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DEVELOPEMENT OF AN ISOTOPIC DEPLETION METHOD FOR REACTOR CORE CALCULATIONS

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ABSTRACT

We will discuss in details two methods which can be used to generate the properties of the pseudo-actinides (pseudo-isotopes) for simplified ^{235}U and ^{238}U depletion chains. Using physical considerations, we derive relations for the time and space dependence of the cross sections, decay constants and fission yields for the pseudo-isotopes. The effect of the creation of these pseudo-actinides on the criticality of a thermal power reactor is investigated.

I. INTRODUCTION

The operation of a nuclear power reactor necessarily implies the consumption or burnup of reactor fuel by fission and capture. A complete treatment of burnup in core calculations requires the knowledge of the microscopic cross sections and the burnup properties associated with all the nuclides which may be present in the fuel. In principle, such an analysis involves the solution of the neutron and nuclide field equations. Because of the large number of isotopes generally present in the depletion chain and of the fact that the isotopic composition of the fuel depends on the regional neutron flux, such calculations are possible in practice only for lattice cells where the number of fuel elements remains small. As a result, it is nearly impossible to follow explicitly the concentration of every isotope in every fuel element independently in practical reactor calculations.

Many approximations could be considered in order to simplify the problem.[1, 2] Here we will discuss one technique that can be used to reduce the number of heavy nuclide isotopic concentrations that must followed in core burnup calculations. We will combine the heavy isotopes into a few pseudo-isotopes. This choice relies on the fact that all the heavy isotopes have a significant effect on the nuclear characteristics of the reactor. Their destruction by radioactive decay or neutron capture leads to the creation of a new heavy isotopes. In addition the fissile isotopes are responsible for the energy production in the reactor and the generation of fission products not originally present in the fuel.

Here we will assume that the fuel elements to be considered are made up of natural or enriched uranium which initially contains only the $^{235}\mathrm{U}$ and $^{238}\mathrm{U}$ isotopes. The scenario that has been considered consists in treating separately the $^{235}\mathrm{U}$ and $^{238}\mathrm{U}$ depletion chains. We will modify the general $^{235}\mathrm{U}$ depletion chain in such a way that it will include only two isotopes: $^{235}\mathrm{U}$ itself and a pseudo-isotope $^{236}\mathrm{U}$*. Similarly, the general $^{238}\mathrm{U}$ chain will be replaced by a three isotopes decay chain containing $^{238}\mathrm{U}$, $^{239}\mathrm{Np}$ and the pseudo-actinide $^{239}\mathrm{Pu}$* which simulates the effect of $^{239}\mathrm{Pu}$ plus the other isotopes that were originally included in the reference depletion chain.

II. THEORICAL INVESTIGATION

The burnup equation for an isotope i having a concentration $N_i(r,t)$ nuclei per unit volume is given by:

$$\frac{dN_i(r,t)}{dt} + \left(r_{i,a}(r,t) + \lambda_i\right) N_i(r,t) = \sum_{\substack{j=1\\ j\neq i}}^{I} \left(r_{j\rightarrow i}(r,t) + \lambda_{j\rightarrow i}\right) N_j(r,t) \tag{1}$$

where

$$r_{i,a}(r,t) = \sum_{g=1}^{G} \sigma_{i,a}^{g} \phi^{g}(r,t)$$

$$r_{j\rightarrow i}(r,t) = Y_{j\rightarrow i}^{a} \sum_{g=1}^{G} \sigma_{j,a}^{g} \phi^{g}(r,t)$$

$$\lambda_{j\rightarrow i} = Y_{j\rightarrow i}^{\lambda} \lambda_j$$

and $\phi^g(r,t)$ is the neutron flux per unit surface. Here $\sigma_{i,a}^g$ and λ_i are the microscopic absorption cross section and the decay constant of isotope i, respectively. The terms $Y_{j\rightarrow i}^{a}$ and $Y_{j\rightarrow i}^{\lambda}$ are the production yields of isotope i resulting from a neutron absorption or a decay of isotope j. Eq. (1) can also be written as follows:

$$\frac{dN_i(r,t)}{dt} + \left(r_{i,a}(r,t) + \lambda_i\right) N_i(r,t) = P_i(r,t) \tag{2}$$

