# Depletion functions and their use in the calculation of isotope transmutations

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### Abstract

The basic points in the calculation of transmutations of isotopes are analyzed using the so-called "depletion functions". It is shown that conventional criteria used for selecting the most important nuclide chains and for eliminating of the short-lived isotopes from them are sometimes misleading. In particular, the usual neglection of the short-lived nuclides may appear to be incorrect. At small irradiation time $t$ the error introduced by this approximation is about $\varepsilon \approx (n-2)/\lambda_k t$, where $n$ is the number of nuclides in the chain and $\lambda_k$ is the destruction rate of the neglected isotope. At large $t$ $\varepsilon \approx -\lambda_m/\lambda_k$ where $\lambda_m$ is the lowest destruction rate in the chain. As a result, the error does not tend to zero when $t$ goes to infinity unless at least one nuclide is not depleted at all. Simple formulae for the sensitivity of the calculated nuclide concentrations to the adopted values of nuclear constants are obtained. To illustrate the results we consider production of actinides.

### Zusammenfassung

**Verarmungsfunktionen und ihre Verwendung bei der Berechnung von Isotopenumwandlungen**

Die „Verarmungsfunktionen" spielen bei Rechnungen zur Analyse von Isotopenumwandlungen eine grundlegende Rolle. Es wird gezeigt, daß die heute üblichen Kriterien zur Auswahl der wichtigsten Nuklidketten und zur Elimination kurzlebiger Isotope aus ihnen in manchen Fällen irreführen. Insbesondere dürfte die häufig gehandhabte Vernachlässigung sehr kurzlebiger Isotope falsch sein. Der so erzeugte Fehler bei kurzer Bestrahlungszeit $t$ ist ungefähr von der Größe $\varepsilon \approx (n-2)/\lambda_n t$. Hierbei ist $n$ die Anzahl der Kettenglieder und $\lambda_n$ die Zerfallskonstante des vernachlässigten Isotops. Der Fehler geht auch bei unendlich langer Bestrahlungszeit nicht gegen Null, es sei denn, daß ein Glied der Kette überhaupt nicht abgebaut wird. Einfache Formeln werden angegeben, die erkennen lassen, wie empfindlich die berechneten Nuklidkonzentrationen von den angenommenen Nuklidkonstanten abhängen. Zur Demonstration der Ergebnisse wird die Erzeugung von Aktiniden behandelt.

## 1. Introduction

In many problems of nuclear physics beginning from the studies of the stellar evolution [1] up to the design of nuclear reactors [2; 3] it is necessary to calculate transmutations of isotopes. The detailed picture of all possible transitions is usually very complicated. However, it is practically always possible to resolve any such picture into a number of independent linear chains if for each particular nuclide one takes into account only one channel of formation and all channels of destruction[1] [4].

Isotope concentrations in each chain satisfy the equations:

$$dN_1/dt = -\lambda_1 N_1$$
$$dN_i/dt = s_{i-1}N_{i-1} - \lambda_i N_i, \quad i = 2,\ldots,n\,. \quad (1)$$

Here $n$ is the number of nuclides in the chain, $N_i$ is the concentration of the nuclide $i$, $\lambda_i$ is its total destruction rate and $s_i$ is the partial rate of its transformation into the next nuclide. Eqs. (1) can be solved for each depletion chain independently and the total concentration of each nuclide can be obtained by summing the contributions of all chains in which that nuclide appears.

In the simplest case, where $s_i$ and $\lambda_i$ do not change with time and only the first isotope in the chain was present initially (i.e. $N_1(0) = N_1^0$, $N_k(0) = 0$, $k = 2,\ldots,n$) the solution of Eq. (1) is [5]

$$N_n(t) = N_1^0 \left( \prod_{i=1}^{n-1} s_i t \right) D_n\left(\lambda_1 t,\ldots,\lambda_n t\right) \quad (2)$$

and for the arbitrary initial concentrations $N_k(0) = N_k^0$, $k = 1,\ldots,n$

$$N_n(t) = \sum_{k=1}^{n} N_k^0 \left( \prod_{i=k}^{n-1} s_i t \right)$$
$$\cdot\, D_{n-k+1}(\lambda_k t,\ldots,\lambda_n t). \quad (3)$$

Here $D_n(x_1,\ldots,x_n)$ is the so-called "depletion function" (DF)

$$D_n(x_1,\ldots,x_n) \equiv \sum_{i=1}^{n} \frac{e^{-x_i}}{\prod_{\substack{j=1\\j\neq i}}^{n} (x_j - x_i)}. \quad (4)$$

In spite of its simplicity Eq. (4) is not always convenient for the actual calculation of DF. It cannot be applied as it stands in the case where $x_i = x_j$ ($i \neq j$), so that the limiting procedure $x_i \to x_j$ must be performed. If the values $x_i$ and $x_j$ are close to each other severe round-off errors arise in computer calculations due to the approximate cancellation of many nearly equal terms [1; 4–6].

