

PARAMETRIC ANALYSIS OF DOPPLER COEFFICIENT OF REACTIVITY IN DUPIC FUEL BY DRAGON

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ABSTRACT

Doppler coefficient of reactivity (DCR) is a crucial parameter in the evaluation of the reactivity-induced transients for both Light Water Reactor (LWR) and CANDU reactors. DCR of DUPIC (Direct Use of Spent PWR fuel in CANDU reactor) fuel, however, is less negative than natural uranium (NU) CANDU fuel in the fresh condition and shifts toward a positive direction after irradiation. After benchmarking the DRAGON code with 89 group WIMS ENDF/B-V library on calculation of DCR in enriched U₂O fuel and MOX fuel against MCNP-3A results, it was used to evaluate DCR in DUPIC fuel and to clarify the effects of changes in DUPIC fuel composition on DCR. A parametric analysis of DCR in DUPIC fuel shows that the presence of 0.3eV resonance cross section of PU239 plays an important role in shifting DCR toward a positive direction. The sign and magnitude of DCR are influenced by the PU239/U235 ratio in the fuel.

I. INTRODUCTION

Since DUPIC (Direct Use of Spent PWR fuel in CANDU reactor)¹ fuel is made of spent PWR fuel without any wet chemical separation, more fissile material (U235, PU239, and PU241) and fission products exist in the fresh DUPIC fuel than that of natural uranium (NU) fuel. Such complicated fuel composition makes the lattice properties such as Doppler coefficient of reactivity, coolant void coefficient, and kinetics parameters quite different from those of NU fuel.

Doppler coefficient of reactivity (DCR) is a crucial parameter in the evaluation of the reactivity induced transients for both Light Water Reactor (LWR) and CANDU reactors. It is the rate at which reactivity changes with the effective fuel temperature, which is typically defined as:

$$DCR = \left(\frac{1}{K_1} - \frac{1}{K_2} \right) / (T_1 - T_2) \quad (1)$$

where K_1 and K_2 are the lattice infinite multiplication factors corresponding to effective fuel temperature T_1 and T_2 respectively. DCR is generally negative in LWR fuel and its behavior has been studied before. For typical UO₂ fuels, as the fuel temperature increases, resonance absorption in fuel material, especially in U238, increases due to Doppler broadening of the resonance. This leads to a reduction in the resonance escape probability and results in a dominant negative reactivity effect. Because of the special characteristics of CANDU lattice (cluster geometry, use of heavy water as coolant and moderator) and a complicated fuel composition, the characteristics of DCR in DUPIC fuel need to be evaluated.

In this paper, the DRAGON² collision probability code with 89 group WIMS ENDF/B-V library was first benchmarked for the calculation of DCR of enriched U₂O fuel and MOX fuel against MCNP-3A results. Then a parametric analysis of DCR in DUPIC fuel was performed to clarify the effects of changes in fuel composition on DCR. Compared to NU fuel, DCR in DUPIC fuel is less negative than NU fuel in the fresh condition and shifts toward a positive direction after irradiation. It was concluded that the presence of 0.3eV

resonance cross section of PU239 plays a most important role in shifting DCR toward a positive direction. The sign and magnitude of DCR are influenced by the PU239/U235 ratio in the fuel.

II. EVALUATION OF DRAGON CALCULATION FOR DCR

In recent papers, DCR for an infinite lattice of slightly idealized PWR pin cells were calculated using MCNP-3A Monte Carlo code with ENDF/B-V library.^{3,4} The results were used as a set of numerical benchmarks to evaluate the accuracy of DRAGON calculation of DCR. Five enrichments, from natural uranium to 3.9 wt%, and two plutonium cases representative of depleted fuel were calculated using EXCEL T collision probability method in DRAGON with the full 89-group neutron energy structure in the WIMS ENDF/B-V library. The DCR computed by DRAGON for all cases are shown in Table 1 and compared with the results of MCNP-3A, MCNP-4A continuous-energy Monte Carlo codes^{3,5}, WIMS-AECL⁵, CELL-2 pin-cell spectrum code of the EPRI-PRESS reactor physics package⁶, ONEDANT discrete-ordinates code⁷, and CASMO-4⁸. All these codes use cross sections derived from ENDF/B-V library. Table 1 shows that DRAGON calculations of DCR are in excellent agreement with those predicted by the Monte Carlo calculation, and are almost within a single standard deviation associated with the MCNP-3A calculations. It is concluded that the DRAGON lattice code, together with the ENDF/B-V data library, can predict DCR of enriched fuel and MOX fuel with very good accuracy.

