

NTI scale of time axis

= 1/2 linear/logarithmic

NAK Scale of result axis

= 1/2 linear/logarithmic

NMUL number of curves per sheet (maximum 9)

Card 3: Format (1814); only needed if NPLOT \neq 0

NINT(I) Isotope or element identification numbers (NMUL entries)

Note: Repeat section B data NPLOT times.

C: Print control parameters

Card 4: Format (1814)

Output options for single intervals NSTEU(1) Specification of interval

NSTEU(2) Print options

- = 3 number of nuclides
- = 4 activity per isotope
- = 5 activity per element
- = 6 activity per unit volume
- = 7 weight per element
- = 8 weight percentage per element
- = 9 decay power per isotope
- = 10 decay power per element
- = 11 decay power per unit volume
- = 12 biological hazard potential per isotope
- = 12 biological hazard potential per element

Note: Repeat NSTEU(1) and NSTEU(2) for each print required.

At last give "0".

Card 5: Format (18 I4)

Output options for single zones.

NSTEU(1) Specification of zone

NSTEU(2) Print options

- = 1 activity per isotope
- = 2 activity per element
- = 3 decay power per isotope
- = 4 decay power per element
- = 5 biological hazard potential per isotope

Note: Repeat NSTEU(1) and NSTEU(2) for each print required.

At last give "0".

4. THE PROGRAM A K T I N

4.1 General remarks

Another method to save computer time for the program AKTIV is to reduce the size of a problem prior to starting the program AKTIV. This may be done using the program AKTIN which is constructed such as to reduce the number of intervals to be evaluated. The user has to specify how many intervals shall be summarized to form a new larger interval. AKTIN then calculates volume averaged fluxes for the new interval from those resulting from the transport calculation for the fine interval structure. It writes the new fluxes on tape which is subsequently used for input to the AKTIV run.

AKTIN reads the total input specified for the AKTIV run of the unreduced problem. Only a single card has additionally to be prepared containing the information about the reduction procedure. The program then provides a complete new input data set which is adapted to the reduced problem. This data set is produced as punch output and can be directly used as input for AKTIV.

4.2 Input description

Only one additional card has to be defined for input to the program AKTIN:

Card 0: Format (18 I4).

- IA first interval of the new macro-interval
- IE last interval of the new macro-interval

Note: Repeat this two-integer combination for each macro-interval to be defined.

IO = 0 characterizing the end of this card.

The remainder of the input is identical to that described in section 2.6.

ACKNOWLEDGEMENTS:

The authors gratefully acknowledge the many helpful discussions with W.H. Köhler, J. Ebberink and A. Merkel (Fa. Interatom) in the course of collecting and evaluating the necessary data. They wish to thank B.F. Maskewitz (RSIC) for her help in getting the cross-section data. They are also indebted to E. Fisser and J. Cox for assistance during the testing phase.

REFERENCES

- [1] Steiner, D.: "The neutron-induced activity and decay power of the niobium structure of a D-T fusion reactor blanket".

 ORNL-TM-3094 (1970).
- [2] Steiner D.: "The nuclear performance of vanadium as a structural material in fusion reactor blankets". Nucl. Fus. 14 (1974), 33-34.
- [3] Dudziak, D.J., Krakowski, R.A.: "Radioactivity induced in a theta-pinch fusion reactor". Nucl. Technol. 25 (1975), 32-55.
- [4] Badger, B. et al.: "UWMAK-I, a Wisconsin toroidal fusion reactor design". Univ. of Wisconsin, Report UWFDM-68 (Vol. I 1974, Vol. II 1975).
- Price, W.G., jr.: "Activation and afterheat in a fusion power reactor". MATT-106, 1973.
- Nigg, D.W., Davidson, J.N.: "The induced activity and decay power of the structure of a stainless steel fusion reactor blanket". Proc. 1st Top. Meet. on the Technol. of Contr. Fus., San Diego 1974.
- [7] Gruber, J.: "The activation of a fusion reactor blanket with low lithium inventory and a vanadium base alloy as structural material". HMI-B202 (1976).
- Powell, J.R. et al.: "Minimum activity blankets for commercial and experimental power reactors". IAEA Workshop on Fus. React. Des. Probl., Culham 1974.
- [9] Badger, B. et al.: "UWMAK-III, a high performance noncircular tokamak power reactor design". Univ. of Wisconsin, Report UWFDM-150 (1976).
- [10] Perry, R.T., Gorenflo, H., Dänner, W.: "INDRA, a program system for calculating the neutronics and photonics characteristics of a fusion reactor blanket". IPP 4/137 (Jan. 1976).

- [11] Raeder, J.: "Systemstudien für Fusionskraftwerke", Reaktortagung Mannheim 1977, 965-968.
- [12] Dänner, W.: "Nukleare Eigenschaften von Lithium-Edelstahl-Blankets", Reaktortagung Mannheim 1977, 993-996.
- [13] Bell, B.J., Adams, R.K.: "MATEXP, a general purpose digital computer program for solving ordinary differential equations by the matrix exponential method". ORNL-TM-1933 (Aug. 1967).
- Dänner, W.: "Fundamental material for stainless steel activation calculations". Projekt Systemstudien im Bereich Technologie des IPP, Internal Report No. 6 (April 1976).
- [15] Seelmann-Eggebert, W., Pfenning, G., Münzel, H.: "Karlsruher Nuklidkarte", 4. Auflage (1974), Gersbach und Sohn Verlag, München.
 - [16] Lieser, K.H.: "Kernchemie", pp 598-602, Verlag Chemie, GmbH, Weinheim/Bergstr.
 - [17] Erste Strahlenschutzverordnung vom 24.6.1960, Bundesgesetzblatt I, S. 430; Neufassung vom 22.10.1965, Bundesgesetzblatt I, S. 1653.
 - [18] A. Merkel: private communication
 - [19] Lederer, M., Hollander, J.M., Perlman, S.: "Table of isotopes". 6th ed., John Wiley and Sons, Inc., New York (1967).
 - [20] Radiation Shielding Information Center (ed.): "MONTAGE-400, 100-group neutron activation cross-section data for fusion reactor structure and coolant materials". DLC-33(Nov. 1976).
 - [21] Brockmann, H., Ohlig, U.: private communication