

Input description for BIOPATH

**Jan-Erik Marklund
Ulla Bergström
Ove Edlund**

Studsvik Energiteknik AB, 1980-01-21

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This report concerns a study which was conducted for the KBS project. The conclusions and viewpoints presented in the report are those of the author(s) and do not necessarily coincide with those of the client.

A list of other reports published in this series is attached at the end of this report. Information on KBS technical reports from 1977-1978 (TR 121) and 1979 (TR 79-28) is available through SKBF/KBS.

Abstract

The computer program BIOPATH describes the flow of radioactivity within a given ecosystem after a postulated release of radioactive material and the resulting dose for specified population groups.

The present report accounts for the input data necessary to run BIOPATH.

The report also contains descriptions of possible control cards and an input example as well as a short summary of the basic theory.

Performed within a joint research program in cooperation with SKBF/KBS.

<u>Table of contents</u>	Page
1. SUMMARY	2
2. GENERAL	3
2.1 Basic equations	3
2.2 Program versions	4
3. CONTROL CARDS	5
4. INPUT DATA	6
4.1 Main input data	6
4.2 Source data from file 4	25
4.3 Additional input data for BIOPATH-2	27
5. INPUT EXAMPLE	46
6. REFERENCES	47
7. EXHIBITS	49

1. SUMMARY

Two versions of BIOPATH, BIOPATH-1 and BIOPATH-2 have been defined. The main difference is that BIOPATH-2 can handle transfer matrices that vary with time. A short summary of the basic theory for BIOPATH is given in chapter 2.

The control cards needed to run the versions are discussed in chapter 3.

In chapter 4 the input data for both versions are presented. BIOPATH-2 needs some additional input data compared to BIOPATH-1, in order to specify the integration method to be used and the time dependence of the transfer coefficients.

An example of a possible set of input data is presented in chapter 5.

2. GENERAL

The program BIOPATH computes the activity and dose in a set of compartments after a release of a radioactive nuclide in one or more of the compartments. The word "compartments" denotes some part of the geosphere, e.g. the groundwater, a well, the atmosphere or the oceans.

2.1 Basic equations

The release and flow of the nuclide between the different compartments is described by the differential equation

$$(1) \quad \underline{y}' = A\underline{y} + \underline{g}$$

where $y_i(t)$ is the amount of the nuclide, and the source term $g_i(t)$ is the release rate of the nuclide in compartment "i" at time t. The matrix elements a_{ij} ($j \neq i$) are called transfer coefficients and give the increase rate of the nuclide in compartment "i" due to the presence of a unit amount of the nuclide in compartment "j".

Conservation of matter gives that

$$(2) \quad \sum_i y'_i = -\lambda \sum_i y_i + \sum_i g_i$$

where λ is the decay constant of the nuclide. This also follows from the condition

$$(3) \quad \sum_i a_{ij} = -\lambda \quad \text{or}$$

$$(4) \quad a_{jj} = -\lambda - \sum_{i \neq j} a_{ij}$$

(Note that the matrix A is read transposed by the input routines, so that the summation should be done horizontally and not vertically for the input data).

When the amounts of the nuclide are known, the activity and dose are computed through multiplication by appropriate factors.

The amount, activity and dose of the daughter nuclides is obtained in the same way, using the amount of mother nuclide times a decay factor as source term and using appropriate transfer coefficients and decay constant.

More details are given in /1/.

2.2 Program versions

Two versions exist, here named BIOPATH-1 and BIOPATH-2.

BIOPATH-1 uses the EISPACK subroutine package /2/ for solving the differential equation (1). It can only handle constant transfer coefficients. The version BIOPATH-2 may handle also transfer coefficients that vary with time. It uses the IMPEX and EULER integration routines /3,4,5,6,7/.

The IMPEX package has proved one of the best for solving stiff differential equations /8/.

(Whether a differential equation should be considered stiff or not depends on the ratio between the largest and smallest eigenvalue to the matrix A in (1), in other words involving processes with time-scales which differ by many orders of magnitude. This is often the case for BIOPATH problems).

3. CONTROL CARDS

The control cards to be used depend to a great extent on the user and on the computer being used. In exhibit 1 is shown one example for the CYBER 172 installation at STUDSVIK. The example shows one submit file SUBIO, that uses the control card file BIOPATH in order to compute the results and another submit file SUPLOT, which plots the information saved on TAPE20. Both SUBIO and SUPLOT presently reside on the archive-file OABIO4 which may be attached by the control card:

```
CALL,BIOPATH,L=JEM(VERS=OABIO4)
```

The control card file BIOPATH, which is shown on exhibit 2 resides on the procedure library under user=JEM. The file BIOPATH presupposes that common input data, source data for BIOPATH-1 and additional data for BIOPATH-2 are stored on indirect access permanent files named DATA, SOURCE and DIMP respectively.

The control card file KONTO, which is used both by SUBIO and SUPLOT contains normal accounting and controlling cards:

```
/NØSEQ  
JOB,T100.NAME ADDRESS  
USER,uuu,PW.  
CHARGE,xxxxx,yyy.
```

(Here uuu,PW, xxxxx and yyy depend on user specification).

4. INPUT DATA

The input routines have been compiled from different sources, therefore the principles used are not the same for all data. The input data may be subdivided into three different groups

- Main input data
- Source data from file 4 (only BIOPATH-1)
- Additional data for BIOPATH-2

Below follows a detailed description of the data belonging to each of these groups.

4.1 Main input data

The main input data is read either from file 1 or from file input, which normally are equivalent. The format is normally free. Exceptions are cards of type 1.1, 1.2, 1.3 and 1.21.

Note that contrary to standard assignments all variables beginning with "M", are real except the variables MATID and MODE. Also the variables KD(17,17), and KONC are real. The variables ACTONLY, ARITM and TOTMOD are integers.

The input data is read by the following 31 READ statements

Type_1.1 Format: 8A10

READ(1,123) TEXT

TEXT : Some special heading for identification of
 the calculation

Ex: U234/RA226 ALT1 KBS1A07 15/2 1979

Type_1.2 Format: A6,5I2, 1PE10.7,1PE10.2

READ(1,304) TIDUNIT,LOKAL,NHAV,KBS,ACTONLY,NPLOT,
 CONVFAC,TRANFAC

TIDUNIT : The time unit in which you want to express
 doserates

Ex: ' MONTH', ' YEAR', ' DAY', ' HOUR', ' '

(Blank means year)

LOKAL : The type of alternative you want to choose
 in the calculation

Ex: 1 = Alternative 1

 2 = Alternative 2

 3 = Alternative 3

NHAV : This number determines if you want to cal-
 culate the consequences of an accident with
 a short release time or not

Ex: 1 = Accident with short release time

 0 = Accident without a short release
 time

KBS : This number controls the collective dose
 calculation

Ex: 2 (Normal)

ACTONLY : If you only want to calculate the activity in the different compartments at different times you are able to control that with this number

Ex: 1 = Only the activity is calculated
2 = Also the dose is calculated

NPLOT : With this number you are able to save and plot the results

Ex: 0 = Saved and plotted
1 = Only saved
2 = Neither saved nor plotted

CONVFAC : A conversion constant

Ex: 1.0E09

TRANFAC : Another constant which expresses the fraction of the decay of a parent, that generates the daughter studied in the calculation.

