ON THE DIFFERENCE BETWEEN DRAGON AND WIMS-AECL CALCULATIONS OF THE COOLANT VOID REACTIVITY

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Abstract

A difference in the shape of the burnup dependence of the coolant void reactivity (CVR) has been observed between DRAGON and WIMS-AECL calculations. This paper discusses the root cause of the difference and assesses the impact on burnup and full-core reactor calculations. A Fortran procedure has been developed to run WIMS-AECL as necessary in order to mimic DRAGON burnup calculations with leakage effects included. The comparison of standard WIMS-AECL results and simulated DRAGON results demonstrated that the difference is due to different definitions of CVR. If the same CVR definition is used, then the results of both WIMS-AECL and DRAGON analyses are essentially indistinguishable. The discrepancies in the fuel composition and cell-averaged two-group cross sections that are due to differences in WIMS-AECL and DRAGON leakage treatments are insignificant.

1. Introduction

A coordinated research project funded by Atomic Energy of Canada Limited (AECL) and the National Science and Engineering Research Council (NSERC) was granted to École Polytechnique de Montréal to undertake research on independent reactor physics methods that can be applied to ACR® calculations[#]. The research results obtained by École Polytechnique have been presented in a number of progress reports and conference papers over the past few years. A difference between the results of WIMS-AECL[a] [1] and DRAGON [2] calculations of the coolant void reactivity (CVR) for an ACR-type lattice has been observed and reported in [3]. Figure 1 (taken from Reference [3] as Fig. 5) presents the burnup dependence of CVR as calculated by the two codes. Reference [3] suggests that the difference may be due to leakage effects. In support of this, Figure 2 (taken from Reference [3] as Fig. 8) presents the DRAGON calculated CVR values with and without leakage.

In this paper the difference between DRAGON and WIMS results is further investigated and the possible impact on the burnup dependence of fuel composition as well as the full-core reactor calculations is evaluated. A Fortran procedure has been developed to run WIMS as necessary in order to mimic the DRAGON method of leakage calculation. Section 2 describes the steps of this procedure and compares the results of CVR calculations carried out by the standard WIMS approach and the simulated DRAGON method.[b] To understand the difference, this section also discusses the mathematical formulae that are applied to calculate CVR using the results of WIMS and DRAGON lattice calculations. Section 3 discusses the atom density of two crucial

[#] ACR® (Advanced CANDU Reactor) is a registered trademark of Atomic Energy of Canada Limited.
[a] For the sake of simplicity the code WIMS-AECL will be referred to as WIMS.
[b] "Simulated DRAGON method" means WIMS calculations using a leakage method similar to DRAGON.

nuclides (^{235}U and ^{239}Pu) and the relative discrepancy between the results obtained by the simulated DRAGON method and the standard WIMS approach. Section 4 compares cell-averaged two-group cross sections and presents the relative discrepancy between the results calculated by the two methods considered.

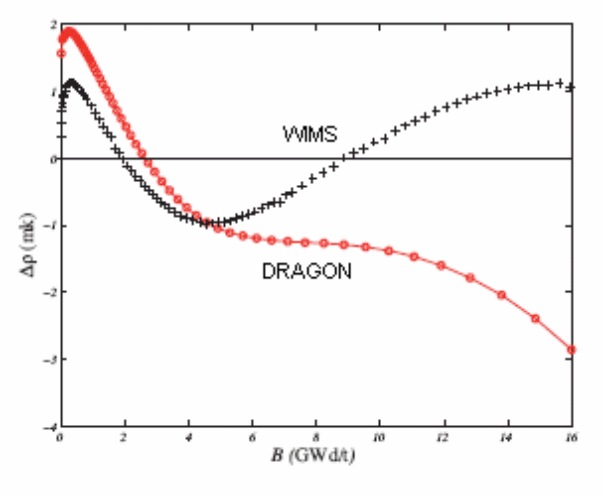

Figure 1 DRAGON versus WIMS results of CVR calculations for an ACR-type lattice (taken from Reference [3]).

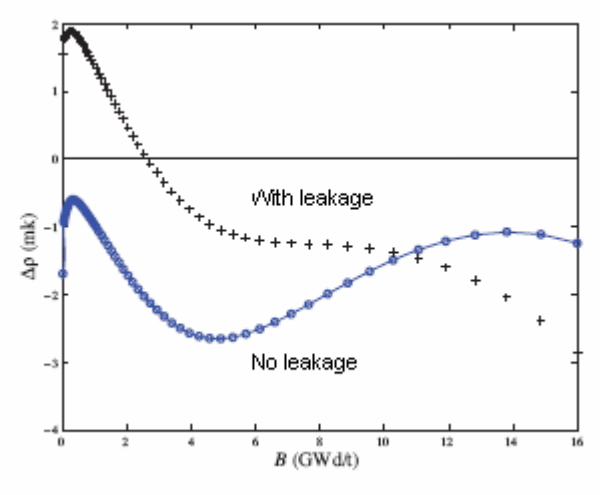

Figure 2 DRAGON results of CVR calculations with and without leakage (taken from Reference [3]).