Now let us consider the case where N of the I isotopes will be combined to form an equivalent pseudo-isotope p. From the point of view of the neutron flux equation, this equivalence between the pseudo-isotope and its constituents can be ensured by imposing that the contribution of the pseudo-isotope to the regional macroscopic cross sections is identical to the sum of the individual contributions of the isotopes included in it. If $N_p(r,t)$ and $\sigma_{p,x}^g(r,t)$ are the concentration and the microscopic cross section of the pseudo-isotope, then we may write

$$N_p(r,t)\sigma_{p,x}^{g}(r,t) = \sum_{i=1}^{N} \sigma_{i,x}^{g} N_i(r,t) \tag{3}$$

where the index x represents a type of interaction (absorption, fission, etc.). From the point of view of the nuclide depletion equation, the fictitious isotope p should obey the following burnup equation:

$$\frac{dN_p(r,t)}{dt} + \left(r_{p,a}(r,t) + \lambda_p(r,t)\right) N_p(r,t) = P_p(r,t) \tag{4}$$

where the parameter $\lambda_p(r,t)$ represents the decay constant of the pseudo-isotope p which is given by:

$$\lambda_p(r,t)N_p(r,t) = \sum_{i=1}^{K} \lambda_i N_i(r,t) \tag{5}$$

where $i = 1, K$ refers to the isotopes in p which deplete by radioactive decay to an isotope not included in p. The contribution from the other decaying isotopes of p add up to 0 (each depletion is compensated by a production). The parameter $P_p(r,t)$ is the production rate of the isotope p. As we will see later its definition will depend on the method adopted for the combination of our actinides. Finally, the fission yield $Y^f_{p\to i}$ must be calculated in such a way as to preserve the production rate of the fission-products

$$Y^f_{p\to i}(r,t)N_p(r,t)r_{p,f}(r,t) = \sum_{j}^{N} Y^f_{j\to i}N_i(r,t)r_{j,f}(r,t) \tag{6}$$

Note that the fission yields, the constant decay and the microscopic cross sections associated with the pseudo-isotope, p all depend explicitly on time and space.

II.1 Selecting the Pseudo-Isotope Concentration

The first and simplest option consists in assuming that the concentration $N_p(r,t)$ of the pseudo-isotope p is identical to the total isotopic concentration (TIC) of the N isotopes:

$$N_p(r,t) = \sum_{i=1}^{N} N_i(r,t) \tag{7}$$

In this case, the pseudo-isotope microscopic cross sections must represent the average microscopic cross sections of the N isotopes combined. The production rate $P_p(r,t)$ is then given by:

$$P_p(r,t) = \sum_{i=1}^{M} P_i(r,t) \tag{8}$$

where $i = 1, M$ refers to a parent isotope not included in p. The production of an isotope in p which also has it parent in p is compensated by the destruction of the parent isotope. As an example, assume that isotope i in p produces by decay or absorption the isotope j of p. Then, the rate at which isotope j is produced is identical to the rate at which isotope i depletes. Accordingly, this reaction will have no effect on the explicit concentration of the pseudo-isotope.

A second option consists in assuming that the concentration of the pseudo-isotope will be identical to the concentration of the isotope which has the largest concentration:

$$N_p(r,t) = \max_{i=1,N} N_i(r,t) \tag{9}$$

In this case, the microscopic cross section of the pseudo-isotope is equal to that of the isotope having the dominant isotopic concentration (DIC) plus a correction term that includes the contribution of all the other isotopes in p.[3] The production rate $P_p(r,t)$ of the pseudo-isotope is then given by:

$$P_p(r,t) = P_k(r,t) \tag{10}$$

where the index k refers to the isotope having the dominant isotopic concentration. In fact, if one assumes that k (the dominant isotope) is the first in a long chain that will be reduced to a single isotope p, then the production or destruction rate of the pseudo-isotope will be controlled directly by the production or destruction rate of k.

II.2 Approximations

Solving the depletion equations for the pseudo-isotope is very difficult since the decay constant and the microscopic absorption cross section now depend explicitly on time and space. In order to simplify the problem additionnal approximations have to be considered.

