FEWGROUP BURNUP CALCULATIONS USING TIME DEPENDENT MICROSCOPIC CROSS SECTIONS

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ABSTRACT

The main drawback of using lattice cell codes in the daily calculation of burnup dependent fewgroup homogenized fuel cross sections is the extensive computer effort that it requires. Many options for speeding up this process can be considered including a reduction of the number of energy groups to be treated in the successive transport solution required at the various burnup steps. Here, we suggest a method for generating time dependent fewgroup microscopic cross sections and discuss how they can be used for fuel depletion calculations.

I. Introduction

The generation of fewgroup burnup dependent cell macroscopic cross sections for core diffusion calculations is one of the main goal of lattice cell codes such as WIMS–AECL[1] and DRAGON[2]. The general calculation scheme considered for such calculations relies on a two step process. The transport equation is first solved for the neutron field distribution at specific time steps using pre-determined nuclide field distributions. The changes in nuclide composition between two different time steps being controlled by the depletion equations which are solved assuming that the neutron flux distribution remains relatively constant during the evolution period.

The main problem of using this method for day to day analyzes is that it involves a repetitive solution of the transport equation, this generally being the most time consuming part in a lattice code calculation. Many options for speeding up this process have been considered including a reduction of the number of energy groups or a simplification of the geometry to be treated in the successive transport solution required at the various burnup steps. The main drawback with the use of a simplified geometry is that the resulting cell model generally gives rise to a totally different problem. Moreover, such a simplification of the geometry is difficult to automatize in lattice codes which can analyze a large variety of different geometry. Accordingly, we will concentrate our efforts on reducing the number of groups used for the transport solution.

In order to be able to condensed the multigroup microscopic cross sections, the neutron flux spectrum must first be known. This flux spectrum depends on burnup as well as on the spatial location inside the cell. The solution therefore consists in pre-calculating approximate multigroup neutron flux distributions that can be used for the fewgroup condensation.

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Such an option is already automated in the code WIMS–AECL.[1] The condensation flux is computed for a simplified cell using the initial nuclide field distribution in the reference cell. This works very well for the cases where the number of condensed energy groups remains relatively large. However, when a condensation to a very small number of energy groups is considered, the simulation errors at the end of the burnup cycle can become very important.

Here, we propose to generate time dependent fewgroup microscopic cross sections based on two condensation fluxes each being representative of the state of the reactor at a specific time step. These cross sections will then be used for the fewgroup flux calculation as well as in the solution of the depletion equations. We expect that the variations in the neutron flux spectrum resulting from burnup can be partially accounted for in the time dependence of the microscopic cross sections. This should result in a method which permits a reliable evaluation fuel isotopic contents at the end of the burnup cycle even in the cases where a very small number of groups is considered.

In Section II of this paper paper we will discuss how the fewgroup time dependent microscopic cross sections can be generated. The performance of the method will be considered in Section III. Finally, we will conclude.

II. Fewgroup Time Dependent Microscopic Cross Sections

Let us consider the typical burnup calculation scheme used in most lattice codes. For the case where an homogeneous cell containing I isotopes of known concentration $N_i(t)$ at time t is to be analyzed, the first step consists of solving the transport equation for the neutron flux distribution using:

$$\left[\vec{\Omega}\cdot\vec{\nabla}+\Sigma^g(t)\right]\phi^g(t)=Q^g(t) \tag{1}$$

where the macroscopic cross section $\Sigma^g(t)$ is defined as

$$\Sigma^g(t)=\sum_{i=1}^{I}N_i(t)\sigma_i^g \tag{2}$$

with σ_i^g the multigroup microscopic cross section associated with isotope i. The term Q^g generally includes fission and scattering sources and is therefore also dependent on t via the isotopic concentrations N_i.

In order to evaluate the concentration of the various isotopes in this cell as a function of time, one has to solve a set of I depletion equations of the form:

$$\frac{dN_i(t)}{dt}=\sum_{j=1}^{I}\left[\lambda_j\alpha_{j\rightarrow i}+\sigma_{j,x}^g\beta_{j\rightarrow i,x}\phi^g(t)\right]N_i(t) \tag{3}$$

where λ_j is the decay constant of isotope j, $\sigma_{j,x}^g$ is the microscopic cross section associated with reaction x for isotope j, $\alpha_{i\rightarrow i}=\beta_{i\rightarrow i,x}=-1$, and the constants $\alpha_{j\rightarrow i}$ and $\beta_{j\rightarrow i,x}$ for $i\neq j$ represent the production yield of isotope i resulting from a decay (α) or neutron collision (β) with isotope j.

This set of coupled differential equations is generally solved over the complete burnup cycle represented by T using a quasi-static algorithm. Accordingly, the period T is subdivided into micro time steps $\Delta t_k = t_{k+1} - t_k$ during which the neutron flux $\phi^g(t)$ can be assumed to remain relatively constant. As a result Eq. (3) can be solved for $N_i(t_{k+1})$ using the flux distribution at the beginning of the time interval (t_k). As we mentioned above, this approximation is only valid when the depletion period is relatively short. This implies that the time consuming computation of instantaneous neutron flux distributions must be repeated at a fairly large number of micro time steps. This scheme can be accelerated either by reducing the number of micro time steps or by accelerating the solution of the transport equation. Here we will concentrate on the second of these options.