2. Coolant void reactivity calculation

In addition to the effective neutron multiplication factor k_{eff}, another quantity, namely *reactivity* (ρ) is also commonly used to characterize quantitatively the degree of criticality of a reactor. There is no universally accepted definition of reactivity and different authors define it in different ways, which may lead to different numerical values for a particular reactor assembly. The following definition [4] is commonly used in reactor design calculations:

$$\rho \equiv 1 - \frac{1}{\lambda} \tag{1}$$

where λ is the number (the eigenvalue k_{eff}) that yields a nontrivial solution (the eigenfunction) of the equation that describes the steady-state neutron flux distribution. This equation is usually approximated by a set of linear algebraic equations, so that, instead of an eigenfunction, the solution is actually the eigenvector of this set of equations. It is worth mentioning that the eigenvalue λ can also be interpreted as the ratio of the neutron-production rate to the neutron-loss (absorption and leakage) rate assuming that reaction rates are calculated using the neutron flux distribution specified by the eigenvector of the set of linear equations.

According to Reference [4], there can be some confusion about the term reactivity. People often refer to "the reactivity of a control rod" or "the coolant void reactivity". What is meant in such cases is the change in reactivity of the reactor when such a reactor perturbation (insertion of a

control rod or coolant voiding) takes place. Thus, the coolant void reactivity actually represents the difference between the reactivity of the perturbed (voided) reactor state and the reactivity of the reference (cooled) reactor state, i.e.,

$$\Delta\rho_{cvr} \equiv \rho^{void} - \rho^{cool} \tag{2}$$

Since $\lambda = k_{eff}$, the coolant void reactivity can be expressed as follows:

$$\Delta\rho_{cvr} = \frac{1}{k_{eff}^{cool}} - \frac{1}{k_{eff}^{void}} \tag{3}$$

The reference case usually represents an equilibrium reactor state (critical reactor) so that $k_{eff}^{cool} = 1 \Rightarrow \rho^{cool} = 0$ and the coolant void reactivity takes the following form:

$$\Delta\rho_{cvr} = 1 - \frac{1}{k_{eff}^{void}} \tag{4}$$

Owing both to insufficient accuracy of numerical methods and the uncertainty of nuclear data, the numerical value of the neutron multiplication factor k_{eff}^{cool} usually differs somewhat from unity. Therefore, Eq. (3) is more suitable for practical calculations because it cancels a part of the CVR bias that is due to numerical approximations and nuclear data uncertainty.

2.1 CVR calculation using WIMS

The above formalism, except Eq. (4), can also be applied to lattice calculations. In this case, the steady-state neutron flux distribution is described by the two-dimensional neutron transport equation. The eigenvalue $\lambda = k_{\inf}$ can be interpreted as the ratio of the neutron-production to neutron-absorption rates assuming that reaction rates are calculated using the eigenvector of the transport equation. Accordingly, the lattice coolant void reactivity can be expressed in the following form similar to Eq. (3):

$$\Delta\rho_{cvr}^{latt} = \frac{1}{k_{\inf}^{cool}} - \frac{1}{k_{\inf}^{void}} \tag{5}$$

This quantity is not a design parameter, however, it is useful in scoping studies to make choices between various fuel bundle configurations.

To understand the difference between WIMS and DRAGON results, it is useful to describe a few steps in the WIMS solution. The first step is to get the solution of the multigroup two-dimensional transport equation, which consists of the eigenvalue (the infinite neutron multiplication factor $k_{\inf}$) and the corresponding eigenvector (the neutron flux distribution). The neutron flux distribution is then used to calculate cell-averaged cross sections and diffusion constants. In order to take into account the finite reactor size effects, the code performs the leakage calculation either using the diffusion equation or B_1 equation for a bare homogeneous reactor of cylindrical shape. Thus, according to input specified bucklings, the code produces k_{eff} and the energy-dependent flux distribution. The user has three options for treating leakage in burnup calculations: (1) critical buckling, (2) user specified buckling, and (3) zero buckling

($k_{\inf}$ spectrum). In standard WIMS calculations, similar to other lattice codes such as UK WIMS9 [5] and HELIOS [6], the burnup calculation is performed using the neutron flux distribution for a critical reactor. To this end, the code performs a critical buckling search and renormalizes the two-dimensional neutron flux distribution in each energy group according to the energy dependent flux distribution of the homogeneous critical reactor.

The coolant void reactivity is calculated by Eq. (5) using $k_{\inf}$ values as obtained from the transport solutions of the cooled and voided lattice states (using infinite lattice spectrum).

