Paper — Abstract No.: 21; Topic No.: 5 (Oral Presentation)
July 11, 2003

Nuclear Science and Technology Division (94)

Continuous-energy Version of KENO V.a for Criticality Safety Applications

Michael E. DUNN,* N. Maurice GREENE and Lester M. PETRIE

*Oak Ridge National Laboratory,** P.O. Box 2008, Oak Ridge, Tennessee 37831-6370, USA*
(865) 574-5260, dunnme@ornl.gov

Submitted to
The 7th International Conference on Nuclear Criticality Safety (ICNC2003),
October 20–24, 2003,
Tokai Research Establishment
Japan Atomic Energy Research Institute,
Tokai-mura, Japan

Organized and sponsored by
Japan Atomic Energy Research Institute,
Atomic Energy Society of Japan

Co-sponsored by
Japan Nuclear Cycle Development Institute

In Cooperation with
Japan Atomic Industrial Forum, Inc.,
The Federation of Electric Power Companies,
Central Research Institute of Electric Power Industry,
Nuclear Power Engineering Cooperation,
OECD/Nuclear Energy Agency

http://nucefwww.tokai.jaeri.go.jp.icnc2003/

*Corresponding author, Tel.+1-865-574-5260, Fax +1-865-574-3527, E-mail: dunnme@ornl.gov

**Managed by UT-Battelle, LLC, for the U.S. Department of Energy under contract No. DE-AC05-00OR22725.

Continuous-energy Version of KENO V.a for Criticality Safety Applications

Michael E. DUNN,* N. Maurice GREENE and Lester M. PETRIE
*Oak Ridge National Laboratory,** P.O. Box 2008, Oak Ridge, Tennessee 37831-6370, USA*

KENO V.a is a multigroup Monte Carlo code that solves the Boltzmann transport equation and is used extensively in the criticality safety community to calculate the effective multiplication factor of systems with fissionable material. In this work, a continuous-energy or pointwise version of KENO V.a has been developed by first designing a new continuous-energy cross-section format and then by developing the appropriate Monte Carlo transport procedures to sample the new cross-section format. In order to generate pointwise cross sections for a test library, a series of cross-section processing modules were developed and used to process 50 ENDF/B-6 Release 7 nuclides for the test library. Once the cross-section processing procedures were in place, a continuous-energy version of KENO V.a was developed and tested by calculating 21 critical benchmark experiments. The point KENO–calculated results for the 21 benchmarks are in agreement with calculated results obtained with the multigroup version of KENO V.a using the 238-group ENDF/B-5 and 199-group ENDF/B-6 Release 3 libraries. Based on the calculated results with the prototypic cross-section library, a continuous-energy version of the KENO V.a code has been successfully developed and demonstrated for modeling systems with fissionable material.

KEYWORDS: Monte Carlo, continuous energy, KENO V.a

1. Introduction

Monte Carlo (MC) methods are used extensively to model complex nuclear systems because such methods have the capability to solve the integral form of the Boltzmann transport equation with little or no approximations. Typically, MC methods are classified according to whether a continuous-energy or multigroup representation of the cross-section data is used to solve the transport equation. In general, continuous-energy or pointwise methods are preferred because the continuous-energy treatment avoids many of the assumptions and approximations inherent in multigroup methods. KENO V.a[1)] is a multigroup MC code that is used throughout the world to analyze fissionable systems for criticality safety applications. The KENO series of codes is developed and maintained at the Oak Ridge National Laboratory (ORNL) as part of the SCALE[1)] (Standardized Computer Analyses for Licensing Evaluation) system. The objective of this work is to develop and test a new version of KENO V.a that utilizes pointwise cross sections to model the radiation transport.