Ex: 0.57 (SR91 → y91m)

Type_1.3 Format: A10

READ(1,1010) KAELLA

KAELLA : Identification. Presently not used by the program.

Type_1.4 Format: Free

READ(1,*) MA, (MV(J), J=1,3), (MM(J), J=1,3), (MK(J), J=1,3),

1 (MC(J), J=1,3), (MR(J), J=1,3), (MG(J), J=1,3),

2 (MF(J), J=1,4), (BV(J), J=1,3)

MA : The inhalation rate of a normal human being

Unit: (M**3/YEAR)

Ex: 9438. (25.8M**3/DAY)

(MV(J),J=1,3): The individual annual consumption of drinking water.

Unit: (Litres/year)

Ex: 438., 0., 438. (1.2L/DAY, 0.L/DAY, 1.2L/DAY)

(MM(J),J=1,3): The individual annual consumption of milk.

Unit: (Litres/year)

Ex: 183., 0., 131. (0.5L/DAY, 0.L/DAY, 0.36L/DAY)

(MK(J),J=1,3): The individual annual consumption of meat.

Unit: (Kg/year)

Ex: 52.5, 0., 45.6 (1 kg/week, 0. kg/week, 0.8 kg/week)

(MC(J),J=1,3): The individual annual consumption of cereals.

Unit: (Kg/year)

Ex: 61.1, 0., 118. (0.17kg/day, 0.kg/day, 0.32kg/day)

(MR(J),J=1,3): The individual annual consumption of rootfruits.

Unit: (Kg/year)

Ex: 83.2, 0., 82. (1.6kg/week, 0.kg/week, 1.57kg/week)

(MG(J),J=1,3): The individual consumption of vegetables.

Unit: (Kg/year)

Ex: 121., 0., 118. (10kg/month, 0.kg/month, 9.8kg/month)

(MF(J),J=1,4): The individual annual consumption of fish

Unit: (Kg/year)

Ex: 50., 20., 22., 50.

(BV(J),J=1,3): The daily average irrigation rate.

Unit: (L/(M**2*DAY))

Ex: 0.4, 0., 0.

The three numbers in the arrays above corresponds to the regional, intermediate and global ecosystems respectively.

Type_1.5 Format: Free

1 READ(1,*) MVK,MKB,TAETB,TAETG,ME,DEP,TIM1,TIM2,TIM3,
TIM4,MEB,MEV

MVK : The daily average consumption of water for
 a cow.

Unit: (L/DAY)

Ex: 30.0

MKB : The daily average consumption of foodstuff
 for a cow.

Unit: (Kg/DAY)

Ex: 30.0

TAETB : The average value of foodstuff produced per
 squaremeter.

Unit: (Kg/M**2)

Ex: 0.03

TAETG : The average value of vegetables produced
 per squaremeter

Unit: (Kg/M**2)

Ex: 1.5

ME : The annual consumption of eggs

Unit: (Number/year)

Ex: 220.

DEP : Deposition velocity

Unit: (M/DAY)

Ex: 259.

- TIM1 : The annual number of hours used for bathing
Unit: (hours/year)
Ex: 30.
- TIM2 : The annual number of hours used for sunbath
on the beach
Unit: (hours/year)
Ex: 90.
- TIM3 : The annual number of hours used for work
with fishing tackle
Unit: (hours/year)
Ex: 90.
- TIM4 : The annual number of hours during which you
are exposed to radiation from contaminated
ground
Unit: (hours/year)
Ex: 8760.
- MEB : The daily consumption of cereals for a hen
Unit: (kg/day)
Ex: 0.07
- MEV : The daily consumption of water for a hen
Unit: (L/day)
Ex: 0.18

Type_1.6

Format: Free

READ(1,*) REAM,REMM,BADM,STRM,FISKM,MARKM

- REAM : The internal weighted total body dose conversion factor for inhalation for the parent nuclide
Unit: (rem/ci)
Ex: 2.71E06 (U234)
- REMM : The internal weighted total body dose conversion factor for ingestion for the parent nuclide
Unit: (rem/ci)
Ex: 1.14E05 (U234)
- BADM : The external dose conversion factor for bathing for the parent nuclide
Unit: (rem/hour)
Ex: 1.4
- STRM : The external dose conversion factor for the parent-nuclide due to visit on a contaminated beach
Unit: (rem/hour)
Ex: 0.6
- FISKM : The external dose conversion factor for the parent-nuclide due to work with contaminated fishing tackle
Unit: (rem/hour)
Ex: 0.003
- MARKM : The external dose conversion factor for the parent-nuclide due to visit on the contaminated ground
Unit: (rem/hour)
Ex: 0.006

Type_1.7

Format: Free

READ(1,*) FVM,FCM,FGM,FRM,FFM,FMM,FKM,FEM

- FVM : The concentration factor (soil-foodstuff)
for the parent nuclide
Unit: (Dimensionless)
Ex: 2.5E-03 (U234)
- FCM : The concentration factor (soil-cereals) for
the parent nuclide
Unit: (Dimensionless)
Ex: 2.5E-03 (U234)
- FGM : The concentration factor (soil-vegetables)
for the parent nuclide
Unit: (Dimensionless)
Ex: 2.5E-03 (U234)
- FRM : The concentration factor (soil-rootfruits)
for the parent nuclide
Unit: (Dimensionless)
Ex: 2.5E-03 (U234)
- FFM : The concentration factor (water-fish) for
the parent nuclide
Unit: (Dimensionless)
Ex: 10., 10., 10.
- FMM : The ratio between the activity concentration
for the parent nuclide in 1 liter milk and
the daily ingested amount of the activity
by a cow
Unit: (Day/l)
Ex: 5.0E-04 (U234)

FKM : The ratio between the activity concentration for the parent nuclide in 1 kg meat and the daily ingested amount of activity by a cow
Unit: (day/kg)
Ex: 5.0E-03 (U234)

FEM : The ratio between the activity concentration for the parent nuclide in one egg and the daily ingested amount of activity by a hen
Unit: (day/egg)
Ex: 1.0E-04 (U234)

Type_1.8 Format: Free

READ(1,*) READ,REMD,BADD,STRD,FISKD,MARKD

READ : The internal weighted total body dose conversion factor for inhalation for the daughter nuclide
Unit: (rem/ci)
Ex: 2.71E06 (RA226)

