

STATUS AND PRELIMINARY TESTING OF CONTINUOUS-ENERGY KENO V.a AND KENO-VI

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ABSTRACT

KENO V.a and KENO-VI are three-dimensional (3-D) multigroup Monte Carlo computer codes that solve the static Boltzmann transport equation. They are used to perform evaluations of 3-D physical systems containing fissile material. As part of an ongoing effort by Oak Ridge National Laboratory to maintain and enhance the capabilities of the SCALE code system, continuous-energy versions of KENO V.a and KENO-VI have been developed and are undergoing testing and evaluation. Parallel to the development of the continuous-energy versions of KENO is the development of the cross-section data needed by these codes. The AMPX cross-section processing system of computer codes has been enhanced to process ENDF/B data and generate continuous-energy cross-section data for use in the continuous-energy versions of KENO. A preliminary continuous-energy cross-section library has been developed that contains 50 isotopes/nuclides, each at one temperature. The sample problem sets contained in SCALE 5 were used for testing and evaluation of the preliminary continuous-energy library used in conjunction with both continuous-energy KENO V.a and KENO-VI. This paper describes the continuous-energy versions of KENO V.a and KENO-VI, presents results for the sample problem sets, and identifies some areas where work is still ongoing.

Key Words: continuous energy, KENO-VI, KENO V.a, Monte Carlo

1 INTRODUCTION

Monte Carlo 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, Monte Carlo methods are classified according to whether the cross-section data used to solve the transport equation are used in the continuous-energy or multigroup format. In general, continuous-energy methods are preferred because the continuous-energy treatment avoids many of the assumptions and approximations inherent in multigroup methods. KENO V.a [1] and KENO-VI [2] are multigroup Monte Carlo codes that are used throughout the world to analyze systems containing fissile material 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 [3] (Standardized Computer Analyses for Licensing Evaluation) system. New continuous-energy versions of both KENO V.a and KENO-VI, CE-KENO V.a and CE-KENO-VI [4], have been developed that do not contain the cross-section processing limitations inherent in the multigroup versions of the codes. The objective of this paper is to compare the results produced using CE-KENO V.a and CE-KENO-VI with those from their multigroup counterparts for respective sets of sample problems.

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One of the primary objectives in the development of these new versions of KENO is to create a set of continuous-energy codes completely independent of any other continuous-energy Monte Carlo code (e.g., MCNP, MONK, and VIM). This entails both new codes that perform the radiation transport and new cross-section data that are processed independent of the data used in other continuous-energy codes. Using the KENO series of codes as a starting point for the continuous-energy codes ensures independence of the radiation transport methodology. The independence of the continuous-energy data is ensured by developing a set of modules using the AMPX-2000 series of cross-section data processing codes [5] to produce the required continuous-energy cross-section libraries.

Using the versions of the KENO V.a and KENO-VI codes contained in SCALE 5 as starting points for the continuous-energy versions of these codes greatly simplified their development. The geometry handling, random walk techniques, and most data management used in the KENO codes remains unchanged. The majority of the changes center on cross-section data storage, manipulation, and use. Several new modules were created to process and use the continuous-energy data. Many of these modules could be plugged directly into the KENO codes, replacing the multigroup versions of the modules, while others perform functions specific to the continuous-energy cross-section format utilized. The object was to make the user interface to the continuous-energy versions of KENO as similar as possible to that of the multigroup versions.

A new continuous-energy cross-section library was developed for the new continuous-energy codes based on the ENDF/B-6 Release 7 evaluation.[6] The ENDF data are voluminous and in a format unsuitable for use directly in radiation transport codes. 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 code system has been developed, maintained, and enhanced over the last 30 years to generate cross-section data for the transport codes developed at ORNL. AMPX-2000, the latest version of the AMPX code system, is a modular system that processes the full range of ENDF/B formats through ENDF/B-6 used to describe the physics associated with neutron, gamma, and coupled neutron-gamma interactions up to 20 MeV. Multiple AMPX-2000 processing modules have been specifically developed to generate cross-section data in the new continuous-energy format. The essential components of a continuous-energy KENO cross-section library include the following: (1) average number of neutrons (delayed and prompt) produced by fission, $\nu(E)$; (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. Some continuous-energy radiation transport codes have the ENDF laws and procedures programmed in the code. 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 AMPX-2000 processes the raw ENDF/B data into a continuous-energy library, the burden of treating the ENDF formats lies solely on the AMPX-2000 cross-section generation code, and not on the transport code.