For both the DIC and TIC methods, we will assume that the time dependence of the microscopic absorption cross sections associated with the pseudo-isotope p is linear.[3] Then for each region r of the cell, we may write:

$$\sigma^g_{p,x}(r,t) = a^g_{p,x}(r) + b^g_{p,x}(r)t \tag{11}$$

where the coefficients $a^g_{p,x}(r)$ and $b^g_{p,x}(r)$ will be determined using a least square fit method. We will also associate with the pseudo-isotopes a time and space independent decay constant. We will therefore replace $\lambda_p(r,t)$ by its time and space average $\overline{\lambda}_p$ defined as:

$$\overline{\lambda}_p = \frac{1}{V}\frac{1}{T}\int_V dr \int_0^T \lambda_p(r,t)dt \tag{12}$$

where T is the period of operation of the reactor. Finally, we will associate with the pseudo-isotope time and space independent fission yields of the form

$$\overline{Y}^f_{p\to i} = \frac{1}{T}\frac{1}{V}\int_V dr \int_0^T Y^f_{p\to i}(r,t)dt \tag{13}$$

II.3 Selecting the Pseudo-Isotopes for CANDU Fuel

The next problem we face is that of selecting the number of pseudo-isotopes to consider and their contents. Here our selection process will be based on two different consideration: minimizing the computation time required to solve the depletion problem and generating new depletion chains which simulate as closely as possible the original chains.

From the physical point of view, we will assume that $^{235}\mathrm{U}$ and $^{238}\mathrm{U}$, which are the main actinides present in fresh CANDU fuel, will be treated explicitly. Moreover, the coupling between the $^{235}\mathrm{U}$ and $^{238}\mathrm{U}$ depletion chains being relatively weak, we will assume that the concentration of the isotopes in the $^{238}\mathrm{U}$ depletion chain are nearly independent of the $^{235}\mathrm{U}$ concentration. We will therefore associate to each of these chains one pseudo-isotope. Now let us discuss how each of these isotopes can be selected and what additional isotopes will be required in both chains.

Let us first consider the $^{235}\mathrm{U}$ depletion chain. The simplest option one may consider consists in replacing all the isotopes of the $^{235}\mathrm{U}$ chain by a single pseudo-isotope: $^{235}\mathrm{U}$*. This pseudo-isotope should be dominated by $^{235}\mathrm{U}$ which is fissile for thermal neutrons and has a relatively large concentration in CANDU type fuels. The problem with this choice is that the cross sections associated with the pseudo-isotope $^{235}\mathrm{U}$* are approximated using Eq. (11). As a result, the general time dependent behavior of the cross section should be reproduced relatively well. However, slight differences between the microscopic cross section of the pseudo-isotope given by the least square method and the exact microscopic cross section of the pseudo-isotope, especially at the origin (t=0), will generate large errors in the contribution of $^{235}\mathrm{U}$* to the macroscopic cross sections (especially fission) since it has a large concentration. The next best alternative is to replace the complete $^{235}\mathrm{U}$ depletion chain by a two isotopes depletion chain:

$$^{235}\mathrm{U} \xrightarrow{n,\gamma} {}^{236}\mathrm{U}^*$$

Here the pseudo-isotope $^{236}\mathrm{U}$* will include the effects of the remaining isotopes in the original chain, such as $^{236}\mathrm{U}$ and $^{237}\mathrm{Np}$. Such a depletion chain has the advantage of following explicitly the depletion of $^{235}\mathrm{U}$. The pseudo-isotope being initially absent from the cell, its initial contribution to the macroscopic cross section will vanish, therefore avoiding the problem generated by the use of $^{235}\mathrm{U}$* as the pseudo-isotope. In addition, the concentration of $^{236}\mathrm{U}$* will remain smaller (using both the TIC and DIC method) than that of $^{235}\mathrm{U}$ during the complete burnup period. As a result, the numerical errors introduced by the various approximations we considered should not affect strongly the macroscopic fuel cross section.

