

**KERNFORSCHUNGSZENTRUM
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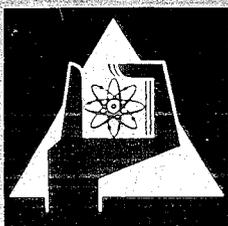
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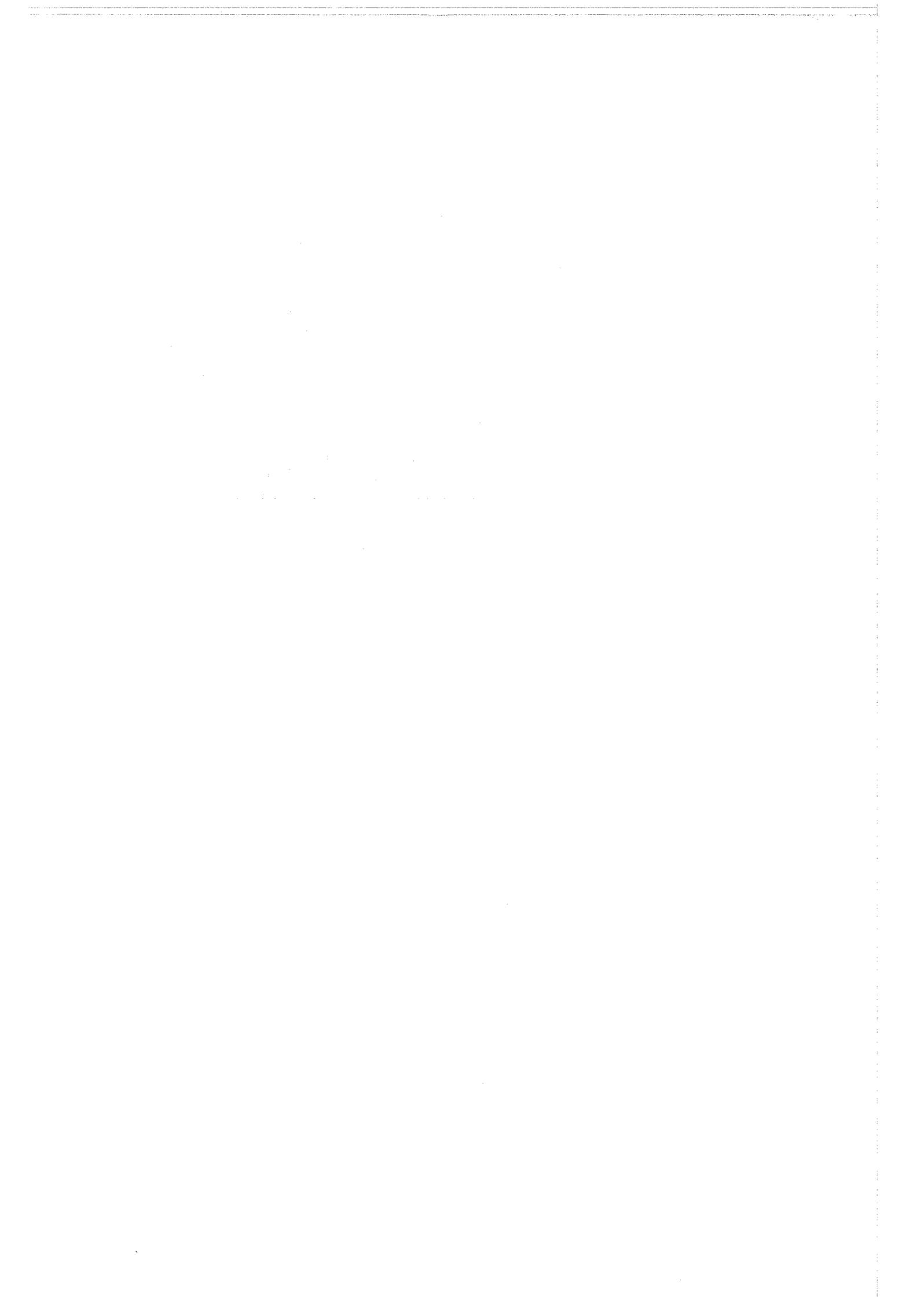
P Y G M Y

A Zero-Dimensional Burn-up Program for Fast Reactors

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PYCMY

A Zero-Dimensional Burn-up Program for Fast Reactors^X

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X

Work performed within the association in the field of fast reactors between the European Atomic Energy Community and Gesellschaft für Kernforschung m.b.H. Karlsruhe.

Abstract

PYGMY is a refined and extended version of the zero-dimensional burn-up code PYRE, which calculates the changes of reactivity, neutron spectrum, and isotopic concentrations with time, taking into account management operations and allowing for a very general isotopic scheme. The code is written in Fortran IV for the IBM 360. An input description and a sample case are presented. Results of a calculation of the transplutonium build-up, including the berkelium and californium isotopes, in thermal fluxes of $5 \cdot 10^{13} - 3 \cdot 10^{16} \text{ cm}^{-2} \text{ sec}^{-1}$ are presented.

I. Introduction

The code PYRE /17 calculates the time dependence of reactivity, power, neutron spectrum, and isotope concentrations for a constant flux or power, taking into account capture, decay and fission product build-up. The version PYGMY has been extended to include

1. the influence of management operations such as shut-down times, different power levels, and charging and discharging of different batches;
2. the possibility of performing pure irradiation calculations excluding the determination of reactivity and neutron spectrum;
3. the calculation of the activity of the individual batches;
4. the influence of (n,2n)-processes;
5. branching of isotopic chains in one process, e.g. competing β^- and β^+ decay;
6. a better numerical procedure for the integration of the isotopic equations;
7. automatic adjustment of step length.

A description of the code performance will be given in the next section.

Section III provides an input description, section IV the input and results of a sample case. In section V the results of a calculation of the transplutonium build-up in a thermal spectrum of $5 \cdot 10^{13} - 3 \cdot 10^{16}$ $\text{cm}^{-2} \text{sec}^{-1}$ are presented. 40 isotopes including the elements berkelium and californium have been taken into account in these calculations.

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II. Description of the code

1. Input

In its present version, the program handles up to 40 time dependent isotopes; this number can be easily enlarged by altering the related dimensions. The information on one isotope is collected in two cards of the input (K3 and K5) including all information on transitions leading from this isotope to other isotopes. An exemption is made for the fission process; here, the fission rate is summarized over all isotopes, and from this, the formation of the fission products is derived using the individual values of β . Decay, capture, and (n,2n)-products which shall not be taken into account must not be specified anywhere in the input.

Only down-scattering is admitted. In order to keep the input as small as possible, only sub-diagonals with non-zero elements have to be specified. The number of these sub-diagonals is NXCM; for the ABN-set NXCM is 10 if hydrogen is included or less if only heavier elements are present.

2. Calculation of reactor characteristics

The first step of the burn-up calculation consists of the determination of breeding ratio, reactivity or buckling, total neutron flux or power, neutron spectrum, some reaction rates, and the activity. In the case of pure irradiation calculations, the determination of reactivity or buckling and of the spectrum is omitted. It is possible to determine either the buckling for a constant reactivity or the reactivity for a constant buckling, which may either be given as input or be determined from a desired value for k_{eff} at time zero. The average cross sections used for the burn-up may be collapsed either with the spectrum pertaining to the present k_{eff} or with a spectrum for $k_{\text{eff}}=1$. The spectrum in the output is the spectrum used for the collapsing of the cross sections.

One may choose whether to keep the power or the total flux constant with time, that is constant between two management operations. In the case of irradiation calculations, the spectrum is kept constant too and has to be specified by the user. It needs not to be normalized to the total flux.

3. Management

The input for management is organized in such a way that for each time at which operations take place first the point of time and then all desired operations such as discharging, recharging and changes of power or flux and time step length are specified. The point of time has to coincide with the end of some time step; thus, it is not possible to define step lengths of 10 days and then to require the first management operation at 25 days, but instead one can change the step length after 20 days to 5 days and then perform the management operation at 25 days.

It is possible to treat several charges in one reactor. The burn-up calculations are performed separately for each charge, while the criticality calculations are done for the homogenized charges. On input, a number and a volume is assigned to each charge. The sum of all charge volumes should equal the core volume, or else the homogenized material densities are suitably condensed or diluted. On discharging, one has only to specify the number of the charge and the volume to be discharged; thus, it is possible to discharge only part of a batch. Numbers of completely discharged batches may be reused for new batches, but if this is done with numbers of charges which are not completely discharged the data of the old charge are deleted and a warning is issued.

If any management operation takes place the program continues with a new criticality calculation; otherwise, a burn-up calculation ensues.

In order to ensure a correct end of the calculation, especially if other cases follow up, one should discharge the core wholly at the last point of time.