2 MULTIGROUP AND CONTINUOUS-ENERGY KENO DIFFERENCES

In an effort to allow experienced KENO users to easily convert existing KENO input files to the new continuous-energy KENO input format, one of the design objectives for the new code is to minimize the number of changes to the KENO input files. From a user interface perspective, the changes are essentially transparent. There are three differences between multigroup and point problem inputs: (1) energy group structure, (2) continuous-energy file, and (3) unique data file. The number of energy groups and group structure are needed to tabulate calculated quantities such as flux and leakage. The number of groups is specified in the parameter data using the keyword “ngp=” followed by an integer. The energy group structure is then read from a file containing the energy boundaries for all the existing cross-section libraries in SCALE 5. If the number of groups is not specified, the code defaults to 44 energy groups having the same group boundaries as those contained in the 44GROUPNDF5 multigroup master library in SCALE 5. It is possible to update this file to include any group structure desired.

The mixing table data are the primary difference between the multigroup and continuous-energy versions of KENO V.a and KENO-VI. The continuous-energy library used for this problem is specified using the keyword “lib=” followed by the directory containing the point library data in the mixing table data block. There is a separate file in the directory containing the cross-section data for each nuclide/isotope. Data are entered in the mixing table by first specifying the keyword “mix=” followed by the mixture number, just as in the multigroup versions of KENO. Data for the mixture are then entered in sets of three numbers consisting of the nuclide/isotope ID, the atom density, and the temperature. Data for the mixture continue until either the keyword “mix=” is again specified or the mixing table data are terminated. It is possible to specify data not in the library or to replace data in the library by specifying the keyword “f=” followed by a unique file number after the nuclide ID number. In this case the specified file must be in the directory where the problem is being executed.

The multigroup versions of KENO require the cross-section data to be preprocessed into a problem-dependent working format library. By default BONAMI [7] is used to process the unresolved-resonance data and NITAWL-III [8] is used to process the resolved-resonance data prior to using the cross-section data in KENO. Since CE-KENO uses continuous-energy cross-section data, no preprocessing is required. The data in the continuous-energy library are stored as discrete points, typically with a tolerance of 0.1%, with the exception of the unresolved-resonance data. Because of the statistical nature of the unresolved parameters used to describe the unresolved-resonance region, probability tables are used to provide cross-section probability distribution functions for energy ranges at specific temperatures within the unresolved region [9].

3 ANALYSIS

All the KENO V.a and KENO-VI sample problems in the relevant sample problem sets from SCALE 5 were used for the preliminary testing of both multigroup and continuous-energy versions of KENO V.a and KENO-VI with the following exceptions. Sample problem 5 was not used because it contains differential albedo data and there are currently no continuous-energy albedo data. Sample problem 17 was not used because it is an adjoint problem and CE-KENO does not currently contain an adjoint option. Each problem tracked 2.5 million particles, 5000 particles per generation, with 510 generations skipping the first 10 generations. For these sample

problems, less than 10 generations are required for the initial source to converge. This ensured the statistics were such that the standard deviation was well under 0.1%.

All calculations were performed on a DEC Alpha XP1000 workstation. The multigroup KENO problems used the 238GROUPNDF5 cross-section master library with BONAMI to perform the unresolved-resonance-range processing and NITAWL-III to perform the resolved-resonance-range processing. The continuous-energy KENO problems used a preliminary 50-nuclide/isotope library generated by AMPX-2000 from ENDF/B-6 Release 7 data. The continuous-energy library includes all uranium and plutonium isotopes; thermal data for H in H₂O and H in CH₂; and other structural and absorber material such as boron, iron, and aluminum. Windows PC versions of CE-KENO V.a and CE-KENO-VI have also been compiled for testing and evaluation with the 50-nuclide/isotope continuous-energy library.