III. FUEL COMPOSITION OF DUPIC FUEL

A 17x17 French standard 900 MWe PWR fuel assembly was used as the reference feed material to the DUPIC fuel cycle in this study.⁹ The initial enrichment of the reference spent PWR fuel is 3.2 w/o. To clarify the effects of changes in fuel composition on DCR, two DUPIC fuel types, corresponding to two different discharge burnup of spent PWR fuels, were studied in this paper:

- 1) DUPIC-A: corresponding to 30000 MWD/T discharge burnup of spent PWR fuel
- 2) DUPIC-B: corresponding to 35000 MWD/T discharge burnup of spent PWR fuel

In assessing the Doppler effect on the lattice infinite multiplication factors of DUPIC fuel, the contribution of isotopes in the fuel that are sensitive to fuel temperature should be considered. Since the discharge burnup of spent PWR fuels are different, the contributions of isotopes in two DUPIC fuel types are much different, as shown in Table 2.

For DUPIC fuel, the number densities of U235 and U238 decrease with burnup. Because of both buildup and depletion effect, the reduction in number density of PU239 is slower than that of U235. Hence the PU239/U235 ratio in DUPIC fuel increases gradually with burnup as shown in Figure 1. Since DUPIC-B fuel is made of spent PWR fuel with higher discharge burnup, the PU239/U235 ratio in DUPIC-B fuel is larger than that in DUPIC-A fuel for any burnup steps. As will be seen later, the sign and magnitude of DCR in DUPIC fuel is strongly dependent on PU239/U235 ratio which varies with fuel types and irradiation.

IV. CHARACTERISTICS OF DCR IN DUPIC FUEL

The burnup dependent DCR of two DUPIC fuels were calculated by DRAGON with 89-group ENDF/B-V library and compared with that of NU fuel in Figure 2. For a given lattice geometry design, DCR depends on the fuel composition in DUPIC fuel, i.e., fuel types and fuel irradiation. The following characteristics of DCR are clarified from the results shown in Figure 2:

- 1) DCR is negative for both NU and DUPIC fuels in fresh condition. It tends to exponentially increase and even changes sign from negative to positive after a period of irradiation.

- 2) Compared to DUPIC-A fuel, the DCR shifts toward a more positive direction in DUPIC-B fuel, which has a higher PU239/U235 ratio.
- 3) The DCR in fresh DUPIC fuel is less negative than in fresh NU fuel. However the DCR in NU increases more rapidly with irradiation than in DUPIC fuels and makes the DCR curves crossover each other around 2000 MWD/T.

V. PARAMETRIC ANALYSIS OF DCR IN DUPIC FUEL

In order to have some insight into the physical significance of the DCR calculation, the four-factor formula was used as follows:

$$K_{\infty} = \epsilon \eta f p \quad (2)$$

where p is the resonance escape probability, ϵ is the fast-fission factor, f is the thermal utilization factor, and η is the reproduction factor. If K -infinity is expressed in terms of Equation (2), then the DCR can be approximated as:

$$DCR \approx \frac{1}{K_{\infty}} \frac{\partial K_{\infty}}{\partial T} = \frac{1}{p} \frac{\partial p}{\partial T} + \frac{1}{\epsilon} \frac{\partial \epsilon}{\partial T} + \frac{1}{f} \frac{\partial f}{\partial T} + \frac{1}{\eta} \frac{\partial \eta}{\partial T} \quad (3)$$