4. Burn-up calculation

The numerical procedure used by PYRE for the integration of the isotopic equations has been discarded in favor of one with better convergence. As in PYRE, the system of differential equations, which shall be denoted by

$$\dot{\vec{N}} = \underline{A} \vec{N} \quad (1)$$

is approximated by

$$\frac{\vec{N}_i - \vec{N}_{i-1}}{\Delta t} = \underline{A} \frac{\vec{N}_i + \vec{N}_{i-1}}{2} \quad (2)$$

$$\Delta t = t_i - t_{i-1}$$

An iterative procedure is needed for the solution of (2). For PYRE, the iteration

$$\vec{N}_i^k = \vec{N}_{i-1} + \frac{\Delta t}{2} \underline{A} (\vec{N}_{i-1} + \vec{N}_i^{k-1}) \quad (3)$$

has been chosen, but this tends to diverge for too big time steps. For PYGMY, (2) is rewritten as follows

$$\left(\underline{E} - \frac{\Delta t}{2} \underline{A}\right) \vec{N}_i = \left(\underline{E} + \frac{\Delta t}{2} \underline{A}\right) \vec{N}_{i-1} \quad (4)$$

\underline{E} = unitary matrix

or

$$\underline{M} \vec{N}_i = \vec{R} \quad (5)$$

With

$$\underline{M} = \underline{D} - \underline{L} - \underline{U}$$

\underline{D} being a diagonal, \underline{L} a lower triangular, and \underline{U} an upper triangular matrix, the iterative procedure has been chosen to be

$$\vec{N}_i^k = (1-w) \vec{N}_i^{k-1} + w (\underline{D} - \underline{L})^{-1} (\underline{U} \vec{N}_i^{k-1} + \vec{R}) \quad (6)$$

with $w = 1$. With $w \neq 1$, an over- or under- relaxation method could be employed, but up to now no procedure for estimating w exists. The

convergence of (6) is the better the more zero-elements are contained in U. It is therefore recommendable to arrange the isotopes in the order of their formation, beginning with the fissile and fertile isotopes and ending with the fission products.

The user may employ the automatic step length adjustment. One has then to specify the maximum number of micro-steps into which one time step may be subdivided. At the start of the calculation and after each management operation, this number is used for the burn-up calculation, whereas for all subsequent time steps, the number of micro-steps is reduced if the change of isotopic concentrations in the last micro-step does not exceed 3%. This ensures an accuracy of at least .1%. Of course, if the maximum number of micro-steps has to be employed, this accuracy cannot be guaranteed.

A redetermination of neutron spectrum and power or flux level over the time interval is not achieved by use of the automatic step length adjustment. If these quantities change appreciably over one time step, smaller steps should be employed.

If no automatic step length adjustment is used, the number of micro-steps is taken to be 4 at the start and after each management operation and 1 for all subsequent steps.

5. Output

One can choose a full or a partial output. The partial output comprises:

- a. Start: All information on isotopes and processes linking them; messages on the type of calculation; data of the initial loading.
- b. Burn-up: Reactivity, breeding ratio, total power and flux, buckling, reaction rates; the homogenized atom densities and activities of all isotopes; the group dependent spectrum and fission source.

- c. Management: Messages on changes of power, flux, or spectrum; number and volume of discharged batches and their activity; number and volume of recharged batches.

Besides, a complete listing of the input is provided. The full output gives the following additional information:

- a. Start: The fission spectrum and a list of the isotope dependent microscopic group cross sections.
- b. Burn-up: Macroscopic group cross sections, isotope dependent spectrum averaged cross sections, and composition and activity of individual charges.
- c. Management: Composition and activity of individual discharged batches.

The output tends to become very lengthy for a big number of time steps. Therefore, one can use NPRT to get output only after every NPRT time steps and at the end of each case. The messages concerning management are excluded from this automatism.

III. Input description

The input comprises a first part which is only concerned with the definition of the isotopes, the linking processes, and the group cross sections. With the data of the first part, an arbitrary number of cases may be run. The second part of the input comprises the data for the different cases.

As for the notation, Kn defines a set of data starting on a new card and Sn a logical decision concerning the further sequence of data cards.

The input is unformatted; this requires that each data set defined by Kn must start with a card containing no blank in column 1 while subsequent cards of the same set must have a blank in column 1.

The character of the numbers is given by their names in the data lists: Names starting with I-N indicate fixed point numbers, while all other names indicate floating point numbers if not explicitly stated as hollerith constants.

K1	NG	Number of groups $\overline{\leq 26}$
	NXCM	Number of subdiagonals in the scattering matrix with elements $\neq 0$ $\overline{\leq 10}$
	NBE	Number of burnable isotopes
	NNE	Number of non-burnable isotopes
	NP	= 0 full print = 1 partial print
S2	for each burnable isotope K3-K5	
K3	HØLN	Hollerith name (up to 4 characters)
	ATW	Atomic weight
	THALF	Half life for unstable isotopes $\overline{\text{days}}$ 0 for stable isotopes
	FE	Energy released per fission $\overline{\text{MeV}}$
	BETA	0 for fissile or fertile isotopes Yield for fission products

NUMT Total number of time steps
 NPRT Number of intervals between prints (e.g. =1: print every time, =2: print every other time)
 NAUT (=0: no step length adjustment
 =1: internal step length adjustment)
 MAX Maximum number of micro-steps per time interval (power of 2)
 H Initial step length /days/
 VØL Core volume /liters/
 G1 Initial power /M wt/ for NFP=0
 Initial flux /cm⁻²sec⁻¹/ for NFP=1
 G2 k_{eff} for NØP=0,2
 B² for NØP =1
 S15 if NSP=1 K16, otherwise K17
 K16 (SP(I),I=1,NG) Neutron spectrum
 K17 LBS Number of fertile isotopes 1<LBS<10
 (LBSN(I),I=1,LBS) For each fertile isotope its number given
 by the order in K3
 IBL Number of fissile isotopes 1<IBL<10
 (IBLN(I),I=1,IBL) For each fissile isotope its number given by
 the order in K3
 K18 MI Initial number of charges
 S19 for each charge K20
 K20 NCH Number of the charge
 VØLCH Volume /liters/
 (DN(I),I=1,NBE+NBE) Isotope densities /cm⁻³.10⁻²⁴/ in the
 order given by K3 and K7
 S21 for each point of time at which management operations shall
 take place K22 - K31, then next case
 K22 TI Point of time /days/
 NDIS Number of wholly or partly discharged batches

NRE Number of recharged batches
 NIF { =1, if power, flux, neutron spectrum, or step
 length is changed
 =0 otherwise
 S23 if NIF=1 K24 - K26, otherwise S27
 K24 G1N New power $[M \text{ wt}]$ for NFP=0
 New flux $[cm^{-2} \text{ sec}^{-1}]$ for NFP =1
 HN New step length $[days]$
 S25 if NSP=-1 K26, otherwise S27
 K26 (SPN(I),I=1,NG) New spectrum
 S27 if NDIS>0 K28, otherwise S29
 K28 for all discharged batches
 NCHDIS Number of batch
 VØLDIS Volume to be discharged $[liters]$
 S29 if NRE=0 S30-K31, otherwise next point of time
 S30 for every new batch K31
 K31 NCHN Number of batch
 VØLN Volume $[liters]$
 (DNN(I),I=1,NBE+NNE) Isotope densities $[cm^{-3} \cdot 10^{-24}]$ in the
 order given by K3 and K7
 K32 0 Constant
 K33 $\alpha \text{ NUFIN } \alpha$ Constant

For a calculation on the Karlsruhe 360/65 the following job control cards have to be added:

```
//EXEC FHG,LIB=NUSYS,NAME=PYGMY,REGION,G=200K
//G.FTO3FCO1 DD UNIT=SYSDA,SPACE=(200,(200))
```

Typical running times are 12 sec for the sample case described in the next section and 92 sec for one flux value in the 40-materials case from chapter V.

An example for the input is provided by the sample problem.

IV. Input and results of the sample problem

A wholly artificial case has been constructed for the sample problem, but in the processes linking the isotopes a certain similarity to realistic cases has been maintained (see fig. 1). Thus, the 7 materials MATA-MATG constitute the fissile and fertile isotopes, P0I1-P0I4 are the fission products, and STR1 and STR2 are structure materials. The five isotopes MATA-MATE can be interpreted as isotopes of one element with MATD and MATC being isomeric nuclei; MATC has a competing γ , β^- and β^+ -decay, the last two transitions leading to the next higher and next lower element. The capture transition leading from MATF to MATE can be interpreted as a transition leading to very short lived isotope which decays into MATE and which is omitted because of its short life time.

The hypothetical reactor is at first loaded with one charge and operates at full power (1000 Mwt) for 80 days. It is then shut down for 10 days, and after two days shut-down time half of the original charge is replaced with a new charge. At T=90 days it is started up again for 80 days at half power and afterwards wholly discharged. The input for this case is given below.

```

2 1 11 2 0
αMATAα 200. 0 200. 0 0 1 0
αMATBα 1.
αMATBα 201. 0 200. 0 0 2 1
αMATCα .8 αMATDα .2 MATA 1.
αMATCα 202. 10. 200. 0 3 1 0
αMATDα .9 αMATFα .06 αMATGα .04 αMATEα 1.
αMATDα 202. 0 200. 0 0 1 1
αMATEα 1. αMATBα 1.
αMATEα 203. 0 200. 0 0 0 1
αMATDα 1.

```

α MATF α 202. .1 200. 0 0 1 0

α MATE α 1.

α MATG α 202. 0 200. 0 0 0 0

α PØI1 α 80. 1. 0 .06 1 0 0

α PØI2 α 1.

α PØI2 α 80. 0 0 .01 0 1 0

α PØI3 α 1.

α PØI3 α 81. 0 0 .03 0 1 1

α PØI4 α 1. α PØI2 α 1.

α PØI4 α 82. 50. 0 0 0 0 0

α STR1 α 50. α STR2 α 2.