REMD : The internal weighted total body dose conversion factor for ingestion for the daughter nuclide
Unit: (rem/ci)
Ex: 1.14E05 (RA226)

BADD : The external dose conversion factor for bathing for the daughter nuclide
Unit: (rem/hour)
Ex: 1.4

STRD : The external dose conversion factor for the daughter nuclide due to visit on a contaminated beach
Unit: (rem/hour)
Ex: 0.6

FISKD : The external dose conversion factor for
the daughter nuclide due to work with
contaminated fishing tackle
Unit: (rem/hour)
Ex: 0.003

MARKD : The external dose conversion factor for
the daughter nuclide due to visit on the
contaminated ground
Unit: (rem/hour)
Ex: 0.006

Type_1.9

Format: Free

READ(1,*) FVD,FCD,FGD,FRD,FFD,FMD,FKD,FED

FVD : The concentration factor (soil-foodstuff)
for the daughter nuclide
Unit: (Dimensionless)
Ex: 3.1E-04 (RA226)

FCD : The concentration factor (soil-cereals) for
the daughter nuclide
Unit: (Dimensionless)
Ex: 3.1E-04 (RA226)

FGD : The concentration factor (soil-vegetables)
for the daughter nuclide
Unit: (Dimensionless)
Ex: 3.1E-04 (RA226)

FRD : The concentration factor (soil-rootfruits)
for the daughter nuclide
Unit: (Dimensionless)
Ex: 3.1E-04 (RA226)

- FFD : The concentration factor (water-fish)
for the daughter nuclide
Unit: (Dimensionless)
Ex: 15., 50., 50.
- FMD : The ratio between the activity concentra-
tion for the daughter nuclide in 1 liter
milk and the daily ingested amount of the
activity by a cow
Unit: (day/l)
Ex: 8.0E-03 (RA226)
- FKD : The ratio between the activity concentra-
tion for the daughter nuclide in 1 kg
meat and the daily ingested amount of
activity by a cow
Unit: (day/kg)
Ex: 9.0E-04 (RA226)
- FED : The ratio between the activity concentra-
tion for the daughter nuclide in one egg
and the daily ingested amount of activity
by a hen
Unit: (day/number of egg)
Ex: 1.0E-06 (RA226)

Type_1.10

Format: Free

READ(1,*) REGF,FISKF,BADF,REDF,FINT

REGF : The number of inhabitants, who are living
in the regional area
Ex: 18000

FISKF : The number of inhabitants, who are bathing
in the regional area
Ex: 1.0E07

BADF : The number of fishermen, who are working
with fishing tackles in the region
Ex: 1000

REDF :

FINT : Critical group regarding fish consumption
in the intermediate and regional ecosystem
Ex: 1200

Type_1.11

Format: Free

READ(1,*) W,MF,A,(KONC(I),I=1,3)

W : The capacity of the well (superficial ground
water
Unit: (l/year)
Ex: 60000

MF : The mass of the soil in the local area
Unit: (kg)
Ex: 2.0E07

A : The size of the local area

Unit: (M**2)

Ex: 25000

(KONC(I),
I=1,3) : Factors with which you are able to choose
how the activity are divided between the
different compartments

Unit: (Dimensionless)

Ex: 1.0 1.0 1.0

Type_1.12 Format: Free

READ(1,*) (IA(I),I=1,7)

(IA(I),I=1,7): These numbers are the indices of the
compartments included in the regional
ecosystem. The value of the numbers
depends on the choice of the dose equa-
tions and are specific for every separa-
te ecosystem

Ex: 5,2,4,6,6,7,4

Type_1.13 Format: Free

READ(1,*) (IB(I),I=1,7)

(IB(I),I=1,7): Similar numbers as for type 1.12, but
for the intermediate ecosystem

Ex: 5,2,4,6,8,9,4

Type_1.14 Format: Free

READ(1,*) (IC(I),I=1,7)

(IC(I),I=1,7): Similar numbers as for type 1.12, but
for the global ecosystem

Ex: 10,16,15,16,11,17,15

Type_1.15 Format: Free

READ(1,*) (ID(I),I=1,7)

(ID(I),I=1,7): Similar numbers as for type 1.12, but
for the local ecosystem

Ex: 1,7,0,0,0,0,0

Type_1.16 Format: Free

READ(1,*) (M(I),I=1,17)

(M(I),I=1,17): The masses of the compartments

Unit: (kg)

Ex: 2.5E8,8.6E11,1.0E7,2.5E12,4.8E14,
1.25E10,5.0E8,2.2E16,3.7E13,4.4E18,
2.0E19,1.4E21,3.6E16,1.8E15,4.4E17,
6.0E19,2.0E15

Type_1.17 Format: Free

READ(1,*) STRTT,FIN

STRTT : The earth population at the time of the
start of the release.

Ex: 6.0E09

FIN : The assumed upper limit of the earth popula-
tion

Ex: 1.0E10

Type_1.18 Format: Free

READ(1,*) ARITH,TOTMOD,TMAX

Note: These values are not used when IMPEX or EULER is used.

The effect of leaking radioactivity in the ecological systems wants generally to be predicted at different times for a long time in the future. The different times can be given in two ways:

1. In arithmetic series
2. In geometric series

ARITH : This number means how many arithmetic series you want to use.

Ex: 2

TOTMOD : This number means the total number of series (arithmetic+geometric) you want to use

Ex: 3

TMAX : This number means the time at which you want to stop the calculation.

Ex: 9.37E06

Type_1.19 Format: Free

READ(1,*) (STRT(I),STEG(I),I=1,ARITH)

Note: These values are not used when IMPEX or EULER is used

(STRT(I),
STEG(I),

I=1,ARITH): These numbers means the start times and time steps for the arithmetic series

Ex: 0.,8.98E06,8.98E06,2.0E03

Type_1.19.2 Format: Free

This card is read only if ARITH=TOTMOD in the card type 1.18 (see before).

READ(1,*) (NSTEP(I),STRT(I),FINISH(I),I=NNN,TOTMOD)

NSTEP(I) means the number of the time steps between the start time STRT(I) and final time FINISH(I) in the geometric serie I.

Type_1.20 Format: Free

READ(1,*) NDEL,JJU,KTID

NDEL, : These three numbers have to do with the
JJU, outputlist in the calculation
KTID

Ex: 2,10,2

Type_1.21 Format: 8A10

READ(1,123) (COMID(I),I=1,N)

COMID : This vector means only the names of the different compartments

Ex: Grundvatt1Grundvatt2Grundvatt3Jord

Atmsreg	Ytvatten	Sediment	Östersjön
Ösjösed	Atmosfär	Wellmixed	Deep sea
Sediment2	Biota	Jord	Grungvglob
Sediment1			

Type_1.22 Format: 8A10

READ(1,123) (TIT(i),i=1,8)

TIT : Identification, used only when printing
 input data.