2.2 CVR calculation using DRAGON

Unlike WIMS, the leakage effects in DRAGON are accounted for by the DB^2 correction of the absorption ($\widetilde{\Sigma}_a = \Sigma_a + DB^2$) and total cross sections ($\widetilde{\Sigma}_t = \Sigma_t + DB^2$), where D denotes the group-dependent diffusion coefficient and B is the geometric buckling. Depending on the choice of D, the code offers three alternative options: (1) the homogeneous B_1 model, (2) the heterogeneous B_1 model with anisotropic streaming, and (3) the heterogeneous B_1 model with isotropic streaming. Thus, DRAGON solves a transport equation with 3D leakage included so that its eigenvalue has the meaning of k_{eff}. The related $k_{\inf}$ is calculated as the ratio of neutron-production rate to neutron-absorption rate. However, it should be emphasized that, except in the special case $B = 0$, this $k_{\inf}$ value differs from the eigenvalue of the two-dimensional transport equation because the reaction rates are calculated with a neutron flux distribution that represents the eigenvector of the DB^2-corrected transport equation. Therefore, for clarity, denote the DRAGON calculated CVR as follows:

$$\Delta\widetilde{\rho}_{cvr}^{latt} = \frac{1}{\widetilde{k}_{\inf}^{cool}} - \frac{1}{\widetilde{k}_{\inf}^{void}} \tag{6}$$

Since the DRAGON transport solution depends on the geometric buckling, it is an open question which buckling values should be used in order to calculate CVR. The following two options are usually suggested for use:

Option A: Use critical buckling for the cooled state and impose the same buckling value on the voided state.

Option B: Use critical bucklings for both cooled and voided states.

These two options are further investigated and discussed in the following sections.

2.3 Simulation of the DRAGON method using WIMS

Among various alternative options, WIMS can also solve the DB^2-corrected transport equation. However, this WIMS option cannot be used in the same manner as in DRAGON. A Fortran procedure had to be written to run WIMS as necessary in order to mimic the DRAGON burnup calculation with leakage effects included using the homogeneous B_1 model.

For each burnup step the following WIMS calculations are carried out:

a) Cooled lattice calculation to get cell-averaged diffusion coefficients and critical buckling of the cooled state. This calculation produces $k_{\inf}^{cool}$ that is used in the standard WIMS CVR calculation.

b) Voided lattice calculation to get cell-averaged diffusion coefficients and critical buckling of the voided state. This calculation produces $k_{\inf}^{void}$ that is used in the standard WIMS CVR calculation.

c) Cooled lattice calculation using DB^2-corrected cross sections with critical buckling of the cooled state. This calculation produces $\widetilde{k}_{\inf}^{cool}$ to be used for CVR calculation by the simulated DRAGON method.

d) Voided lattice calculation using DB^2-corrected cross sections either with critical buckling of the cooled state (option A) or voided state (option B). This calculation produces $\widetilde{k}_{\inf}^{void}$ to be used for CVR calculation by the simulated DRAGON method.

e) For comparison, the calculation of the next fuel composition is performed using either DB^2-corrected model with critical buckling of the cooled state or the standard WIMS method.

2.4 Simulated DRAGON results versus standard WIMS results

Two series of WIMS simulations have been carried out to check the DRAGON method of CVR calculation using options A and B as specified in Section 2.3. The ACR-type lattice cell considered is the same as in Reference [3]. It is a light water cooled lattice of 24 cm lattice pitch and a large calandria tube to reduce the amount of moderator associated with each cell. The fuel bundle consists of 43 elements containing a central poisoned pin surrounded by low enriched fuel pins. Figure 3 presents the geometric model of the lattice cell.

Figure 4 compares the standard WIMS results with simulated DRAGON results based on option A (the critical geometric buckling of the cooled state is imposed on the leakage calculation of the voided state). Both methods produce very close results so that the CVR curves almost coincide with each other. This might be expected because in both cases the coolant void reactivity is defined in a similar manner, i.e., the CVR value is obtained as the difference in the reactivity of the perturbed (voided) state and the equilibrium (cooled) state. A slight difference that can be observed between these two curves is due to different definitions of $k_{\inf}$. The WIMS value of $k_{\inf}$ represents the eigenvalue of the 2D transport equation, while in the case of the DRAGON simulation it is an arbitrarily introduced quantity, which is equal to the ratio of neutron-production rate to neutron-absorption rate calculated with a neutron flux distribution that represents the eigenvector of the DB^2-corrected transport equation instead of the original 2D transport equation.