The relative changes in four factors upon fuel temperature variation from 641K to 941K, i.e., the right hand side of Equation (3), were given in Figure 3 for DUPIC-A fuel. We observed that, after irradiation, the relative change in thermal reproduction factor with fuel temperature, i.e., $1/\eta \cdot \partial \eta / \partial T$, increases (positive direction) while changes in other factors are not much significant. Therefore, DCR tend to shift toward a positive direction with burnup and will become positive after a period of irradiation. It should be understood that the four-factor formula was used here only as a means for expressing the results of detailed multi-group transport calculations and of understanding their physical significance. The lattice infinite multiplication factor and the corresponding four factors were derived entirely from multi-group transport calculations. Overall, the following three effects are regarded as main effects on DCR in DUPIC fuel:

1) Effect of epi-thermal resonance of U238

As other typical UO₂ fuels, U238 is the major constituent of the DUPIC fuel as shown in Table 3. When the fuel temperature increases, epi-thermal resonance absorption of U238 increases due to Doppler broadening of the resonance. This leads to a reduction in the resonance escape probability p and makes a dominant negative contribution to DCR. That's why DCR is generally negative in fresh DUPIC and NU fuels. Since U238 depletion with fuel irradiation is very small, $1/p \cdot \partial p / \partial T$ keeps almost constant with irradiation as shown in Figure 3.

2) Effect of 0.3 eV resonance of Pu239

The resonance in the PU239 cross section will affect considerably DCR. When the fuel temperature increases, thermal resonance fission in Pu239 increases due to Doppler broadening of the resonance. This results in an increase of the thermal reproduction factor η and makes a significant positive contribution to DCR. Therefore the DCR in fresh DUPIC fuel is less negative than in fresh NU fuel.

$1/\eta \cdot \partial \eta / \partial T$ is very sensitive to the fuel composition, especially the amounts of U235 and Pu239 present in the fuel, i.e. PU239/U235 ratio. Physically, if we assume that the thermal neutron spectra in the DUPIC fuel is independent on fuel composition and irradiation, the higher the PU239/U235 ratio, the more neutrons will be

produced due to thermal fission of PU239. The increased thermal resonance fission rates of PU239 with fuel temperature thus contribute to a positive increase of $1/\eta \cdot \partial\eta/\partial T$.

Since PU239/U235 ratio in DUPIC fuel increases with irradiation, $1/\eta \cdot \partial\eta/\partial T$ thus increases with burnup accordingly as shown in Figure 3. We conclude that the large (positive) increase in $1/\eta \cdot \partial\eta/\partial T$ causes DCR to change sign after irradiation. Interestingly enough, the variation of PU239/U235, $1/\eta \cdot \partial\eta/\partial T$, and DCR with irradiation in DUPIC fuel show similar trends as illustrated in Figures 1 to 3.

Similarly, the higher PU239/U235 ratio in DUPIC-B fuel makes the DCR shifts faster toward a positive direction than that in DUPIC-A fuel. Compared with DUPIC fuels, the PU239/U235 ratio in NU fuel increased much faster with irradiation. This results in DCR of NU fuel shift toward a positive direction more rapidly with irradiation than in DUPIC fuels and makes the DCR curves crossover each other as shown in Figure 2.

Though PU241 also has a resonance at 0.3eV like PU239, both its resonance cross section and content are smaller than that of PU239 so that the positive contribution of PU241 on DCR is much smaller than that of PU239.

3) Thermal Neutron spectrum effect

Since the thermal neutrons are dominant in the heavy water-moderated fuel lattice, the variations in the thermal neutron spectrum effect are important. For DUPIC fuels, the higher fissile material (U235, PU239 and PU241) contents and the presence of resonance absorption in plutonium isotopes at low energy (PU239 and PU241 resonance absorption at 0.3eV, PU240 resonance absorption at 1eV) make the neutron spectrum harder than that of NU fuel as shown in Figure 4. Compared with NU fuel, it was seen that in DUPIC fuel:

- a. The thermal neutron flux decreases largely
- b. The dipped thermal neutron flux is further dipper at a resonance width of 0.3eV
- c. The thermal neutron spectra in two DUPIC fuels are almost identical

After depletion, the neutron spectra tend to soften to make the thermal neutron flux increase, and the reduced content of PU239 tends to recover the dip of the thermal neutron flux at 0.3eV resonance width as shown in Figure 5. These will increase the thermal resonance fission rate of PU239 and make a positive contribution to DCR.