1. 0

5. 10. 15. 20. 0 0

600. 650. 1500. 660. 0 .01

.1 4. .3 12. .05 0

0 15. 0 20. 0. .01

2. 8. 6. 15. 0 0

400. 600. 900. 615. 0 .01

15. 30. 40. 35. .02 0

800. 1200. 2000. 1210. 0 .01

1. 10. 3. 18. 03 0

0 15. 0 25. 0 .01

.5 7. 1.5 15. 0 0

0 4. 0 10. 0 .01

.05 .1 .1 4. 0 0

0 .4 0 5. 0 .01

0 0 0 5. 0 0

0 0 0 5. 0 .01

0 1. 0 10. 0 0

0 2000. 0 2010. 0 .01

0 4. 0 10. .1 0

0 4000. 0 4010. 0 .01

```

0 300. 0 320. 0 0
0 10000. 0 10020. 0 .01
0 20. 0 30. 0 0
0 15. 0 20. 0 2.5
0 0 0 20. 0 0
0 0 0 25. 0 3.
1
1 0 1 12 1 1 32 20. 12000. 1000. .001
1 2 3 1 3 4
1
1 12000. .004 .02 0 0 0 0 0 0 0 0 0 0 .005 .05
80. 0 0 1
0 1.
82. 1 1 1
0 4.
1 6000.
2 6000. .006 .02 0 0 0 0 0 0 0 0 0 .007 .045
90. 0 0 1
500. 20.
170. 2 0 0
1 6000. 2 6000.
0
 $\alpha$ NUFIN $\alpha$ 

```

The time dependence of the homogenized materials is given in fig. 2; other results are listed in table 1.

V. Formation of transplutonium isotopes in a thermal spectrum

The formation of transplutonium isotopes, including the Bk- and Cf-isotopes, has been calculated using a total of 40 isotopes. Fig. 3 shows the isotopes and the processes linking them. (n,2n)-processes have not been taken into account as their contribution is negligible in a thermal spectrum. Of course, the isotopic scheme depends upon the nature of the problem to be solved. Thus, for the smaller flux values, decay transitions override the capture transitions, so that some isotopes to the lower right edge of the scheme in fig. 3 (Pu^{244} , Pu^{245} , Am^{249} , Bk^{251}) could be dropped without any loss of accuracy. On the other hand, for a high flux, only Bk^{251} turns out to be superfluous.

The neutron spectrum has been chosen to represent the FR2-spectrum and the group cross sections were partly taken from irradiation calculations recently done for an experiment at this reactor [2]. As far as possible they are one group cross sections condensed from the 26-group-ABN-set; all other cross sections were taken from either the book of E.K. Hyde [3] or the chart of the nuclides [4] and corrected for the spectrum and flux depression in the sample. Some values had to be guessed. This, of course, limits the accuracy of the results especially for the higher isotopes; for Bk and Cf absolute numbers have a big error and only relative results are meaningful, but this is inherent in such calculations at the present state of knowledge.

Flux values of $5 \cdot 10^{13}$ - $3 \cdot 10^{16} \text{ cm}^{-2} \text{ sec}^{-1}$ are examined[‡]; the management is always the same: a sample is irradiated for 180 days and then the dying-away of the activity is observed during another 35 days with zero flux.

[‡] the lower value being the flux in the FR2, the highest value lying a little above the fluxes currently discussed for high flux reactors.

The initial composition of the sample is given below:

U ²³⁵	2.7·10 ²⁰	nuclides
U ²³⁸	3.7·10 ²²	nuclides
Pu ²³⁹	1.45·10 ²²	nuclides
Pu ²⁴⁰	1.3·10 ²¹	nuclides
Pu ²⁴¹	1.3·10 ²⁰	nuclides
Pu ²⁴²	6.4·10 ¹⁸	nuclides
<hr/>		
Total	5.3·10 ²²	nuclides

The results are summarized in fig.'s 4-10.

The first four figures show the amount of the four transplutonium elements formed after 180 days of irradiation as function of the flux. There is an optimum flux value for the formation of Am and Cm above which the amount of nuclides decreases again because it is used up for the generation of the higher elements. This optimum value increases for the higher elements and therefore is above the range of flux values under consideration. The same holds for the different isotopes of one element^{*}; the wavy structure of some curves for the lower isotopes (Am²⁴¹, Am²⁴², Am^{242m}) results from the fact that basically two isotopes contribute to the build-up: Pu²³⁹ and U²³⁸. For the lower fluxes the main contribution comes from Pu²³⁹ and this dies away with increasing fluxes. For a further increase a similar curve originating from U²³⁸ overlaps.

Fig. 8 shows the increase with time of Cf-nuclides for the two most extreme fluxes. The relative increase is much bigger for the lower flux values; for example the ratio $N_{\text{Cf}}(180\text{d})/N_{\text{Cf}}(170\text{d})$ is ~ 1.6 for $\phi = 5 \cdot 10^{13} \text{ cm}^{-2} \text{ sec}^{-1}$ versus ~ 1.15 for $3 \cdot 10^{16} \text{ cm}^{-2} \text{ sec}^{-1}$. Thus, the optimum irradiation times tend to be higher for the low fluxes than

^{*} especially the isotope contributing most of the sum tends to be one with higher atomic number for the higher fluxes.

for the high fluxes, but, looking at the absolute values of N_{Cf} for low fluxes, one can conclude that even longer irradiation times will not appreciably improve the output of the higher elements.

Fig.'s 9 and 10 show the time and flux dependent behaviour of the activity. From fig. 9 one finds that the activity can be divided into a short, a medium, and a long lived term. The isotopic contribution to the different terms depends upon the flux too and can be found from both figures. In figure 10, isotopes with a half life of less than 1 day are represented by dashed lines, the others by solid lines. The groups are:

1. Short lived term ($T_{1/2} < 5$ h): U^{239} for all flux values and Pu^{243} for medium fluxes.
2. Medium lived term ($T_{1/2} = 2.35$ d): Np^{239} for all fluxes.
3. Long lived term ($T_{1/2} > 160$ d): Pu^{241} for low and medium fluxes, Cm^{242} for medium fluxes only, and Cm^{244} for medium and high fluxes.

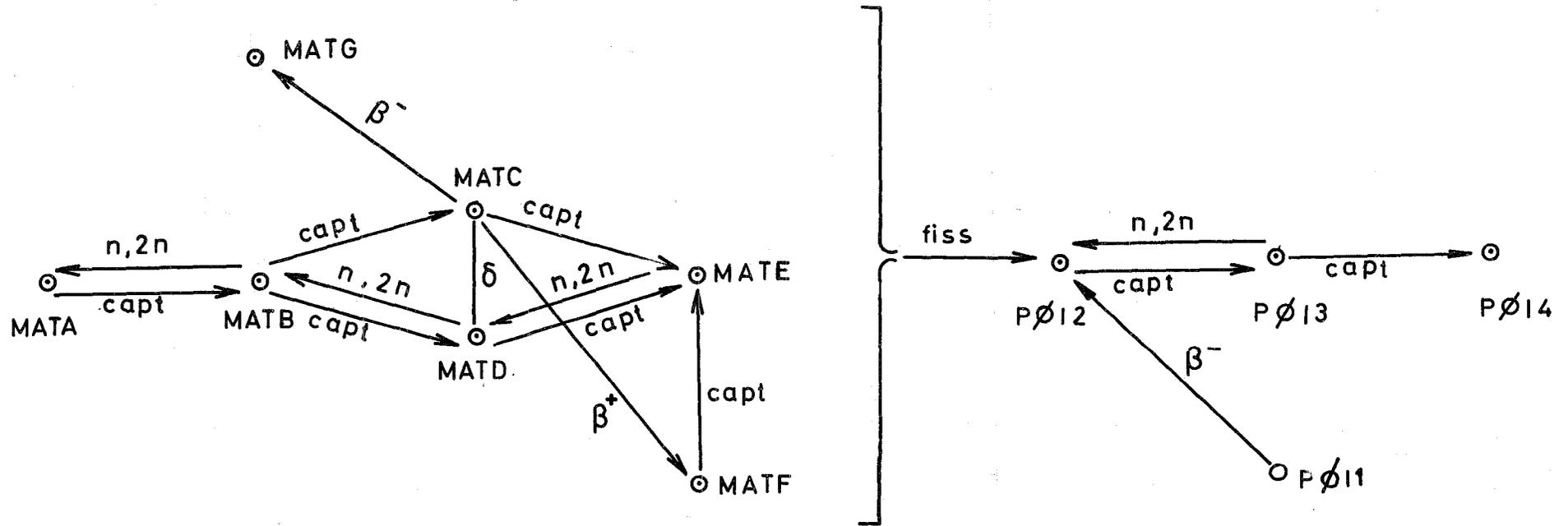
The calculations presented demonstrate the good performance of PYGMY. Checks on the accuracy have shown that even for the highest fluxes steps of 10 days with a subdivision into 64 intervals are adequate. It is intended to include the integration procedure in one- and two-dimensional codes to ensure a high flexibility in regard to isotopic combinations.