The $^{238}\mathrm{U}$ depletion chain will be reduced to three isotopes: $^{238}\mathrm{U}$ as a main fertile isotope, $^{239}\mathrm{Np}$, which is not a fissile isotope for thermal neutrons, and finally the pseudo-isotope $^{239}\mathrm{Pu}$* which will be the main fissile isotope for thermal neutron in this chain. The $^{239}\mathrm{Pu}$* will include the effects of the other isotopes of the original chain, namely $^{239}\mathrm{Pu}$, $^{240}\mathrm{Pu}$ and $^{241}\mathrm{Pu}$ which play an important role both in energy production and in the neutronic balance. The main reasons why we selected here a three isotopes depletion chain are the following. First and foremost, $^{238}\mathrm{U}$ is not fissile by thermal neutrons. Since $^{238}\mathrm{U}$ is the dominant isotope in this chain, all the cross sections associated with a single isotope $^{238}\mathrm{U}$* would therefore reproduce the general features of $^{238}\mathrm{U}$ except for fission. As a result, the rate of evolution of $^{238}\mathrm{U}$* in the cell would be similar to that of $^{238}\mathrm{U}$, which means that the thermal part of the fission cross section of $^{238}\mathrm{U}$* would require a strong time dependence to be able to simulate the apparition of the main fissile actinide ($^{239}\mathrm{Pu}$). Since the dependence on time of the $^{239}\mathrm{Pu}$ concentration is far from linear, a linear approximation for the thermal fission cross section would then be insufficient. The second option we could have considered is to combine all the secondary isotopes in the $^{238}\mathrm{U}$ depletion chain into a single pseudo-isotope denoted $^{239}\mathrm{Np}$* as we did for the $^{235}\mathrm{U}$ chain. However, the problem is that the concentration of $^{239}\mathrm{Np}$ is generally lower than the concentration of the $^{239}\mathrm{Pu}$, which is the dominant secondary isotope here. In addition, it is not fissile by thermal neutrons. As a result we would then need to generate a pseudo-isotope $^{239}\mathrm{Np}$*, which is fissile for thermal neutrons while being produced directly by $^{238}\mathrm{U}$. It would therefore be impossible to take into account the delay in the production of the first fissile isotope ($^{239}\mathrm{Pu}$) by thermal neutrons. Hence, our choice for the simplified decay chain:

$$^{238}\mathrm{U} \xrightarrow{n,\gamma} {}^{239}\mathrm{Np} \xrightarrow{\lambda} {}^{239}\mathrm{Pu}*$$

which should reproduce the main features of the original $^{238}\mathrm{U}$ depletion chain.

Finally, to simplify the process of selecting the isotopes to be combined, we have assumed that the $^{238}\mathrm{U}$ and $^{235}\mathrm{U}$ depletion chains were decoupled. In fact, even if these two chains are coupled, this coupling generally remains weak: the isotopes of the $^{238}\mathrm{U}$ chain which are produced directly by an isotope of the $^{235}\mathrm{U}$ chain are $^{238}\mathrm{U}$ $^{239}\mathrm{Np}$ and $^{239}\mathrm{Pu}$. However, the production rate of these isotopes from $^{235}\mathrm{U}$ is significantly lower than their production rates from $^{238}\mathrm{U}$, hence they can be neglected.

III. RESULTS AND DISCUSSION

III.1 Methods of Calculation

The numerical work required to determine the properties of the pseudo-isotope is divided into three parts. A reference calculation, is first performed in transport theory using the code DRAGON,[4] and a reference multigroup microscopic cross section library and its associated depletion chain. All the default isotopes were included in the burnup problem solved by DRAGON, and the reference concentrations of the heavy isotopes to be combined are evaluated as well as the reference effective multiplication constant k_{eff}^{REF} at the different burnup steps. For a given region and energy group, the resulting time dependent cross sections of the pseudo-isotopes are then fitted to the form given in Eq. (11) using a least-square method. Finally, one determines the average value of the fission yield and of the decay constant of the pseudo-isotope given by Eqs. (12) and (13). These tasks are required for the generation of a new library, that contains all the nuclear properties of the pseudo-isotope, (initial concentration, microscopic cross section, constant decay, ...), and of course the properties of the other isotope that were not combined. The results obtained using this library containing pseudo-isotopes will be compared with those obtained in the reference calculation.

Table 1. Energy limits for the few groups cross section libraries

Condensed group number g	2-groups library		6-groups library	
	Upper energy	Lower energy	Upper energy	Lower energy
1	10 MeV	4.0 eV	10 MeV	0.82085 MeV
2	4.0 eV	0.0 eV	0.82085 MeV	5530.8 eV
3			5530.8 eV	4.0 eV
4			4.0 eV	0.625 eV
5			0.625 eV	0.1 eV
6			0.1 eV	0.0 eV

The main library we used for our calculations is the WIMS-AECL Winfrith 69 group cross section library.[5] These cross sections were first condensed to produce 2- or 6- group libraries to further simplify the problem (see Table 1). We also considered two different cells, namely the standard CANDU-6 fuel cell and a simplified 3 region annular fuel cell (an homogenized version of the CANDU-6 cell with the fuel located in the central region).