VI. CONCLUSION

Doppler coefficient of reactivity (DCR) is a generic safety feature of the nuclear fuel in the case of reactivity induced transients because it is an important response to the fuel temperature changes. In view of reactor safety and verification of nuclear analysis code for a practical utilization of DUPIC (Direct Use of Spent PWR fuel in CANDU reactor) fuel in CANDU reactors, DRAGON calculation of DCR was benchmarked against Monte Carlo results. The calculation showed that DRAGON calculations of DCR are almost within a single standard deviation associated with the MCNP-3A calculations. It is concluded that DRAGON lattice code, together with the ENDF/B-V data library, can predict DCR of enriched fuel and MOX fuel with very good accuracy.

Because of the significant fraction of fissile plutonium in the DUPIC fuel, the DCR in DUPIC fuel is less negative than natural uranium (NU) CANDU fuel in the fresh condition and shifts toward a positive direction after irradiation. A parametric study made by DRAGON with ENDF/B-V library showed that the presence of 0.3eV resonance cross section of PU239 plays an important role in shifting DCR toward a positive direction. When the fuel temperature increases, thermal resonance fission of Pu239 increases due to Doppler broadening

of the resonance. This leads to an increase of the thermal reproduction factor with temperature ($1/\eta \cdot \partial\eta/\partial T$) and makes a significant positive contribution to DCR. The magnitude and sign of the DCR are influenced by the PU239/U235 ratio in the fuel. If the thermal neutron spectra in the fuel rod are identical, DCR tends to shift toward a more positive direction for the fuel with a higher PU239/U235 ratio. As the PU239/U235 ratio increases with irradiation, the DCR in DUPIC fuel tends to shift toward a positive direction with irradiation and will become positive after a period of irradiation.

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Table 1: Comparison of Doppler Coefficient of Reactivity (mk/K) among DRAGON and some selected transport theory lattice codes with cross section derived from ENDF/B-V library

Enr. (wt%)	MCNP-3A	MCNP-4A	DRAGON 89-Group	WIMS-AECL (DSN) 89-Group	CELL-2 97-Group	ONEDANT 69-Group	CASMO- 4 40-Group
0.711	-0.054±0.008	-0.055±0.003	-0.060	-0.058	-0.056	-0.057	-0.055
1.6	-0.036±0.003	-0.034±0.002	-0.037	-0.036	-0.036	-0.036	-0.034
2.4	-0.027±0.003	-0.028±0.002	-0.030	-0.029	-0.030	-0.029	-0.028
3.1	-0.026±0.002	-0.028±0.001	-0.027	-0.027	-0.027	-0.026	-0.025
3.9	-0.024±0.002	-0.025±0.002	-0.026	-0.025	-0.024	-0.025	-0.024
Pu Con. (a/o)	MCNP-3A		DRAGON 89-Group	WIMS-AECL (DSN) 89-Group	CELL-2 97-Group		
1.0	-0.037±0.004		-0.037	-0.036	-0.042		
2.0	-0.034±0.003		-0.034	-0.033	-0.038		

Table 2: Variation of Isotopic Number Density ($1.0 \times 10^{20} \text{ cm}^{-3}$) with Burnup for DUPIC fuels

Burnup (MWD/T)	DUPIC-A		DUPIC-B	
	0	14737	0	14737
U235	2.47	0.61	1.99	0.44
U238	230.34	227.80	229.28	226.63
PU239	1.42	0.80	1.46	0.78
PU241	0.19	0.21	0.22	0.22