4 RESULTS

There are two distinct sets of results: one for KENO V.a contained in Table I and a second for KENO-VI contained in Table II. Table III contains the results for the first 25 sample problems using MCNP [10] and cross-section data derived from ENDF/B-6, revision 2 data and a comparison with the continuous-energy KENO V.a and KENO-VI results. Table I compares the multigroup and continuous-energy version of KENO V.a. In the 31 sample problems analyzed (33 total minus sample problems 5 and 17), there are only 10 distinctly different sample problems. The remaining sample problems are variations of other sample problems that test program options. For most sample problems, CE-KENO V.a results are from 0 to -0.3% of the multigroup KENO V.a results. As shown in Table III, these sample problems range from 0.36% high to -0.22% low when compared to MCNP results, which is within 2 standard deviations. There are five exceptions to this generalization. The calculated k_{eff} values using CE-KENO V.a are from 0.35 to 0.85% higher than the multigroup results in sample problems 15, 16, and 18. These sample problems are thermal problems—two UO₂F₂ solutions and one water-reflected sphere—containing enriched uranium. These are not the only thermal problems utilizing highly enriched uranium; therefore, no trend is readily observable. For sample problems 15 and 16, the MCNP results compare well with the multigroup results, which are significantly lower than the continuous-energy results. Sample problem 18 is just the opposite, with the MCNP result being 0.9% higher than the continuous-energy result. These anomalies could be a result of the different libraries used but further investigation is warranted.

The fourth anomaly is sample problem 33, low-enriched-uranium annular billets partially submerged in water. This is the only sample problem utilizing low-enriched uranium. The resulting calculated k_{eff} value is 6.3% high, indicating a problem with the AMPX-processed U-238 continuous-energy cross-section data. Further work needs to be done on the U-238 cross-section data to identify the exact cause of the problem.

Table I. KENO V.a results

Sample Problem	Description	M.G. $k_{eff} (\pm\sigma)$	C.E. $k_{eff} (\pm\sigma)$	% Δk_{eff}
1	case 2c8 bare	0.99819 (0.00058)	0.99515 (0.00053)	-0.304
2	2c8 bare with 8 unit types	0.99819 (0.00058)	0.99515 (0.00053)	-0.304
3	2c8 15.24 cm paraffin refl	0.99740 (0.00056)	0.99473 (0.00061)	-0.267
4	2c8 15.24 cm para - auto refl	0.99682 (0.00059)	0.99529 (0.00057)	-0.153
6	one 2c8 unit (single unit)	0.74417 (0.00045)	0.74264 (0.00052)	-0.153
7	bare 2c8 using spec. reflector	0.99846 (0.00048)	0.99648 (0.00058)	-0.198
8	infinitely long 2c8 cylinder	0.93928 (0.00048)	0.93737 (0.00048)	-0.191
9	infinite array of 2c8 units	2.28793 (0.00040)	2.26284 (0.00040)	-2.509
10	2c8 bare write restart	0.99819 (0.00058)	0.99515 (0.00053)	-0.304
11	2c8 bare read restart data	0.99819 (0.00058)	0.99515 (0.00053)	-0.304
12	4 aqueous 4 metal arrays	1.00167 (0.00068)	0.99978 (0.00069)	-0.189
13	two cuboids in a cyl. annulus	0.99611 (0.00057)	0.99541 (0.00058)	-0.070
14	u metal cylinder in annulus	0.99426 (0.00050)	0.99429 (0.00053)	0.003
15	small water reflected sphere on Plexiglas collar	0.99625(0.00052)	1.00462 (0.00049)	0.837
16	uo2f2 infinite slab k-inf	0.99115 (0.00038)	0.99467 (0.00064)	0.352
18	1f27 demonstration of options	1.01261 (0.00067)	1.02109 (0.00069)	0.848
19	4a-4m array of arrays-prob 12	1.00001 (0.00062)	0.99895 (0.00065)	-0.106
20	triangular pitched array	0.99570 (0.00073)	0.99267 (0.00061)	-0.303
21	partially filled sphere	0.99619 (0.00051)	0.98928 (0.00053)	-0.691
22	2c8 bare w/ 3 nested holes	0.99808 (0.00056)	0.99582 (0.00047)	-0.226
23	2c8 bare as zhemicylinders	0.99753 (0.00055)	0.99570 (0.00056)	-0.183
24	2c8 bare as xhemicylinders	0.99717 (0.00051)	0.99636 (0.00045)	-0.081
25	2c8 bare as yhemicylinders	0.99806 (0.00054)	0.99539 (0.00063)	-0.267
26	2c8 bare as zhemicylinders	0.99752 (0.00049)	0.99557 (0.00050)	-0.195
27	2c8 bare as xhemicylinders	0.99867 (0.00047)	0.99599 (0.00051)	-0.268
28	2c8 bare as yhemicylinders	0.99750 (0.00056)	0.99608 (0.00053)	-0.142
29	bare 3.4420" radius sphere	0.99476 (0.00047)	0.99426 (0.00051)	-0.050
30	prob 29 with zhemispheres	0.99523 (0.00056)	0.99440 (0.00057)	-0.083
31	prob 29 with xhemispheres	0.99539 (0.00057)	0.99459 (0.00052)	-0.080
32	prob 29 with yhemispheres	0.99493 (0.00052)	0.99396 (0.00047)	-0.097
33	critical triangular pitched array of annular rods	0.99385 (0.00051)	1.05657 (0.00051)	6.272