One of the most efficient way to speed up the instantaneous flux distribution evaluation is to reduce the number of energy groups treated in the transport equation. The energy condensation process that leads to the generation of time dependent fewgroup microscopic cross sections is:

$$\sigma_i^G(t) = \frac{1}{\phi^G(t)} \sum_{g \in G} \phi^g(t) \sigma_i^g \tag{4}$$

where

$$\phi^G(t) = \sum_{g \in G} \phi^g(t) \tag{5}$$

and each macro group G contains a varying numbers of micro groups g.

The main problem with this scheme is that the microscopic cross sections are now time dependent and will be affected by the change in the flux spectrum resulting from the depletion process. Because of the form of Eq. (4), we might expect that the dependence of σ_i^G on t is weaker than the dependence of ϕ^g on t. In fact, for the case where σ_i^g is relatively flat in the macro group G, this dependence vanishes, and a unique set of condensed microscopic cross sections can be generated using the initial flux distribution in the cell. Typically, this is the behaviour observed when the number of micro groups included in a macro group is relatively small. However, in the cases where the macro groups are composed of a large number of micro groups, this approximation is no longer valid. We therefore have to take into account, at least approximately, the effect of the changing flux spectrum on the cross sections.

Here we will assume that the condensed fewgroup microscopic cross sections vary linearly with time for macro time steps $\Delta T_K = T_{K+1} - T_K$ much larger than the micro times steps Δt_k required for the depletion calculation. We will therefore consider that for $T_K \leq t \leq T_{K+1}$ we can use the relation:

$$\sigma_i^G(t) = \sigma_{i,0}^G + \sigma_{i,1}^G (t - T_K) \tag{6}$$

where

$$\sigma_{i,0}^G = \frac{\sum_{g \in G} \sigma_i^g \phi^g(T_K)}{\sum_{g \in G} \phi^g(T_K)} \tag{7}$$

$$\sigma_{i,1}^G = \frac{1}{(T_{K+1} - T_K)} \left(\frac{\sum_{g \in G} \sigma_i^g \phi^g(T_{K+1})}{\sum_{g \in G} \phi^g(T_{K+1})} - \sigma_{i,0}^G \right) \tag{8}$$

and

$$\Delta T_K = \sum_{k \in K} \Delta t_k \tag{9}$$

The problem is still incomplete since the evaluation of $\sigma_{i,1}^G$ requires the knowledge of $\phi^g(T_{K+1})$. However, a first approximation for the flux at time T_{K+1} can be obtained by solving the depletion equation over a macro rather than a micro time step using the quasi-static approach. As a result the overall change in the flux spectrum should be partially accounted for in the fewgroup microscopic cross sections.

A solution of the burnup problem can then be considered using these fewgroup time dependent microscopic cross sections for the smaller micro time steps. As a result the full group transport equation would need to be solved only for a very small number of large burnup steps, while most of the micro time steps will involve computing only the fewgroup neutron flux distributions.

This approximation scheme was programmed in the lattice code DRAGON for the case where a general heterogeneous cell is considered. The derivation of the time dependent fewgroup microscopic cross-section library associated with a macro time step as well as the use of this library to generate the macroscopic cross sections required for each micro time steps were automated.

One of the main concerns about this method that can be brought forward is related to perturbations calculations. The fewgroup time dependent microscopic cross sections should be adequate when the properties of the various materials present in the cell are not modified during burnup. However, when temperature perturbations are considered or if coolant voiding takes place in the cell, the fewgroup cross sections computed using the method described above may be entirely inadequate.

This problem can be easily by-passed in DRAGON, since the computed nuclide field distribution at any specific time step can be used to update either the fewgroup or the multigroup macroscopic cross-sections. As a consequence, the effect of perturbations at specific micro or macro time steps can be evaluated using the full library group structure even if the successive transport calculations leading to this point in time were preformed based on the fewgroup cross-section library. Another option is to derive additional few-group libraries for perturbed cell based on the approximate nuclide composition obtained for a reference cell at the end of each macro time step.

III. Numerical results

Here we will consider the burnup of a CANDU cell for 300 days at a power of 31.9713 kw/kg. The fewgroup microscopic cross sections were generated using a single macro time step $\Delta T = 300$ days assuming that the neutron flux spectrum remains constant during this period. Starting from the 69 groups Winfrith WIMS-AECL library, three different fewgroup time dependent microscopic cross-section libraries were generated corresponding to a condensation to 2, 4 and 18 groups (see Table 1 for the energy limits associated with the individual group in the resulting fewgroup libraries). A unique set of microscopic cross section was generated for each of the isotopes present in the coolant, the moderator and the individual structure materials. Similarly, we generated for each of the fuel ring an independent set of microscopic cross sections.