Literature

- [1] W.W. Little, R.W. Hardie: Pyre- A Multigroup Burn-up code for Fast Reactors; BNWL-54, 1965
- [2] E. Waibel: private communication
- [3] E.K. Hyde et al.: The Nuclear Properties of the Heavy Elements, Vol. III; Prentice-Hall, 1964
- [4] Nuklidkarte, Gersbach u. Sohn, München, 1968

Table 1: Results of the sample problem

	T/_days_7	k _{eff}	Power/_Mwt_7	Breeding ratio	Total flux /_cm-2sec-1_7	Group 1 flux /_cm-2sec-1_7	Group 2 flux /_cm-2sec-1_7	Mean activity /_C/ccm_7
full power	0	1.0293	1000.	.5181	1.7919·10 ¹³	1.6989·10 ¹³	9.2934·10 ¹¹	0
	20.	1.0287	1000.	.5182	1.7929·10 ¹³	1.7000·10 ¹³	9.2988·10 ¹¹	31.775
	40.	1.0281	1000.	.5183	1.7940·10 ¹³	1.7009·10 ¹³	9.3022·10 ¹¹	38.678
	60.	1.0275	1000.	.5183	1.7949·10 ¹³	1.7019·10 ¹³	9.3053·10 ¹¹	40.419
	80.	1.0269	1000.	.5183	1.7959·10 ¹³	1.7028·10 ¹³	9.3082·10 ¹¹	40.872
shut-down →								
power	80.	1.0269	0	.5183	0	0	0	40.872
	81.	1.0269	0	.5183	0	0	0	36.327
	82.	1.0269	0	.5183	0	0	0	32.981
reloading →								
zero	82.	.9943	0	.4769	0	0	0	16.491
	86.	.9943	0	.4769	0	0	0	12.132
	90.	.9943	0	.4769	0	0	0	9.174
start-up →								
half power	90.	.9943	500.	.4769	8.6596·10 ¹²	8.3000·10 ¹²	3.5958·10 ¹¹	9.174
	110.	.9941	500.	.4769	8.6616·10 ¹²	8.3019·10 ¹²	3.5965·10 ¹¹	17.385
	130.	.9938	500.	.4769	8.6634·10 ¹²	8.3037·10 ¹²	3.5971·10 ¹¹	18.916
	150.	.9936	500.	.4769	8.6653·10 ¹²	8.3055·10 ¹²	3.5977·10 ¹¹	19.301
	170.	.9934	500.	.4769	8.6671·10 ¹²	8.3073·10 ¹²	3.5982·10 ¹¹	19.401



⊙ STR 1

⊙ STR 2

Fig.1 : Material transitions for sample problem

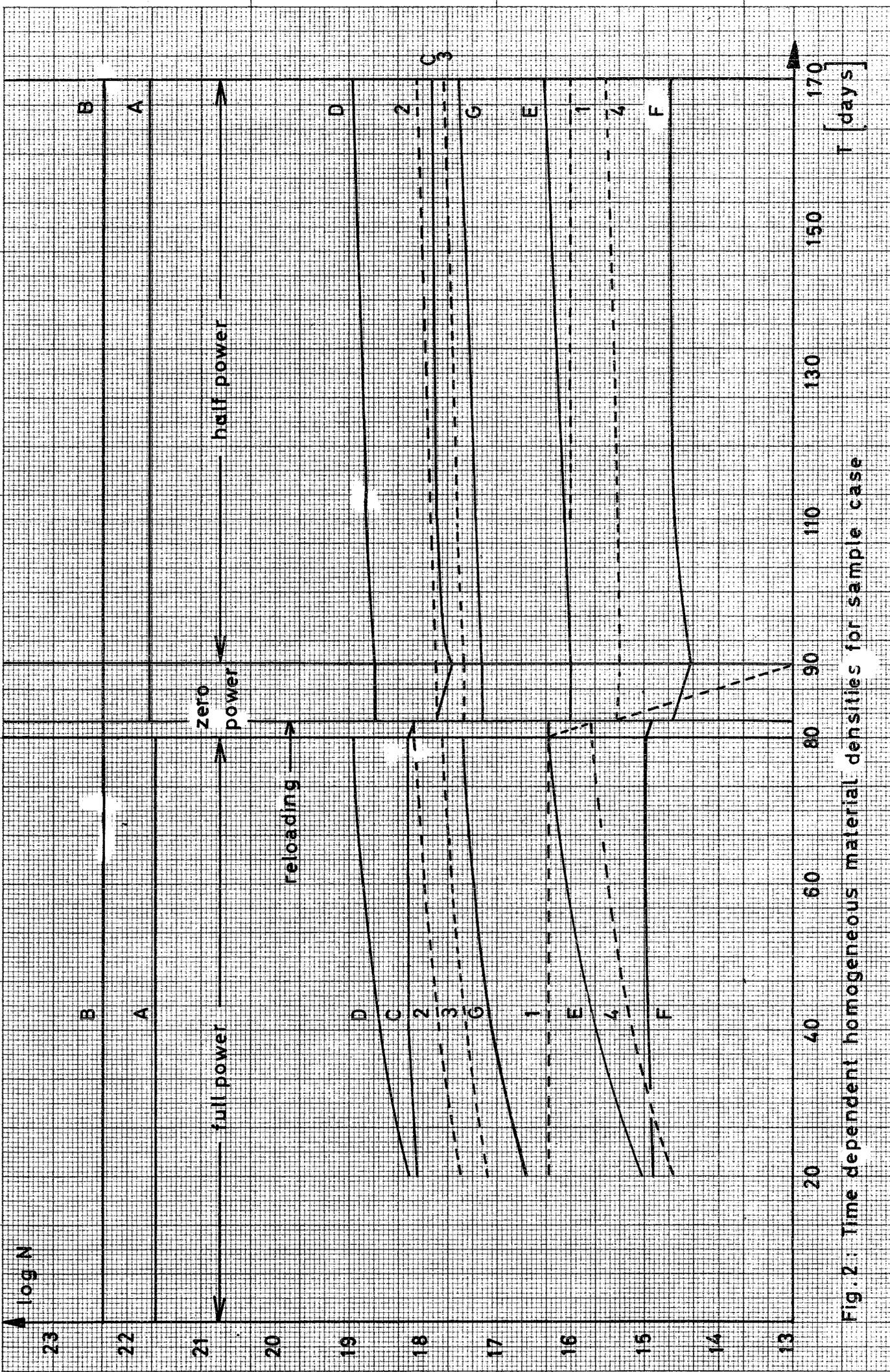


Fig. 2: Time dependent homogeneous material densities for sample case

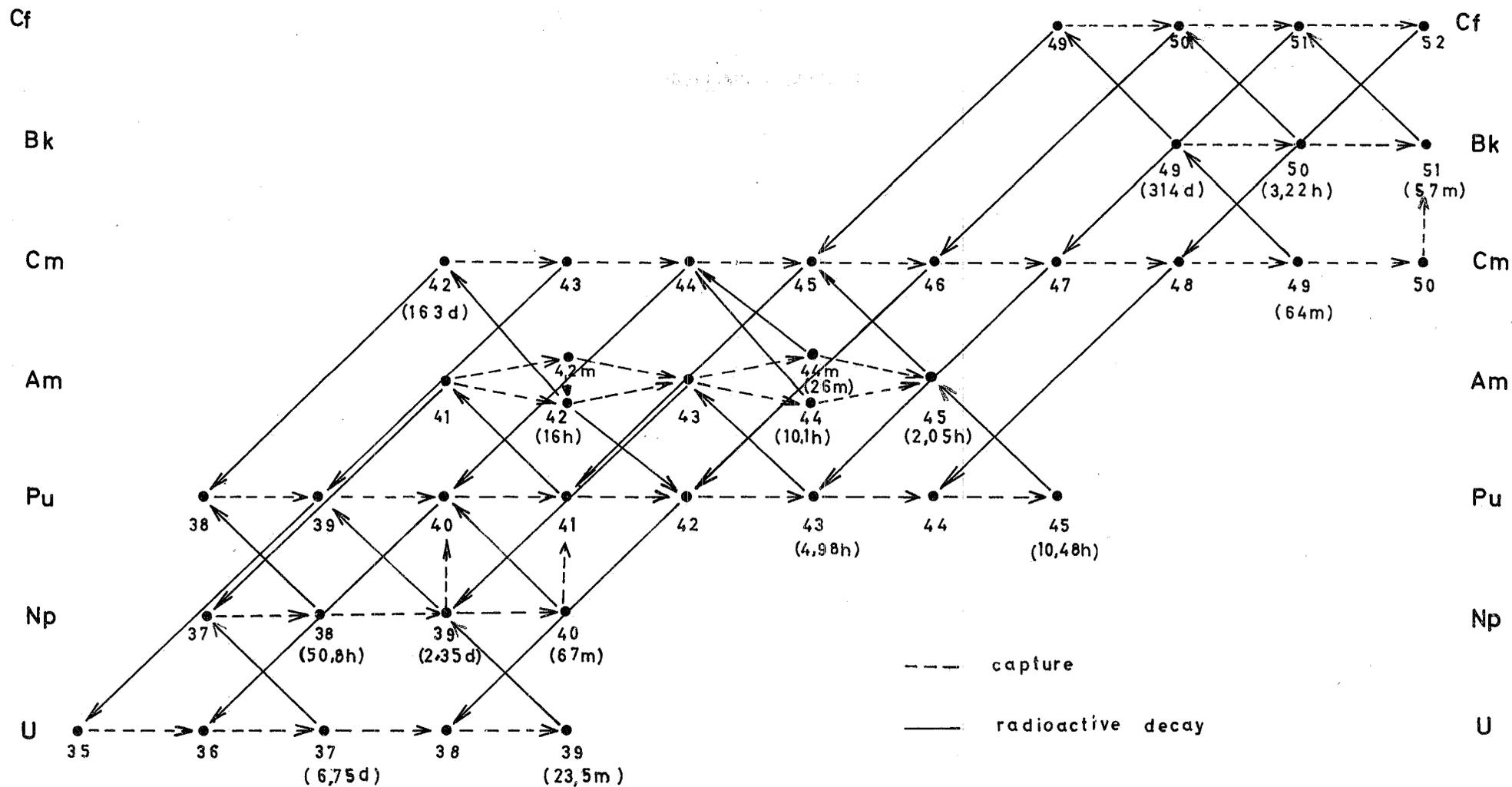


Fig.3: Isotopic scheme used for the calculation of the generation of transplutonium isotops .