Table II. KENO-VI results

Sample Problem	Description	M.G. Result $k_{eff} (\pm\sigma)$	C.E. Results $k_{eff} (\pm\sigma)$	$\% \Delta k_{eff}$
1	case 2c8 bare	0.99791 (0.00052)	0.99643 (0.00048)	-0.148
2	case 2c8 bare with 8 unit types	0.99791 (0.00052)	0.99643 (0.00048)	-0.148
3	case 2c8 15.24 cm paraffin refl	0.99731 (0.00056)	0.99408 (0.00059)	-0.323
4	case 2c8 15.24 cm paraffin refl	0.99636 (0.00059)	0.99483 (0.00060)	-.0153
6	one 2c8 unit (single unit)	0.74432 (0.00046)	0.74246 (0.00056)	-0.186
7	bare 2c8 using spec. reflector	0.99830 (0.00049)	0.99560 (0.00056)	-0.270
8	infinitely long 2c8 cylinder	0.93787 (0.00045)	0.93748 (0.00050)	-0.039
9	infinite array of 2c8 units	2.28889 (0.00041)	2.26336 (0.00039)	-2.555
10	case 2c8 bare write restart	0.99791 (0.00052)	0.99643 (0.00048)	-0.148
11	case 2c8 bare read restart data	0.99791 (0.00052)	0.99643 (0.00048)	-0.148
12	4 aqueous 4 metal mixed units	1.00142 (0.00062)	0.99878 (0.00059)	-0.264
13	two cuboids in a cyl. annulus	0.99556 (0.00052)	0.99588 (0.00047)	-0.032
14	u metal cylinder in an annulus	0.99535 (0.00060)	0.99280 (0.00061)	-0.255
15	small water reflected sphere on plexiglas collar	0.99656 (0.00053)	1.00471 (0.00071)	0.815
16	uo2f2 infinite slab k-infinity	0.99105 (0.00035)	0.99430 (0.00055)	0.325
18	1f27 demonstration of options	1.01193 (0.00066)	1.02211 (0.00063)	1.018
19	4a-4m array of array-prob 12	1.00167 (0.00066)	0.99918 (0.00063)	-0.249
20	triangular pitched array	0.99547 (0.00075)	0.99283 (0.00063)	-0.264
21	partially filled sphere	0.99626 (0.00050)	0.98900 (0.00051)	-0.726
22	2c8 bare w/ 3 nested holes	0.99791 (0.00044)	0.99604 (0.00050)	-0.187
23	2c8 bare as zcylinders	0.99822 (0.00054)	0.99567 (0.00048)	-0.255
24	case 2c8 bare as x-rotated cylinders	0.99736 (0.00050)	0.99610 (0.00062)	-0.126
25	case 2c8 bare as y-rotated cylinders	0.99847 (0.00049)	0.99603 (0.00052)	-0.133
26	bare 3.4420" radius sphere	0.99448 (0.00057)	0.99486 (0.00051)	0.038
27	critical triangular pitched array of annular rods	0.99362 (0.00058)	1.05699 (0.00049)	6.337