An explicit burnup calculation over a set of 15 non-uniform micro time step (1, 5, 10, 20, 30, 50, 70, 90, 110, 130, 150, 200, 250 and finally 300 days) was then performed using the resulting fewgroup time dependent libraries and compared to a reference calculation for the same micro time steps but using the original 69 group library. Note that for the fewgroup calculations, the depletion over the macro time step, the generation of the time dependent library, and the burnup over the micro time steps were performed in a single DRAGON run.

The errors on K_∞ in mk at the various micro time steps for the 2-, 4- and 18-group calculations are presented in Fig. 1 for the cases where time dependent microscopic cross sections were considered ($\Sigma(t)$) as well as for the case where time independent microscopic cross sections were generated using the initial multigroup flux distribution inside to core ($\Sigma(0)$). As one can see, both 18 group results are within 1.5 mk of the reference. This is expected since the 18 group library is such that it retains most of the feature present in the 69 group library. The main differences can be observed when 2 group calculations are considered. In the case where a condensation using only the flux spectrum at $t = 0$ is used, the error in reactivity for this cell can reach 8 mk. However, when time dependent cross sections are computed using the approximation method described above, the errors in reactivity are reduced to a maximum of 2.3 mk this being comparable to the 18 group calculations with constant cross sections.

One can easily understand the reason for such improvements in the computed reactivity by looking at Fig. 2. As we expect, the use of time dependent cross sections that take into account approximately the final neutron flux spectrum, results in a much better simulation for the ratio of the thermal to the total flux in the cell. In fact, after reaching a maximum of 0.5 % at mid-burnup the errors in the thermal flux decrease to less than 0.1 % at the end of the cycle. These errors are a direct consequence of the apparition of Plutonium in the core. The thermal fission cross section $\nu\Sigma_f^2$ is initially controlled by ^{235}U alone but, as the cell burns, the contribution from Plutonium becomes more and more important. In fact, the error in the cell averaged $\nu\Sigma_f^2$ increase linearly with time when constant microscopic cross sections are considered reaching 40 % for the 18 group calculation (see Fig. 3). However, when time dependent cross sections are considered, the maximum error observed for a 2 group calculation is less than 20% over the whole burnup range.

Finally, looking at Fig. 4 to Fig. 7, where the errors on the concentration of ^{235}U, ^{239}Pu, ^{241}Pu and ^{135}Xe as a function of time are presented, we see that our method can follow the nuclide field distribution in the core quite accurately. In addition, starting with the isotopic concentration obtained using the 2-group time dependent cross sections model at $t = 300$ days we have evaluated the void reactivity effect at the end of the burnup cycle to 11.56 mk. A full 69 group burnup results in a value of 11.37 mk.

As one can see, even for the 2 group calculations the errors remain relatively low. On the other hand, the collision probability calculation only requires 3 seconds for the 2 group cross sections while 80 seconds were required for the same calculation using a 69 group library. This gain is partially compensated by the two additional 69 group transport calculations which are required condensation purpose.

IV. Conclusions

We have shown that it is possible to generate, using a very crude approximation, time dependent microscopic cross sections which can be used to study the burnup of a cell based on fewgroup transport calculations. Here, all the calculations were performed in the original cell geometry. Additional studies are required to see if these calculations could be further simplified while still keeping the same level of accuracy by considering either a simplified cell for the evaluation the condensation flux or by considering a simplified cell for the transport calculations required at the micro time steps.

ACKNOWLEDGMENTS

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REFERENCES

[1] J.V. Donnelly, *"WIMS-CRNL, A User's Manual for the Chalk River Version of WIMS"*, AECL-8955, Atomic Energy of Canada Limited, January 1986.

[2] G. Marleau, A. Hébert and R. Roy, *"New Computational Methods Used in the Lattice Code DRAGON"*, Topical Meeting on Advances in Reactor Physics, Charleston, SC, March 8–11 1992; see also G. Marleau, A. Hébert and R. Roy, *"A User's Guide for DRAGON"*, Report IGE–174 Rev.1, École Polytechnique de Montréal, March 1996.

Table 1: Energy limits associated with the individual group for the 2-, 4- and 18-group libraries.

Library	group	$E_{\min}$ (eV)	group	$E_{\min}$ (eV)
2-groups	1	4.000×10^{0}	2	0.000×10^{0}
4-groups	1	5.530×10^{3}	2	4.000×10^{0}
	3	6.250×10^{-1}	4	0.000×10^{0}
18-groups	1	3.679×10^{6}	2	8.210×10^{5}
	3	6.734×10^{4}	4	5.530×10^{3}
	5	4.805×10^{1}	6	2.770×10^{1}
	7	9.877×10^{0}	8	4.000×10^{0}
	9	1.071×10^{0}	10	9.960×10^{-1}
	11	6.250×10^{-1}	12	3.500×10^{-1}
	13	2.200×10^{-1}	14	1.000×10^{-1}
	15	5.000×10^{-2}	16	3.000×10^{-2}
	17	1.500×10^{-2}	18	0.000×10^{0}