Ex: TH230+U234,KBS.

Type_1.23 Format: 8A10

READ(1,123) MATID

MATID : Identification, used only when printing in-
 put data.

Ex: UDATA

Type_1.24 Format: Free

READ(1,*) NEKV,ALMOD,EPS

NEKV : Number of equations (= compartments)

Ex: 17

ALMOD : λ , i.e. $\ln 2/T^{1/2}$, where $T^{1/2}$ = half-life,
 for the parent nuclide.

Ex: 2.13276E-5 (U235)

EPS : Constant, used in SOURCM and SOURCD (only
 EISPACK), in order to check if the quotient
 between two numbers is close to 1. It is used
 to determine the accuracy in the calculation.

Ex: 1.E-6

Type_1.28, 1.29

These data are read only if DOT= .TRUE. and are similar to type 1.26 and 1.27, except that they refer to the daughter nuclide instead of the parent nuclide.

4.2 Source data from file 4 (BIOPATH-1)

When the EISPAC -version of BIOPATH is used, the source data for the mother are read from file 4 two times, first in SOURCM and then in CITO. In SOURCM the data are used to compute the source term of the differential equation, in CITO to compute the release of activity for printing purposes and for storage in the vector $TOT(i), i=1,2,\dots,NSP-1$.

The input is read through the following four READ statements. The format is free. Cards of type 2.2 to 2.4 are read only if $NCG > 0$.

Type_2.1

READ(4,*) NCG

NCG : Number of releases

Ex: 1

Type_2.2

READ(4,*) (IFF(i),i=1,NCG)

IFF(i) : The identification number(s) of the release compartment(s).

Ex: 1

Type_2.3

READ(4,*) NG(i)

NG(i) : Number of time table entries for release i

Ex: 4

Type_2.4

READ(4,*) (TG(i,j),G(i,j),j=1,NG)

TG(i,j) : Time

G(i,j) : Corresponding release

Ex: See ref /9/

The values form a time-table in which linear interpolation is made.

Note that the first time in the time entries, when the release is different from zero must correspond with a time in the time entries, when the activity concentration is calculated given in card type 1.19.1 and 1.19.2.

4.3 Additional input data for BIOPATH-2

Input data are read from file 7. An example is shown in exhibit 3. The input format is either free or based on module 4, i.e. I4 and E8.0, except for the A-formats and for the data under directive PARAMETERS(80I1).

Input is controlled by directives. Only the first three characters of each directive are significant. The rest of the card may be used for comments on input data. The directives presently available are:

1. RESTART (Presently not used)
2. TITLE (Only output)
3. LIMITS
4. INTEGRATION
5. IMPLICIT PARAMETERS
6. LONG (Presently not used)
7. SOURCES
8. MATRICES
9. VARIATIONS
10. AIJ
11. INPUT FILE FOR SOURCE DATA
12. REWIND FILE 7
13. NO REWIND OF FILE 7
14. PRESENT DATA
15. OUTPUT PARAMETERS (Only for test purposes)
16. PARAMETERS (Only for test purposes)
17. REST (Only for test purposes)
18. STOP (Mainly for test purposes)
19. START (Only directive card)
20. END (Only directive card)

Only directives 2,4,7,8,9,10,19 and 20 are normally used. The input data up to a START-directive constitute a data set which is considered by the program as one unit. As a rule the sequence of directives within a data set is immaterial, with some exceptions:

- a) If restart data are used to define the start conditions, the RESTART directive should precede the other directives.

- b) The START directive is the last directive in each data set and an END directive, which terminates the integration, should be placed after the last START directive for each nuclide (mother and daughter(s)).

The cards following the directive are described below.

4.3.1 _RESTART_directive (Presently not used)4.3.2 _TITLE_directive Format 13A6,A2

An arbitrary title could be given. The program will then print date and time of run.

4.3.3 _LIMITS_directive

Upper limit for time usage (lowest of this limit and time limit set by JOB-card is used)

Type_1 Format E8.0

Pos 1-8: t_{\max}^C = execution time limit (In decimal CP-seconds).

Standard value = 1000 s (Initially set by the program).

4.3.4 _LONG-TIME_MODEL (Presently not used)

Type_1

Pos 1-4: ILO = Long-time parameter
-1 means not long-time model
1 means use long-time model with old values of parameters
2 as 1, but read new values of long-time parameters

Type_2 Long-time parameters

Pos 1-8: HKRIS = maximum IMPEX time-step allowed across critical points. Standard value = 10s.

Card 2 is read only if ILO=2.

4.3.5 INTEGRATION_card Format: 4I4,8E8.0

Here the conditions affecting integration routines are determined.

Type

- Pos 1-4: Integration method:
- 1 means Euler method
 - 2 means Explicit method (DIFSYS)
 - 3 means Implicit method (IMPEX)
 - 4 means Implicit method (GEAR, only some versions)
- Pos 5-8: n_s . If Euler integration is used each n_s timestep is printed. If other methods are used each n_s result is written into the restart file 11. ($n_s=0$ or blank gives the same output as $n_s=1$).
- Pos 9-12: i_{hit} . If $i_{hit}=1$, no effort is made by the implicit method to hit the final time specified.
- Pos 13-16: Not used.
- Pos 17-24: t_{start} seconds. Starting time. Ignored at restart.
- Pos 25-32: t_{end} seconds. Final time. The executions stops when $t > t_{end}$.
- Pos 33-40: Δt seconds. Initial timestep. When using implicit method Δt should be less than $(t_{end}-t_{start})/4$, or else the step will be set to $(t_{end}-t_{start})/4$.

Pos 41-48: ϵ = max allowed global error. Ignored for EULER integration.

Pos 49-64: Not used.

Pos 65-72: Δt_{\min} = minimum timestep for implicit integration. Integration is cut off if IMPEX tries to use timesteps shorter than Δt_{\min} .

Pos 73-80: Δt_{\max} = maximum timestep for implicit integration. If no value is given, the program uses $\Delta t_{\max} = 1000 * \text{the value given in Pos 33-40}$.

4.3.6 _IMPLICIT PARAMETERS

The directive is used to modify the procedures used to compute the implicit solution. Pos 1-8 are not used in BIOPATH. Normally the standard values initially set by the program are sufficient.

Card_1

Format: 8I4,3E8.0

Pos 1-4: m_{fast} = method used for jacobian elements.

Pos 5-8: JACOB = method used during jacobian computation.

Pos 9-12: n_{ero} . If $ero_{min} < ero < ero_{max}$, n_{ero} iterations are allowed before the jacobian is recomputed.

