

## COMPARISON OF CANDU DUPIC PHYSICS CODES WITH MCNP

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### Abstract

Computational benchmark calculations have been performed for CANDU DUPIC fuel lattice and core using a Monte Carlo code MCNP-4B with ENDF/B-V library. The eigenvalues of the DUPIC fuel lattice have been predicted by an integral transport code WIMS-AECL using ENDF/B-V library for different burnup steps and lattice conditions. The comparison has shown that the eigenvalues match those of MCNP-4B within 0.20%  $\Delta k$  difference between WIMS-AECL and MCNP-4B results. The calculation of a 2-dimensional CANDU core loaded with DUPIC fuel has shown that the eigenvalue predicted by a diffusion code RFSP using lattice parameters generated by WIMS-AECL matches that of MCNP-4B within 0.12%  $\Delta k$  and the largest bundle power prediction error is around 7.2%.

### 1. Introduction

Currently, a physics design study on the Direct Use of Spent PWR Fuel in CANDU (DUPIC)<sup>1</sup> is being carried out by Korea Atomic Energy Research Institute (KAERI) and Atomic Energy of Canada Limited (AECL). Most of CANDU physics calculations are performed with an integral transport code WIMS-AECL<sup>2</sup> for the lattice calculation and a diffusion code RFSP<sup>3</sup> for the core simulations. Though there have been a series of benchmark tests<sup>4-6</sup> on these two codes, most of them are restricted to CANDU natural uranium fuel system. In order to develop a new fuel to be used in an existing CANDU reactor, the design tool should produce accurate results and, therefore, the validation of these codes for the specific fuel type is necessary to provide confidence in the calculation results.

DUPIC fuel is made of spent PWR fuel and the fuel composition is completely different from either UO<sub>2</sub> or Mixed Oxide (MOX) fuel. The criticality experiment data are not readily available for the DUPIC fuel which contains all the actinides and fission products. Nonetheless, it is still necessary to perform a validation test of the design tools for future licensing of the fuel. In order to assess the applicability of CANDU physics code to the DUPIC fuel and core design study, a computational benchmark test using a Monte Carlo code MCNP-4B<sup>7</sup> has been performed because its solution method is superior. For a consistent comparison between WIMS-AECL and MCNP-4B, ENDF/B-V nuclear data was used for both codes.

## 2. Code Description

WIMS-AECL is being used to generate all the CANDU physics parameters including the composition of the DUPIC fuel. It performs multigroup transport calculation for a lattice and produces flux distribution, eigenvalues and reaction rates. For the solution method, the collision probability method is chosen to model the 2-dimensional geometry of the CANDU DUPIC lattice exactly.

RFSP is a 3-dimensional diffusion code used for CANDU core analysis. It performs a wide variety of calculations such as time-average, instantaneous and refueling simulations based on the solution of the finite-difference form of the neutron diffusion equation in two energy groups. RFSP incorporates the lattice parameters generated by WIMS-AECL by interpolating them for specific data points of fuel burnup, fuel temperature and coolant density.

MCNP-4B is a general-purpose, continuous-energy, generalized geometry, time-dependent, coupled neutron- photon-electron Monte Carlo transport code system. The criticality calculation is embedded in MCNP to estimate the multiplication factor. The local parameters such as particle or energy current and flux across a surface, flux or energy deposition averaged over a volume, and flux at the point can be extracted via a tally option.

## 3. DUPIC Lattice Calculation

### *Reference DUPIC Fuel*

The reference DUPIC fuel contains 1.55 wt% of fissile material ( $^{235}\text{U}$ ,  $^{239}\text{Pu}$ , and  $^{241}\text{Pu}$ ) and 0.75 wt% of fission products at fresh condition. Currently, the center pin of a DUPIC fuel bundle is poisoned by natural dysprosium in order to reduce the coolant void reactivity. The DUPIC fuel lattice is composed of 43 fuel pins in a cluster form.