III.2 Comparison Between the TIC and the DIC Methods

The TIC and DIC methods were first compared to study the effect of creating $^{236}\mathrm{U}$* for the $^{235}\mathrm{U}$ depletion chain and $^{239}\mathrm{Pu}$* for the $^{238}\mathrm{U}$ chain. These tests were performed using the simple cell with the 2-group condensed library.

Let us first discuss the individual effects of $^{236}\mathrm{U}$* and $^{239}\mathrm{Pu}$* on the cell reactivity. One can find in Table 2 the errors in k_{eff} resulting form the creation of $^{236}\mathrm{U}$* by the combination of $^{236}\mathrm{U}$ and $^{237}\mathrm{Np}$. The first thing to note is that both the TIC and the DIC methods perform very well, the maximum error in k_{eff} being 0.03 mk and 0.08 mk respectively.

Table 2. Error in k_{eff} after the generation of $^{236}\mathrm{U}$*, $^{239}\mathrm{Pu}$* or $^{236}\mathrm{U}$*+$^{239}\mathrm{Pu}$*

		$^{236}\mathrm{U}^*$		$^{239}\mathrm{Pu}^*$		$^{236}\mathrm{U}^* + {}^{239}\mathrm{Pu}^*$	
t (days)	k_{eff}^{REF}	$\Delta k_{\mathit{eff}}^{TIC}$	$\Delta k_{\mathit{eff}}^{DIC}$	$\Delta k_{\mathit{eff}}^{TIC}$	$\Delta k_{\mathit{eff}}^{DIC}$	$\Delta k_{\mathit{eff}}^{TIC}$	$\Delta k_{\mathit{eff}}^{DIC}$
0	1.117660	0.00	0.00	0.00	0.00	0.00	0.00
20	1.077957	0.00	0.00	-5.88	-3.69	-3.74	-3.85
50	1.078323	0.00	0.00	-11.88	-4.26	-7.62	-4.59
90	1.062512	0.00	0.00	-16.78	-0.36	-12.84	-.74
110	1.051623	0.00	0.00	-19.44	1.78	-16.60	1.43
130	1.039970	0.00	-0.01	-22.69	3.54	-21.43	3.24
150	1.028045	0.00	-0.01	-26.65	4.70	-27.44	4.47
200	0.998825	0.00	-0.02	-39.22	4.96	-47.52	4.91
250	0.972693	0.00	-0.04	-55.37	1.31	-74.07	1.52
300	0.950394	-0.03	-0.08	-73.12	-4.76	-99.88	-4.31

The fact that the two techniques are equivalent is not surprising for the following reason. The concentration of $^{236}\mathrm{U}$ is large compared with that of $^{237}\mathrm{Np}$. As a result, the ratio of the computed concentration of $^{236}\mathrm{U}$* to that evaluated in the reference calculation should remain very close to 1 for both the TIC and DIC method. This behavior can be easily observed in Table 3 where C^{TIC} and C^{DIC} are defined as

$$C^{TIC}(r,t) = \frac{N_p^{TIC}(r,t)}{N_p^{REF}(r,t)}$$

$$C^{DIC}(r,t) = \frac{N_p^{DIC}(r,t)}{N_p^{REF}(r,t)}$$

respectively. As expected both C^{TIC} and C^{DIC} remain almost equal to unity.

Table 3. Variation of C^{TIC} and C^{DIC} for ^{236}U* or $^{239}\mathrm{Pu}$ as a function of time

	^{236}U*		$^{239}\mathrm{Pu}$*	
t (days)	C^{TIC}	C^{DIC}	C^{TIC}	C^{DIC}
0	1.00	1.00	1.00	1.00
20	0.99	0.99	0.96	1.01
50	0.99	0.99	0.91	1.02
90	0.99	0.99	0.86	1.03
110	0.99	0.99	0.84	1.04
130	0.98	0.98	0.82	1.04
150	0.98	0.98	0.81	1.05
200	0.98	0.98	0.79	1.05
250	0.97	0.97	0.78	1.06
300	0.97	0.96	0.77	1.06

The error in reactivity are also small because these two isotopes have very low concentrations and relatively small absorption cross sections. As a results their contribution to the fuel macroscopic cross section remains small. In addition, they are not fissile for thermal neutrons and hence their role in the the neutron balance is not considerable.

