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Abstract

KENO V.a and KENO-VI are Monte Carlo codes that solve the multigroup form of the Boltzmann transport equation. These codes are part of the SCALE system of codes and are used for performing criticality calculations of systems with fissionable material. In general, continuous-energy Monte Carlo methods are preferred because such an approach avoids many of the assumptions inherent in the multigroup treatment. On the other hand, continuous-energy treatment is much more demanding in terms of computer storage space for data, memory requirements, and calculation speed. Continuous-energy versions of KENO V.a and KENO-VI have been created and are being extensively tested. Generation of ENDF/B-VI continuous-energy cross sections is explained, and the results of the validation and verification of the codes and the data are presented.

Introduction

SCALE[1] (Standardized Computer Analyses for Licensing Evaluation) is a computer code system that is widely used and accepted around the world for criticality safety analyses. It is a modular code system that utilizes individual programs for performing one or more of the required calculations for a desired analysis result. The Monte Carlo codes KENO V.a and KENO-VI are used to calculate the multiplication factor of fissile systems, as well as the flux distributions throughout the system. KENO V.a and KENO-VI differ in their treatment of the geometric modeling of the problem; KENO-VI is not the next version of KENO V.a., but rather incorporates more general geometric modeling capabilities. As such, both codes are maintained and improved continuously. KENO V.a contains simpler geometric modeling capabilities and therefore runs much faster, while still allowing complex geometries to be modeled using simple geometric shapes. KENO-VI allows more complex geometric modeling and runs longer than KENO V.a. Current versions of both codes employ a multigroup scheme to treat the energy dependence of the transport equation; but recently, much effort has been devoted to add a continuous-energy scheme to treat the energy dependence of the transport equation in these codes.

Cross-Section Processing for Continuous-Energy KENO

A cross-section processing system is used to process ENDF (Evaluated Nuclear Data File) data and generate nuclear data libraries that can be accessed by radiation transport codes. At Oak Ridge National Laboratory (ORNL), the AMPX[2] code system has been used since the early 1970s to process the full range of ENDF/B formats used to describe the physics associated with neutron, gamma, and coupled neutron-gamma interactions up to 20 MeV. To facilitate the development of an independent transport capability, a new continuous-energy cross-section library structure has been designed for KENO, and multiple AMPX processing modules have been developed to generate cross-section data in the new pointwise format. All new AMPX modules have been written in accordance with the free-form FORTRAN 90/95 standard. The details of the continuous-energy library format are beyond the scope of this paper. However, the essential components of a KENO cross-section library include the following: (1) average number of neutrons (delayed and prompt) produced by fission, $\bar{\nu}(E)$; (2) one-dimensional (1-D) continuous-energy cross sections as a function of temperature, $\sigma(E, T)$; (3) two-dimensional (2-D) pointwise joint probability distributions that describe the energy and angle of particles emerging from a collision, $f(E \rightarrow E', \mu)$; and (4) probability tables for sampling the cross sections in the unresolved-resonance region. The

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following discussion provides an overview of the cross-section processing development effort that was performed to support the development of the continuous-energy capability in KENO.

For the KENO CE development, existing AMPX modules were used to process the ENDF/B collision kinematics data and generate energy and angle distributions for secondary particles in a general pointwise format. AMPX is used to process S(α, β) data for thermal moderators for elastic and inelastic scattering (n,2n), etc., and free-gas S(α, β) data for materials not having thermal scattering law data. The free-gas S(α, β) data are also postprocessed to generate pointwise kinematics distributions that can be used in a variety of transport applications. As for the 1-D continuous-energy cross sections, the AMPX-generated pointwise kinematics data can be post-processed for a specific transport application. In particular, the kinematics data have been successfully postprocessed with additional AMPX modules to generate multigroup transfer matrices for group-dependent cross-section libraries that can be used by various multigroup transport codes (e.g., XSDRNPM, KENO V.a, KENO-VI, etc.).

Additional AMPX modules were developed to postprocess the pointwise collision kinematics data and generate continuous-energy joint (i.e., coupled in energy and angle) probability density functions (PDFs) and cumulative distribution functions (CDFs). In AMPX, all of the pointwise kinematics data are exported in the lab system frame of reference, and the joint PDFs and CDFs that are generated for KENO CE are also in the lab system. By adhering to the lab coordinate system, KENO CE does not have to transform between different coordinate systems during the random walk; however, the energy and angle distributions for elastic and discrete-level inelastic scattering become more complex in the lab system. For example, an angular distribution that is isotropic in the center-of-mass system is anisotropic in the lab system. In addition, the secondary energy distribution as a function of exit angle cosine in the lab system can be double-valued (i.e., two possible exit energies with respect to a single angle cosine) for certain incident energies above threshold for discrete inelastic-level reactions. Likewise, a similar double-valued distribution is observed for elastic scattering with hydrogen in the lab system if the actual mass ratio is used (i.e., A = 0.99917 as opposed to A = 1.0). In the generation of joint PDFs and CDFs for KENO CE, special attention is exercised in the construction of the secondary angle and energy distributions in the lab system. The KENO CE cross-section format provides the flexibility to represent secondary angle and energy distributions with either equal probable or nonequal probable bins.

