

Development and Testing of Code for Automatic Generation of Multi-Temperature Continuous-Energy Neutron Cross-Section Libraries (Post-print)

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Abstract

A code for automatically generating multi-temperature continuous-energy neutron cross-section data libraries, designated as AMTND, was developed to address the requirements of reactor core design coupled with thermal-hydraulic analysis. The code provides point-wise cross-sections at arbitrary temperatures for Monte Carlo neutron transport programs such as MCNP. To ensure that the nuclear data generated by AMTND meets the validation requirements of critical benchmark experiments, a computational performance comparison with NJOY was conducted, demonstrating the superior efficiency of AMTND. Additionally, Doppler coefficient benchmark tests were performed to evaluate the code's accuracy, yielding results that provide preliminary verification of its reliability.

Full Text

Preamble

Development and Testing of a Code for Automatic Generation of Multi-Temperature Continuous-Energy Neutron Cross-Section Libraries

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Abstract: A code for automatically generating multi-temperature continuous-energy neutron cross-section data libraries, designated AMTND, was developed to support reactor core design coupled with thermal-hydraulic analysis. The code can provide point-wise cross sections at any temperature for Monte Carlo neutron transport programs such as MCNP. To ensure that the nuclear data produced by AMTND satisfies critical benchmark experiments, a comparison of processing time between AMTND and NJOY was performed, demonstrating superior efficiency. The code's accuracy was further validated through Doppler coefficient benchmark tests, with results providing preliminary verification of its reliability.

Keywords: Reactor design, Temperature Doppler coefficient, Critical benchmark experiments

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Introduction

Nuclear data libraries form the foundation of neutronic design for nuclear reactors. In core design, various reactor parameters must be calculated, including reactivity coefficients during transitions from cold zero-power to hot zero-power and hot full-power states. The design process also involves iterative coupling with thermal-hydraulic analysis, where each set of thermal-hydraulic parameters must correspond to an appropriate set of reactor design parameters. Consequently, numerous nuclear databases for real-time temperature conditions must be generated when calculating these core parameters. Based on domestic and international reactor design studies and operational experience, this paper describes the design and development of an Automatically generated Multi-Temperature continuous-energy Neutron cross-section Data library code, abbreviated as AMTND.

II. Design of AMTND

A. Background

The Monte Carlo neutron transport code MCNP is widely recognized as a precise and mature tool for reactor design and analysis. Point-wise continuous-energy cross-section data in ACE format is suitable for use by the MCNP family of Monte Carlo codes and other programs capable of reading this library format. When using MCNP to calculate temperature-dependent parameters in reactor core design, nuclear data at corresponding temperatures must be produced to ensure accuracy, which is computationally intensive. The IAEA released a nuclear data processing package called SIGACE that can broaden ACE format data from 300 K to higher temperatures based on FENDL2.1 nuclear data, but it produces errors when processing some heavy nuclei, such as incorrect values

for the nuclear data' s location parameter JXS array.

B. Doppler Broadening

In neutron calculations, the effective cross section for a material at temperature T is defined as the cross section that yields the same reaction rate for stationary target nuclei as the real cross section does for moving nuclei. In many cases of interest, the target motion is isotropic and the velocity distribution can be described by the Maxwell-Boltzmann function. Therefore, the standard form of the Doppler-broadened cross section is as follows:

$$\sigma(T, \nu) = \int_{-\infty}^{\infty} dV \sigma(V) V^2 [e^{-\alpha(V-\nu)^2} - e^{-\alpha(V+\nu)^2}]$$

where $\alpha = M/(2kT)$, $V = |v - v'|$, k is Boltzmann' s constant, M is the target mass, v is the velocity of the incident particles, v' is the velocity of the target, and $\sigma(T, v)$ is the cross section for nuclides.

C. Preparation of MCNP Input Files

The MCNP input file is prepared by writing information about radionuclide species and their temperatures required for neutron transport calculations without interfering with MCNP' s normal operation. For example:

```
82208.83c 3.91128E-3 $ t=356.9 K
```

This represents a material card in the MCNP input file. The information appears to the left of the '\$' character, while comments appear to the right. "82208" represents the radionuclide type, where the first two digits indicate the proton number and the last three digits indicate the nuclide mass. "83c" is the database identifier, which can be defined according to user needs. To distinguish normal radionuclides from temperature-dependent ones, the temperature-dependent radionuclide is deliberately assigned the default identifier "*1.c". "t=356.9 K" specifies the nuclide temperature. All letters are case-insensitive.