Previous work[2)] has focused on the development of a prototypic version of KENO V.a that performs the random walk using continuous-energy MCNP[3)] cross sections. Although the previous work successfully demonstrated the use of MCNP cross sections with the KENO V.a transport package, the prototypic KENO V.a is not available for widespread distribution and is limited to ENDF (Evaluated Nuclear Data File) data prior to Version 6.[4)] Because the format and structure of the MCNP cross-section data inherently dictate the transport procedures used in the random walk, the previously developed continuous-energy KENO V.a is not completely independent from the MCNP transport procedures. For criticality safety applications that do not have applicable benchmarks experiments, completely independent calculational methods are essential for establishing and verifying subcritical limits. By using MCNP cross-section data, the previously developed pointwise version of KENO V.a could not provide an independent verification of systems having fissionable material. As a result, this work has focused on the development of a production-level continuous-energy version of KENO V.a that is completely independent of other pointwise MC codes (e.g., COG, MCNP, MONK, RACER, TART, VIM, etc.). The research initially focused on the design and development of a continuous-energy cross-section format for KENO that necessitated the development of new continuous-energy cross-section processing modules. The second phase of the research focused on the development of a pointwise version of KENO V.a

*Corresponding author, Tel.+1-865-574-5260, Fax +1-865-574-3527, E-mail: dunnme@ornl.gov

**Managed by UT-Battelle, LLC, for the U.S. Department of Energy under contract No. DE-AC05-00OR22725.

that uses the continuous-energy data to perform the radiation transport.

2. Cross-Section Processing Development

The nuclear data within the ENDF system are voluminous in nature and cannot be used directly in radiation transport codes. As a result, a cross-section processing system must be used to process the ENDF data and generate nuclear data libraries that can be accessed by radiation transport codes. At ORNL, the AMPX[5] 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. In order to facilitate the development of independent transport procedures, 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 of the new AMPX modules and point KENO V.a 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 point KENO cross-section library include the following: (1) average number of neutrons (delayed and prompt) produced by fission, $\bar{\nu}(E)$; (2) 1-dimensional (1-D) continuous-energy cross sections as a function of temperature, $\sigma(E, T)$; (3) 2-D pointwise joint probability distributions that describe the energy and angle of particles emerging from a collision, $f(E \rightarrow E', \mu)$; (4) probability tables for sampling the cross sections in the unresolved-resonance region. The following discussion provides an overview of the cross-section processing development effort that was performed to support the development of a continuous-energy version of KENO V.a.

Although the current point KENO development represents a complete redesign from the "ground up" (i.e., redesigning the base cross-section format and associated transport procedures), a significant amount of cross-section processing work had already been completed prior to the development of point KENO. Beginning in the mid 1990s, the AMPX code system was completely redesigned to process the latest ENDF/B formats through Version 6.[5] The latest version of the cross-section processing system (AMPX-2000) can be used to generate a variety of multigroup and/or continuous-energy cross-section libraries. The preceding and concurrent AMPX-2000 development effort has provided the foundation for a significant portion of the continuous-energy KENO development. As a result, the point KENO cross-section development did not have to begin with the base ENDF/B data formats. A majority of the cross-section processing work for point KENO involved the development of new modules to post-process data from existing AMPX modules to generate MC data libraries.

Because AMPX-2000 is extremely modular in construction (i.e., more than 80 distinct processing modules), cross-section processing sequences can be tailored for a specific application. Moreover, if cross-section data have already been processed from ENDF/B files for a specific application, an AMPX sequence can be developed to post-process the existing data for another application. As a result, the ENDF/B files do not have to be accessed multiple times to generate cross-section libraries for different radiation transport codes. As an example, one of the newest additions to SCALE is a continuous-energy 1-D discrete ordinates capability (CENTRM) that is used to calculate pointwise neutron spectra for generating problem-dependent resonance self-shielded multigroup cross sections.[6, 7] Prior to the Point KENO development, AMPX-2000 was used to generate prototypic 1-D temperature-dependent continuous-energy cross-section data [i.e., $\sigma(E, T)$] for CENTRM using ENDF/B-5 and ENDF/B-6 Release 7 evaluations. After the point KENO library format was defined, additional AMPX processing modules were developed and tested for post-processing the 1-D temperature-dependent data that served as the foundation for the prototypic CENTRM cross-section libraries. Note that point KENO data are not generated directly from CENTRM data; rather, the temperature-dependent data used to generate CENTRM cross sections can be stored in a general format and post-processed for a specific transport code.