In my recent paper [7] (hereafter I) it is shown that DF are closely connected with the divided differences of the function $f(x) = \exp(-x)$ and a number of new expressions and inequalities for DF is obtained. Here we shall apply these results to the analysis of the following key points in the calculation of isotope transmutations[2].

1) Estimates of the isotope production in a linear chain.
2) Selection of the most important nuclide chains.
3) Elimination of the short-lived nuclides.
4) Estimation of the sensitivity of the calculated nuclide densities to the adopted values of nuclear constants.

## 2. Basic relations for depletion functions (DF)[3]

DF are strictly positive and symmetrical in all arguments. The following recursion relations hold

$$D_1(x_i) = e^{-x_i}, \quad i=1,\ldots,n$$

$$D_n(x_1,\ldots,x_n) = \quad (5)$$

$$\frac{D_{n-1}(x_1,\ldots,x_{i-1},x_{i+1},\ldots,x_n) - D_{n-1}(x_1,\ldots,x_{j-1},x_{j+1},\ldots,x_n)}{x_i - x_j}$$

Eq. (5) gives us the expression for the partial derivative

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[1] The only exception is the case of recycling (i.e. the formation of a parent nuclide from one of its daughters). Here we assume that this effect is negligible.

[2] More detailed exposition can be found in [8].

[3] Other relations, proofs and references as well as the FORTRAN-IV subroutine DEPLET for calculating DF without the loss of accuracy at nearly equal values of $x_1,\ldots,x_n$ can be found in I.

$$\frac{\partial}{\partial x_i} D_n(x_1,\ldots,x_n) = -D_{n+1}(x_1,\ldots,x_n,x_i). \quad (6)$$

In the case where some of the arguments $x_1,\ldots,x_n$ coincide

$$D_n(\overbrace{x_1,\ldots,x_n}^{n}) = \frac{e^{-x_1}}{(n-1)!} \quad (7)$$

$$D_n(\overbrace{x_1,\ldots,x_1}^{n-1},x_2) = e^{-x_2}\gamma^*(n-1,\ x_1-x_2). \quad (8)$$

Here $\gamma^*(n,x)$ is the modified incomplete gamma function (see Appendix).
The following sequence of inequalities is valid

$$0 < D_n(x_1,\ldots,x_n) \leqslant \frac{1}{(n-1)!}, \quad (9)$$

$$(x_i \geqslant 0, \quad i=1,\ldots,n),$$

$$\frac{1}{(n-1)!} \exp\left(-\frac{1}{n}\sum_{i=1}^{n} x_i\right) \leqslant D_n(x_1,\ldots,x_n) \leqslant \quad (10)$$

$$\leqslant \frac{1}{n!}\sum_{i=1}^{n} \exp(-x_i),$$

$$e^{-x_k}\gamma^*\left[n-1,\ \frac{1}{n-1}\sum_{\substack{i=1\\i\neq k}}^{n}(x_i-x_k)\right] \leqslant$$

$$\leqslant D_n(x_1,\ldots,x_n) \leqslant \frac{e^{-x_m}}{n-1}\sum_{\substack{i=1\\i\neq m}}^{n}\gamma^*(n-1,x_i-x_m) \quad (11)$$