Pos 13-16: m_{recomp} = maximum number of recomputations of jacobians for each point.

Pos 17-20: m_{iter} = maximum number of iterations for each point

Pos 21-24: m_{stv} = method used for start value computation

0 means quadratic extrapolation through three last points

1 means linear extrapolation by least square points fit through three last points

2 means linear extrapolation through two last points

3 means linear extrapolation through last and third last point

Note, that the points used are by necessity un-smoothed, and may therefore contain relatively great errors of different signs.

Pos 24-28: n_{rmp} = number of old jacobians saved (0 or 1). Usually 0 should be used.

Pos 29-32: M_{inc} = minimum number of steps until increase of stepsize is allowed.

Pos 33-40: β_{rmp} = jacobian underrelaxation factor. If $\beta_{rmp} > 0$ instead of the new jacobian, a weighted average between the old jacobian and the new is used:

$$J = (1 - \beta_{rmp}) J_{new} + \beta_{rmp} J_{old}$$

Pos 41-48: ero_{min} = acceptable inverse convergence rate. If $ero < ero_{min}$, the old jacobian will be used.

Pos 49-56: ero_{max} = not acceptable inverse convergence rate. If $ero > ero_{min}$, a new jacobian will be computed.

Pos 57-64: BIWF = Factor for computing error weights
 in implicit method $w_i = \text{BIWF}/|y_i| +$
 $+ (1-\text{BIWF})\min(w_i, 1/|y_i|)$

The inverse convergence rate is computed as

$$\text{ero} = \text{SQRT}((\sum (w_i \Delta y_i^n)^2) / (\sum (w_i \Delta y_i^{n-1})^2))$$

If convergence is not achieved within the iterations specified by m_{recomp} and m_{iter} , the procedure backs one steps and restarts with half the earlier stepsize.

If no data have been given, the following values are used:

0, 0, 0, 8, 2, 0, 0, 0, 0., 0.2, 0.2, 0.

4.3.7 _SOURCES Format: Free

Reads source data for mother nuclide.

Card_1

NCG : Number of compartments containing sources
($0 \leq \text{NCG} \leq 17$).

Card_2

IFV(i), i=1, NCG: Compartment indices

Card_3A

NG(i) : Number of time table entries for source i

Card_3B

TGV(j,i), GV(j,i), j=1, ..., NG(i): Table containing
time and source strength for source i.

Data of type 3A and 3B are repeated NCG times in order
3A, 3B, 3A, 3B etc corresponding to i=1, 2, ..., NCG.

4.3.8 MATRICES Format: Free

Under this directive two matrices AI1(i,j) and AI2(i,j) are specified.

Card_1

JUA1 = File index for AI1
 = -2 means AI1(i,j) is set = AD(i,j)
 -1 - " - AM(i,j)
 0 means no action
 >0 means READ(JUA1,*) ((AI1(i,j),i=1,N),
 j=1,N)

JUA2 = Same action as JUA1, but for AI2 instead
 of AI1.

KUA1 = Treatment index for AI1
 >0 means set AI1(i,i) such that $\sum_j AI1(i,j)=0$
 <0 means set
 AI1(i,i) = -DCM (KUA1= -1),
 AI1(i,i) = -DCD (KUA1= -2) or
 AI1(i,i) = $\sum_j AI1(i,j)$ (KUA1< -2)
 Then set AI1(i,j)=0 for j≠i.

KUA2 = Same action as KUA1, but for AI2.

Card_2_and_3

These data are read only if JUA1 > 0 or JUA2 > 0, see above.

Comment: By using e.g. KUA1=1 and KUA2=-3, AI1 will contain the transfer coefficients and AI2 the decay constant. It will then be easy to modify AI1 without affecting the decay constant.

4.3.9 VARIATIONS Format: FreeCard 1

NVA = Number of new models of variation for the
 coefficient matrix A(i,j)

IVAA = Index of the model of variation applied to
 AI1(i,j) and AI2(i,j). If IVAA=0, A(i,j)
 is set to AI1(i,j).

If NVA \leq 0, data of type 2 and 3 are not read.

Card 2

i = Index of the model of variation to be speci-
 fied. First value =1 and max value =9. Must
 be increasing with "1" for each new model.
 (It is though possible to do e.g. in the
 following way:

 First specify models 1, 2, 3, 4. Then after
 some time change models 3 and 4 and add
 models 5, 6, 7 by specifying models 3, 4, 5,
 6, 7 etc. This could be a way to overcome
 the limitation to 9 values.)

MEVA(i) = Method of variation (see below and exhibit 2).
 (0 \leq MEVA(i) \leq 6 specifies the value of FA1).

FA2M(i) = Method for FA2
 <0 means FA2 = 1-FA1
 \geq 0 means FA2 = FA2M(i)

TA1(i) = Start time for periodical variations
 (Methods MEVA(i)=1,2 or 3).

PERIOD(i) = Length of period (Only valid for
MEVA(i)=1,2 or 3)

NT(i) = Number of table values.
NT(i) \geq 2 if MEVA(i) = 4 or 5.
NT(i) = 0 for other values of MEVA(i).

Card_3

These data are read only when MEVA(i) = 4 or 5. The data define a time table for the factor of variation.

TAA(L) = Time entry

TAB(L) = Corresponding value of FA1.

The data are repeated NT(i) times in the order TAA(1), TAB(1), TAA(2), ..., TAB(NT(i))

Methods of variation (Compare exhibit 3)

The following are allowed values of M=MEVA(i):

M=0 means FA1=1

M=1 means stepwise periodicity:

$$FA1=1 \text{ for } TA1+n \cdot DTA12 \leq t < TA1+(n+0.5)DTA12$$

$$FA1=0 \text{ for } TA1+(n+0.5)DTA12 \leq t < TA1+(n+1)DTA12$$

M=2 means linear periodicity, i.e. linear interpolation between

$$\left. \begin{array}{l} FA1=1 \text{ for } t=TA1+n \cdot DTA12 \\ FA1=0 \text{ for } t=TA1+(n+0.5)DTA12 \end{array} \right\} n=0,1,\dots$$

M=3 means sinusoidal periodicity:

$$FA1 = [\cos[(t-TA1) \cdot 2\pi / DTA12] + 1] / 2.$$

- M=4 means that $FA1 = TAB(L)$ for $TAA(L) \leq t < TAA(L+1)$
(Compare cards of type 3 above).
- M=5 means that FA1 is obtained through linear interpolation in the table defined by TAA(L), TAB(L).
- M=6 means that FA1 is obtained by a user-supplied function FA1F(META,T)
- M \geq 7 means that $A(i,j)$ and $\partial(A(i,j))/\partial y$ are computed by user supplied subroutines UF(M,17,T,A) and UDFDY(M,17,T,Y,A) (Compare subroutines VARA and DFDY).