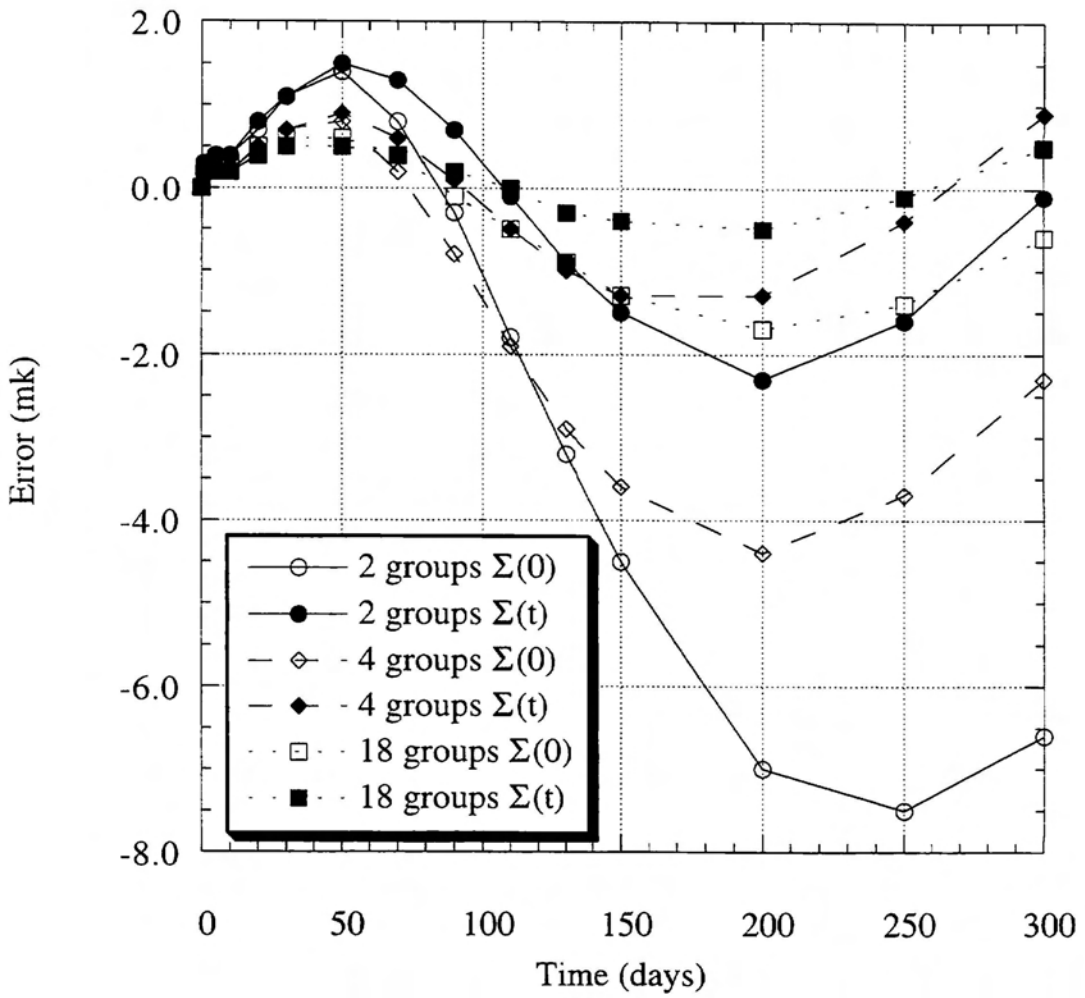

Figure 1: Error on K_{eff}.