Each of these inequalities is more restrictive than the previous one. The right-hand side of Eq. (9) is close to the exact value only if all the arguments $x_1,\ldots,x_n$ are small. The interval of the possible variation of DF, allowed by Eqs. (10), (11) decreases with the decrease in the scatter of $x_1,\ldots,x_n$ while their absolute values may be large. In order to minimize this interval in Eq. (11) one should first substitute $x_k = x_m = x_{min}$ and then $x_k = x_m = x_{max}$ ($x_{min}$ is the smallest argument of DF and $x_{max}$ is the largest one). In this way two lower and two upper bounds on DF are obtained and it is easy to choose the most restrictive limitations among them.
For small scatter of arguments a good estimate of DF is provided by the linear combination of the lower and upper bounds in Eq. (10)

$$D_n(x_1,\ldots,x_n) \approx \quad (12)$$

$$\frac{1}{n+1}\left[\frac{n}{(n-1)!}\exp\left(-\frac{1}{n}\sum_{i=1}^{n}x_i\right) + \frac{1}{n!}\sum_{i=1}^{n}\exp(-x_i)\right]$$

## 3. Estimates of the isotope production in a linear chain

In order to demonstrate how Eqs. (9)–(11) can be used let us estimate the production of Cf-250 from Cm-246 via the chain shown in Fig. 1. Using the parameters from [9] for the irradiation time $T = 1$ year we obtain the values of $s_i T$ and $\lambda_i T$ listed in the Table.
The exact value of Cf-250 concentration is $N_5 = 7.2 \cdot 10^{-5}$. Eqs. (9) and (10) give $0 < N_5 \leqslant 8.6 \cdot 10^{-4}$ and $3.4 \cdot 10^{-5} \leqslant N_5 \leqslant 3.4 \cdot 10^{-4}$ respectively. Eq. (12) gives the estimate $N_5 \approx 8.5 \cdot 10^{-5}$. Substituting in Eq. (11) $x_k = x_m = 0.073$ and using Eq. (A.2) or the table of $\ln \gamma^*(n,x)$ from I, we obtain $4.8 \cdot 10^{-5} \leqslant$
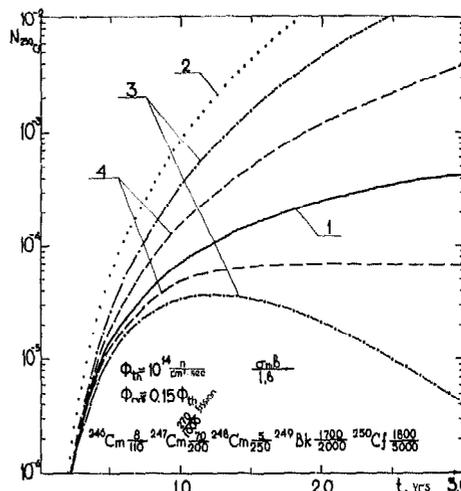


Fig. 1: The use of inequalities (9)–(11) for estimating the production of Cf-250 from Cm-246; data from Ref. [9] (β-decays and resonance shielding are neglected) 1 – exact solution, 2 – Eq. (9), 3 – Eq. (10), 4 – Eq. (11)

$N_5 \leqslant 2.5 \cdot 10^{-4}$. If we choose $x_k = x_m = 8.05$ the result is $4.4 \cdot 10^{-5} \leqslant N_5 \leqslant 1.5 \cdot 10^{-4}$. Finally, we come to the following bounds $4.8 \cdot 10^{-5} \leqslant N_5 \leqslant 1.5 \cdot 10^{-4}$.
The time dependence of Cf-250 concentration together with the lower and upper bounds given by Eqs. (9)–(11) is shown in Fig. 1. At small $t$ one can use simple estimates (9) and (10) while at large $t$ only inequalities (11) are sufficiently restrictive.

## 4. Selection of the most important nuclide chains

Since the number of all possible paths going to a given nuclide is usually very large one would like to neglect those paths along which only a small fraction of the flow travels. Usually the chains which are reached from the seed isotope due to a small branching are believed to be insignificant. For example, an unstable nuclide instead of decay may capture a neutron and jump into another chain. If this nuclide is short-lived such chains are neglected without any further consideration, in particular, because neutron cross sections for radioactive isotopes are usually unknown[4].
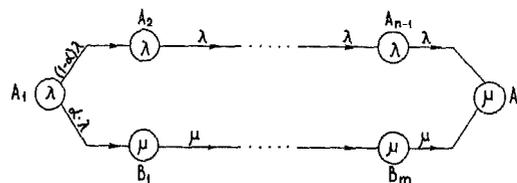


Fig. 2: Two nuclide chains contributing to the production of the isotope $A_n$ from $A_1$

