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Reactivity Coefficient Calculation of CANDU Fuel Lattices by MCNP

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ABSTRACT

The reactivity coefficient calculations have been performed for the standard and advanced CANDU fuels using a Monte Carlo code MCNP-4B in order to validate lattice codes WIMS-AECL and HELIOS. New MCNP libraries were generated from ENDF/B-VI in order to consider the full isotopic composition and the temperature effect. The lattice codes were benchmarked by MCNP for the major safety parameters of the CANDU fuel lattices. For WIMS-AECL, the difference of the infinite multiplication factor increases as the fuel burnup increases with the maximum value of 7.58mk for DUPIC fuel at discharge burnup. The void coefficient and Doppler constant agree with those of MCNP within 1.67σ and 3.31σ, respectively. For HELIOS, the infinite multiplication factors agree with those of MCNP calculations with slightly smaller difference compared with WIMS-AECL and the void and Doppler constant are slightly larger than those of WIMS-AECL for both fuel lattices.

I. INTRODUCTION

The standard Canada deuterium uranium (CANDU) fuel bundle has 37 fuel pins which are made of natural uranium. The physics design and analysis of natural uranium CANDU fuel are typically performed by a lattice code POWDERPUFS-V (PPV)[1] which has been developed based on series of physics measurements. However, the application of PPV is limited to the natural uranium fuel because of empirical correlations implemented. Recently, advanced CANDU fuel development programs are conducted, which includes 43-element fuel bundle, recovered uranium (RU), slightly enriched uranium (SEU), mixed oxide (MOX) and direct use of spent pressurized water reactor fuel in CANDU reactors (DUPIC). For the advanced CANDU fuel analysis, a transport code WIMS-AECL[2] is widely used and a newly developed code HELIOS[3] also has the potential of future uses because both codes have the capability of modelling the two-dimensional fuel cluster geometry.

However, the criticality experiment data that can be used for benchmarking such advanced fuels in the heavy water environment are not readily available yet. Especially for the DUPIC fuel which contains all the actinides and fission products, it is even more difficult to perform the criticality measurement because of the radiation emission and the complexity of the fuel composition. Nonetheless, it is still required to validate the physics calculations for such fuels in order to prove the credibility of the physics design and analysis. Fortunately, a Monte Carlo code MCNP[4] has been used as an alternative way of benchmarking lattice codes for key safety parameters such as the burnup reactivity swing, void coefficient and Doppler constant. For example, Mosteller et al.[5] has used MCNP for the benchmark calculation of the pressurized water reactor (PWR) fuel Doppler constant and Rhanema et al.[6] applied MCNP to the benchmark calculation of the boiling water reactor (BWR) fuel lattice. These works have encouraged to use MCNP for the benchmarking of the CANDU fuel lattices especially for the DUPIC fuel which is considered to be one of the most complex fuel types ever made.

II. MCNP LIBRARY GENERATION

The public MCNP cross-section libraries have limited number of isotopes and temperature data, which is not sufficient to analyze the irradiated fuel such as DUPIC. Therefore new cross-section libraries were generated for the isotopes considered in the DUPIC fuel composition based on ENDF/B-VI. This section describes the procedure of generating MCNP cross-section library.

III.A Data Processing

All the application codes used for the reactor physics analysis including MCNP are not able to access the evaluated data files directly.[7] Therefore, the evaluated data should be processed into an appropriated data form such as an ACE format for MCNP code. There are several codes that convert the ENDF into libraries useful for the practical application calculations. For example, NJOY[8] nuclear data processing system is widely used to produce working libraries for the transport codes. The NJOY system consists of many independent modules such as RECONR, BROADR, UNRESR, HEATR, THERMR, GROUPR, ACER, etc. The data processing procedure is composed of the reconstruction of ENDF into the pointwise ENDF (PENDF), the production of the groupwise ENDF (GENDF) using the PENDF and the weighting spectrum, and the recompilation of PENDF and GENDF into an appropriate library format for the transport code. In this study, the up-to-date NJOY97.62 version is used and the library generation is performed on the HP9000 C180EG workstation under HP-UX 10.20 operating system.

III.B Temperature Data

The temperature-dependent neutron cross-section libraries have been generated for six data points: 293.16, 342.16, 561.16, 673.16, 960.16 and 1473.16K. Using the MAKXSF cross-section processor which is included in MCNP code package, the cross-section libraries are combined for the specified temperatures and named as 'en6t292', 'en6t342', 'en6t562', 'en6t672', 'en6t962', and 'en6t142'. The nuclide identification numbers (ZAID) are designated by ending with .21c, .22c, .23c, .24c, .25c, and .26c, respectively. The trailing "2" on the data library name generally indicates that the file is in a binary format. For the thermal scattering law data, MCNP cross-section library is not made for the specific temperature and, therefore, the two temperature data were generated using the nearest temperature data and interpolated to the specific temperature. The NJOY input parameter for the fractional tolerance is set to be 0.001, which results in a library of ~40 Mega-bites.