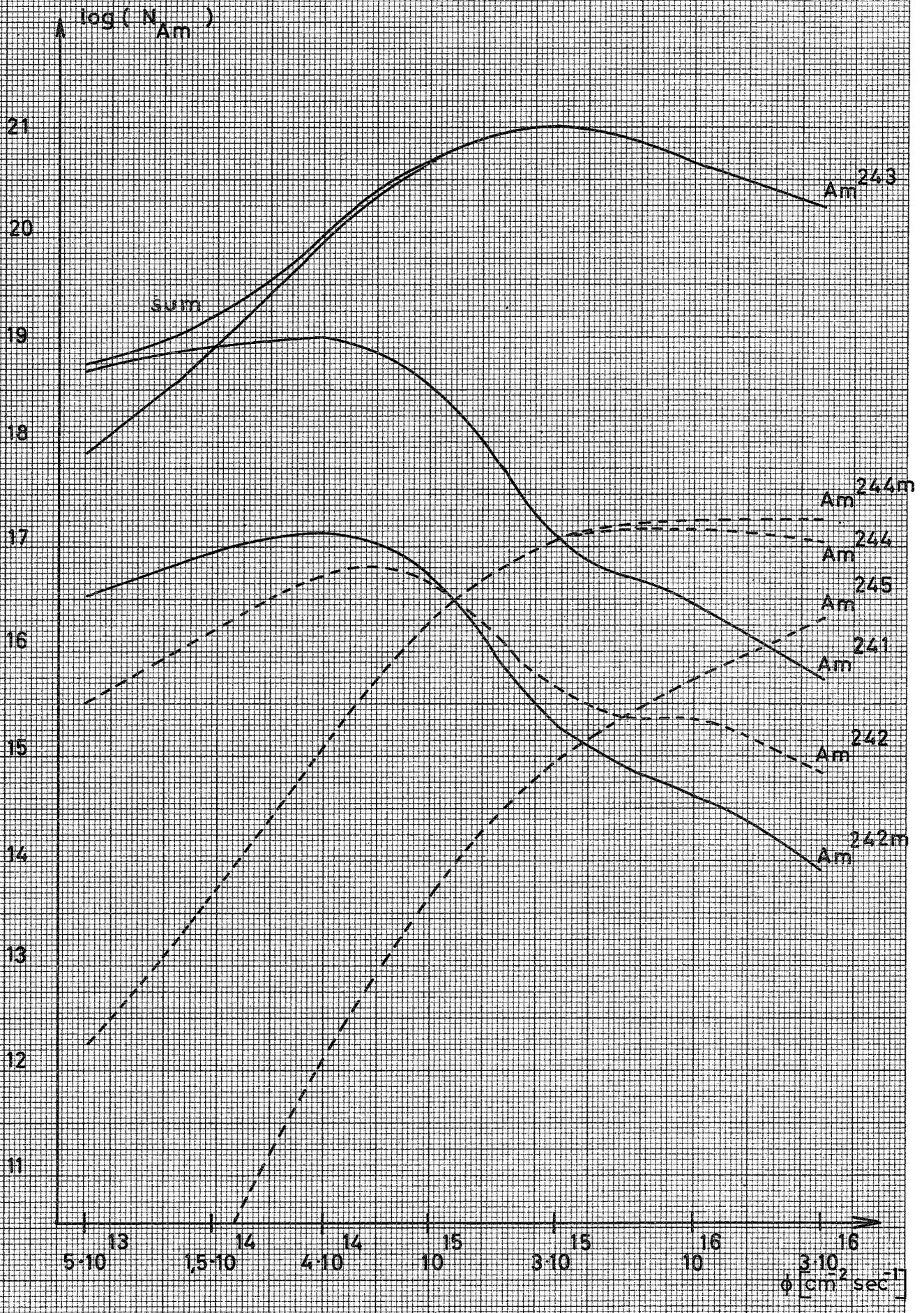


Fig 4. Generation of americium isotops as a function of the flux

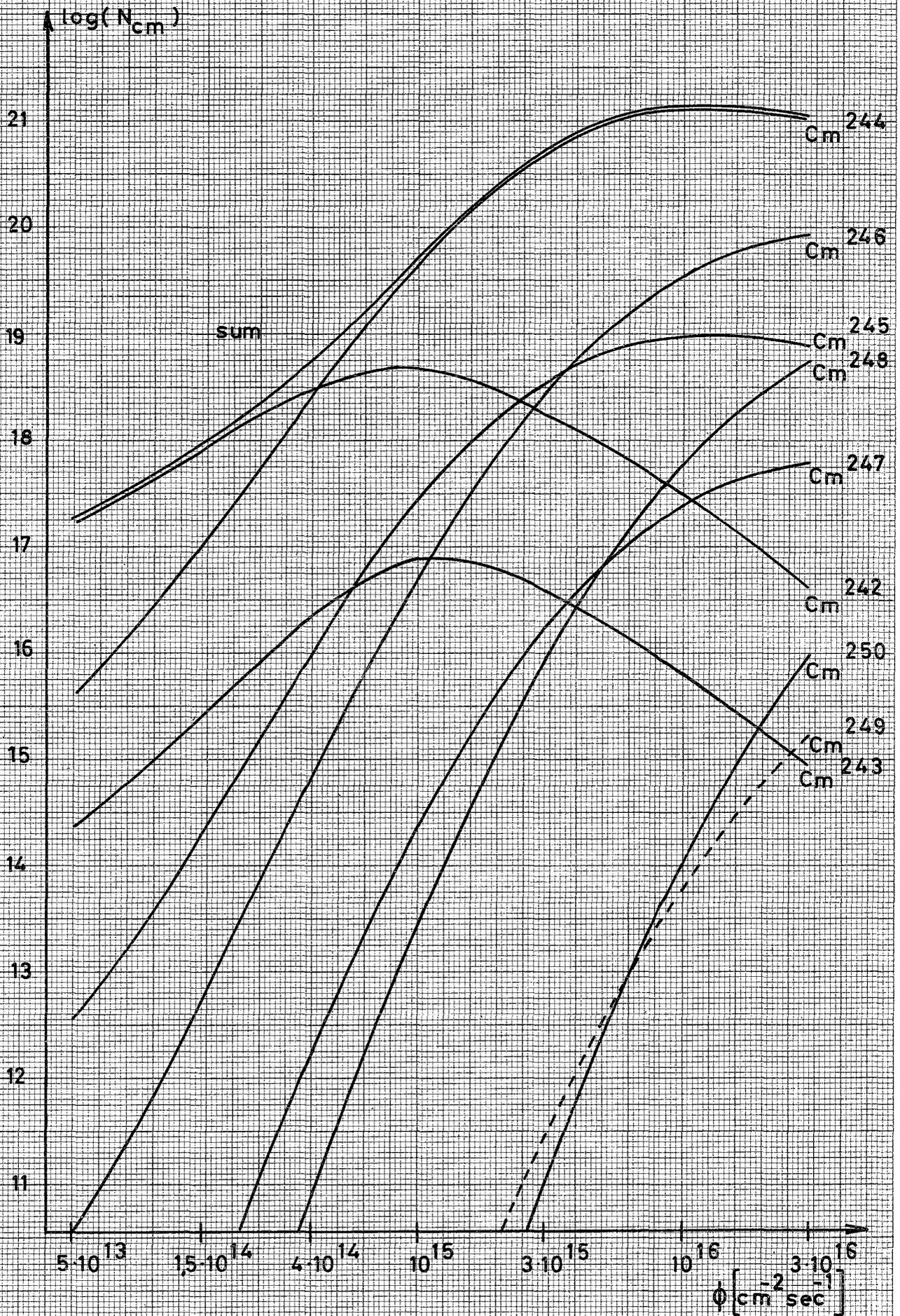


Fig. 5: Generation of curium isotops as a function of the flux