Let us compare the contributions of two nuclide chains $A$ $(A_1,\ldots,A_n)$ and $B(A_1,B_1,\ldots,B_m,A_n)$ into the production of the isotopes $A_n$ from $A_1$ (see Fig. 2). Assuming that only $A_1$ was present initially we obtain using Eqs. (2) and (8)

$$\frac{N_A(t)}{N_B(t)} = \quad (13)$$

$$\frac{1}{\alpha}\cdot\frac{(\lambda t)^{n-2}}{(\mu t)^m}\cdot\frac{e^{-\mu t}\gamma^*(n-1,\lambda t-\mu t)}{e^{-\lambda t}\gamma^*(m+1,\mu t-\lambda t)}.$$

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[4] Note that for estimates of unknown thermal neutron cross sections one can use the statistical approach developed in our recent paper [10].

Here $N_A$ and $N_B$ denote the number of $A_n$ nuclei produced via the branches $A$ and $B$ respectively. If the relations $\mu \gg \lambda$, $\mu t - \lambda t \gg \max (m, n)$ hold, Eq. (A.5) gives

$$\frac{N_A(t)}{N_B(t)} \approx \frac{1}{\alpha} \frac{(\lambda t)^{n-2}}{(n-2)!} \, . \tag{14}$$

Hence, in the time interval

$$(\lambda/\mu) \cdot \max (m, n) \ll t \ll [\alpha \, (n-2)!]^{1/(n-2)}$$

the branch $B$ gives the main contribution into $A_n$ production. For example, in the case where $n = 7$, $m = 10$, $\mu/\lambda = 10^4$ this interval is noticeable even for an extremely small branching ratio $\alpha = 10^{-7}: 0.001 \ll t \ll 0.1$.

Thus, one cannot neglect a branch where transitions occur rapidly, even if it is longer than the main path and the corresponding branching ratio is small[5]. The contribution of any such branch should be estimated reliably using, for instance, the inequalities (9)–(11).
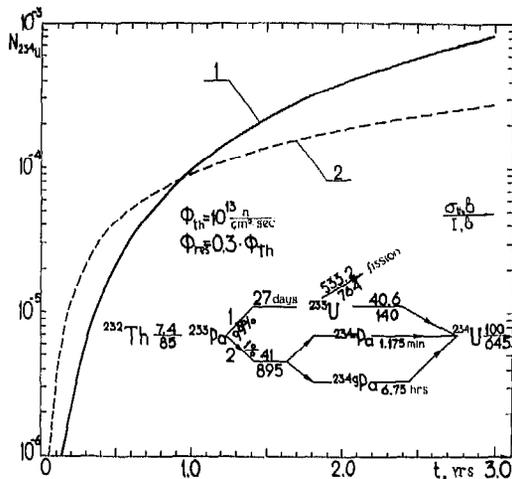


Fig. 3: Comparison of the contributions of two chains into the production of U-234 from Th-232; data from the KORT library [12]

As an example, let us compare the production of U-234 from Th-232 through the two paths shown in Fig. 3. The short-lived Pa-233 decays into U-233 with 99 % probability. Only in 1 % of cases it captures a neutron and turns into Pa-234. However, Pa-234 decays into U-234 directly, while U-233 must at first capture a neutron (and avoid fission, which follows 91 % of captures). As a result, for a neutron irradiation in times less than a year the main flow goes through the Pa-234 path and even after three years this branch contributes more than 30 %.

## 5. Elimination of short-lived nuclides

It is always assumed in nuclide inventory calculations as well as in the analysis of radioactive chains that short-lived nuclides achieve equilibrium concentrations rapidly and thus can be neglected. The question is: which isotopes in a particular problem are sufficiently short-lived? The commonly used criterion is $\lambda_k t > C$ ($3 \leq C \leq 20$), where $\lambda_k$ is the destruction rate of the short-lived nuclide [2; 13–15]. If this criterion is fulfilled the isotope is deleted from the chain, so that in the reduced chain the $(k-1)$ nuclide is directly transformed into the $(k+1)$ one (the factor $s_k$ in Eq. (2) is replaced by $s_{k-1} \cdot s_k/\lambda_k$). The underlying assumption is that the error decreases as $\exp(-\lambda_k t)$ and at $t \sim C/\lambda_k$ it becomes negligible [13; 14]. We shall demonstrate here that this assumption is wrong.