Table III. KENO V.a and KENO-VI vs. MCNP results

Sample Problem	Description	MCNP Result $k_{eff} (\pm\sigma)$	KENO V.a vs. MCNP $\% \Delta k_{eff}$	KENO-VI vs. MCNP $\% \Delta k_{eff}$
1	case 2c8 bare	0.9957 (0.0017)	-0.05	0.07
2	2c8 bare with 8 unit types	0.9957 (0.0017)	-0.05	0.07
3	2c8 15.24 cm paraffin refl	0.9975 (0.0019)	-0.22	-0.27
4	2c8 15.24 cm para - auto refl	0.9975 (0.0019)	-0.22	-0.27
6	one 2c8 unit (single unit)	0.7447 (0.0013)	-0.21	-0.23
7	bare 2c8 using spec. reflector	0.9934 (0.0018)	0.31	0.22
8	infinitely long 2c8 cylinder	0.9350 (0.0016)	0.23	0.25
9	infinite array of 2c8 units	2.2643 (0.0022)	0.15	-0.09
10	2c8 bare write restart	0.9957 (0.0017)	-0.06	0.07
11	2c8 bare read restart data	0.9957 (0.0017)	-0.06	0.07
12	4 aqueous 4 metal arrays	0.9995 (0.0026)	0.02	-0.07
13	two cuboids in a cyl. annulus	0.9929 (0.0019)	0.25	0.30
14	u metal cylinder in annulus	0.9943 (0.0018)	0.00	-0.15
15	small water reflected sphere on Plexiglas collar	0.9991 (0.0022)	0.55	0.56
16	uo2f2 infinite slab k-inf	0.9911 (0.0022)	0.35	0.32
18	1f27 demonstration of options	1.0302 (0.0027)	-0.91	-0.81
19	4a-4m array of arrays-prob 12	0.9995 (0.0026)	-0.06	-0.03
20	triangular pitched array	0.9933 (0.0029)	-0.07	-0.05
21	partially filled sphere	0.9926 (0.0018)	-0.33	-0.36
22	2c8 bare w/ 3 nested holes	0.9922 (0.0019)	0.36	0.38
23	2c8 bare as zhemicylinders	0.9957 (0.0017)	0.00	0.00
24	2c8 bare as xhemicylinders	0.9928 (0.0018)	0.35	0.33
25	2c8 bare as yhemicylinders	0.9974 (0.0018)	-0.20	-0.14

Finally, sample problem 9, an infinite array of bare highly enriched cylinders, has a calculated k_{eff} value that is 2.5% low. However, examining the MCNP results show a difference of only 0.15% compared to the continuous-energy results. This indicates a difference in the base ENDF/B-5 vs. ENDF/B-6 cross-section libraries and not a problem with the processed continuous-energy library.

Table II compares the multigroup and continuous-energy versions of KENO-IV. In the 25 cases analyzed (27 total minus sample problems 5 and 17), there are 11 distinctly different sample problems. The remaining sample problems are variations of other sample problems that test program options. Most of these sample problems are the same as those in Table I, but set up using KENO-VI geometry. The trends in these sample problems follow those present in Table I, with the calculated k_{eff} values for most CE-KENO-VI sample problems calculating from the same to as much as 0.32% lower than multigroup KENO-VI sample problems. As shown in Table III, excluding sample problems 15-18, these sample problems range from 0.38% high to -0.22% low when compared to MCNP results, which is within 2 standard deviations. The five anomalous sample problems present in Table I are repeated for the corresponding sample problems in Table II.

5 CONCLUSIONS

Both CE-KENO V.a and CE-KENO-VI have been tested over a range of problems that include most of the geometry and parameter options in KENO. CE-KENO V.a and CE-KENO-VI produce consistent results, which indicates that remaining problems are not with the transport process but with the APX-2000 processed cross-section data. For fast systems using highly enriched uranium, CE-KENO calculates no more than 0.32% below standard KENO. This indicates that, for these types of systems, multigroup KENO and continuous-energy KENO produce consistent results. The 2.5% low value for an infinite system of enriched uranium is the result of the different base ENDF/B cross-section data. The 6.3% high value for the low-enriched-uranium system indicates there are some definite problems with the AMPX-2000 processed uranium cross-section data that need to be investigated and corrected.

With regard to future development, additional testing for a wide variety of benchmarks will be performed. Moreover, work is ongoing to improve the calculational efficiency of the code. The continuous-energy versions of the codes currently run substantially slower than the multigroup versions. Several changes to both the codes and the cross-section libraries are ongoing that will significantly improve the running times. Also, significant work is needed to evaluate and expand the continuous-energy library. Although additional research is needed and planned, continuous-energy versions of the KENO V.a and KENO-VI codes have been successfully developed and demonstrated for modeling systems with fissionable material.

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