### *Lattice Condition*

Comparisons have been made among three different burnup states of the DUPIC fuel: 0, 7453 and 15040 MWD/T which represent the fresh, equilibrium and discharge burnup, respectively. The fuel composition at each burnup step is obtained from the WIMS-AECL depletion calculation. There are 20 actinides and 45 fission products in ENDF/B-V library of WIMS-AECL. But, the isotopes not occurring in the MCNP-4B library ( $^{232}\text{U}$ ,  $^{236}\text{Pu}$ ,  $^{239}\text{Np}$ ,  $^{133}\text{Xe}$ ,  $^{134}\text{Cs}$ ,  $^{139}\text{La}$ ,  $^{144}\text{Nd}$ ,  $^{146}\text{Nd}$ ,  $^{150}\text{Nd}$ ,  $^{148}\text{Sm}$ ,  $^{153}\text{Sm}$ ,  $^{151}\text{Pm}$ ,  $^{155}\text{In}$ ,  $^{166}\text{Er}$ ,  $^{167}\text{Er}$ , and a pseudo fission product) are not considered as fuel constituents for consistent comparison between WIMS-AECL and MCNP-4B.

Three lattice conditions such as cold (reference), voided and hot states are modelled for each burnup state. For the cold condition, the temperature of all the material in a lattice is 300 K. It is also assumed

that the densities of the coolant and the moderator are those of normal operating condition. In a voided condition, the coolant density is reduced from 0.807859 g/cc to 0.0001 g/cc. In a hot condition, the fuel temperature is increased to 900 K to get the temperature effect.

### ***Comparison***

The calculations have been performed for the DUPIC fuel lattice to get the eigenvalues and the relative pin power of each case. The MCNP-4B calculation is done with 2,000 particles per cycle and a total of 500 cycles. The results are summarized in Table 1 in which the numbers in parenthesis are the difference with the MCNP-4B calculation. For the nine cases (3 burnup states  $\times$  3 lattice conditions), the maximum deviation of  $k_{\infty}$  is 0.20%  $\Delta k$  which is considered to be sufficiently small.

## **4. CANDU DUPIC Core Calculation**

### ***DUPIC Core Model***

The only difference between the existing natural uranium and DUPIC fuel CANDU-6 core is the fuel type and, therefore, the geometry model of the DUPIC core is the same as that of the natural uranium fuel core.

Because of on-power refueling operation and bi-directional refueling scheme of the CANDU reactor, the fuel burnup distribution is not symmetric in both the radial and axial directions. This disables the use of reflective boundary conditions. But a full core model including reactivity devices will cost too much, especially for MCNP-4B and, therefore, it has been decided to simplify the core model using the average burnup distribution obtained by RFSP full core calculation.

### ***Simplified Core Model***

Several simplifications have been made for geometry, burnup distribution, and temperatures of the DUPIC core in order to lighten the computational burden in MCNP-4B calculation.

- The reactivity devices and structural materials are not included in a core model.
- A 2-dimensional quarter core model is used.
- The average fuel burnups are 7,964 and 7,206 MWD/T for the inner and outer core, respectively.
- The temperature of the system is 300 K.

### ***Comparison***

The MCNP-4B criticality calculation has been carried out to get the eigenvalue and the power distribution for the DUPIC fuel core. The MCNP-4B results are obtained after completing 120 cycles with 100,000 particles per cycle. The final multiplication factor of MCNP-4B calculation is  $1.03825 \pm 0.00024$  and

the difference of multiplication factor between RFSP and MCNP-4B calculations is only 0.12%  $\Delta k$ . But, the difference of the bundle power prediction, shown in Fig.1, is relatively large for the peripheral region. The maximum difference is 7.2% for the bundles located on the periphery.