For the reduced chain Eq. (2) takes the form

[5] *Ward et al.* [11] considered various branching points in the s-process heavy element synthesis network. In particular, they have paid attention at the similar relative-delay effect of alternative capture paths passing through cross sections of different size and underlined the importance of the paths passing through large cross sections.

$$N_n^{(r)}(t) = N_1^0 \cdot \frac{s_k}{\lambda_k} \tag{15}$$

$$\prod_{\substack{i=1 \\ i \neq k}}^{n-1} (s_i t) D_{n-1} (\lambda_1 t, \dots, \lambda_{k-1} t, \lambda_{k+1} t, \dots, \lambda_n t).$$

Taking into account the recursion relations (5) we obtain

$$N_n(t) = \frac{1 - \delta}{1 - \frac{\lambda_m}{\lambda_k}} \, N_n^{(r)}(t)$$

$$\delta = \frac{D_{n-1}(\lambda_1 t, \dots, \lambda_{m-1} t, \lambda_{m+1} t, \dots, \lambda_n t)}{D_{n-1}(\lambda_1 t, \dots, \lambda_{k-1} t, \lambda_{k+1} t, \dots, \lambda_n t)} \, , \tag{16}$$

where $\lambda_m$ is the lowest destruction rate in the chain. As the time passes the value of $\delta$ tends to zero. It is evident from Eq. (16) that unless one of the nuclides in the chain is not depleted at all ($\lambda_m = 0$) the error from replacing $N_n(t)$ by $N_n^{(r)}(t)$ does not tend to zero at $t \to \infty$.

This result can be easily understood if one takes into account that elimination of a short-lived nuclide from the chain shifts the time scale for the following isotopes by $\Delta t \sim 1/\lambda_k$

$$N_n(t) \approx N_n^{(r)}(t - 1/\lambda_k) \, . \tag{17}$$

At large $t$ only one exponent survives in Eq. (4) and $N_n(t)$ is proportional to $\exp (-\lambda_m t)$. For $\lambda_m \ll \lambda_k$ Eq. (17) is reduced to Eq. (16) with $\delta = 0$.

The exact expression for the time-dependent part of the error can be obtained in the simple case where all nuclides except the short-lived one have equal destruction rates (i.e. $\lambda_i = \lambda$, $i \neq k$). Eqs. (7), (8) and (16) give

$$\delta = (n-2)! \, e^{\lambda t - \lambda_k t} \, \gamma^*(n-2, \lambda t - \lambda_k t). \tag{18}$$

Using Eq. (A.6) we obtain for $\lambda_k t - \lambda t \gg n$

$$\delta = \frac{n-2}{\lambda_k t - \lambda t}$$

$$\cdot \left[ 1 - \frac{n-3}{\lambda_k t - \lambda t} + \frac{(n-3)(n-4)}{(\lambda_k t - \lambda t)^2} - \dots \right] \tag{19}$$

Hence, in this case $\delta$ is almost proportional to the length of the chain and inversely proportional to the irradiation time. For small $t$ ($\lambda_i t \ll 1$, $i \neq k$) this result is model-independent. It can be easily derived from Eq. (17) and the commonly used approximate solution of Eq. (1) [2] which for the reduced chain has the form

$$N_n^{(r)}(t) \approx \frac{s_k}{\lambda_k} \left( \prod_{\substack{i=1 \\ i \neq k}}^{n-1} s_i \right) \frac{t^{n-2}}{(n-2)!} \, . \tag{20}$$

For $\lambda_k t \gg n$ we have

$$N_n(t) \approx \frac{s_k}{\lambda_k} \left( 1 - \frac{n-2}{\lambda_k t} \right) N_n^{(r)}(t) \, , \tag{21}$$

which is similar to Eq. (19) ($\lambda_k \gg \lambda$). For $n = 7$ and $\lambda_k t = 20$ the error will be about 25 %. Thus, the commonly used criterion $\lambda_k t > C$ cannot provide sufficient accuracy.