In addition to the 1-D cross-section processing capabilities, one of the novel and robust features of the latest AMPX system is the treatment of the collision kinematics that provide secondary energy and angle distributions for particles emerging from a reaction of interest. In AMPX, a uniform kinematics structure (i.e., data have the same structure independent of reaction type) has been developed to describe all possible secondary energy-angle distributions including thermal scattering collisions. Because of the uniformity in the collision kinematics data, pointwise cross-section libraries can be produced that are independent of ENDF laws and procedures. Some continuous-energy radiation transport codes have the ENDF laws and procedures programmed in the code. Unfortunately, as changes are made to the ENDF formats, the radiation transport code and associated cross-section processing code system must be updated to process the new ENDF laws and procedures. Because of the novel AMPX processing procedures, the burden of treating the ENDF formats in the transport code has been transferred solely to the cross-section generation code.

For the point KENO 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(", $) data for thermal moderators in addition to secondary energy and angle distributions for particles emerging from collisions [e.g., elastic scattering, (n,2n), (n,3n), etc.]. In addition, AMPX can be used to generate free-gas S(", $) data for materials not having thermal scattering law data. The free-gas S(", $) data are also post-processed 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 post-processed 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.).

For the current work, additional AMPX modules were developed to post-process 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 point KENO are also in the lab system. By adhering to the lab coordinate system, point KENO 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 point KENO, special attention is exercised in the construction of the secondary angle and energy distributions in the lab system. The point KENO cross-section format provides the flexibility to represent secondary angle and energy distributions with either equal probable or nonequal probable bins.

For resonance isotopes in a neutron cross-section evaluation, the unresolved-resonance region is an energy region in which the experimental resolution is inadequate for determining the resonance parameters of individual resonances. As a result, energy-averaged unresolved-resonance parameters are typically provided for the unresolved region. Because of the statistical nature of the unresolved parameters, probability tables can be used to provide cross-section probability distribution functions for energy ranges at specific temperatures within the unresolved region. Prior to the point KENO development, a new AMPX-2000 module was developed to generate probability tables for the unresolved region using an MC approach.[8] As opposed to using the conventional "ladder" approach,[9] AMPX uses MC procedures to sample pairs of resonances for each spin sequence around the reference energy provided in the ENDF/B evaluation. The resonance spacings are sampled from a Wigner spacing distribution, and the parameters for each resonance are sampled from a Chi-square distribution. In addition, the Dyson and Mehta Δ_3-statistics test[10, 11] is used to determine the number of resonances to sample in the probability table calculation. Using the sampled resonance parameters, the total, capture, fission, and elastic scattering cross sections are calculated at the reference energy using the single-level Breit-Wigner formalism[4] with appropriate treatment for temperature effects. Cross-section probability tables are generated based on the different MC estimates of the total and corresponding partial reactions.

As indicated above, different AMPX modules are used to generate each component of a point KENO library for a specific nuclide, and a subsequent module was developed to combine the different components to create a point KENO cross-section file for each nuclide.

3. Radiation Transport Development

KENO V.a has been used extensively in the nuclear community to model fissionable systems for various criticality safety applications. In an effort to allow experienced KENO users to easily convert existing KENO input files to the new point KENO input format, one of the design objectives for the new code is to minimize the number of changes to the user interface. From a user interface perspective, the changes are essentially transparent, except for the material format specifications used in a problem. This phase of the research focused on the development of a stand-alone pointwise version of KENO V.a. Future work will focus on the development of a new CSAS (Criticality Safety Analysis Sequence) module for SCALE that integrates the material information processing capabilities that are available in SCALE with the material specification requirements of the pointwise version of KENO V.a.