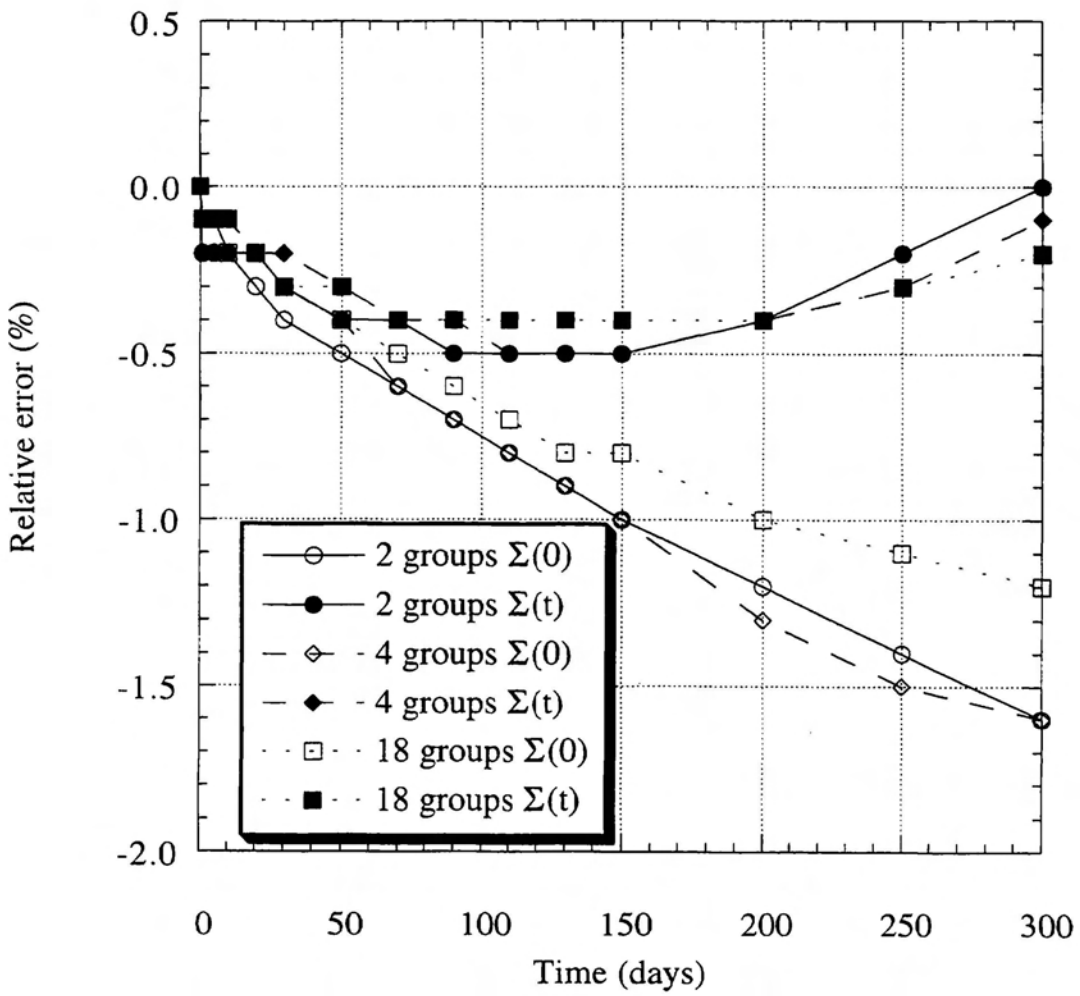

Figure 2: Relative error on the ratio of the thermal to the total flux.

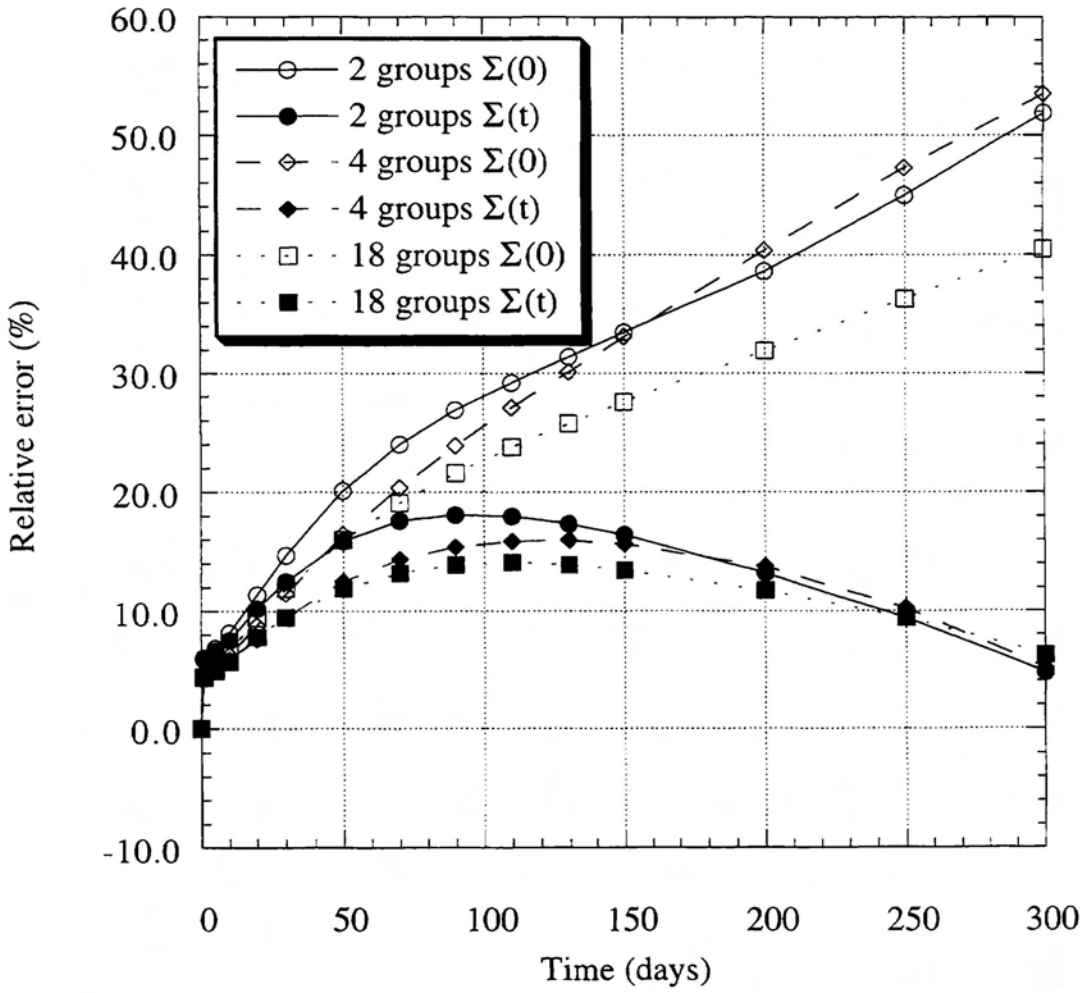

Figure 3: Relative error on cell averaged thermal fission cross section.