Let us consider the influence of Np-239 on the production of Pu-239 from U-238 as an example (Figs. 4, 5). Due to the short lifetime ($T_{1/2} = 2.35$ d) Np-239 is often neglected (see e.g. [4; 16].). The error of this approximation after three months of irradiation in the constant flux is about 10 %. It is comparable to the difference between the one- and two-dimensional
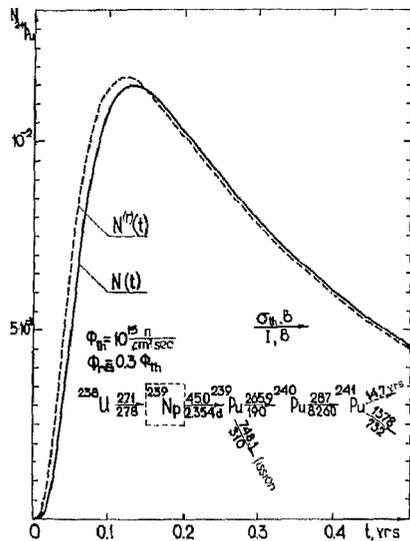
Fig. 4: The influence of Np-239 on the production of Pu-241 from U-238; — Np-239 is taken into account; – – – – Np-239 is neglected
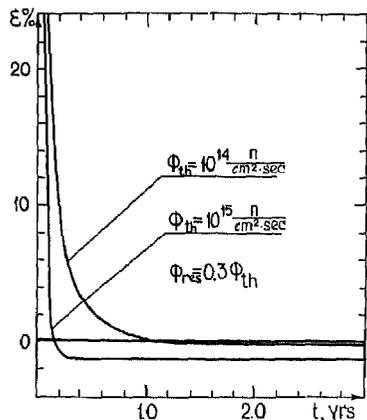


Fig. 5: The relative error due to elimination of Np-239, $\varepsilon = (N^{(r)}-N)/N$

calculation of the plutonium production in nuclear reactors [16]. Hence, Np-239 is non-negligible in such calculations. At large $t$ the error is determined only by the ratio of U-238 and Np-239 destruction rates and does not depend on the particular plutonium isotope considered.

## 6. Discussion

Simple estimates show that the two sources of potential error considered in Secs. 4,5 can be responsible for the reported discrepancies between the measured and calculated concentrations. For example, the comparison of the extensive fission-product absorption calculations (using EPRI-CINDER code and data libraries [4]) with the experiment [17] has revealed that "values calculated for the epithermal quantities are consistently (about 10–25 %) lower than measured values; these discrepancies greatly exceed any consideration of the tacit inclusion of fast absorption in measured values" [5]. This trouble seems to be due to the fact that all nuclides with half-lifes < 4 hours were assumed to decay instantaneously. Assuming $\Phi \sim 10^{14}$ n/cm$^2$sec and $\sigma \sim 10^3$ b we see that all the paths having branching rations less than $10^{-3}$ have been neglected. The examples of Sec. 4 show that some important chains could be lost. On the other hand, the typical irradiation time in the experimental was about 400 hours and there are about 10 nuclides in each chain. Eq. (21) gives the estimate of the error $\varepsilon = (N^{(r)}-N)/N \approx 11.5\%$ per neglected nuclide (for $T_{1/2} = 4$ hours). In absorption calculations this error could be still more enhanced by the large values of epithermal cross

sections for some isotopes. However, the comparison with the experiment shows that for epithermal absorbers the first source of error is more important.

In s-process nucleosynthesis calculations, where very long chains are considered (about 150 isotopes produced via successive neutron captures), the error connected with the elimination of the short-lived nuclides can be large even at $\lambda_k t \sim 10^3$. The total irradiation time in s-process is about $2 \cdot 10^3$ yrs. In the unbranched s-process calculations isotopes having $T_{1/2} \lesssim 1$ yr are usually neglected [6]. Eq. (21) shows that the elimination of a nuclide with $T_{1/2} = 1$ yr over-estimates the last nuclide density by $\varepsilon \approx 10\%$. If there are ten such isotopes the total error can exceed 100 %.

## 7. Sensitivity of nuclide densities to the physical constants

Sensitivity studies in nuclide inventory calculations were performed by a number of authors. Wilson et al. [15] varied numerically each of the parameters involved, making a lot of separate calculations. Sola [18; 19] derived many explicit formulae for the sensitivities of particular actinide and fission product concentrations. Rudik et al. [3; 9; 20–22] developed a general perturbation theory for depletion equations. Here we shall derive several simple relations which enable one to estimate sensitivities in practical problems.