To utilize continuous-energy cross sections, modifications were made to the input processing routines in KENO V.a. Several new subroutines were developed to read and process the new pointwise cross-section library structure that is discussed in the previous section. In the stand-alone version of KENO V.a, the user must specify a mixing table that defines the mixtures for a problem. Moreover, each mixture has a

nuclide specification along with the appropriate atomic number density. In point KENO, the user has the capability to specify different nuclides from different evaluation sources. As a result, the user has more control and flexibility with the new material specification options relative to the multigroup versions of KENO. Regarding other changes to the user interface, additional parameters have been defined that are specific to the continuous-energy transport. For example, the user has the option to disable the probability table treatment if the impact of the unresolved-resonance region treatment is to be investigated for the problem. Also, the user must specify an energy group structure that is used to tabulate calculated quantities (e.g., flux, leakage, etc.) during the random walk. In addition, the current group-dependent biasing schemes (e.g., roulette and splitting) in KENO V.a are maintained in the continuous-energy version of the code. Because the pointwise version of KENO uses the existing KENO V.a geometry package, existing KENO V.a geometrical models can be used in the new continuous-energy version of KENO V.a. Future work will also focus on the development of a pointwise version of KENO-VI.

Because the cross-section library format dictates the random walk procedures, the cross-section processing development, which is described in the previous section, provided the foundation for the subsequent point KENO radiation transport development. For the first generation in a calculation, an estimate of the initial source distribution is made based on the nature of the problem. The six start-type options that are available in the multigroup version of KENO are maintained in the continuous-energy version of the code; however, the starting energy distribution is sampled from a continuous-energy fission spectrum, P(E), of the fissionable isotope present in the mixture. If N fissionable isotopes are present in the mixture, the i^{th} fissionable isotope to sample is selected from a relation of the form

$$\sum_{j=1}^{i-1} \Sigma_f^j < R \sum_{j=1}^{N} \Sigma_f^j \le \sum_{j=1}^{i} \Sigma_f^j \ , \qquad (1)$$

where R is a random number between 0 and 1 and Σ_f^j is the macroscopic fission cross section. Linear-linear interpolation is used to determine intermediate cross-section values between energy grid points. In general, the starting direction cosines are sampled uniformly from an isotropic distribution. In the first generation of the MC simulation, fission points are generated that will serve as the source distribution for the next generation. The source distribution for each successive generation is generated from the fission points from the preceding generation.

Once the starting distribution is sampled, the next collision site in a mixture is sampled from the following CDF:

$$F(x) = 1 - e^{-\Sigma_t^{mix}(E)\,x} \ , \qquad (2)$$

where x is the spatial variable and $\Sigma_t^{mix}(E)$ is the macroscopic total cross section for a mixture at energy E. If any of the isotopes in the mixture have probability-table data and the incident energy is in the unresolved region of the isotope, the macroscopic total cross section for the mixture is adjusted based on the sampled probability table. Because the pointwise collision treatment is modeled on a per-nuclide basis, the total cross section and corresponding partial reactions (i.e., elastic scattering, fission, and capture) from the probability table are stored for each isotope that is sampled during the collision site selection.

At each collision site, the collision is modeled by selecting the i^{th} isotope/nuclide in the mixture from the following equation (energy variable suppressed):

$$\sum_{j=1}^{i-1} \Sigma_t^j < R \sum_{j=1}^{N} \Sigma_t^j \le \sum_{j=1}^{i} \Sigma_t^j \ , \qquad (3)$$

where Σ_t^j is the macroscopic total cross section for the j^{th} isotope/nuclide in the mixture. Once the collision nuclide is selected, the nonabsorption, absorption, and fission probabilities are calculated. Absorption is modeled implicitly by reducing the particle's weight by the nonabsorption probability. Depending on the particle's weight, splitting, roulette or both are performed as necessary. In the pointwise random walk, an explicit collision treatment is modeled, and the k^{th} reaction is selected from NR possible nonabsorption reactions based on the microscopic cross-section data for the target nuclide:

$$\sum_{j=1}^{k-1} \sigma_j < R \sum_{j=1}^{NR} \sigma_j \le \sum_{j=1}^{k} \sigma_j \ , \qquad (4)$$

where σ_j is the cross-section value for the j^{th} nonabsorption reaction at incident energy E.