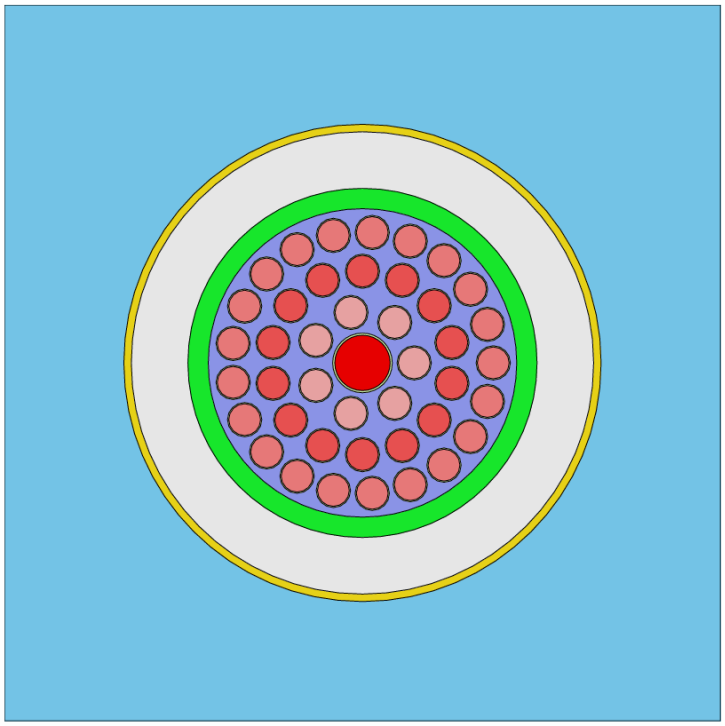

Figure 3 Geometric configuration of the ACR lattice

Figure 5 compares standard WIMS results with simulated DRAGON results based on option B (the critical geometric buckling used in both cooled and voided states). Comparison between Figure 5 and Figure 2 shows that the curve shapes of the original DRAGON results [3] and simulated DRAGON results are almost identical within the burnup range considered here. Thus, the DRAGON results obtained with option B initiated the issue of differing CVR results. The explanation of the root cause of the difference is as follows.

A reactor is critical (in an equilibrium state) when the geometric buckling is equal to the material buckling. Using critical geometric buckling in both cooled and voided states (option B) means that we consider two different equilibrium states. Consequently, in this case, instead of a change in reactivity, the coolant void reactivity represents a difference in the reactivity of two different equilibrium states. This is in contradiction with the notion of the coolant void reactivity as the change in reactivity due to a reactor perturbation (coolant voiding) that occurs over a very short period of time.

As stated above, the infinite neutron multiplication factor $\widetilde{k}_{\text{inf}}$ calculated by DRAGON differs from the eigenvalue k_{inf} of the neutron transport equation. In order to get a quantitative measure of this difference, Figure 6 presents a comparison of the values of the infinite neutron multiplication factor as calculated by the simulated DRAGON method and the standard WIMS method.

When option A is considered, the difference $\widetilde{k}_{\text{inf}} - k_{\text{inf}}$ is almost identical for both cooled and voided states, and ranges from about –15 mk for the fresh fuel to about 0 for the burnt fuel. Since cooled and voided states yield almost the same difference, this option produces CVR

values that are very close to the WIMS values. WIMS and DRAGON agree when zero buckling is used as shown in Reference [3]. This paper indicates that a good agreement can be achieved for the case of cooled critical buckling. Therefore, it is expected that similar agreement would be obtained with intermediate buckling values as well.

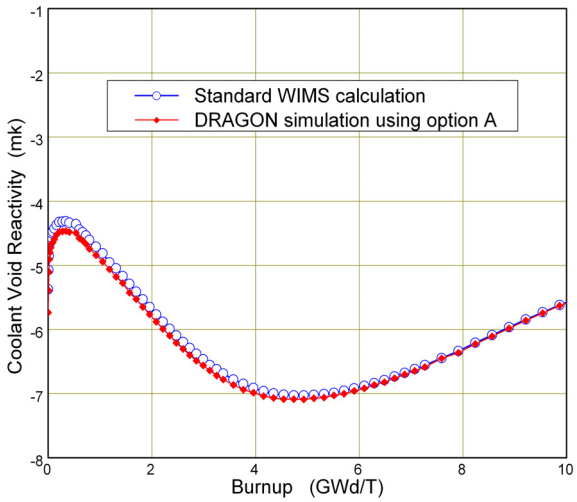

Figure 4 WIMS versus simulated DRAGON results obtained with option A (the critical buckling of cooled state imposed to voided state).