The same study was repeated for $^{239}\mathrm{Pu}$*. Again, one can find in Table 2 the error in k_{eff} obtained using the TIC and DIC method. In this case very large errors are observed when the TIC method is considered reaching a maximum error of -73.12 mk. On the other hand, the errors are reduced substantially if the DIC method is used even if they still remain relatively large. This is not surprising since $^{239}\mathrm{Pu}$* includes $^{239}\mathrm{Pu}$, $^{240}\mathrm{Pu}$ and $^{241}\mathrm{Pu}$. All three isotopes have large absorption microscopic cross section, while both $^{239}\mathrm{Pu}$ and $^{241}\mathrm{Pu}$ are fissile. Finally the concentration of these three isotope is also of the same order of magnitude.

This behavior of C^{TIC} and C^{TIC} as a function of time can be found in Table 3. One can see that C^{DIC} remains almost equal to unity while C^{TIC} decreases by nearly 25 % over the full period of burnup. These differences are expected for the following reasons.

For the TIC method, the production of the pseudo-isotope $^{239}\mathrm{Pu}$* should differ from the reference production rate of $^{239}\mathrm{Pu}$, since, in addition to being produced by the $^{239}\mathrm{Np}$ with the same constant decay it is also produced by neutron capture in $^{239}\mathrm{Np}$ (see Eq. (8)). The destruction rate of $^{239}\mathrm{Pu}$* on the other hand will be controlled by the product of its concentration and microscopic cross section. The rate at which $^{239}\mathrm{Pu}$* disappears will be determined by the total concentration of the isotopes included in it. On the other hand, the microscopic absorption cross section of the pseudo-isotope $^{239}\mathrm{Pu}$* represents the average microscopic cross section of all the isotopes combined. Accordingly, if all the isotopes in $^{239}\mathrm{Pu}$* had the same cross section, the depletion rate of $^{239}\mathrm{Pu}$* would be substantially larger than the depletion rate of $^{239}\mathrm{Pu}$. As a consequence the increase in the production rate of $^{239}\mathrm{Pu}$* due to neutron capture in $^{239}\mathrm{Np}$ is insufficient to compensate the increase in its depletion rate.

For the DIC method, the total production rate of the pseudo-isotope $^{239}\mathrm{Pu}$* is identical to the reference production rate of $^{239}\mathrm{Pu}$, since they are both produced only via radioactive decay of

$^{239}\mathrm{Np}$ (see Eq. (10)). Similarly, the destruction process for $^{239}\mathrm{Pu}^*$ and $^{239}\mathrm{Pu}$ will be identical. Their destruction rates will therefore be identical provided their microscopic absorption cross sections are also identical. Here the microscopic cross section of the $^{239}\mathrm{Pu}^*$ is equal to the cross section of $^{239}\mathrm{Pu}$ plus a correction term which includes the effects of the other isotopes combined. For the reaction chain we considered, this correction can be shown to be relatively small (an increase of the order of 5 % over 300 days) and as expected the concentration of the pseudo-isotope is almost equal to the concentration of $^{239}\mathrm{Pu}$ as shown in Table 3.

For all the calculations that will follow, we are going to consider only the DIC method for the case where both the $^{236}\mathrm{U}^*$ and $^{239}\mathrm{Pu}^*$ are used simultaneously (see Table 2). This seems to be the most promising method, because, on one hand, the results obtained by this method are better that those obtained by the TIC method and on the other hand, this method can be applied for both the $^{235}\mathrm{U}$ chain and $^{238}\mathrm{U}$.

III.3 Geometry Effect

The proposed method was used to verify weather or not the error in k_{eff} is affected by the type of geometry used. In this case, we have considered two types of geometry: a three region annular cell with the fuel located at the center and a CANDU-6 cell composed of 13 regions. The fuel being located at four different regions in the CANDU fuel cluster, four sets of microscopic cross sections will be associated with each pseudo-isotope.

Table 4. Comparison of errors in k_{eff} for two geometry

t	Δk_{eff} (mk)	
(day)	SIMPLE cell	CANDU cell
0	0.00	0.00
20	-3.8	-4.34
50	-4.59	-5.66
9	-0.74	-2.22
110	1.43	-0.19
130	3.24	1.50
150	4.47	2.66
200	4.91	3.07
250	1.52	-0.05
300	-4.31	-5.21

Table 4 shows that the errors in k_{eff} do not vary enormously by changing the type of geometry. This is because each region in a cell calculation is treated locally. Hence, we conclude, that the precision of the DIC method is not affected by the choice of geometry.