D. Programming of AMTND

AMTND integrates both database library production and neutron transport calculations into a single process. The flow chart of AMTND is shown in Fig. 1 [Figure 1: see original paper]. The program operates through the following sequence: First, AMTND reads radionuclide species information, database identifiers, and temperatures from the material card of the MCNP input file, while automatically merging identical information for all nuclides and storing it in a temporary structure array. Second, AMTND encapsulates radionuclide species information, radionuclide identification numbers, and evaluation database names (with 408 nuclides from HENDL-ADS) in a structure array. Using the radionuclide species information obtained from the MCNP input file and the radionuclide ID number,

the corresponding evaluation database name can be located in this structure array. Third, based on the information about radionuclide species, radionuclide ID numbers, database identifiers, and temperatures obtained above, AMTND automatically generates a Doppler broadening input file. Fourth, AMTND calls Doppler broadening modules, which read the Doppler input file and evaluation database files to generate ACE format files and corresponding index files. Finally, the ACE format files and index files are merged into the original database, making the new database usable by MCNP.

III. Testing and Discussion

The testing of AMTND focused primarily on data accuracy and computational efficiency in generating nuclear data. Three test cases were conducted as follows.

A. Critical Benchmark Experiments

Critical benchmark testing addresses both thermal and fast reactor data. In this test, ten fast reactor experiments released by the Organization for Economic Cooperation and Development (OECD) were selected from the “International Handbook of Evaluated Criticality Safety Benchmark Experiments.” The radionuclide evaluations were taken from HENDL-ADS at a temperature of 293.6 K. Based on criticality calculations using MCNP with data produced by AMTND, the overall agreement of k_{eff} between experimental measurements and computed values shown in Table 1 was very good, with some deviations between calculation results and experimental values smaller than those produced by NJOY.

B. Time Consumed by Nuclear Data Generation

As shown in Table 2, AMTND demonstrates significant improvement over NJOY99 in generating actinide nuclei data libraries, with an average speedup ratio of 1.37 and a maximum speedup ratio of 1.61.

C. SEFOR Doppler Benchmark

The SEFOR reactor was designed to provide Doppler measurements in an environment representative of an operating LMFBR with respect to neutron spectrum, fuel temperature range, reactor composition, and fuel microstructure. The standard SEFOR fuel was a mixed oxide (20% PuO₂, 80% UO₂), in which the Pu contained a minimum of approximately 8% ²⁴⁰Pu, and the U was depleted in ²³⁵U. A one-dimensional spherical model was analyzed in this study. The 1-D SEFOR Doppler benchmark spherical model is shown in Fig. 2 [Figure 2: see original paper], and the spherical model region composition is presented in Table 3. Further details can be found in Ref. [11].

Using the Doppler calculation model, the isothermal Doppler coefficient is computed as:

$$\frac{dk}{dT} = \frac{k_2 - k_1}{\ln(T_2/T_1)}$$

where $T_1 = 677$ K is the average fuel temperature at zero power, $T_2 = 1365$ K is the average fuel temperature at 20 MW, k_1 is the neutron multiplication factor with fuel at T_1 , and k_2 is the neutron multiplication factor with fuel at T_2 .

The radionuclides for the SEFOR model adopted evaluation documents from HENDL-ADS/MC [9]. The results are shown in Table 4. A correction factor of -0.0005 for modeling was obtained due to resonance heterogeneity, subassembly heterogeneity, and other factors [11]. The calculated Doppler coefficient values were -0.0081 ± 0.0011 using NJOY-MCNP and -0.0080 ± 0.0012 using AMTND-MCNP, which compare well with the experimental result of -0.0080 ± 0.0010 .

IV. Conclusion

In this work, an automatic code for generating continuous-energy neutron cross-section data libraries called AMTND was designed and developed. The code was tested through critical benchmark experiments, processing time comparisons for nuclear data generation, and isothermal Doppler coefficient benchmark tests. The results demonstrate the preliminary accuracy and reliability of the code. Further verification will be required in future work.

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