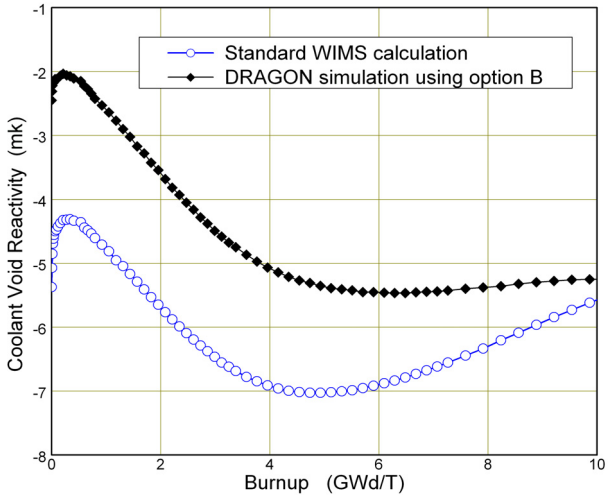

Figure 5 WIMS versus simulated DRAGON results obtained with option B (critical buckling in both cooled and voided lattice states).

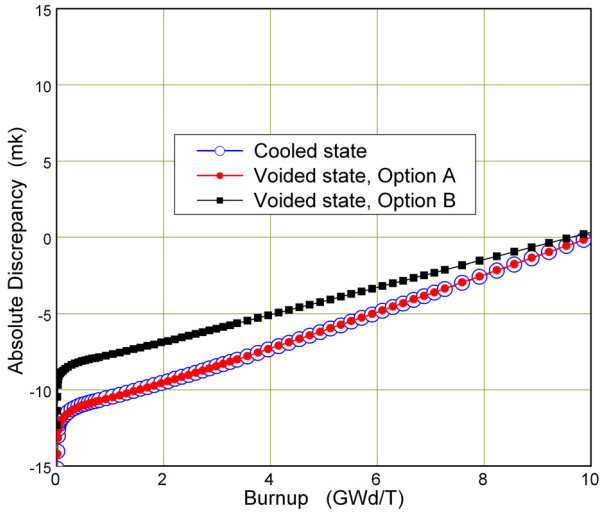

Figure 6 Absolute difference between the DRAGON-type infinite neutron multiplication factor $\tilde{k}_{\text{inf}}$ and the eigenvalue k_{inf} of the transport equation as calculated by WIMS.

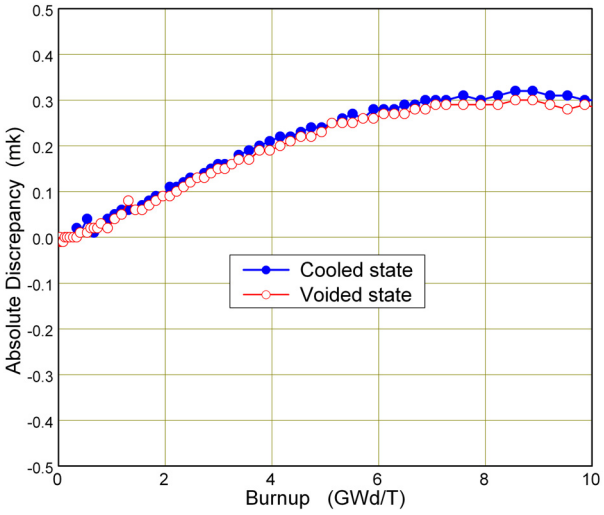

Figure 7 Absolute difference between k_{inf} values calculated for fuel compositions obtained with simulated DRAGON method and the standard WIMS method.

In the case of the option B, the difference between the curves $\widetilde{k}_{\inf}^{cool} - k_{\inf}^{cool}$ and $\widetilde{k}_{\inf}^{void} - k_{\inf}^{void}$ ranges from about 2.5 mk for the fresh fuel and decreases with irradiation to about 0 for the burnt fuel. Thus, this is the cause of differing CVR results.

Figure 7 compares the eigenvalues $k_{\inf}$ calculated for fuel compositions obtained with the simulated DRAGON method and the standard WIMS method. The difference in corresponding $k_{\inf}$ values ranges from 0 for the fresh fuel to about 0.3 mk for the burnt fuel. Thus, both burnup calculations, the standard WIMS approach and the simulated DRAGON method, yield very similar fuel composition, which is the subject of consideration in the next section.

3. Fuel isotopics as a function of irradiation

Concerning leakage effects on the change in isotopic composition, it has to be pointed out that the burnup calculation is carried out only for the cooled lattice state. Thus, in both DRAGON options A and B, the fuel isotopic composition should be identical. To get a quantitative measure of (dis)agreement of the fuel composition calculated by the standard WIMS approach and simulated DRAGON method, the atom densities of two crucial fuel nuclides (^{235}U and ^{239}Pu) have been considered.