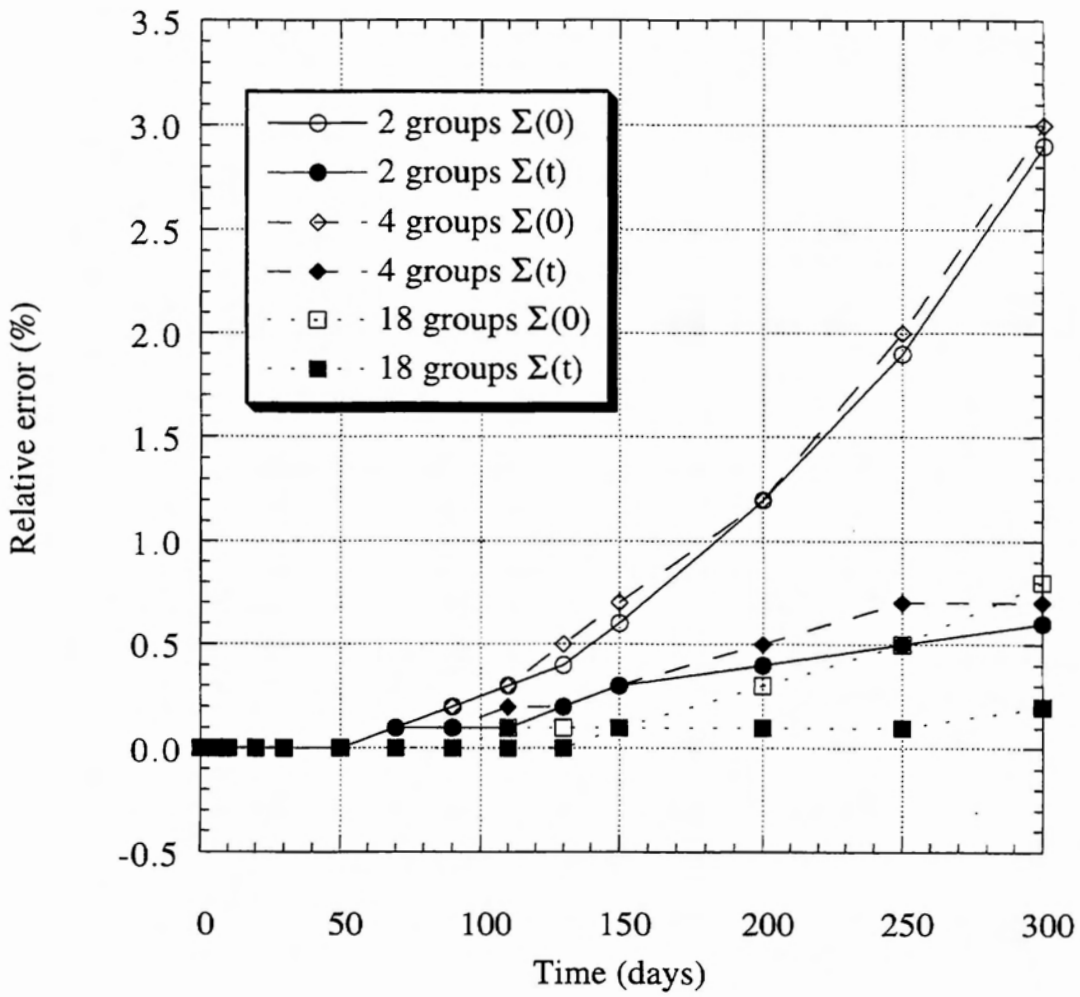

Figure 4: Relative error on ^{235}U concentration.