As noted in the previous section, the point KENO cross-section libraries are prepared by generating tabular joint kinematics distributions in the lab system. Moreover, the coupled distributions are constructed such that the angular cosine, μ, is selected first. Once the angular cosine is sampled, the exit energy is sampled from the conditional probability distribution corresponding to the sampled E and μ. Note that for isotropic angular distributions, the exit cosine is sampled uniformly from !1 to 1, and a single exit energy distribution is sampled for the exiting neutron energy.

For neutron-producing reactions other than fission [e.g., (n,2n), (n,3n), etc.], the weight of the exiting neutron is adjusted by the reaction multiplicity to account for the additional neutrons. In other words, nonfission neutron-producing reactions provide a source for the current generation. The fission treatment in point KENO is implicit in nature. At each collision site, the code determines whether fission occurs and how many fission points are generated based on the fission probability. For each fission point generated, the angle cosine and energy of the fission neutron are sampled from the kinematics distribution, which is generally isotropic in nature. The fission points are stored in a "fission bank" which serves as the source for the next generation.

In each generation, all of the histories are tracked until death or the particle leaks from the system. When the specified number of histories is complete for the current generation, an estimate of the eigenvalue of the system is made in addition to other requested quantities (e.g., flux, leakage, etc.). Subsequently, the next generation is processed based on the source estimate from the previous generation. The calculation is complete when all of the specified number of generations have been processed.

4. Testing

Using the AMPX modules developed specifically for this work, prototypic point KENO cross sections were generated for 50 ENDF/B-6 Release 7 nuclides (i.e., includes all the uranium and plutonium isotopes, in addition to thermal data for H in H_2O and H in CH_2). In an effort to demonstrate and test the computational capability of point KENO, 21 critical benchmarks were selected from the work by Bowman et. al.[12] and modeled with the continuous-energy version of KENO V.a. A brief description of each benchmark is provided in Table 1, using the case designation specified in Ref. 12. The first 13 benchmarks in Table 1 involve light-water-reactor (LWR)-type UO_2 fuel pin lattices with various absorber and reflector configurations. The next four benchmarks in Table 1 (i.e., cas82 through cas85) are the "green block" experiments that involve 2–3 wt % enriched homogenized uranium in paraffin blocks. Cases cas86 through cas88 involve uranyl fluoride and uranyl nitrate solutions at 93.2 wt % enrichment, and cas91 consists of uranyl fluoride solution at 4.89 wt % enrichment.

The new version of point KENO was used to model each of the benchmarks presented in Table 1, and the calculated results for each benchmark are provided in Table 2. All of the calculations were performed on a DEC Alpha XP1000 workstation. For comparison purposes, the 21 benchmarks were modeled with the multigroup version of KENO V.a using the 238-group ENDF/B-5[1] and 199-group ENDF/B-6 Release 3[13] cross-section libraries. The 199-group and 238-group libraries are general-purpose data libraries with adequate group structures for most fast and thermal criticality safety applications. One limitation of the 199-group library is the method used for self-shielding the resonances in the resolved region. The 199-group library was generated using NJOY 91,[14] and full-energy-range Bondarenko factors are provided in the library to perform resonance self-shielding. As a result, the narrow resonance approximation is used throughout the resonance region with the 199-group library. The failure of the narrow resonance approximation in the resolved region is observed for the 199-group library with the green block cases in Table 2 (i.e., cas82 through cas85), and these results are consistent with the results provided in Ref. 12. As noted in Ref. 12, the narrow resonance approximation in the 199-group library provides too much self-shielding of the ^{238}U capture cross section and the capture cross section is too low, thereby causing an overprediction in k_{eff}. In contrast, the 238-group results and point KENO results are closer to critical compared with the 199-group values because of improved modeling of the resonance self-shielding of the ^{238}U capture cross section. The point KENO results for the remaining cases in Table 2 are consistent with the multigroup KENO V.a results and demonstrate the computational capability of the new continuous-energy version of KENO V.a.