Figures 8 and 9 show the atom density of ^{235}U and the relative discrepancy, respectively, while Figures 10 and 11 show the atom density of ^{239}Pu and the relative discrepancy, respectively, as calculated by both methods. Pin-average values are given for each ring of fuel pins as well as the cluster-average atom density. As the average bundle burnup at each step is slightly different in standard WIMS and simulated DRAGON calculations, it is easier to present the results by plotting them as functions of the irradiation time. An irradiation period of 309 days corresponds to a burnup of 10 GWd/T initial heavy elements. WIMS and simulated DRAGON results are in very good agreement so that visually no difference can be observed.

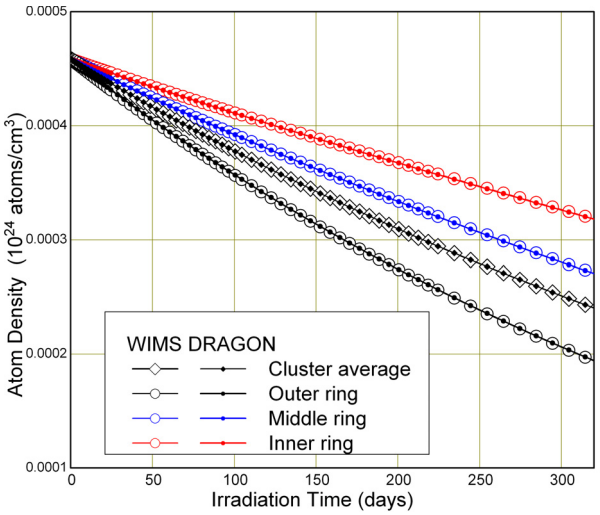

Figure 8 Atom density of ^{235}U calculated by WIMS and simulated DRAGON method.

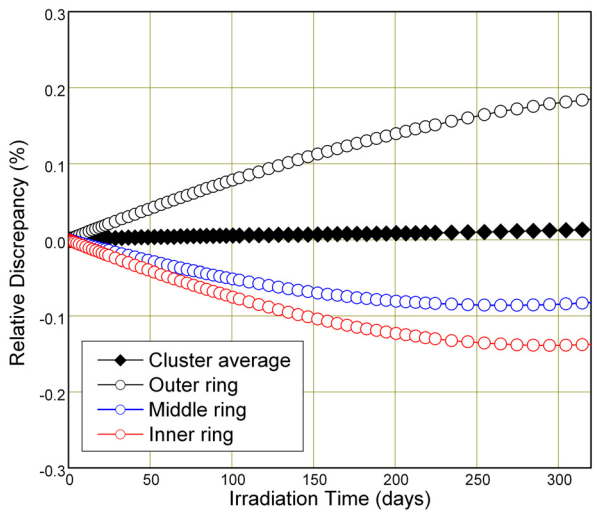

Figure 9 Relative discrepancy in ^{235}U atom density.

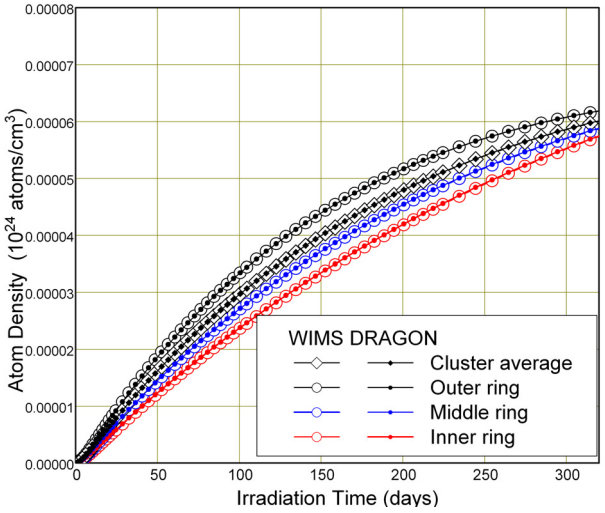

Figure 10 Atom density of ^{239}Pu calculated by WIMS and simulated DRAGON method.

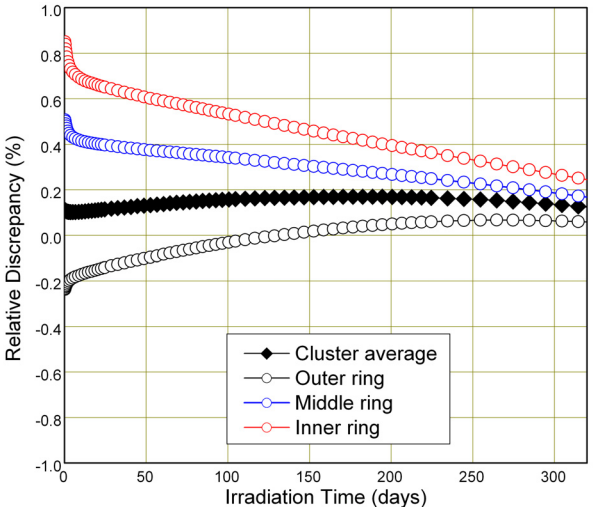

Figure 11 Relative discrepancy in ^{239}Pu atom density.