III.4 Effect of Group Condensation

The main goal of this study was to make sure that our module could deal with different energy group structures. We studied the effect of changing the number of condensed energy group on the errors in k_{eff} due to the presence of the pseudo-isotopes. The CANDU-6 cell geometry is used in this case.

Table 5. Comparison of errors in k_{eff} for two library energy group structure

t (day)	Δk_{eff} (mk) 2 groups	6 groups
0	0.00	0.00
20	-4.34	-4.03
50	-5.66	-4.83
90	-2.22	-0.89
110	-0.19	1.24
130	1.50	2.98
150	2.66	4.17
200	3.07	4.68
250	-0.05	2.72
300	-5.21	-0.03

The results presented in Table 5 indicate that the error in reactivity is not affected enormously by the number of group considered, as the errors remain of the same magnitude for the two cases.

III.5 Library Effect

In addition to using the WIMS-AECL Winfrith library, we also repeated our calculations using the 89 groups ENDF/B-V and ENDF/B-VI based WIMS-AECL library. For both libraries, the ^{235}U and ^{238}U chains, which are initially coupled, had to be broken down into two independent chain as described in Section II. One can see in Table 6 that the errors in k_{eff} remain of the same magnitude regardless the type of library used. This indicates that the coupling between the ^{235}U and ^{238}U chain remains weak and can be neglected as we suggested before.

III.6 Effect of Time Step Width in Burnup

The microscopic cross sections of the pseudo-isotopes, as shown in Eq. (3), depend on the concentrations of the isotopes to be combined. These concentrations are obtained by a reference calculation for a given number of burnup time steps. Here, we will show that, using the approximation in Eq. (11) for the cross sections does not strongly depends on the size and the number of time steps used for the generation of the simplified decay chain. We have considered the cases where the library containing a simplified chain was obtained using our standard 16

Table 6. Comparison of errors in k_{eff} for three different libraries

t (day)	Δk_{eff} (mk) Winfrith	ENDF/B-V	ENDF/B-VI
0	0.00	0.00	0.00
20	-4.34	-4.30	-1.83
50	-5.66	-5.78	-1.17
90	-2.22	-4.55	2.26
110	-0.19	-1.31	3.63
130	1.50	0.13	4.16
150	2.66	0.89	4.28
200	3.07	0.51	2.58
250	-0.05	-3.81	-2.31
300	-5.21	-4.52	-4.41

burnup steps and a case where 30 shorter time steps were considered. The results shown in Table 7 indicate that the k_{eff} is nearly independent of the specific number of steps chosen for the reference calculation used to generate the simplified library.

Table 7. Comparison of errors in k_{eff} for different burnup steps

t (day)	Δk_{eff} (mk) long steps	short steps
0	0.00	0.00
20	-4.34	-4.35
50	-5.66	-5.75
90	-2.22	-2.02
110	-0.19	0.01
130	1.50	1.70
150	2.66	2.85
200	3.07	3.07
250	-0.05	0.15
300	-5.21	4.81

IV. CONCLUSIONS

The main conclusions are:

- The DIC method can be used for both the generation of pseudo-actinide in ^{235}U chain and ^{238}U chain. This is not the case for the TIC method.
- By using DIC method, the concentration of the pseudo-isotopes created is nearly equal to the concentration of their associated dominant isotopes.
- This method can be applied to simple as well as to more complex geometries, where the microscopic cross sections associated with a pseudo-isotope are region dependent.
- The coupling between the ^{238}U and ^{235}U chain can be neglected.
- Assuming a linear time dependence for the pseudo-isotopes cross sections is a good approximation.

In order to improve on the error in reactivity due to the simplification of the depletion chain, additional analysis are required. For example, we need to investigate if a quadratic time dependence for the cross sections of the pseudo-isotopes would improve substantially our results. We will also need to consider the impact of using mixed oxide fuel on our simplified depletion chain since such fuels contains initially $^{239}\mathrm{Pu}$. Similarly we will need to study how our method can be extended to the treatment of the $^{232}\mathrm{Th}$ depletion chain.

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