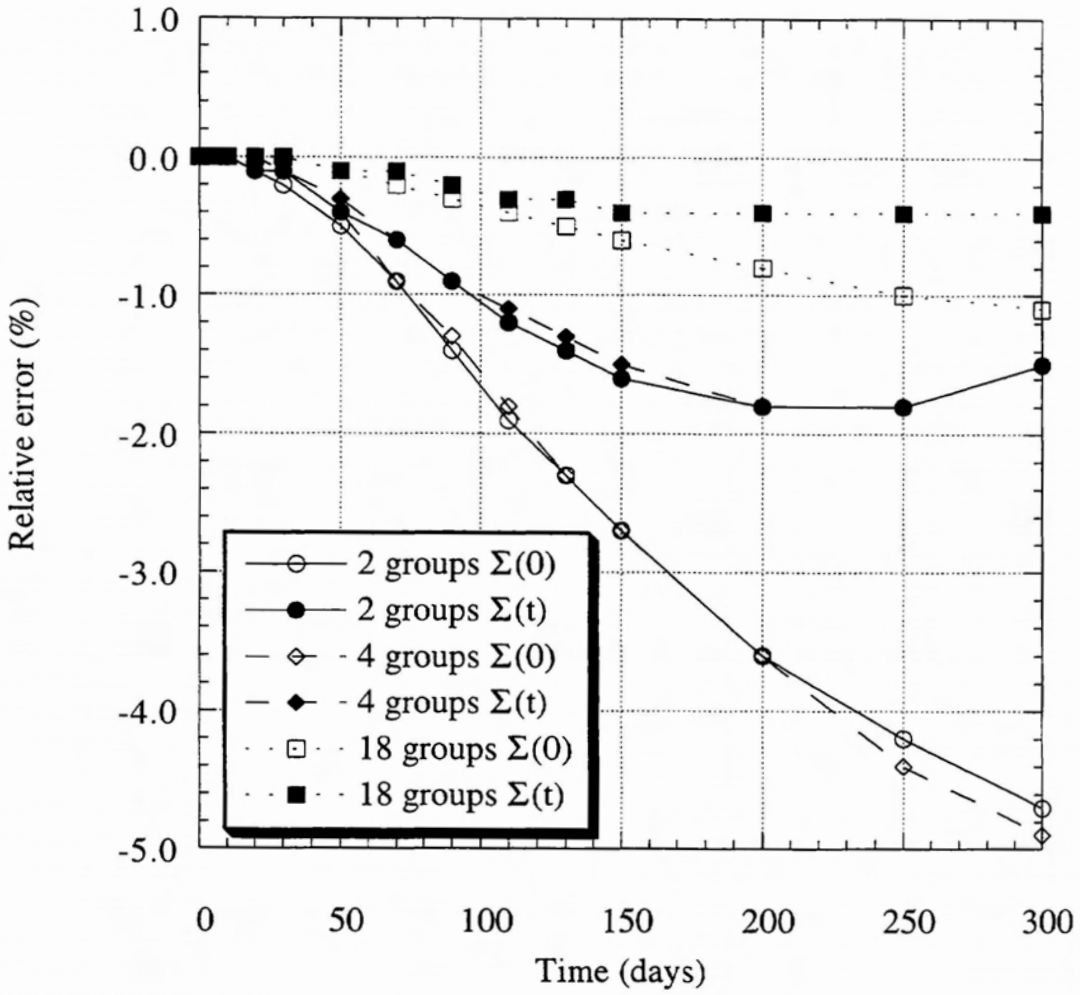

Figure 5: Relative error on ^{239}Pu concentration.