The magnitude of the relative discrepancy in pin-wise density of ^{235}U increases with irradiation from 0 to 0.2%. However, the discrepancy in cluster average density is close to 0 for the entire period of irradiation. The time dependence of the pin-wise discrepancy of ^{239}Pu has an opposite behaviour. It reaches values of up to 1% at the beginning of irradiation and decreases with irradiation to a magnitude of less than 0.3%. This is due to the fact that at the beginning of irradiation the density is very low so that one may expect a larger relative discrepancy between two very small quantities. The relative discrepancy in cluster-average densities remains at a very low level for the entire period of irradiation. The conclusion is that the discrepancy in atom densities calculated by the two methods is insignificant.

4. Cell-averaged two-group cross sections

In order to investigate the possible impact on the full-core reactor calculations, comparison of cell-averaged two-group cross sections are presented in this section. Group condensation has been performed with critical fluxes as calculated by each of the methods considered. Only the results for the cooled lattice state are presented, because the voided case is a perturbed state in which the coolant density is modified without any changes in the fuel isotopic composition. Figures 12 and 13 show the absorption as a function of the irradiation and the relative discrepancies in these cross sections, respectively. Similarly, Figures 14 and 15 show the fission yield (nu∗fission) and Figures 16 and 17 show scattering cross sections.

For all cross sections considered, except the up-scattering cross section, the observed discrepancy is less than 0.1%. The discrepancy in the up-scattering cross section decreases with irradiation from 0.8% to 0.05%. However, as demonstrated in Figure 16, the absolute value of this cross section is very small and it cannot affect the neutron multiplication factor significantly. According to the magnitudes of the discrepancies, as well as the discrepancy in k_{inf} presented in Figure 7 it is expected that the impact on the full-core neutron multiplication factor may be of the order of less than half a mk. Therefore, the change in two-group cross sections due to DRAGON-type leakage is considered as negligible.

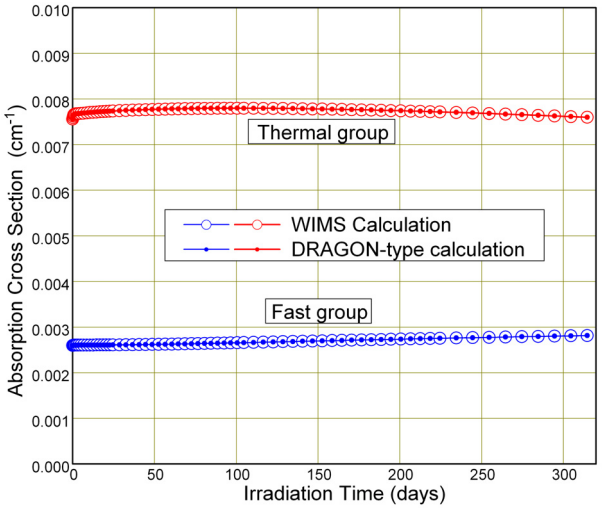

Figure 12 WIMS and simulated DRAGON results of absorption cross section.

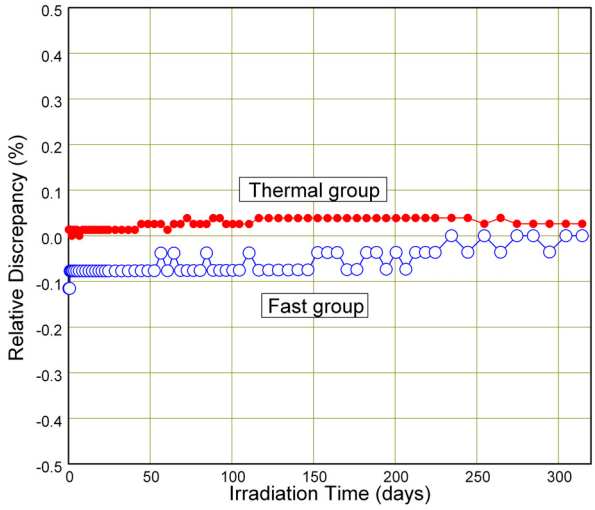

Figure 13 Relative discrepancy in absorption cross section.

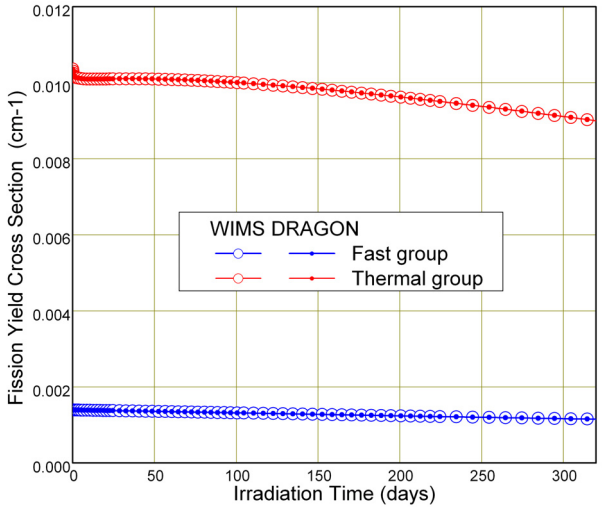

Figure 14 WIMS and simulated DRAGON results of fission yield cross section.