At this point in the development, extensive CPU timing studies have not been performed with the continuous-energy version of KENO V.a; however, timing comparisons relative to the multigroup version of KENO V.a have been performed for the 21 benchmark problems in Table 1. The differences in CPU times between the pointwise and multigroup versions of KENO V.a are directly correlated to the complexity of the problem. Based on testing during the point KENO development and testing with the 21 benchmarks, the multigroup version is ~6 to 133 times faster than point KENO. One of the recognized strengths of the multigroup version of KENO is the speed of the MC simulation. Fast execution times for multigroup KENO V.a are attributed to the "building-block" type of geometry package coupled with the multigroup collision treatment. In the multigroup approach, a collision is modeled with the entire mixture, and the collision treatment does not require the selection of the interacting nuclide or reaction type (i.e., elastic versus nonelastic) as in the continuous-energy approach. As a result, particle collisions in multigroup KENO are treated much faster than in the continuous-energy treatment. The large range of differences in CPU time for the 21 benchmark cases are attributed to the amount of H in H_2O material [i.e., kinematics distributions based on S(", $) data] as either a moderator or reflector. The point KENO particle collision treatment requires

Table 1 Descriptions of selected critical benchmark cases

Case	Enrichment (wt %)	Description	Lattice water/fuel volume ratio*
cas01	2.35	No absorber plates	2.92
cas07	2.35	Uranium reflector	2.92
cas09	2.35	No reflector	2.92
cas19	2.35	Uranium reflector	1.6
cas21	2.35	No reflector	1.6
cas34	2.46	Core XX: 1675 ppm soluble boron	0.999
cas36	2.46	Core IX: No B_4C pins, four pitches between assemblies	1.84
cas37	2.46	Core XIII: 1.6 wt % Boral, one pitch between assemblies	1.84
cas38	2.46	Core XXI: 0.1 wt % Boral, three pitches between assemblies	1.84
cas46	2.35	1.562 cm pitch, 464 ppm soluble boron	1.196
cas47	2.35	1.905 cm pitch, no boron	2.408
cas48	2.35	1.905 cm pitch, 568 ppm soluble boron	2.408
cas50	2.35	2.210 cm pitch, 286 ppm soluble boron	3.687
cas82	2.0	Homogenized uranium in paraffin, unreflected	$H/^{235}U = 293.9$
cas83	2.0	Homogenized uranium in paraffin, plexiglass and paraffin reflector	$H/^{235}U = 406.3$
cas84	3.0	Homogenized uranium in paraffin, plexiglass and paraffin reflector	$H/^{235}U = 133.4$
cas85	3.0	Homogenized uranium in paraffin, unreflected	$H/^{235}U = 133.4$
cas86	93.2	UO_2F_2 solution sphere, no reflector	$H/^{235}U = 1112$
cas87	93.2	UO_2F_2 solution sphere, H_2O reflector	$H/^{235}U = 1270$
cas88	93.2	$UO_2(NO_3)_2$ solution, 142.9 g U/l, cylinder, no reflector	$H/^{235}U = 186$
cas91	4.89	UO_2F_2 solution sphere, 42.54 g ^{235}U/l, Al box, H_2O reflector	$H/^{235}U = 524$

* Unless designated as $H/^{235}U$ ratio.

that the exiting energy and angle be sampled from tabular kinematics distributions. Consequently, the continuous-energy approach requires extensive table searches for the collision treatment. Problems that have extensive thermal collisions require multiple sampling of the H_2O tabular kinematics distributions. For example, problems cas36 and cas37 involve $U(2.46)O_2$ fuel pin lattices that have separation differences of 1 and 4 pitches, respectively. The increased water moderation between assemblies in cas37 leads to ~2.5 times longer point KENO CPU time compared with cas36. As a result, more CPU time is spent sampling the tabulated CDFs in cas37 than in cas36 as a neutron thermalizes in H_2O. Improved CPU times in the point KENO simulation can be obtained by improving the sampling efficiency of the tabular kinematics distributions.