4.3.10 AIJ-variations Format: Free

Allows different a_{ij} to have different types of variation. JUN is presently file 7.

Card_1 = READ(JUN,*)NAIJ

NAIJ = Number of a_{ij} with separate variations.
If NAIJ \leq 0 cards of type 2 are not read,
and any former specification of AIJ-varia-
tions is cancelled.

Cards_2ff = READ(JUN,*)j,i,m_{ij},a_{ij}⁽¹⁾,a_{ij}⁽²⁾

j = Index for A(i,j)

i = Index for A(i,j) i.e. indices for transport
coefficient from compartment j to compart-
ment i.

m_{ij} = Index of any of the models specified under
directive variations

a_{ij}⁽¹⁾ = New value corresponding to AI1(i,j)

a_{ij}⁽²⁾ = New value corresponding to AI2(i,j)

$a_{ij}(t)$ is set to $FA1 \cdot a_{ij}^{(1)} + FA2 \cdot a_{ij}^{(2)}$, where FA1 and
FA2 are determined by MEVA(m_{ij}) and t.

The input data of type 2 are repeated NAIJ times.

Note that

a) The action corresponding to this directive is
applied after any other variation specified, i.e.
it is possible to specify one overall variation
using AI1 and AI2 and then modify it for certain
 a_{ij} 's by the present directive.

b) The diagonal term is automatically modified in a
consistent way, i.e. $\Delta a_{jj} = - \Delta a_{ij}$

4.3.11_ INPUT FILE Format: Free

|J30| = New input file for source data. If positive the file is rewound. (Until this card is read, TAPE 7 is used for source data to version BIOPATH-2)

4.3.12_ REWIND_RESTART_FILE (Presently not used)

No cards needed except directive. The result is that the restart output file (FORTRAN unit 11) is rewound after each creation, i.e. only the latest restart file created will be available. The directive is suitable when restart data is saved on expensive media.

Warning! If the run terminates while writing restart data, the restart file will be unusable.

4.3.13_ NO_REWIND_OF_RESTART_FILE (Presently not used)

No cards except directive. The directive is needed only for terminating the effect of the preceeding directive, since standard is "no rewind".

4.3.14_ PRESENT DATA

No cards except directive. Gives an account of the data presently used.

Note: This is an exception from the rule that action takes place only after reading START directive.

4.3.15_ OUTPUT_PARAMETERS (Presently not used)

Card_1 Format: 40I1

Pos 1-40: K_i $i=1,40$ (usually 0 or 1)

4.3.16 PARAMETER-card Format: 80I1

This card is mainly used by the programmer in order to get more information about program behaviour.

Card_1

Pos 1 : not used

" 2 : =1 gives output of time T in RECOMP

" 3 : not used

" 4 : not used

" 5 : =1 gives output of T and y entering PVAL

" 6 : >0 gives some output for MOTHER in subroutine
SOURCE (Number of lines per call = P6+1)

" 7 : As P6, but for DAUGHTER

" 8 : Test output in subroutine VARA

" 9 : - " -

" 10 : - " -

" 11 : - " -

" 12 : - " -

" 13 : Not used

" 14 : Not used

" 15 : >0 gives output of DY(i), i=1, min(10*P15, N)
in subroutine F

" 16-22: Not used

" 23 : >0 means output in LONG onto file = P23

" 24 : - " - SMOTEX onto file = P24

" 25 : >0 means output in KRIS

- Pos 26 to 31: Not used
- Pos 32 and 33: Gives some output in COPRIN
- Pos 34 to 41: Not used
- Pos 42 : =1 gives output of ϵ and T in routine
ITERAT.
=2 gives output of ϵ , T and of IT, AMAX
and ERO for each iteration in routine
ITERAT.
- Pos 43 : =1 gives output of F1(i), SW(i), W(i),
i=1,N in routine ITERAT.
- Pos 44 : =1 gives output of Jacobian and iteration
matrix in routine RECOMP.
- Pos 45 : =1 gives output of Z(i), i=1,N with format
1P10E11.3
=2 gives output of Z(i), i=1,N with format
1P8E14.6 (routine ITERAT).
- Pos 46 to 49 : Not used
- Pos 50 : Used in the routine FIMPX3 to control
variation of stepsize h:
0 and 1 means variation of h allowed
2 and 3 means constant h
- Pos 51 : =0 or 2 means no trace
=1 means trace of implicit computation
(routine IMPLIC)
- Pos 52 : =1 gives output of IGIT etc on unit 6
(implicit method, routine COPRIN)
- Pos 53 : =1 gives output of y(i), i=1,N on unit 6
=2 gives output of y(i), ERR(i), i=1,N on
unit 6 (implicit method, routine COPRIN)

Pos 54 to 60: Not used

Pos 61-80 are used to gather information on number of calls to different routines. The figures printed represent the number of calls since last time directive PARAMETERS was read. They are printed in the following order:

Pos 61 : Not used

Pos 62 : RECOMP

Pos 63 and 64: Not used

Pos 65 : FVAL

Pos 66 : PRINT

Pos 67 : F

Pos 68 to 71: Not used

Pos 72 : DFDY

Pos 73 : ITERAT

Pos 74 to 80: Not used

4.3.17 TEST

Presently not used.

4.3.18 STOP

Causes an immediate end of execution. Mainly used for test purposes.

4.3.19 START

No cards except directive.

Execution will start, taking into consideration all data up to START directive. If corrections have been made on input data the latest values submitted will be used.

4.3.20 END

No cards except directive.

Will cause a normal end of integration. Used to terminate integration for each nuclide (Mother, daughter).

5. INPUT EXAMPLE

Exhibit 4 shows an example of input data consisting of two files DNP237 and SNP237 respectively.

In this example the dose rates caused by continuous release of the isotope Np237 are calculated as a function of time. More detailed information about the input parameters is possible to get in the input data description, chapter 4 in this report.

The SNP237-file is the release data.

The DNP237-file consists of nuclide specific data among other data.