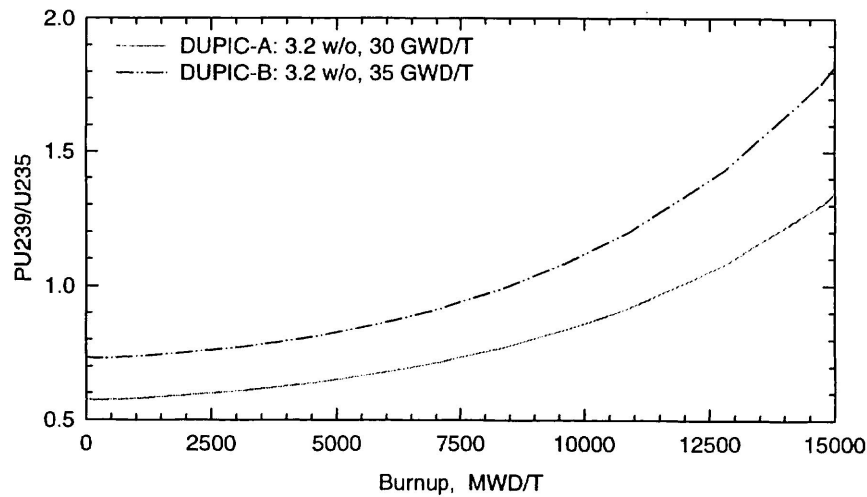


Figure 1: Burnup Dependent PU239/U235 for Two DUPIC Fuel Types

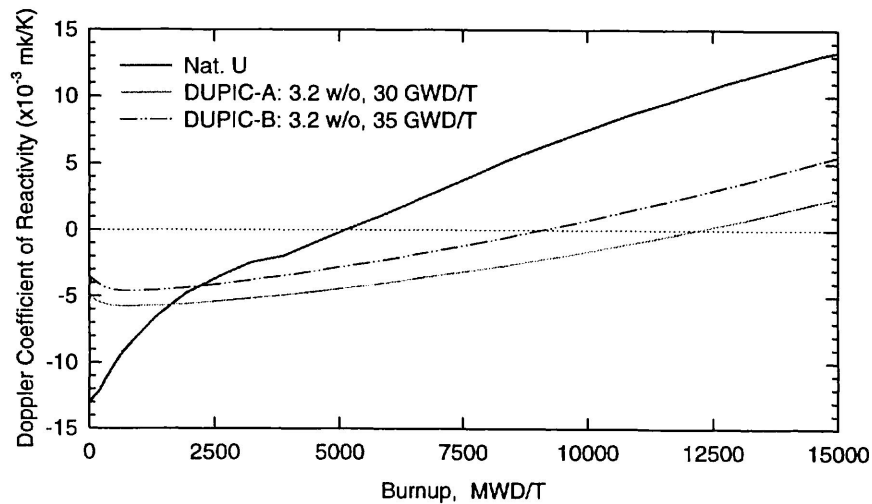


Figure 2: Burnup Dependent Doppler Coefficients of Reactivity for DUPIC and Nat. U Fuels

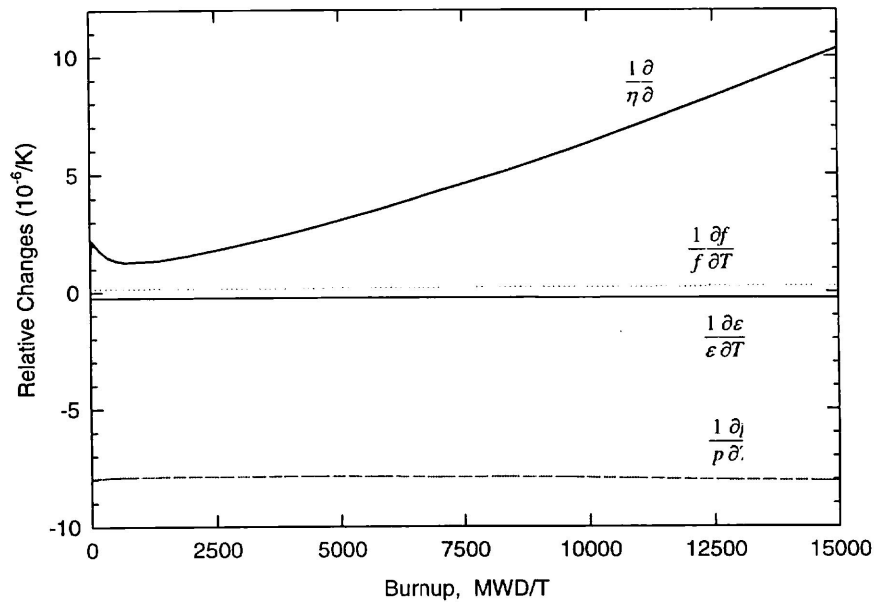


Figure 3: Relative Changes in Four Factors upon Fuel Temperature Variation from 641K to 941K for DUPIC-A Fuel (3.2 w/o, 30 GWD/T)