5. Summary

The objective of the research is to develop and demonstrate a continuous-energy version of the MC code KENO V.a. The initial phase of the research focused on the design and development of a continuous-energy cross-section format and the associated cross-section processing modules for the AMPX-2000 code system. After defining the cross-section format, the transport procedures were developed and implemented in a pointwise version of KENO V.a. Using the processing modules that were developed in the initial phase of the research, 50 ENDF/B-6 Release 7 nuclides were processed with AMPX to create a test pointwise cross-section library. In an effort to demonstrate and test the new transport capability, 21 critical benchmarks have been calculated with the continuous-energy KENO V.a. The point KENO–calculated eigenvalues for the different benchmarks are in agreement with the results obtained with KENO V.a using the 238-group ENDF/B-5 and 199-group ENDF/B-6 Release 3 libraries. In addition, the point KENO results obtained with ENDF/B-6 Release 7 data are in much better agreement with critical than were previously calculated results obtained with the 199-group ENDF/B-6 Release 3 library for the green block experiments. With regard to future development, additional testing for a wide variety of benchmarks should be performed. Moreover, additional work needs to be performed to improve the calculational efficiency of the code. Although

Table 2 Calculated k_{eff} for selected critical benchmark cases

Case	Point KENO ENDF/B-6 Rel. 7	KENO V.a 199-group ENDF/B-6 Rel. 3	KENO V.a 238-group ENDF/B-5
cas01	0.9925 ± 0.0016	0.9947 ± 0.0015	0.9937 ± 0.0015
cas07	1.0048 ± 0.0016	0.9934 ± 0.0016	0.9956 ± 0.0015
cas09	0.9936 ± 0.0014	0.9908 ± 0.0015	0.9956 ± 0.0014
cas19	0.9999 ± 0.0015	0.9937 ± 0.0022	0.9903 ± 0.0014
cas21	0.9955 ± 0.0017	0.9890 ± 0.0017	0.9941 ± 0.0016
cas34	0.9990 ± 0.0018	0.9973 ± 0.0011	0.9925 ± 0.0015
cas36	0.9908 ± 0.0016	0.9896 ± 0.0014	0.9934 ± 0.0014
cas37	0.9975 ± 0.0020	0.9979 ± 0.0020	0.9931 ± 0.0015
cas38	0.9924 ± 0.0015	0.9859 ± 0.0015	0.9901 ± 0.0016
cas46	0.9967 ± 0.0018	0.9948 ± 0.0017	0.9942 ± 0.0014
cas47	0.9959 ± 0.0012	0.9924 ± 0.0010	0.9952 ± 0.0012
cas48	0.9984 ± 0.0012	0.9972 ± 0.0011	0.9981 ± 0.0010
cas50	0.9999 ± 0.0021	0.9973 ± 0.0011	1.0033 ± 0.0014
cas82	1.0027 ± 0.0016	1.0241 ± 0.0015	1.0021 ± 0.0016
cas83	1.0011 ± 0.0019	1.0194 ± 0.0017	0.9992 ± 0.0017
cas84	1.0129 ± 0.0021	1.0357 ± 0.0017	1.0118 ± 0.0017
cas85	1.0137 ± 0.0017	1.0407 ± 0.0020	1.0123 ± 0.0020
cas86	1.0043 ± 0.0016	1.0026 ± 0.0022	1.0088 ± 0.0016
cas87	1.0014 ± 0.0018	1.0015 ± 0.0014	1.0039 ± 0.0013
cas88	0.9981 ± 0.0020	1.0029 ± 0.0025	1.0090 ± 0.0021
cas91	1.0025 ± 0.0014	1.0120 ± 0.0012	1.0064 ± 0.0013

additional research is planned, a continuous-energy version of the KENO V.a code has been successfully developed and demonstrated for modeling systems with fissionable material.