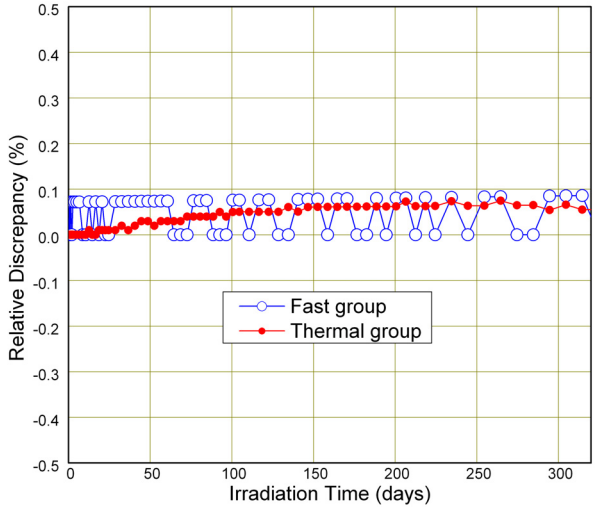

Figure 15 Relative discrepancy in fission yield cross section.

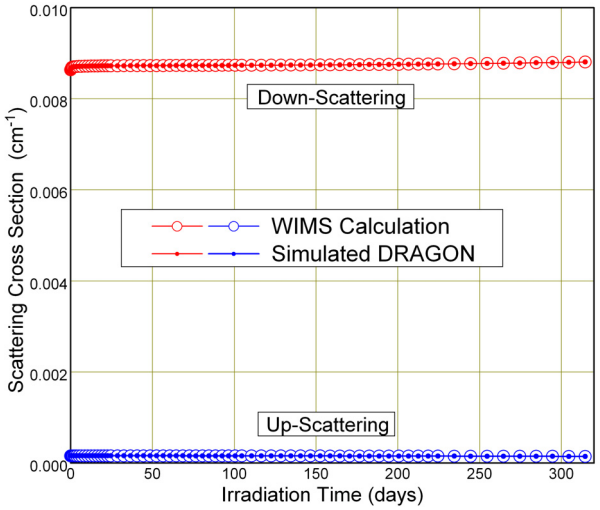

Figure 16 WIMS and simulated DRAGON results of scattering cross section.

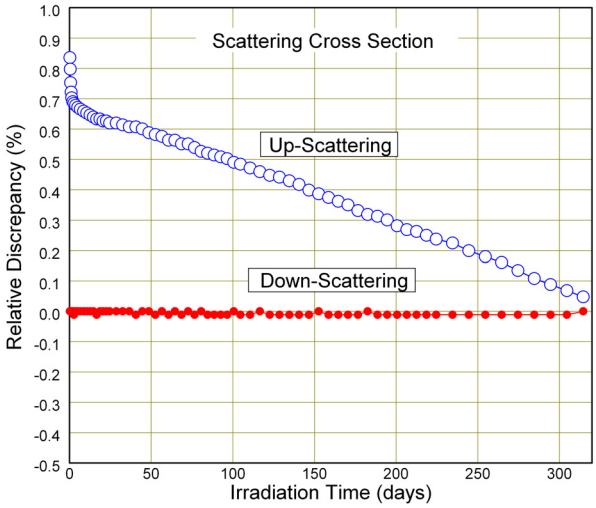

Figure 17 Relative discrepancy in scattering cross section.

5. Conclusions

A simulation of the DRAGON leakage calculation has been carried out in order to clarify the difference in the coolant void reactivity calculated by DRAGON and WIMS. The findings of the comparison of simulated DRAGON results and the corresponding results obtained by the standard WIMS approach are summarized as follows:

- The difference in CVR values is due to different CVR definitions.
- The difference is insignificant if the same CVR definition (option A) is used.
- The change in burnup-dependent fuel composition is insignificant.
- The change in cell-averaged two-group cross sections is negligible.

The lattice CVR is not a design parameter and is only used in scoping studies. It is the full-core CVR that is the relevant design parameter. Based on these findings, the conclusion is that the DRAGON-type leakage calculation is not expected to cause a significant change in the full-core CVR results obtained by full-core diffusion calculations (such as RFSP [7]) using lattice data from a standard WIMS calculation.

5. References

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