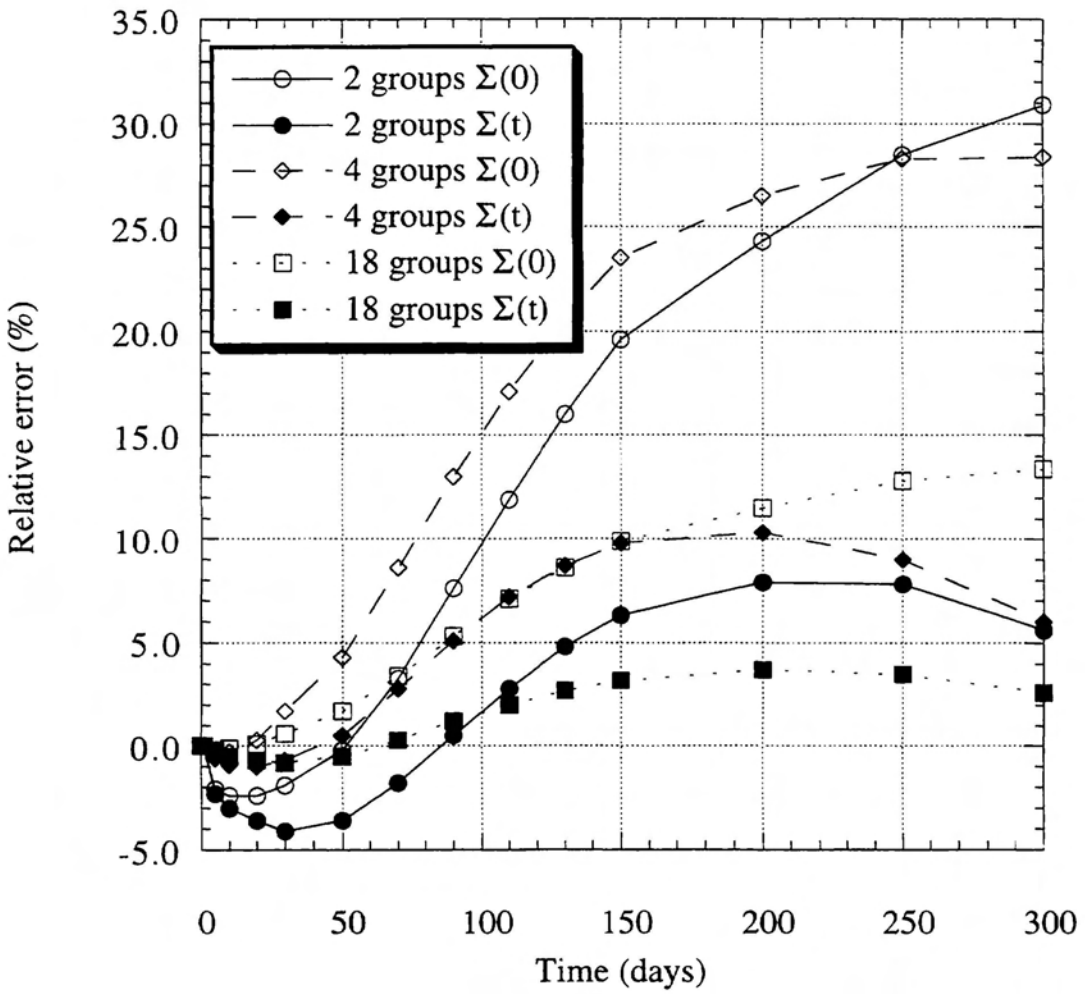

Figure 6: Relative error on ^{241}Pu concentration.

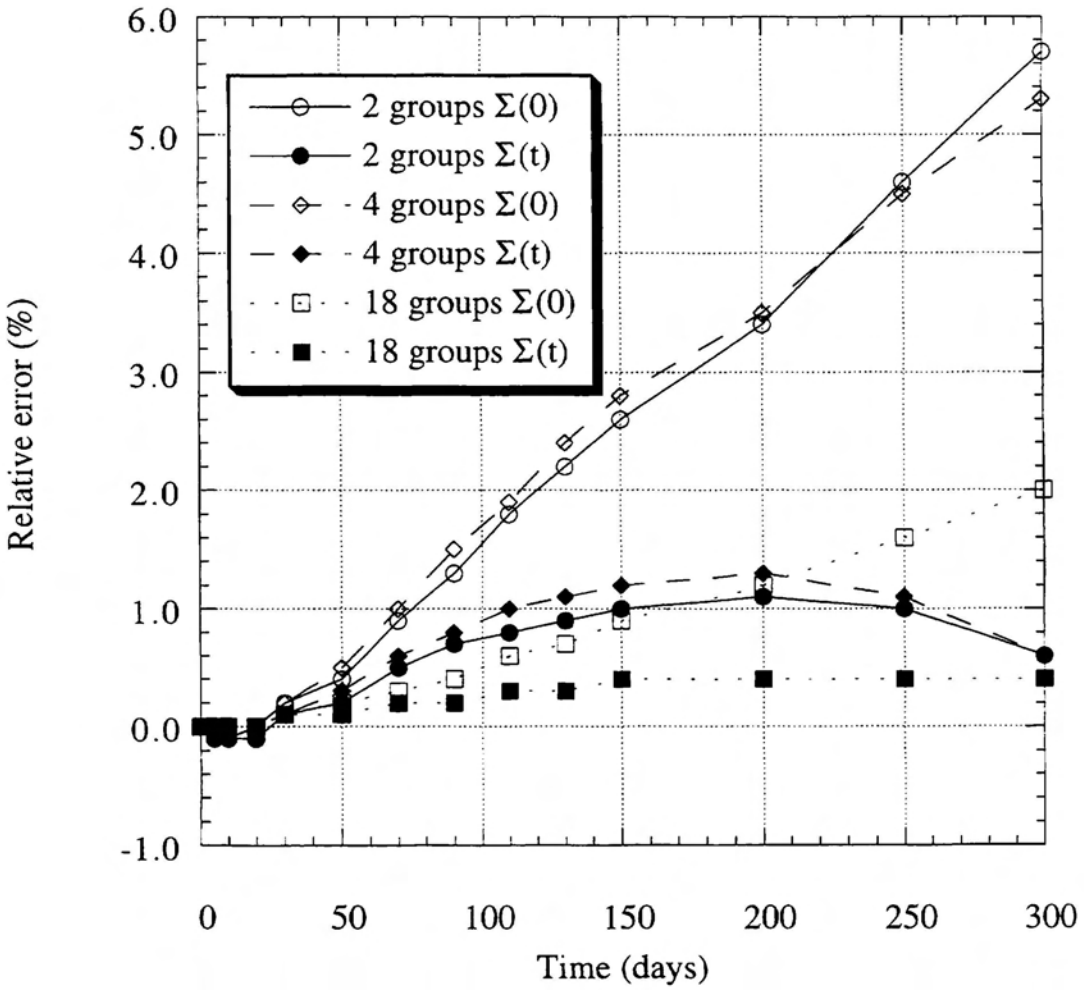

Figure 7: Relative error on ^{135}Xe concentration.