Changes in the KENO Codes

In an effort to allow SCALE users to easily run their existing KENO cases, changes to the input structure have been minimized. The SCALE user simply has to specify the continuous-energy cross-section library in the library input record to execute the continuous-energy versions of KENO V.a and KENO-VI using CSAS (Criticality Safety Analysis Sequence). To allow users the flexibility of using various evaluations as opposed to the default cross sections, additional keywords have been implemented into the SCALE Material Information Processor.[1] In addition, a new parameter has been added to the KENO parameter data to allow binning of integral values such as fluxes and absorptions in one of the existing SCALE multigroup cross-section-library energy group structures or in a user-specified energy-group structure.

Calculations and Results

ENDF/B-VI.7 data for 320 nuclides and isotopes have recently been processed through AMPX to generate continuous-energy cross-section data. Continuous-energy versions of KENO and these newly generated data have been and are continuing to be tested using various problem sets, including sample problems from SCALE and critical benchmark cases. The results for the SCALE sample problems using earlier versions of these codes and data were published previously.[3] The most recent results from the latest versions of the KENO codes using the latest continuous-energy cross sections are listed in Table 1. For comparison purposes, the results of multigroup KENO V.a and continuous-energy Monte Carlo Neutron Particle (MCNP)[4] calculations are also listed in Table 1. In all calculations, the standard deviations are less than 0.003. In all ten cases, the KENO V.a and KENO-VI codes with continuous-energy cross sections yield very similar answers to the multigroup KENO V.a and continuous-energy MCNP codes, indicating that the results from all calculations are in very good agreement.

Table 1. SCALE sample problems

Sample problem	Description	KENO V.a multigroup	KENO V.a continuous energy	KENO-VI continuous energy	MCNP continuous energy
1	Case 2c8 bare	0.9940	0.9934	0.9927	0.9957
3	2c8 15.24 cm paraffin refl	0.9914	0.9935	0.9949	0.9975
6	One 2c8 unit (single unit)	0.7409	0.7411	0.7423	0.7447
9	Infinite array of 2c8 units	2.2586	2.2589	2.2588	2.2643
12	4 aqueous 4 metal arrays	0.9951	0.9976	0.9948	0.9995
13	Two cuboids in a cyl. annulus	0.9883	0.9922	0.9916	0.9929
14	U metal cylinder in annulus	0.9922	0.9963	0.9918	0.9943
15	Small water reflected sphere on Plexiglas collar	0.9983	0.9973	0.9954	0.9991
20	Triangular pitched array	0.9998	0.9919	0.9911	0.9933
21	Partially filled sphere	0.9951	0.9933	0.9943	0.9926

Although code-to-code comparisons are very valuable in providing a basis for verification, they cannot replace actual code validation against experimental benchmarks. As such, the KENO V.a and KENO-VI codes have been used to model and calculate the multiplication factors for more than 300 experimental benchmarks from the *International Handbook of Evaluated Criticality Safety Benchmark Experiments*.[5] Select benchmark k_{eff} values, as well as the calculated k_{eff} values from the multigroup and continuous-energy KENO codes and the continuous-energy MCNP code, are listed in Table 2. In Table 2, SCALE 5.1 results are obtained using the multigroup cross sections that are based on the ENDF/B-VI Rel.7 evaluations, whereas SCALE 6 (pre-release) results are obtained using the continuous-energy cross sections from the same evaluations. The results from MCNP are provided using the continuous-energy cross sections based on the ENDF/B-VI Rel. 8 (Ref. 6) and ENDF/B-VII (beta 3). To demonstrate the differences between the calculated values and the benchmark values, the percent differences are plotted in Fig. 1. Analysis of the trends in Fig. 1 shows that all codes calculate very similar k_{eff} values and demonstrate similar trends.