III.C Pseudo Fission Product Data

The isotopic composition of a CANDU fuel was generated by WIMS-AECL depletion calculation. In WIMS-AECL code, the fission products not included in the burnup chain are represented by a pseudo fission product (PFP). In order to keep the consistency in the isotopic composition, the PFP cross-section data for MCNP library was generated using the average fission product data of the RMCCS library. The PFP data of MCNP library was prepared such that the absorption cross-section is the same as that of the WIMS-AECL PFP. For the HELIOS code, the PFP cross-section was also added to the 190-group master library. Using the HEBE-1.5 code, the master library was converted to an 190-group working library which is used by HELIOS code directly. The consistency of the PFP cross-section data was assessed for MCNP, WIMS-AECL and HELIOS code using the fresh DUPIC fuel composition. The calculations have shown that the reactivity defects due to the PFP are 6.42 ± 0.58mk, 6.33mk and 6.25mk for MCNP, WIMS-AECL and HELIOS code, respectively.

III. BENCHMARK CALCULATION OF CANDU FUEL

The standard CANDU fuel bundle is loaded in a fuel channel (or pressure tube) and the calandria tube surrounds the pressure tube which physically separates the moderator from the coolant. The heavy water is used as both the coolant and moderator material. For the DUPIC fuel lattice, the configuration of the pressure and calandria tube is the same as that of the standard CANDU fuel lattice. However, the DUPIC fuel bundle utilizes the 43-element cluster geometry which has been developed for the advanced CANDU fuels. The fissile content of the reference DUPIC fuel is 1.0 wt% and 0.45 wt% for ^{235}U and ^{239}Pu, respectively. In addition, the center rod of the DUPIC fuel bundle contains natural dysprosium by 4.3 wt%. For both fuel types, the fuel gap was smeared into the clad material and the endcap was not considered.

IV.A Calculation Model

The fuel composition of the CANDU fuel was generated by WIMS-AECL depletion calculation and used for both MCNP and HELIOS. The WIMS-AECL lattice calculation was performed using the 89-group ENDF/B-V library. The HELIOS lattice calculations were performed using the 190-group library which contains the PFP information. For DUPIC fuel lattices, the 1/7 symmetry models was designed and the rotational boundary condition was applied to the circumference direction. For MCNP calculations, the new cross-section libraries of different temperatures were used. The MCNP calculations were done with 4,000 particles per cycle and 1,000 active cycles after 200 inactive cycles.

Under the normal operating condition, the temperatures of the fuel, clad, coolant and moderator are 960.16, 561.16, 561.16 and 342.16K, respectively. The Doppler constant was obtained by changing the fuel temperature from 293.16K to 960.16K such as;

$$\alpha_T(10^{-6}\Delta k/\mathrm{K}) = \frac{(k_{960} - k_{293})}{(960.16\,\mathrm{K} - 293.16\,\mathrm{K})} \times 10^6. \quad (1)$$

The coolant void coefficient was calculated by reducing the coolant density from the nominal value (0.807859 g/cc) to 0.0001 g/cc such as;

$$\alpha_V(mk) = 1000 \times \left[\frac{1}{k_{nominal}} - \frac{1}{k_0} \right]. \quad (2)$$

III.B Natural Uranium Fuel

The validation calculation of lattice codes for the CANDU fuel analysis was performed for the natural uranium first. The physics parameters used for the validation calculations are the burnup reactivity, coolant void reactivity and fuel temperature coefficient. The coolant void reactivity and the fuel temperature coefficient are calculated for 0, 3500 and 7200 MWd/t burnup state which represent the fresh, equilibrium and discharge condition, respectively.

The infinite multiplication factors (k_{∞}) of natural uranium fuel were calculated by the MCNP and compared with the results of WIMS-AECL and HELIOS calculations as given in Table 1 in which numbers in parentheses are the differece with MCNP calculation. Throughout the fuel burnup, the largest difference of k_{∞} is 4.59 and 3.31mk for WIMS-AECL and HELIOS, respectively. Compared with MCNP results, the errors of WIMS-AECL and HELIOS calculation increase as the fuel burns. The void coefficients of WIMS-AECL and HELIOS agree with those of MCNP within 0.95 and 0.93mk, respectively. The maximum difference of Doppler constants between MCNP and WIMS-AECL calculations is $-3.28 \times 10^{-6} \Delta k/\mathrm{K}$ for the fresh state, which is 3.31σ (about 99.9% confidence interval). Generally, the results of WIMS-AECL have shown

somewhat large discrepancies with those of HELIOS and MCNP when the fuel burnup is relatively large.

III.C DUPIC Fuel

The validation calculation of the DUPIC fuel was performed for the same physics parameters as were used for natural uranium fuel. However, because of higher fissile content of the DUPIC fuel, the burnup data used for the reactivity coefficient calculations are 0, 7400 and 14800 MWd/t which represent the fresh, equilibrium and discharge condition, respectively.