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7. EXHIBITS

The following pages contain the figures:

1. Examples of possible control cards
2. Procedure file BIOPATH
3. Methods of variation for FA1 (functions related to the time dependant transfers)
4. Input example

SUBIO

```
1  
2  
3 /JOB  
4 /READ KONTO  
5 CALL,BIOPATH,L=JEM(VERS=2,DATA=DU235,SOURCE=SDU235,INT=DIMP,REP=YES)  
6 /READ STOP  
7 /EOR  
8  
9  
10 /EOF
```

SUPLOT

```
11  
12  
13  
14 /JOB  
15 /READ KONTO  
16 ATTACH,OLDARC=OABIO4.  
17 ARCSEL.RPLOT  
18 GET,TAPE20.  
19 * PLOT RESULT  
20 REWIND(TAPE20)  
21 FILE,TAPE40,RT=K,RT=F,R9=1,FL=1320,MBL=1320.  
22 LDSET(FILE=TAPE40,LIB=PLOTLIB)  
23 RPLOT.  
24 LABEL,T,W,PO=W,L=PLOT1,D=HD,F=S,VSN=A1425.RING  
25 REWIND,TAPE40.  
26 COPYBF,TAPE40,T.  
27 OPCUH,PLOTTA A1425 JEM KONTO D9301  
28 /READ STOP  
29 /EOR  
30 /EOR  
31 /EOF
```

32
33
34
35
36
37
38
39
40 Exhibit 1. Examples of possible control cards

```

BIOPATH
ATTACH,OLDARC=0AB104/NA.
IF(FILE(OLDARC,AS))GOTO,71.
DEFINE,OLDARC=0AB104/CT=P.
LABEL,T,R,P)=P,L=JAN80,VSN=A1426,WRING
SKIPF,T,7.
COPYBF,T,OLDARC.
RETURN,T.
REWIND,OLDARC.
GOTO,72.
71,ATTACH,OLDARC=0AB104.
72,IF(VERS.EQ.3)GOTO,79.
GET,TAPE2=DATA/NA.
IF(FILE(TAPE2,AS))GOTO,72.
72,GET,TAPE4=SOURCE/NA.
IF(FILE(TAPE4,AS))GOTO,74.
74,IF(VERS.EQ.1)GOTO,75.
ARCSEL,A/R1 110,3/R3B10,C/EISP
GOTO,77.
75,ARCSEL,A/R2 310,3/R3B10,C/R4 310
GET,TAPE7=INT.
IF(FILE(TAPE7,AS))GOTO,77.
77,RETURN,OLDARC.
MAP,OFF.
LDSET,PRESET=ZERO.
LOAD,A,B,C.
NOGO,AA.
AA.
IF(SAVE.EQ.YES)SAVE,TAPE20.
IF(REP.EQ.YES)REPLACE,TAPE20.
REWIND,TAPE20.
CATALOG,TAPE20.
79,REWIND,TAPE20.

```

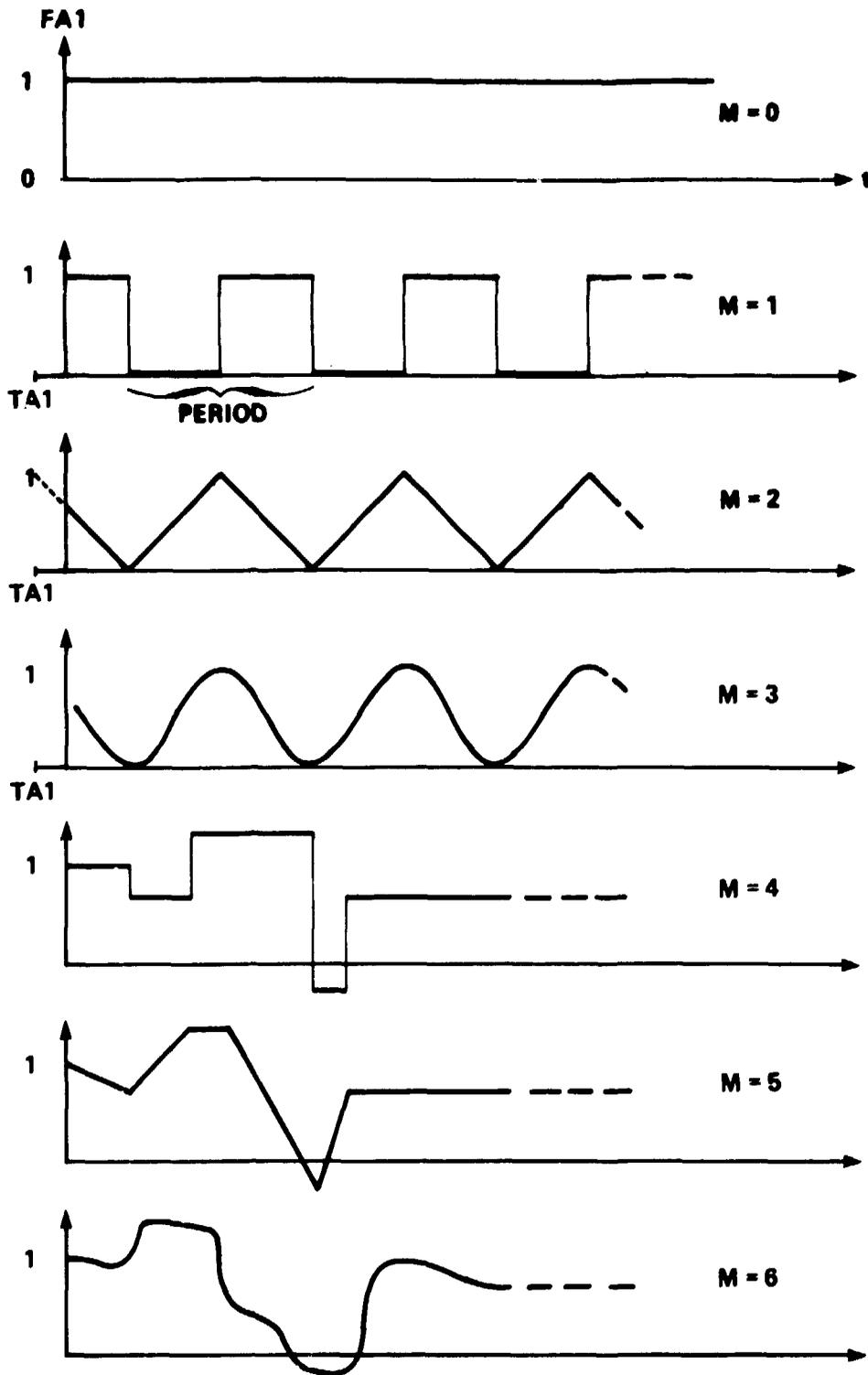


Exhibit 3 Methods of variation for FA1
 (functions related to the time dependant transfers)