Acknowledgments

The work presented in this paper was sponsored by the United States Nuclear Regulatory Commission.

References

1) "SCALE: A Modular Code System for Performing Standardized Computer Analysis for Licensing Evaluation," NUREG/CR-0200, Rev. 6, ORNL/NUREG/CR/CSD-2/R6, Vols. I, II, and III (2000).
2) M. E. Dunn, C. L. Bentley, S. Goluoglu, L. S. Paschal, L. M. Petrie and H. L. Dodds, "Development of a continuous energy version of KENO V.a," Nucl. Technol. **119**, 306–313 (1997).
3) "MCNP — A General Monte Carlo – Particle Transport Code," Version 4C, LA-13709-M, J. F. Briesmeister, Ed., Los Alamos National Laboratory (2001).
4) "ENDF-102 Data Formats and Procedures for the Evaluated Nuclear Data File ENDF-6," BNL-NCS-44945, Rev. 10/91 (ENDF/B-6) (1991).
5) M. E. Dunn and N. M. Greene, "AMPX-2000: A cross-section processing system for generating nuclear data for criticality safety applications," Trans. Am. Nucl. Soc. **86**, 118–119 (2002).
6) M. Williams and M. Asgari, "Computation of continuous-energy neutron spectra with discrete ordinates transport theory," Nucl. Sci. Eng. **121**, 173–201 (1995).
7) S. M. Bowman, D. F. Hollenbach, M. D. DeHart, B. T. Rearden, I. C. Gauld and S. Goluoglu, "An Overview of What's New in SCALE 5," Trans. Am. Nucl. Soc. **87**, 265–268 (2002).
8) M. E. Dunn and L. C. Leal, "Calculating probability tables for the unresolved-resonance region using Monte Carlo methods," Proc. Int. Conf. on the New Frontiers of Nuclear Technology: Reactor Physics, Safety and High-Performance Computing, PHYSOR 2002, Seoul, Korea, Oct. 7–10, 2002, 11C.03.pdf (2002).
9) L. B. Levitt, "The probability table method for treating unresolved neutron resonances in Monte Carlo calculations," Nucl. Sci. Eng. **49**, 450–457 (1972).
10) F. J. Dyson and M. L. Mehta, "Statistical theory of the energy levels of complex systems," J. Math. Phys. **4**, 701 (1963).

11) L. C. Leal and N. M. Larson, “SAMDIST: A Computer Code for Calculating Statistical Distributions for R-Matrix Resonance Parameters,” ORNL/TM-13092 (1995).
12) S. M. Bowman, R. Q. Wright, M. D. DeHart, C. V. Parks and L. M. Petrie, “Recent validation experience with multigroup cross-section libraries and SCALE,” Proc. Int. Conf. on Nuclear Criticality Safety, ICNC’95, Albuquerque, NM, Sept. 17–21, 1995, 2C44 – 2C55 (1995).
13) D. T. Ingersoll, J. E. White, R. Q. Wright, H. T. Hunter, C. O. Slater, N. M. Greene, R. E. MacFarlane and R. W. Roussin, “Production and Testing of the VITAMIN-B6 Fine-Group and the BUGLE-93 Broad-Group Neutron/Photon Cross-Section Libraries Derived from ENDF/B-VI Nuclear Data,” ORNL-6795, NUREG/CR-6214 (1995).
14) R. E. MacFarlane and D. W. Muir, “The NJOY Nuclear Data Processing System–Version 91,” LA-12740-M (1994).