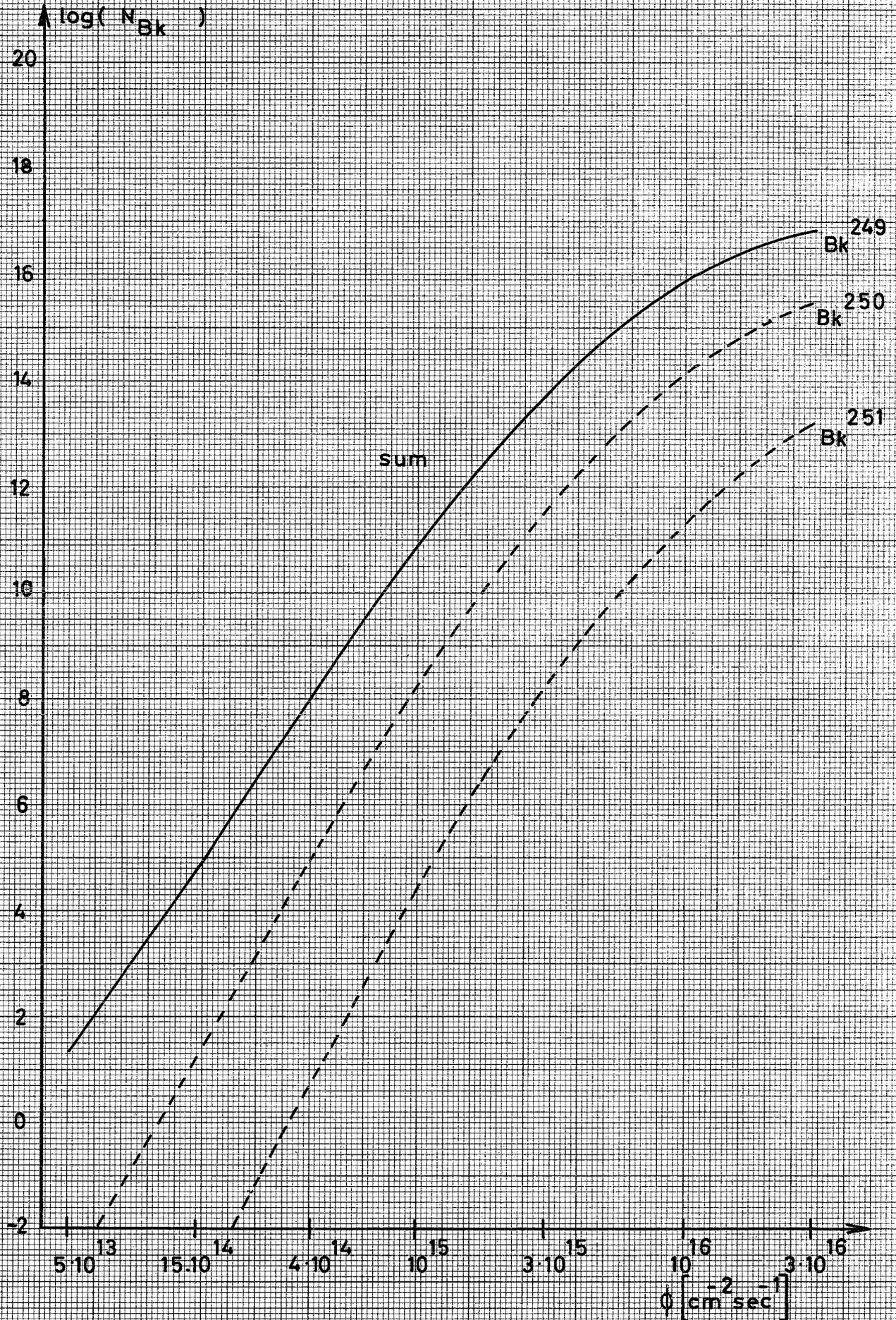


Fig. 5: Generation of berkelium isotops as a function of the flux

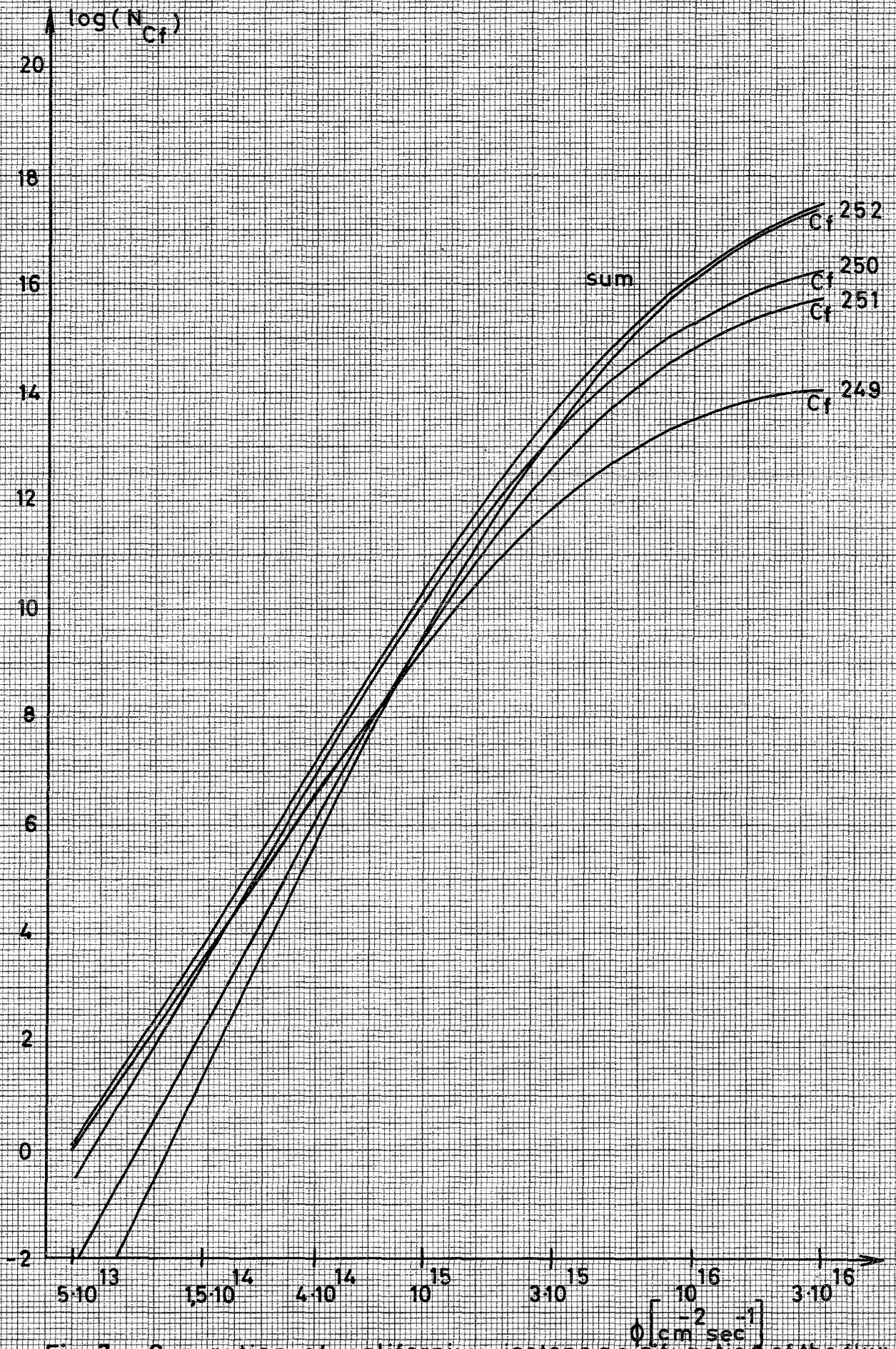


Fig. 7: Generation of californium isotops as a function of the flux