## 5. Discussion

For the lattice calculation, the eigenvalues predicted by WIMS-AECL generally agree with those of MCNP-4B. For example, the burnup reactivity swings are 24.1 and 24.0%  $\Delta k$  for MCNP-4B and WIMS-AECL, respectively. But the comparison of Fuel Temperature Coefficient (FTC) has shown large discrepancy between WIMS-AECL and MCNP-4B calculations. The FTC's of DUPIC fuel at discharge burnup are  $-5.17 \times 10^{-6}$  and  $-2.15 \times 10^{-6}$   $\Delta k/K$  for MCNP-4B and WIMS-AECL, respectively. Such a large difference may be due to the insufficient temperature data of plutonium isotopes in MCNP-4B cross-section libraries used in this study. It should be noted that plutonium is the major fissile nuclide in DUPIC fuel and its contribution to total fission rate is around 75% at the discharge state.

For the core calculation, the bundle powers on the peripheral region are underpredicted for RFSP. This seems to be due to the boundary condition and coarse mesh spacing in the diffusion calculation. It is also probable that the cross-section of reflector (heavy water) affects the bundle powers of the peripheral lattices. At the same time, it is noted that the KCODE calculation by the iterative source of MCNP-4B does not produce a stable result for the DUPIC core. For example, the bundle powers of channels A12 and L22, which are almost on the symmetric position in a quarter core, are different by 2.5% in MCNP-4B calculation while they are the same in RFSP calculation.

## 6. Conclusion and Future Works

The DUPIC lattice and core calculations has been carried out with MCNP-4B in order to ensure the accuracy of DUPIC physics calculations done by other code systems. The criticality calculations of DUPIC fuel lattice have shown that the results of WIMS-AECL and MCNP-4B calculations are in good agreement for various burnup steps and lattice conditions; the largest and average difference are 0.20%  $\Delta k$  and 0.087%  $\Delta k$ , respectively. The 2-dimensional quarter core calculation has also shown an excellent agreement in  $k_{eff}$  prediction between MCNP-4B and RFSP. But the comparison of the reactivity coefficient calculation has shown that the current cross-section library of MCNP-4B is not sufficient yet to take the MCNP-4B calculation as the reference one. For the core calculation by MCNP-4B, it is necessary to perform a lot of independent criticality calculations because the consecutive source distributions are corrected when the system is very large ( $\sim$ large dominance ratio).

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## REFERENCES

1. J.S. Lee et al., "Research and Development Program of KAERI for DUPIC (Direct Use of Spent PWR Fuel in CANDU Reactors)," Proc. of Int. Conf. and Tech. Exh. on Future Nuclear System: Emerging Fuel Cycles and Waste Disposal Options, GLOBAL'93, Seattle, USA, Sept. 1993.
2. J.V. Donnelly, "WIMS-CRNL: A User's Manual for the Chalk River Version of WIMS," AECL-8955, CRNL, 1986.
3. D.A. Jenkins and B. Rouben, "Reactor Fuelling Simulation Program - RFSP: User's Manual for Microcomputer Version," TTR-321, Atomic Energy of Canada Limited, 1993.
4. J.V. Donnelly, "Progress in the Development of WIMS at Chalk River," Sixth Annual Conf. of the Canadian Nuclear Society, Ottawa, Canada, June 1985.
5. D.S. Craig, "A Comparison of Lattice Parameters for CANDU-type Lattices Obtained Using MCNP, WIMS, and WIMS with Resonance Reaction Rates from MCNP," AECL-9778, Atomic Energy of Canada Limited, 1989.
6. D.A. Jenkins and E.G. Young, "Simulation of the 1992 SDS1 Trip Test at Point Lepreau," Proc. of 1994 Nuclear Simulation Symposium, Ontario, Canada, Oct. 1994.
7. J.F. Briesmeister ed., "MCNP-A General Monte Carlo N-Particle Transport Code Version 4A," LA-12625-M, Los Alamos National Laboratory, 1993.