For the DUPIC fuel lattice, the k_∞'s are given Table 2. The differences of the k_∞ between the lattice code and MCNP are less than 7.58 and 2.44mk, for WIMS-AECL and HELIOS, respectively. Compared with MCNP results, the error of WIMS-AECL calculation increases as the fuel burns, which was found for the natural uranium case, too. For the difference of the void coefficient between WIMS-AECL and MCNP is within 1σ for all burnup steps. However, the results of HELIOS has shown somewhat large differences with the maximum error of -0.82mk. For Doppler constant, the maximum errors of WIMS-AECL and HELIOS predictions are 2.16×10^{-6} and $2.32\times 10^{-6}\Delta k/K$, respectively.

IV. CONCLUSION

The reactivity coefficients have been performed for the standard CANDU fuel and DUPIC fuel lattices using a Monte Carlo code MCNP-4B. The benchmark calculations of CANDU fuel lattices using new MCNP libraries have been shown that the void coefficient and Doppler constant by WIMS-AECL calculations are consistent with those of MCNP calculations. For the natural uranium fuel, the k_∞ prediction error of WIMS-AECL is reasonably small. However, for a high burnup fuel like DUPIC, the error is relatively large, which is mainly due to the difference of ENDF/B version. The k_∞ prediction of HELIOS has shown a relatively small error, and the void coefficient and Doppler constant are also consistent with those of MCNP calculations. In general, the results of benchmark calculations for the CANDU fuel lattice have shown that the adequacy of WIMS-AECL library needs to be assessed for the high burnup fuel and the use of HELIOS for CANDU fuel lattice analysis is reasonable.

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Table 1. Comparison of k_{∞} for Natural Uranium Fuel Lattice

Burnup (MWd/T)	Codes	k_{hot}	k_{void}	k_{cold}	$\Delta\rho_v$ (mk)	Doppler ($10^{-4}\ \Delta k/K$)
0	MCNP	1.11776 ±0.00047	1.13846 ±0.00047	1.12869 ±0.00046	16.27 ±0.59	-16.39 ±0.99
	WIMS	1.11678 (-0.00098)	1.13820 (-0.00026)	1.12990 (0.00121)	16.85 (0.58)	-19.67 (-3.28)
	HELIOS	1.11744 (-0.00032)	1.13763 (-0.00083)	1.12943 (0.00074)	15.88 (-0.38)	-17.98 (-1.59)
3980	MCNP	1.04389 ±0.00043	1.06062 ±0.00042	1.04744 ±0.00042	15.11 ±0.57	-5.32 ±0.90
	WIMS	1.04803 (0.00414)	1.06382 (0.00320)	1.05146 (0.00402)	14.16 (-0.95)	-5.14 (0.18)
	HELIOS	1.04709 (0.00320)	1.06161 (0.00099)	1.05067 (0.00323)	13.06 (-2.05)	-5.37 (-0.04)
7228	MCNP	0.98907 ±0.00037	1.00285 ±0.00039	0.98979 ±0.00038	13.89 ±0.54	-1.08 ±0.79
	WIMS	0.99331 (0.00424)	1.00744 (0.00459)	0.99318 (0.00339)	14.12 (0.23)	0.20 (1.27)
	HELIOS	0.99238 (0.00331)	1.00531 (0.00246)	0.99297 (0.00318)	12.96 (-0.93)	-0.89 (0.19)

Table 2. Comparison of k_{∞} for DUPIC Fuel Lattice

Burnup (MWd/T)	Codes	k_{hot}	k_{void}	k_{cold}	$\Delta\rho_v$ (mk)	Doppler ($10^{-4}\ \Delta k/K$)
0	MCNP	1.15099 ±0.00047	1.16371 ±0.00048	1.15865 ±0.00046	9.50 ±0.58	-11.48 ±0.99
	WIMS	1.15222 (0.00123)	1.16505 (0.00134)	1.15972 (0.00107)	9.56 (0.06)	-11.24 (0.24)
	HELIOS	1.14978 (-0.00121)	1.16232 (-0.00139)	1.15770 (-0.00095)	8.95 (-0.11)	-11.87 (-0.39)
7419	MCNP	1.03880 ±0.00041	1.05243 ±0.00041	1.04296 ±0.00040	12.47 ±0.55	-6.24 ±0.85
	WIMS	1.04397 (0.00517)	1.05727 (0.00484)	1.04779 (0.00483)	12.05 (-0.42)	-5.73 (0.51)
	HELIOS	1.03730 (-0.00150)	1.04999 (-0.00244)	1.04301 (0.00005)	11.65 (-0.82)	-8.56 (-2.32)
14825	MCNP	0.91889 ±0.00033	0.93074 ±0.00035	0.91980 ±0.00033	13.86 ±0.52	-1.36 ±0.70
	WIMS	0.92617 (0.00728)	0.93832 (0.00758)	0.92564 (0.00584)	13.98 (0.13)	0.80 (2.16)
	HELIOS	0.91727 (-0.00162)	0.92857 (-0.00217)	0.91932 (-0.00048)	13.27 (-0.59)	-3.07 (-1.71)