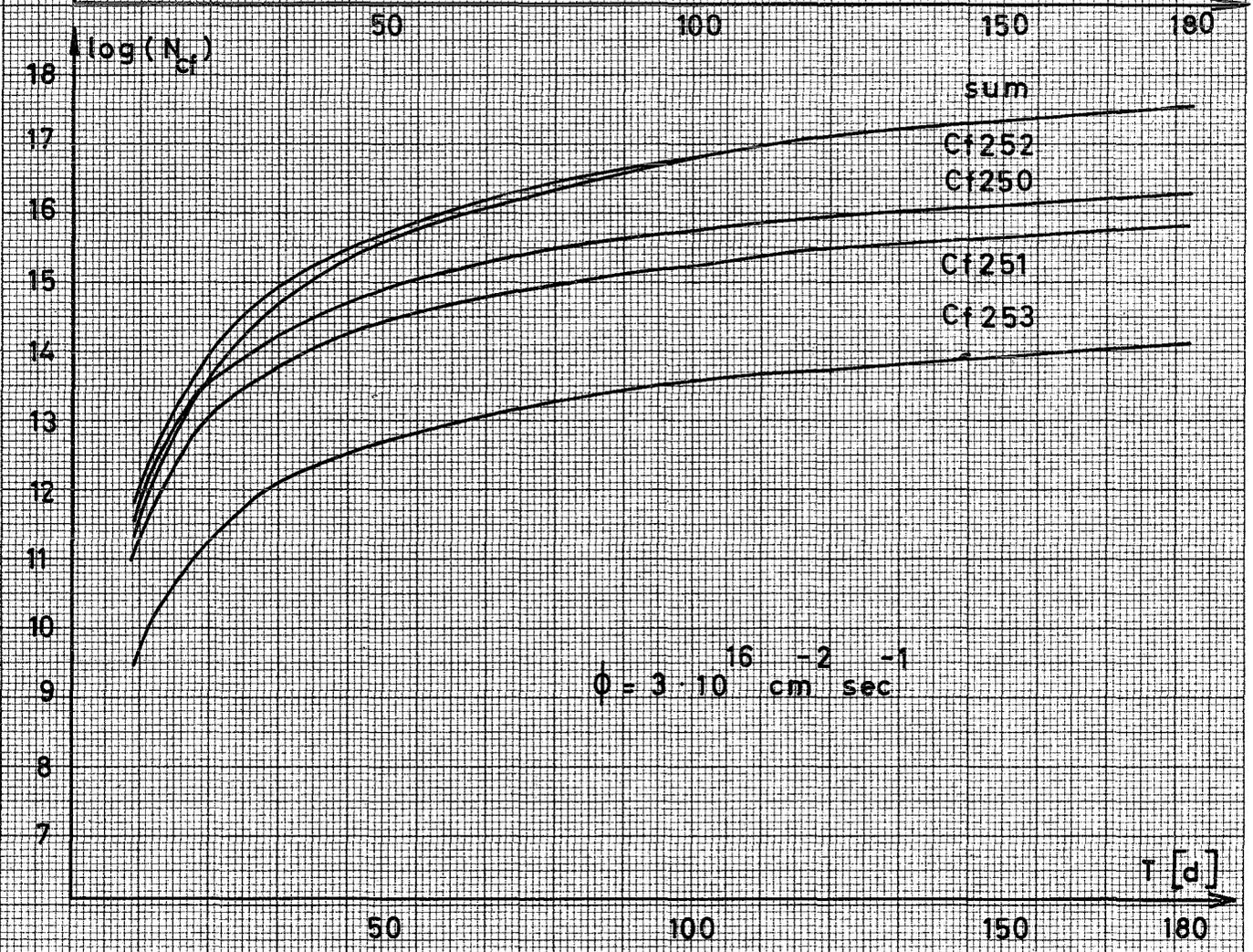
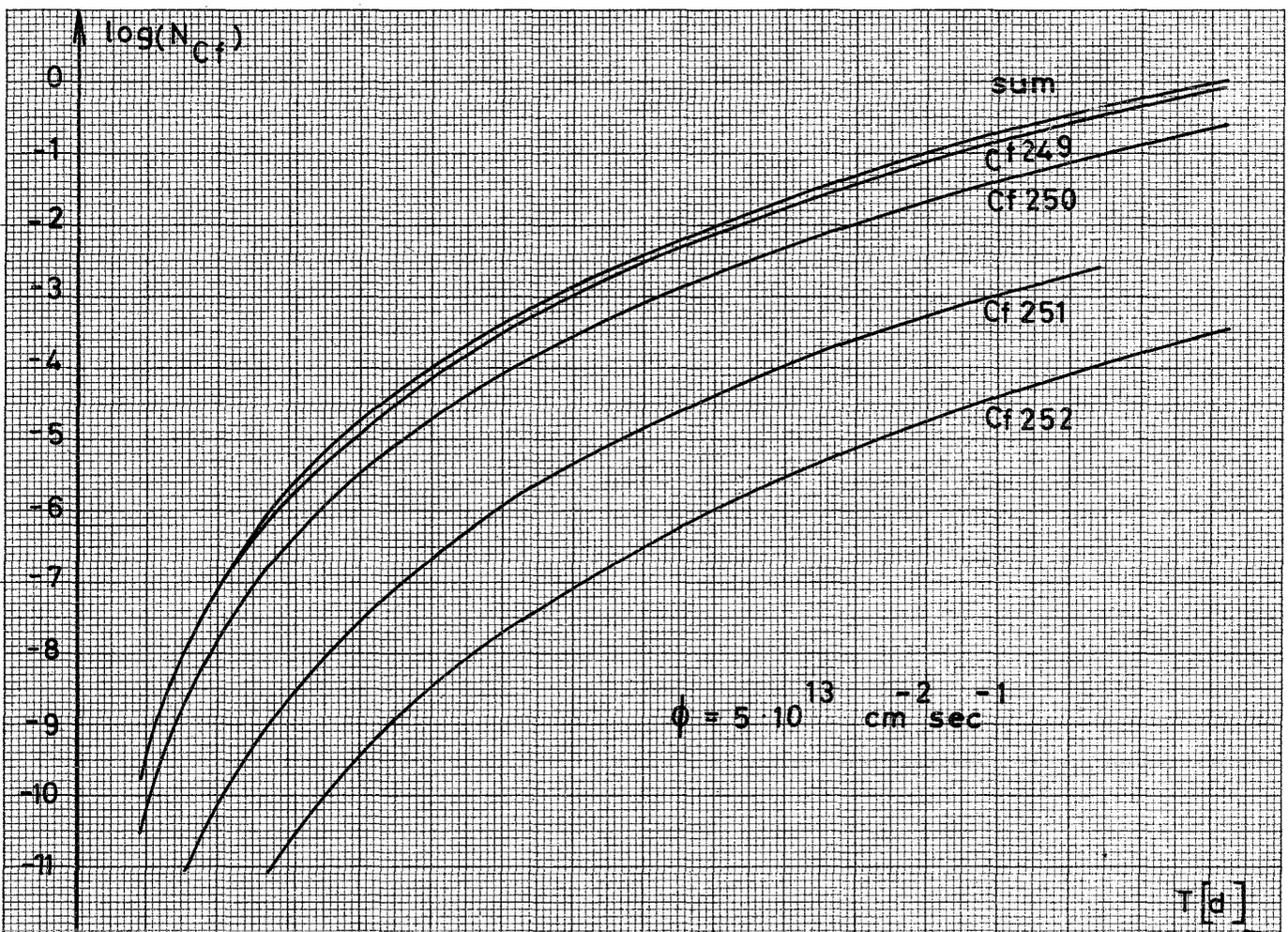


Fig 8 : Time dependent formation of californium

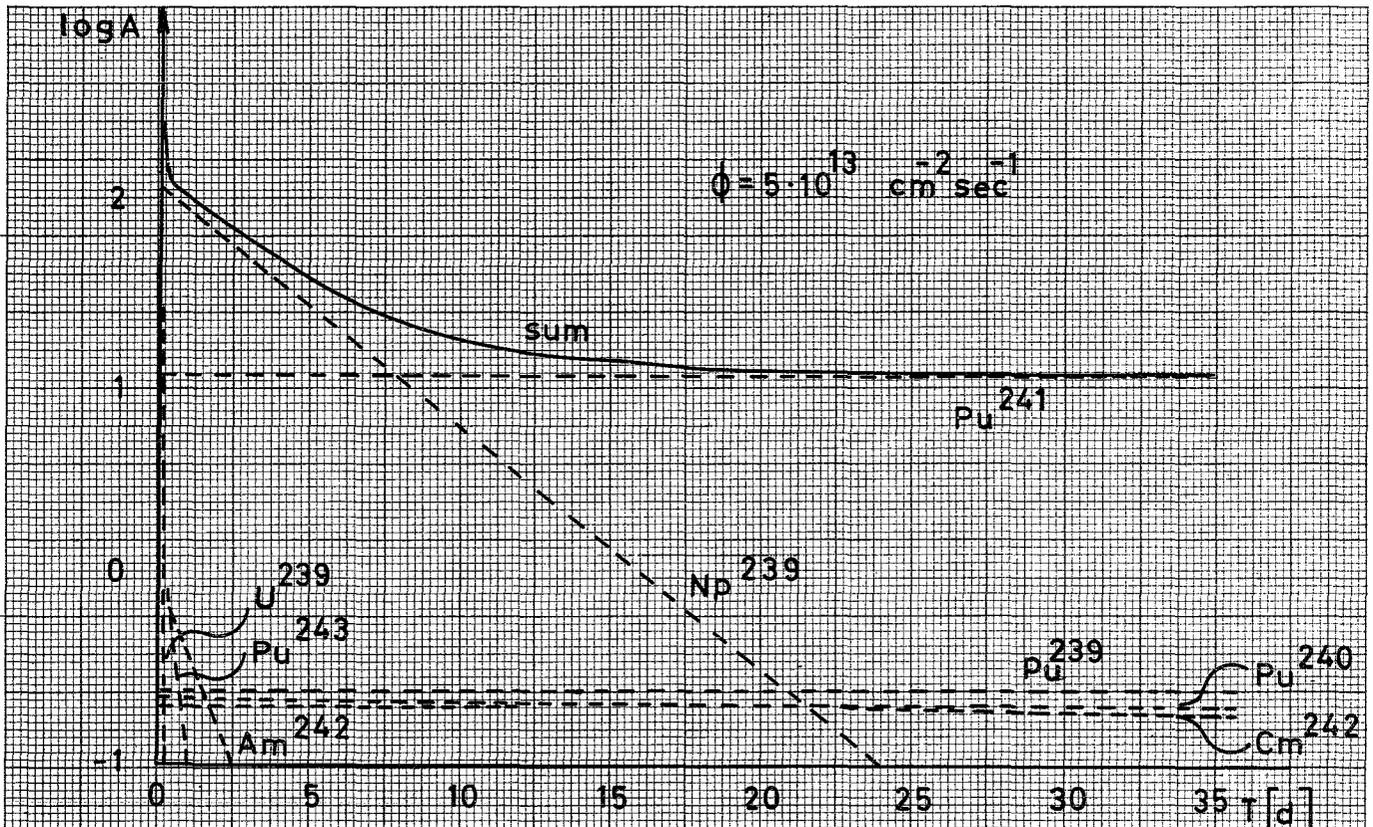
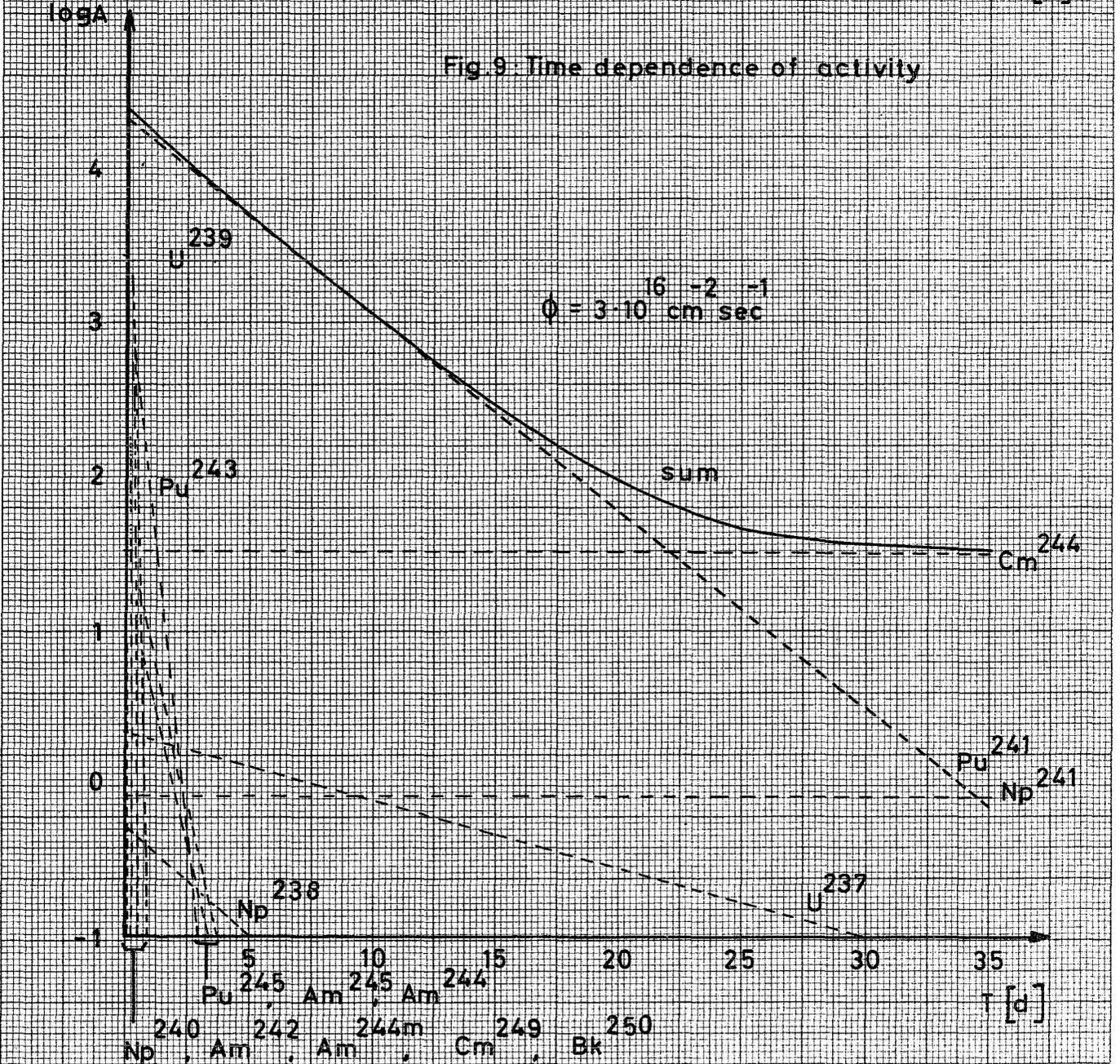