Table 2. Comparison against benchmark values

Benchmark	Benchmark	SCALE 5.1	% diff	SCALE 6 (CE)	% diff	MCNP	% diff
Name	k_{eff}	ENDF/B-VI		ENDF/B-VI		ENDF/B-VI.8	
HST-001.1	1.0004	0.9986	-0.18%	0.9969	-0.35%	0.9994	-0.10%
HST-001.2	1.0021	0.9963	-0.58%	0.9940	-0.81%	0.9963	-0.58%
HST-001.3	1.0003	1.0012	0.09%	1.0004	0.01%	1.0026	0.23%
HST-001.4	1.0008	0.9991	-0.17%	0.9955	-0.53%	0.9986	-0.22%
HST-001.5	1.0001	1.0000	-0.01%	0.9982	-0.19%	1.0005	0.04%
HST-001.6	1.0002	1.0035	0.33%	1.0022	0.20%	1.0035	0.33%
HST-001.7	1.0008	0.9984	-0.24%	0.9966	-0.42%	0.9987	-0.21%
HST-001.8	0.9998	0.9996	-0.02%	0.9967	-0.31%	0.9988	-0.10%
HST-001.9	1.0008	0.9952	-0.56%	0.9919	-0.89%	0.9939	-0.69%
HST-001.10	0.9993	0.9942	-0.52%	0.9924	-0.69%	0.9942	-0.51%
HST-009.1	0.9990	1.0004	0.14%	0.9978	-0.12%	0.9993	0.03%
HST-009.2	1.0000	1.0009	0.09%	0.9986	-0.14%	1.0002	0.02%
HST-009.3	1.0000	1.0004	0.04%	0.9987	-0.13%	0.9998	-0.02%
HST-009.4	0.9986	0.9958	-0.28%	0.9932	-0.54%	0.9950	-0.36%
HST-010.1	1.0000	1.0012	0.12%	0.9997	-0.03%	1.0009	0.09%
HST-011.1	1.0000	1.0055	0.55%	1.0041	0.41%	1.0050	0.50%
HST-011.2	1.0000	1.0017	0.17%	1.0001	0.01%	1.0012	0.12%
HST-012	0.9999	1.0015	0.16%	1.0007	0.08%	1.0015	0.16%
HST-013.1	1.0012	0.9991	-0.21%	0.9982	-0.30%	0.9994	-0.18%
HST-032	1.0015	0.9965	-0.50%	0.9999	-0.16%	0.9989	-0.26%
HST-042.1	0.9957	0.9969	0.12%	0.9961	0.04%	0.9969	0.12%
HST-042.2	0.9965	0.9969	0.04%	0.9961	-0.04%	0.9966	0.01%
HST-042.3	0.9994	0.9969	-0.25%	0.9961	-0.33%	1.0003	0.09%
HST-042.4	1.0000	1.0020	0.20%	1.0007	0.07%	1.0017	0.17%
HST-042.5	1.0000	0.9990	-0.10%	0.9985	-0.15%	0.9992	-0.08%
HST-042.6	1.0000	0.9998	-0.02%	0.9987	-0.13%	0.9998	-0.02%
HST-042.7	1.0000	1.0005	0.05%	1.0001	0.01%	1.0005	0.05%
HST-042.8	1.0000	1.0011	0.11%	1.0002	0.02%	1.0011	0.11%
HST-043.1	0.9986	0.9963	-0.23%	0.9941	-0.46%	0.9959	-0.27%
HST-043.2	0.9995	1.0068	0.73%	1.0051	0.56%	1.0064	0.69%
HST-043.3	0.9990	1.0019	0.29%	1.0010	0.20%	1.0018	0.28%

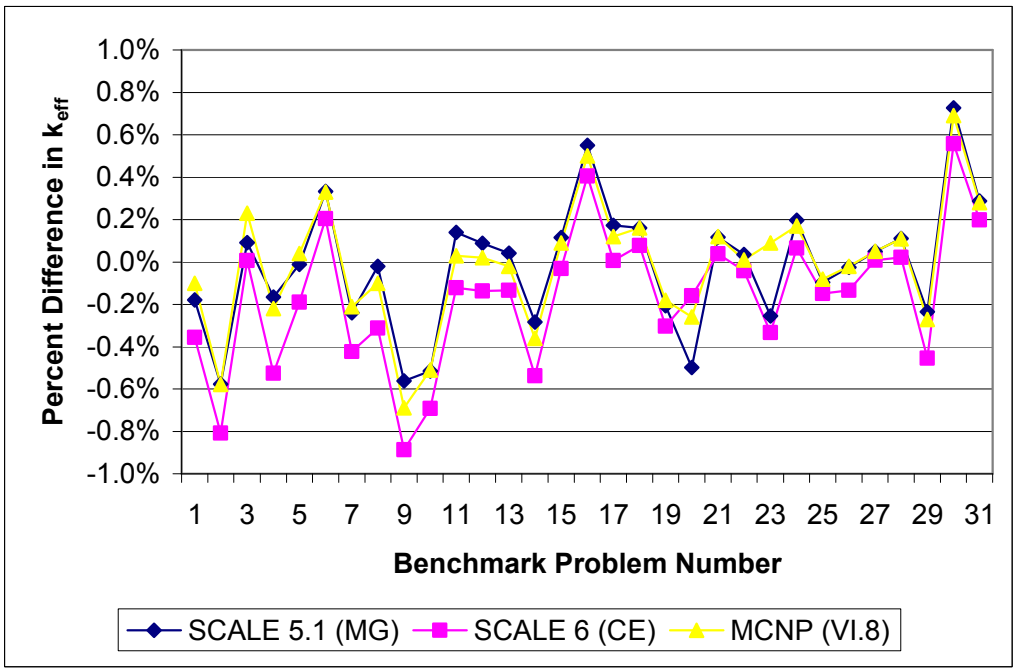

Figure 1. Percent differences in calculated k_{eff} values against benchmark values

Conclusions

Analysis of the results from the latest versions of the continuous-energy KENO V.a and KENO-VI using the latest AMPX-generated cross sections indicates that the new versions of the continuous-energy codes and data calculate the expected multiplication factors accurately. KENO V.a and KENO-VI with continuous-energy capability will be available as part of SCALE 6.

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