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One of the longstanding obstacles to the use of the MCNP Monte Carlo code[1] for reactor-physics calculations has been its requirement for nuclear data libraries at the temperature associated with the application of interest. Recently, however, an auxiliary code, named "doppler," has been developed that uses an existing nuclear data library as the basis for generating a new library at the desired temperature. doppler has simple input and is straightforward to use. Libraries generated with doppler and based on the existing ENDF66 library[2] have been developed for three hot Kritz benchmarks.[3,4] Results obtained from MCNP5 for those hot benchmarks and their cold (i.e., room-temperature) counterparts are presented herein.

For continuous-energy cross sections, doppler starts with library data for a temperature below the desired temperature, and it broadens the resonance cross sections up to the desired temperature using a kernel broadening method identical to the one used in the NJOY[5] processing that created the original data library. For thermal $S(\alpha,\beta)$ tables, doppler works with two sets from the data library with temperatures that bracket the desired temperature, and it interpolates for the new cross sections and (E',μ) emission events. If probability tables for the unresolved resonance range are present, doppler also interpolates for new probability tables at the desired temperature using library data for temperatures above and below the desired value. The new customized data sets are written in the user's working directory, and a modified xsdir file is also created there. The user then can specify new materials, old materials, or a combination of them to be used in subsequent MCNP calculations.

Description of Benchmarks

The benchmarks selected for this study are those from the Kritz-2 series that are documented in Ref. 3: Kritz-2:1, Kritz-2:13, and Kritz-2:19. All three configurations consisted of rectangular lattices of fuel rods immersed in water inside a cylindrical pressure tank, and all three had both cold and hot cases. Kritz-2:1 and Kritz-2:13 employed low-enriched UO_2 fuel, while Kritz-2:19 used mixed-oxide (MOX) fuel. Criticality was achieved by adjusting the height of the water. The temperatures of the hot cases ranged from 235.9 °C to 248.5 °C, and they were pressurized so that the water remained liquid. The lattices were not placed in the center of the pressure tank but instead were placed near its wall. Consequently, the moderator region between the edge of the lattice and the wall of the tank is considerably thinner on the south and west sides of the lattice than on the north and east sides.

Kritz-2:1 contained a 44x44 array of fuel pins enriched to 1.86 wt.% and clad in Zircaloy-2. At room temperature, the radius of the fuel pellets was 0.529 cm, the outer radius of the cladding was 0.6125 cm, and the lattice pitch was 1.485 cm. At cold conditions (19.7 °C), the water contained 217.9 ppm of boron, and the critical axial buckling was 1.475×10^{-3} cm^{-2}. At hot conditions (248.5 °C), the water contained 26.2 ppm of boron, and the critical axial buckling was 6.25×10^{-4} cm^{-2}.

Kritz-2:13 contained a 40x40 array of the same fuel pins as Kritz-2:1. However, the lattice pitch (at room temperature) was increased to 1.635 cm. At cold conditions (22.1 °C), the water contained 451.9 ppm of boron, and the critical axial buckling was 8.01×10^{-4} cm^{-2}. At hot conditions (243.0 °C), the water contained 280.1 ppm of boron, and the critical axial buckling was 5.98×10^{-4} cm^{-2}.

Kritz-2:19 contained a 25x24 array of MOX fuel pins with 1.50 wt.% PuO_2. The remainder of the fuel was depleted UO_2, with 0.16 wt.% ^{235}U. The fuel pins were clad in Zircaloy-2. At room temperature, the radius of the fuel pellets was 0.4725 cm, the outer radius of the cladding was 0.5395 cm, and the lattice pitch was 1.80 cm. At cold conditions (21.1 °C), the water contained 4.8 ppm of boron, and the critical axial buckling was 1.637×10^{-3} cm^{-2}. At hot conditions (235.9 °C), the water contained 5.2 ppm of boron, and the critical axial buckling was 7.15×10^{-4} cm^{-2}.

Analysis and Results

Two sets of continuous-energy nuclear data libraries were generated using doppler. The libraries for the hot UO_2 cases were generated at 245 °C, while the libraries for the hot MOX case were generated at 235 °C. Both sets of libraries were generated using the existing ENDF66 libraries as a starting point.

MCNP5 calculations were performed for the six benchmarks. ENDF66 libraries were used for the cold cases, and the temperature-specific libraries were used for hot cases. All cases were run with 250 generations of 5,000 neutron histories each. The first 50 generations were discarded from the statistics so that the results for each case are based on 1,000,000 active neutron histories. The models are essentially two-dimensional, because they are axially uniform with heights that correspond to the critical axial buckling.

Results from the six calculations are presented in Table 1, along with the benchmark values and values obtained previously[6] with the HELIOS collision-probability code.[7] The HELIOS results are based on nuclear data from ENDF/B-VI release 3 (ENDF/B-VI.3), while the ENDF66 library is based on ENDF/B-VI.6. The changes made between the two releases should have little impact on the results for these benchmarks.[8] However, the resonance integral for ^{238}U in the HELIOS library was reduced slightly from the ENDF/B-VI.3 value, and this reduction has been shown to increase reactivity by approximately 0.003 Δk for low-enriched uranium lattices at room temperature.[9] When allowance is made for this difference, the MCNP5 results are in good agreement with the HELIOS results for all six benchmarks.

Table 1. Comparison of Results for Kritz-2 Benchmarks.

Core	Temperature (°C)	k_{eff}		
		Benchmark	ORNL Helios (ENDF/B-VI.3)	LANL MCNP5 (ENDF/B-VI.6)
Kritz-2:1	19.7	1.0000 ± 0.0008	1.0000	0.9976 ± 0.0007
	248.5	1.0000 ± 0.0008	0.9971	0.9913 ± 0.0007
Kritz-2:13	22.1	1.0000 ± 0.0008	1.0012	0.9982 ± 0.0007
	243.0	1.0000 ± 0.0008	0.9995	0.9931 ± 0.0007
Kritz-2:19	21.1	1.0000 ± 0.0008	1.0013	1.0016 ± 0.0007
	235.9	1.0000 ± 0.0008	1.0003	1.0028 ± 0.0007

Pinwise fission rates also have been computed and compared with measured results. The RMS difference between the calculated means and the corresponding measured values is 2% - 3%, which is comparable to the statistical uncertainty associated with the calculated values.

Conclusions

The doppler code has been developed to produce temperature-specific continuous-energy nuclear data libraries for MCNP. Its input structure is simple, and it is straightforward to use. In this study, it has been employed to generate temperature-specific libraries for hot UO_2 and MOX benchmarks. MCNP5 results using those libraries are in good agreement with results from the HELIOS code after allowance has been made for library differences.

Acknowledgment

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