Most often we are interested in the relative change of $N_n$ $(t)$ which is caused by the variation of some parameter $\alpha$. Following [22] let us define the "influence function" $\varphi_\alpha^{(n)}(t)$ through the relation

$$\frac{N_n(t)}{N_n(t)} = \frac{\Delta\alpha}{\alpha} \, \varphi_\alpha^{(n)}(t). \qquad (22)$$

If $\alpha$ enters into one of the partial reaction rates $s_k$ we have a trivial relation

$$\varphi_\alpha^{(n)} = \frac{\alpha}{s_k} \cdot \frac{\partial s_k}{\partial\alpha} \qquad (23)$$

The case where $\alpha$ enters into one of the total destruction rates $\lambda_k$ is more interesting. Eq. (6) gives

$$\varphi_\alpha^{(n)} = -\alpha t \cdot \frac{\partial\lambda_k}{\partial\alpha} \cdot \frac{D_{n+1}(\lambda_1 t, \ldots, \lambda_n t, \lambda_k t)}{D_n(\lambda_1 t, \ldots, \lambda_n t)} \qquad (24)$$

Due to the symmetry of $D_n$ $(x_1, \ldots, x_n)$ in all its arguments $S_\alpha^{(n)}(t)$ does not depend on the detailed locations of nuclides in the chain.

At small $t$ $(\lambda_i t \ll 1, i = 1, \ldots, n)$ Eqs. (9) and (24) give

$$\varphi_\alpha^{(n)} \approx -\frac{\partial\lambda_k}{\partial t} \cdot \frac{dt}{n} \qquad (25)$$

Using Eq. (25), we obtain similarly to Eq. (16)

where $\qquad \varphi_\alpha^{(n)}(t) = -\frac{\alpha}{\lambda_k} \cdot \frac{\partial\lambda_k}{\partial\alpha} \cdot \frac{1-\delta}{1-\frac{\lambda_m}{\lambda_k}}$

$$\qquad (26)$$

$$\delta = \frac{D_n(\lambda_1 t, \ldots, \lambda_{m-1} t, \lambda_{m+1} t, \ldots, \lambda_n t, \lambda_k t)}{D_n(\lambda_1 t, \ldots, \lambda_n t)}$$

Here $\lambda_m$ is the lowest destruction rate $\lambda_i$ which is not equal to $\lambda_k$. The function $|\varphi_\alpha^{(n)}(t)|$ increases monotonously with the irradiation time $t$. If $\lambda_k < \lambda_m$ (i. e. the $k$th isotope disappears at the lower rate than any other nuclide in the chain) it follows from Eqs. (6) and (26) that arbitrary large negative values of $\varphi_\alpha^{(n)}(t)$ can occur. On the other hand, if $\lambda_m < \lambda_k$, $\varphi_\alpha^{(n)}(t)$ satisfies the inequality

$$0 \geqslant \varphi_\alpha^{(n)}(t) \geqslant -\frac{\alpha}{\lambda_k} \cdot \frac{\partial\lambda_k}{\partial\alpha} \cdot \frac{1}{1-\frac{\lambda_m}{\lambda_k}} \qquad (27)$$

For large $t$, when $\delta \ll 1$, $\varphi_a^{(n)}(t)$ depends neither on $n$ nor on $t$. Hence, it does not matter, which particular isotope is produced by the chain, provided that its destruction rate is not the lowest one (Rudik et al. [9] have arrived at a similar conclusion using Eqs. (2) and (4)).

As an example, let us estimate the sensitivity of Cf-250 production by the chain shown in Fig. 1 to the variation of Cf-250 thermal neutrons capture cross section. For small irradiation time $t = 0.2$ yr Eq. (25) gives

$$\varphi_{\sigma_5}^{(5)}(t) \approx - \sigma'_5 \cdot \mathcal{P}_{th} \cdot t/5 = -0.227. \qquad (28)$$

The exact value $\varphi_{\sigma_5}^{(5)} = -0.194$ [9], the error being about 15 % only, though in this case $\lambda_4 t = 1.3$, $\lambda_5 t = 1.6$ (see Table 1), so that $t = 0.2$ yr is not really small.