Table 1. Comparison of  $k_{\infty}$  for DUPIC Fuel Bundle

Burnup (MWD/T)	$k_{cold}$		$k_{void}$		$k_{hot}$	
	MCNP	WIMS	MCNP	WIMS	MCNP	WIMS
0.0	1.16425 $\pm 0.00081$	1.16414 (-0.009%)	1.17616 $\pm 0.00083$	1.17633 ( 0.014%)	1.15915 $\pm 0.00081$	1.15756 (-0.137%)
7453	1.05415 $\pm 0.00083$	1.05349 (-0.063%)	1.06902 $\pm 0.00080$	1.06724 (-0.167%)	1.04664 $\pm 0.00079$	1.04875 ( 0.202%)
15040	0.92336 $\pm 0.00070$	0.92375 ( 0.042%)	0.93847 $\pm 0.00074$	0.93865 ( 0.019%)	0.92026 $\pm 0.00076$	0.92246 ( 0.130%)

( ) Difference with MCNP

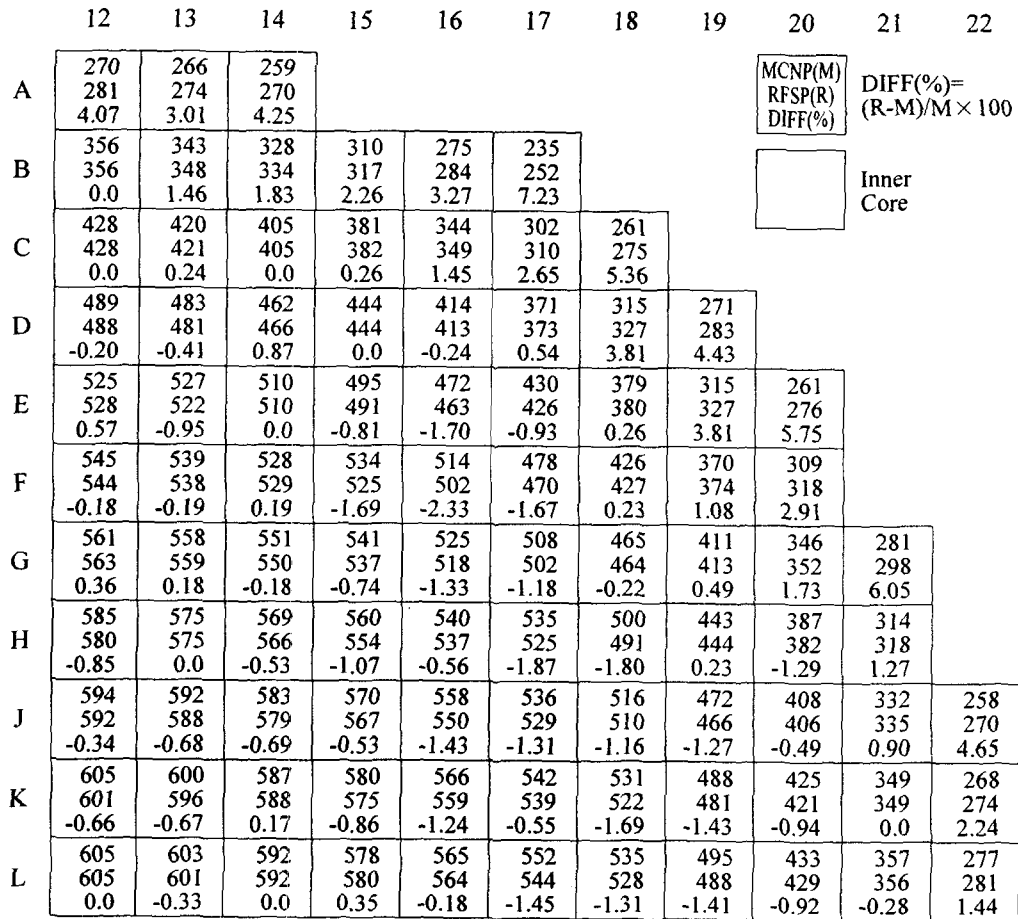


Fig.1. Comparison of Bundle Power Distribution