Fig. 9: Time dependence of activity



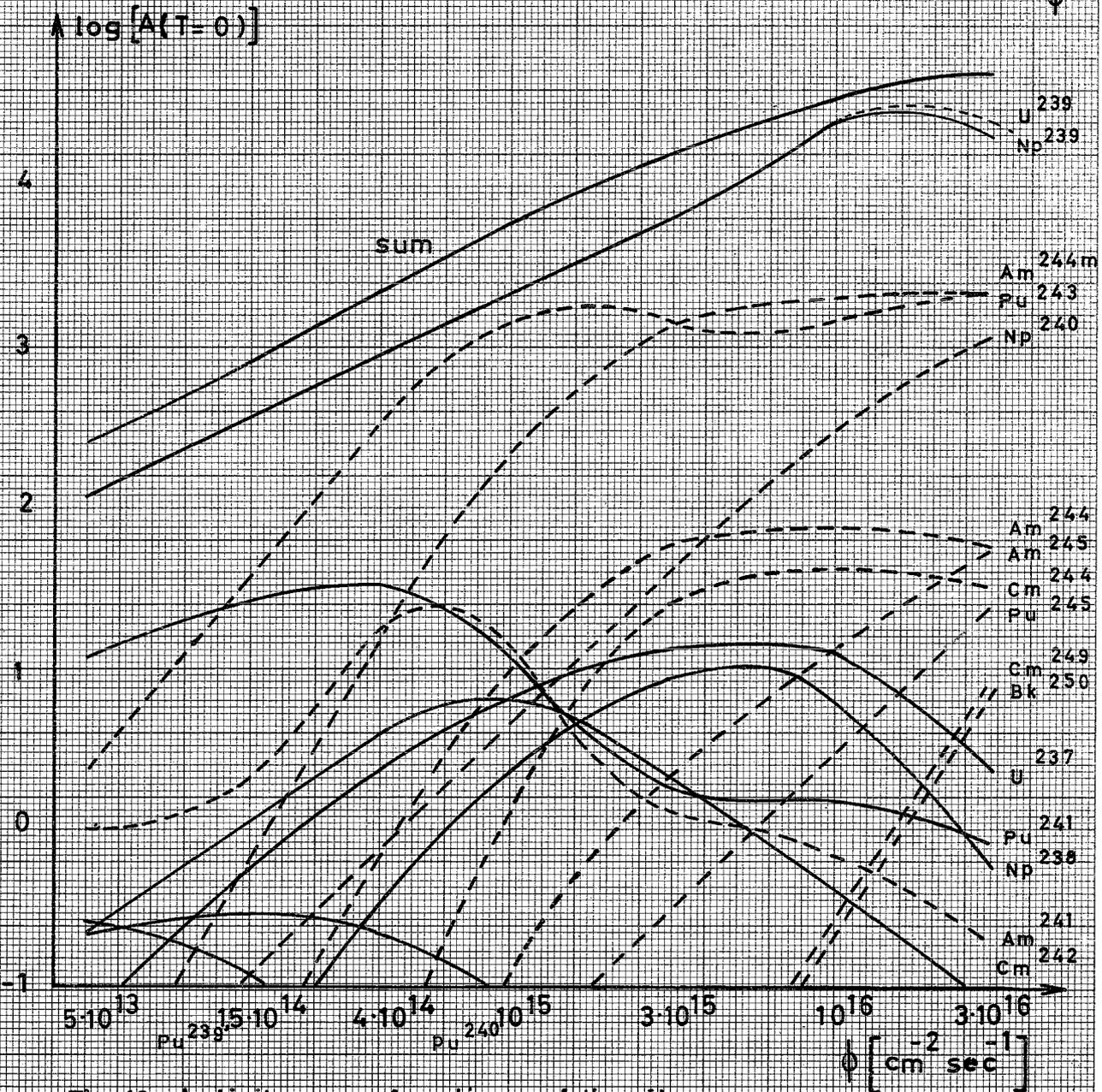
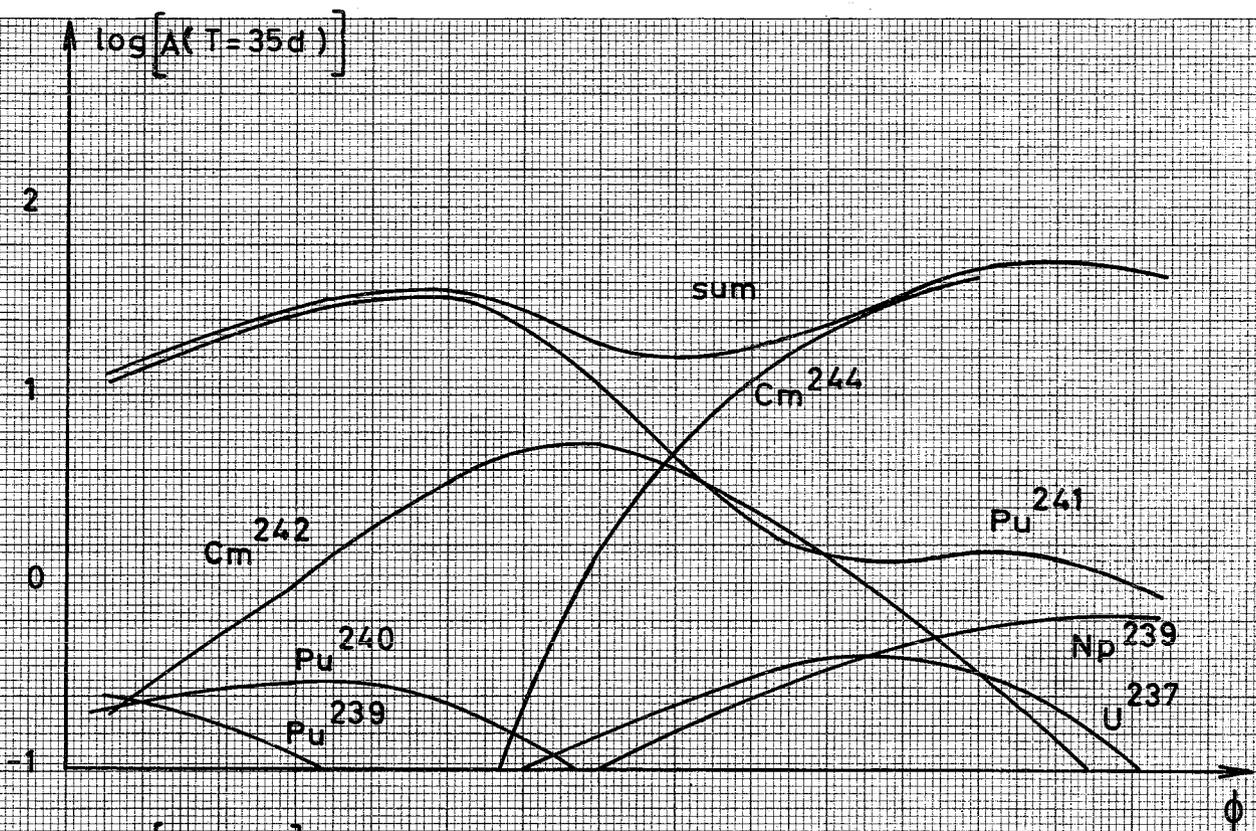


Fig 10 Activity as a function of the flux