**Table 1: Values of $s_i T$ and $\lambda_i T$ for the chain shown in Fig. 1 ($T = 1$ year)**

| Nuclide | $^{246}Cm$ | $^{247}Cm$ | $^{248}Cm$ | $^{249}Bk$ | $^{250}Cf$ |
|---------|-----------|-----------|-----------|-----------|-----------|
| $\sigma_i T$ | 0.0773 | 0.316 | 0.134 | 6.312 | - |
| $\lambda_i T$ | 0.0773 | 1.641 | 0.134 | 6.312 | 8.047 |

The lower bound for $\varphi_{\sigma_5}^{(5)}(t)$ can be obtained using Eq. (27)

$$\varphi_{\sigma_5}^{(5)}(t) \geqslant \qquad (29)$$

$$- \frac{\sigma'_5 \mathcal{P}_{th}}{(\sigma'_5 - \sigma'_1) \cdot \mathcal{P}_{th} + (I_5 - I_1) \mathcal{P}_r} = -0.713.$$

Here $\lambda_m = \lambda_1$ because Cm-246 has the lowest destruction rate. For $t = 6$ yr $\varphi_{\sigma_5}^{(5)} = 0.697$ [9], so that the sensitivity has almost achieved its lower bound.

The time dependence of $\varphi_{\sigma_i}^{(5)}(t)$ is shown in Fig. 6 which demonstrates the validity of simple formulae (25) and (27) in estimating sensitivities.
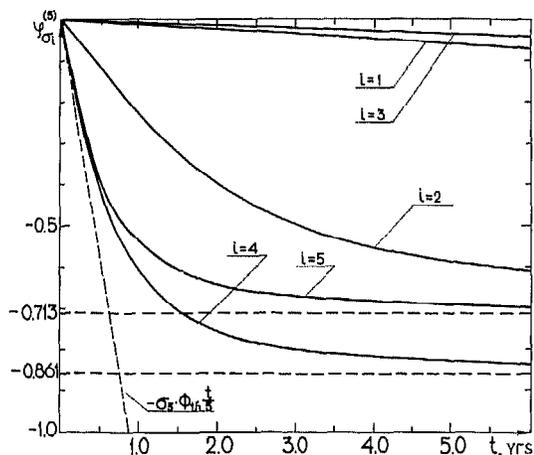


Fig. 6: Time dependence of the sensitivity functions $\varphi_{\sigma_i}^{(5)}(t)$

### Conclusions

The technique of the depletion functions is applied to the problems occurring in nuclide inventory calculations. This technique has three distinct advantages. In the first place it is simpler and more elegant than the other more conventional methods. Second, it allows quick estimates of the rate of isotope production in various problems and its sensitivity to the adopted values of constants. Finally, using depletion functions one can easily analyze the validity of the assump-

tions which are often used without caution. In particular, the error arising when short-lived nuclides are deleted from the chain appears to be surprisingly large.

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**Appendix**

This appendix contains basic relations for the modified incomplete gamma function $\gamma^*(n, x)$. These formulae can be easily derived from the similar relations for $\gamma(n, x)$ [23]. Additional formulae and the table of $\ln \gamma^*(n, x)$ ($1 \leq n \leq 10$, $-100 \leq x \leq 100$) can be found in I.

$$\gamma^*(n,x) = \frac{1}{(n-1)! \, x^n} \int_0^x e^{-t} t^{n-1} dt, \qquad (A.1)$$

$$\gamma^*(n,x) = \frac{1 - e^{-x} e_{n-1}(x)}{x^n}, \qquad (A.2)$$

where $e_n(x) \equiv \sum_{m=0}^{n} x^m/m!$,

$$\gamma^*(n,x) = 1/x \left[ \gamma^*(n-1, x) - \frac{e^{-x}}{(n-1)!} \right] \qquad (A.3)$$

$$\frac{d}{dx} \gamma^*(n,x) = -n \cdot \gamma^*(n+1, x), \qquad (A.4)$$

$$\gamma^*(n,x) = \frac{1}{(n-1)!} \cdot \sum_{m=0}^{\infty} (-1)^m \frac{x^m}{m! \, (m+n)}. \qquad (A.5)$$

The following asymptotic formula is valid

$$\gamma^*(n,x) \underset{|x| \to \infty}{\sim} \frac{1}{x^n} - \frac{e^{-x}}{(n-1)! \, x}$$

$$\cdot \left[ 1 + \frac{n-1}{x} + \frac{(n-1)(n-2)}{x^2} + \dots + \qquad (A.6) \right.$$

$$\left. + \frac{(n-1)\dots(n-k)}{x^k} + R_k(x) \right].$$

Provided that at least $(n-1)$ terms have been taken into account in Eq. (A.6), the remainder $R_k(x)$ has the sign of the first neglected term and does not exceed its absolute value.

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