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Preliminary assessment of Geant4 HP models and cross section libraries by reactor criticality benchmark calculations

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Geant4 [1] is an open source general purpose simulation toolkit for particle transportation in matter. Since the extension of the thermal scattering model in Geant4.9.5 and the availability of the IAEA HP model cross section libraries, it is now possible to extend the application area of Geant4 to reactor modelling. Before version 9.5, Geant4 HP thermal scattering model (i.e. the $S(\alpha, \beta)$ model) supports only three bounded isotopes, namely, H in water and polyethylene, and C in graphite. Newly supported materials include D in heavy water, O and Be in beryllium oxide, H and Zr in zirconium hydride, U and O in uranium dioxide, Al metal, Be metal, and Fe metal. The native HP cross section library G4NDL does not include data for elements with atomic number larger than 92. Therefore, transuranic elements, which have impacts for a realistic reactor, can not be simulated by the combination of the HP models and the G4NDL library. However, cross sections of those missing isotopes were made available recently through the IAEA project "new evaluated neutron cross section libraries for Geant4" [2].

In this work, we assessed the performance of the combination of HP models and the IAEA new HP model libraries by reactor criticality calculation. The Gean4 thermal scattering model was enabled in all cases.

The power iteration method has been used in this work. A K_{eff} estimator similar to the collision estimator in MCNP has been implemented in Geant4.9.5.p02. In the simulations, fission reactions were treated as capture reaction. Secondary neutrons from fission reactions were removed from current simulation cycle. But their histories (i.e. position, direction and energy) were recorded to be used as the primary source particles in the next cycle. At the beginning of a new cycle, a constant number of neutrons were initialised by randomly sampling the histories in the last cycle. A number of inactive calculation cycles were performed until the K_{eff} and fission distribution were converged. K_{eff} were accumulated in the following active simulation cycles. Calculation will

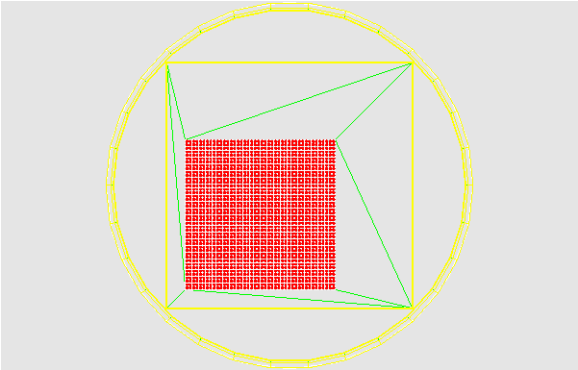

Figure 1: Geant4 simulated core specified in LEU-COMP-THERM-001 case KRITZ 2:1 at 248.5 °C

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Table I: Comparisons of benchmark-model and calculated K_{eff}

benchmark ID	case	benchmark model		Geant4 calculated K_{eff}		
		K_{eff}	uncertainty	ENDF/VII.0	JEFF-3.1	JENDL-4.0
HEU-MET-T-FAST-069	1	0.9994	0.0004	0.99916		
HEU-MET-FAST-059 case 1	2	0.9929	0.0028	0.99221		
HEU-MET-FAST-059 case 2	3	0.9952	0.0016	0.99624		
LEU-MET-THERM-006 case 20	4	1.0000	0.0018	1.00016	0.99983	0.99999
LEU-MET-THERM-006 case 24	5	1.0000	0.0018	1.00162	1.00123	1.00109
LEU-MET-THERM-006 case 28	6	1.0000	0.0018	1.00356	1.00448	1.00318
LEU-COMP-THERM-001 KRITZ 2:1 19.7C	7	1.0000	0.0008	1.00051	0.99984	0.99864
LEU-COMP-THERM-001 KRITZ 2:1 248.5C	8	1.0000	0.0008	0.96417		
LEU-COMP-THERM-007 Case 1	9	1.0000	0.00144	1.00520		
LEU-COMP-THERM-007 Case 2	10	1.0000	0.00081	1.00739		
LEU-COMP-THERM-007 Case 3	11	1.0000	0.00072	1.00638		

stop when the statistical error is lower than a satisfied level. Inactive and active cycles are 200 and 800 in this work, respectively. 10,000 neutrons are simulated in each cycle. The 1 σ uncertainties in all calculations are 0.035% (i.e. 35pcm).

A total of 11 benchmark cases have been selected to calculate from the International Criticality Safety Benchmark Evaluation Project (ICSBEP) handbook. Simulated cases include high enriched U metal fast neutron benchmark (HEU-MET-FAST-059 and HEU-MET-FAST-059), low enriched U metal thermal neutron benchmark (LEU-MET-THERM-006), low enriched UO2 thermal neutron benchmark (LEU-COMP-THERM-007), and low enriched UO2 thermal neutron high temperature benchmark (LEU-COMP-THERM-001).

Calculated K_{eff} for case 1 to case 7 closely agree with benchmark K_{eff}. Different libraries used in case 4 to 6 showed very good consistency. However, Geant4 overestimated the K_{eff} in case 9 to case 11 up to 739pcm; and significantly underestimated the K_{eff} in case 8 by about 3.6%.

Indicated by Mendoza et. al. [2], Geant4 thermal scattering model can behave differently than the $S(\alpha, \beta)$ model in MCNPX. We are now comparing these two models, and investigating if it is necessary to implement a new thermal scattering physics model based on ACE format files (http://www-nds.iaea.org/indltsl/) which is the standard cross section library format in MCNPX. Treatment of cross section Doppler effect in Geant4 will also be examined in the near future. More results will be presented in the conference.

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