NP237 ALT.2 SLAK 26/6
2 0 2 0 2 0.0 0

Exhibit 4A

SLAK
9438.,438.,0.,438.,183.,0.,131.,52.5,0.,45.6,61.1,0.,118.,83.2,0.,82.,121.,
0.,118.,50.,20.,22.,50.,0.4,0.,0.
30.,30.,0.03,1.5,220.,259.,30.,90.,30.,8760.,0.07,0.18
2.5E-3,2.5E-3,2.5E-3,2.5E-3,10.,10.,10.,5.E-6,1.E-2,1.E-4
5.0E8 4.0E7,3.77E1,5.438,8.63,5.438E-2
3.1E-4,3.1E-4,3.1E-4,3.1E-4,50.,50.,50.,8.E-3,9.E-4,1.E-6,
3.76E7,5.75E7,1.59E1,5.53,4.4,5.53E-2
1.8E4,1.E7,1.E7,1.E3,1.2E3,
6E4,2.E7,2.5E4,1.,1.,1.
5 2 4 6 6 7 4,5 2 4 6 8 9 4 ,10 16 15 16 11 17 15,1 7 0 0 0 0 0
2.5E8,8.6E11,1.E7,2.5E12,4.8E14,1.25E10,5.E8,2.2E16,3.7E13,4.4E18,2E19,
1.4E21,3.6E16,1.8E15,4.4E17,6E19,2.E15
6E9,1.E10
2,3,1.0E8
0.0 8.08E6 8.08E6 2.0E3
30 8.3E6 1.0E8
2,10,2
GRUNDVATT1GRUNDVATT2GRUNDVATT3JORD ATMSREG YTVATTEN SEDIMENT 6STEPSJ6N
BISJ6SED ATMOSFAR WELLMIXED DEEP SEA SEDIMENT 2BIOTA JORD GRUNDV6GLOB
SEDIMENT1
NP237 SLAK
NPDATA
17 3.239E-7 1.E-6
FT
3.239E-7
-2.0000003239 0. 0. 0. 0. 2. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.
0. -.0030003239 0. .001 0. .002 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.
0. 0. -3.239E-7 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.
0. .004 0. -.0052004339 1.1E-7 .0012 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.
0. 0. 0. .45 -339.4525003239 .0025 0. 189. 0. 150. 0. 0. 0. 0. 0. 0. 0.
0. 0. 0. .02 0. -58.0200003239 56. 2. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.
0. 0. 0. 0. 0. 1.2 -1.2000003239 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.
0. 0. 0. 0. 0. 0. 0. -2.3430003239 2.3 0. .043 0. 0. 0. 0. 0. 0. 0.
0. 0. 0. 0. 0. 0. 0. .43 -.4300003239 0. 0. 0. 0. 0. 0. 0. 0. 0.
0. 0. 0. 0. .016 0. 0. 0. 0. -18.5160003239 13. 0. 0. 0. 5.5 0. 0.
0. 0. 0. 0. 0. 0. 0. 0. 0. 0. -.1960004939 .11 0. 0. 1.7E-7 0. .086
0. 0. 0. 0. 0. 0. 0. 0. 0. 0. .0008 -.0058003239 .005 0. 0. 0. 0.
0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. .01 -.0100003239 0. 0. 0. 0.
0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. -3.239E-7 0. 0. 0.
0. 0. 0. 0. 0. 0. 0. 0. 0. .000068 .003 0. 0. 0. -.0040683239 .001 0.
0. 0. 0. 0. 0. 0. 0. 0. 0. 0. .00001 0. 0. 0. .00001 -.0000203239 0.
0. 0. 0. 0. 0. 0. 0. 0. 0. 0. .56 0. 0. 0. 0. 0. -.5600003239

The DNP237-file, which contains all inputdata in order to perform the dose calculation.

1
6
102

C.	C.	B.080E+00	1.570E-15	B.080E+00	4.360E-15	B.080E+00	1.170E-14	B.080E+00	3.050E-14
B.090E+00	7.730E-14	B.090E+00	1.910E-13	B.090E+00	9.010E-13	B.100E+00	1.950E-12	B.100E+00	3.790E-12
B.100E+00	7.350E-12	B.110E+00	1.460E-11	B.110E+00	4.560E-11	B.110E+00	9.350E-11	B.120E+00	1.770E-10
B.120E+00	3.230E-10	B.120E+00	6.130E-10	B.120E+00	1.540E-09	B.130E+00	2.930E-09	B.130E+00	5.280E-09
B.130E+00	9.030E-09	B.140E+00	1.550E-08	B.140E+00	3.200E-08	B.140E+00	5.470E-08	B.150E+00	9.330E-08
B.150E+00	1.490E-07	B.150E+00	2.370E-07	B.160E+00	4.210E-07	B.160E+00	6.830E-07	B.160E+00	1.050E-06
B.150E+00	1.350E-05	B.170E+00	2.270E-06	B.170E+00	3.490E-06	B.170E+00	5.100E-06	B.180E+00	7.160E-06
B.180E+00	9.790E-06	B.180E+00	1.310E-05	B.190E+00	1.760E-05	B.190E+00	2.350E-05	B.190E+00	3.020E-05
B.200E+00	3.790E-05	B.200E+00	4.660E-05	B.200E+00	5.670E-05	B.200E+00	6.750E-05	B.210E+00	7.370E-05
B.210E+00	9.010E-05	B.210E+00	1.010E-04	B.220E+00	1.110E-04	B.220E+00	1.200E-04	B.220E+00	1.270E-04
B.230E+00	1.320E-04	B.230E+00	1.350E-04	B.230E+00	1.340E-04	B.240E+00	1.310E-04	B.240E+00	1.250E-04
B.240E+00	1.190E-04	B.250E+00	1.090E-04	B.250E+00	9.920E-05	B.250E+00	8.800E-05	B.250E+00	7.670E-05
B.260E+00	6.550E-05	B.260E+00	5.460E-05	B.260E+00	4.420E-05	B.270E+00	3.630E-05	B.270E+00	2.890E-05
B.270E+00	2.250E-05	B.280E+00	1.700E-05	B.280E+00	1.240E-05	B.280E+00	9.240E-06	B.290E+00	6.740E-06
B.290E+00	4.790E-05	B.290E+00	3.270E-06	B.300E+00	2.100E-06	B.300E+00	1.430E-06	B.300E+00	9.570E-07
B.310E+00	6.210E-07	B.310E+00	3.860E-07	B.310E+00	2.160E-07	B.310E+00	1.370E-07	B.320E+00	8.510E-08
B.320E+00	5.160E-08	B.320E+00	2.920E-08	B.330E+00	1.390E-08	B.330E+00	8.060E-09	B.330E+00	4.640E-09
B.340E+00	2.610E-09	B.340E+00	1.340E-09	B.340E+00	5.210E-10	B.350E+00	2.810E-10	B.350E+00	1.540E-10
B.350E+00	8.250E-11	B.360E+00	3.990E-11	B.360E+00	1.290E-11	B.360E+00	6.440E-12	B.370E+00	3.290E-12
B.370E+00	1.670E-12	B.370E+00	7.440E-13	B.370E+00	1.560E-13	B.380E+00	6.270E-14	B.380E+00	2.610E-14
B.350E+00	9.360E-15	B.390E+00	3.640E-15						

Exhibit 4B

The SNP237-file, which contains the release of the activity at different times.

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