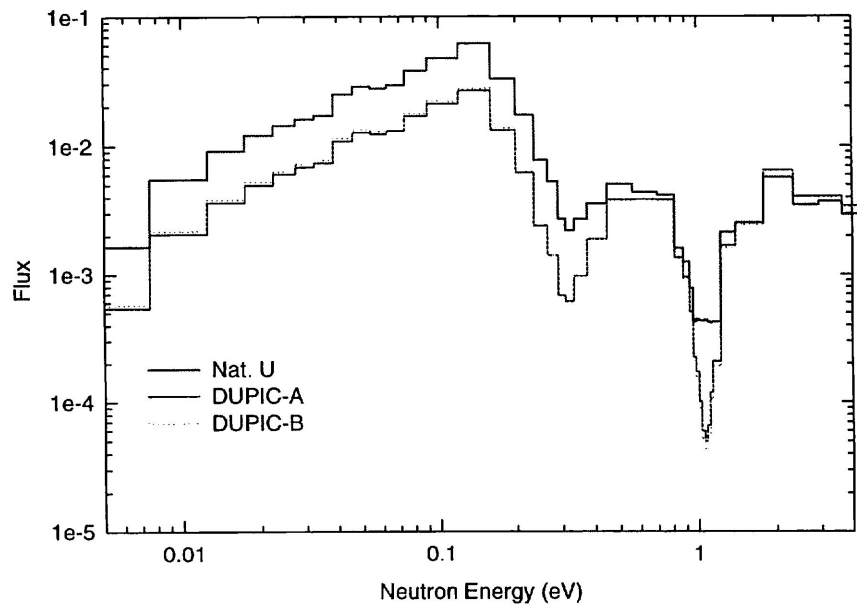


Figure 4: Thermal Neutron Spectra in DUPIC and Nat. U Fuels (0 GWD/T)

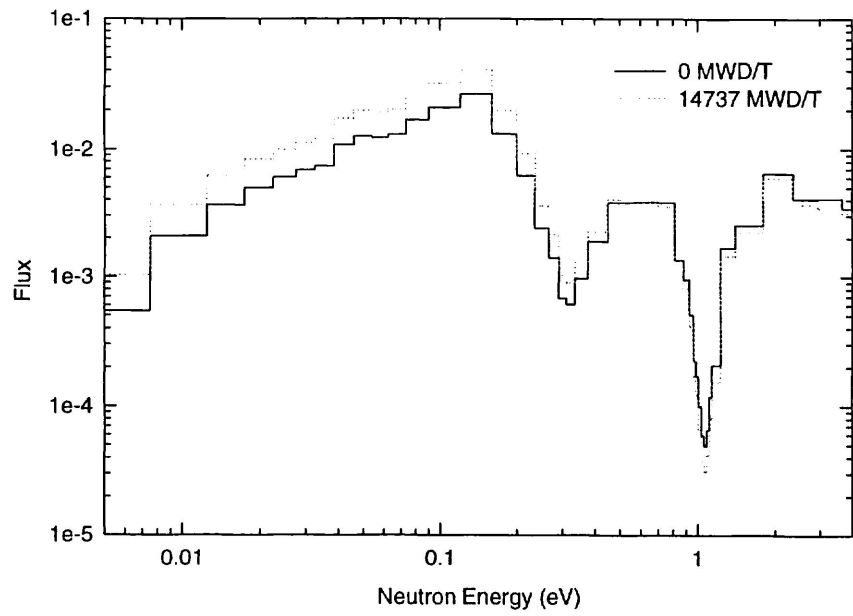


Figure 5: Variation of Thermal Neutron Spectra with Burnup in DUPIC-A Fuel