NECP-Atlas: A new nuclear data processing code

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A B S T R A C T
A new nuclear data processing code called NECP-Atlas is under development at Xi’an Jiaotong University in China. The motivation for the development is to establish a platform to carry out deeper researches on nuclear data processing methods to satisfy the demands on accurate cross sections in the fields of high-fidelity transport simulation and advanced reactor design. The present paper describes the methods used in the current version of NECP-Atlas and demonstrates the performance and accuracy of the code on a variety of benchmarks. At the present time, NECP-Atlas can process ENDF/B-VII.1, ENDF/B-VII.0, CENDL-3.1, JEFF-3.2 and JENDL-4.0 evaluations, and generate WIMS-D and ACE format libraries. The accuracy of the code is comparable with NJOY2016. NECP-Atlas is competent to provide cross sections for deterministic and Monte Carlo transport calculations.

1. Introduction

The nuclear data is one of the most fundamental input quantities for the neutronics analysis of nuclear reactors. Although the evaluated nuclear data files include various nuclear data, neutronics analysis codes do not directly read data from the evaluations. The evaluated nuclear data should be firstly processed into a specific format by the nuclear data processing code, before it can be used by neutronics analysis codes. NJOY (MacFarlane et al., 2016), AMPX (Wiarda et al., 2016) and PREPRO (Cullen, 2017) are well-known nuclear data processing codes. There are also some newly developed nuclear data processing codes. For example, FRENDY has recently developed by Japan Atomic Energy Agency (JAEA) to produce ACE format library for Monte Carlo code (Tada et al., 2017). Ruler developed in China can provide WIMS-D format multi-group library (Liu and Wu et al., 2016). In this paper, a new nuclear data processing code called NECP-Atlas is developed. The motivation for the development is summarized as follows.

Many types of advanced reactors are under research and development (R&D) in China, for example, sodium-cooled fast reactor (IAEA and Yang, 2013) and high-temperature gas-cooled reactor (Zhang et al., 2016). The accurate neutronics analysis is very important in the R&D of advanced reactors. There are several new neutronics analysis codes for advanced reactors under development in China (Zheng et al., 2018; She et al., 2016). Different nuclear data processing methods from the light water cooled reactors are demanded in the neutronics analysis of advanced reactors. However, there is no mature nuclear data processing code in China. Ruler is a domestic nuclear data processing code, which can just produce WIMS-D format library. It hardly satisfies wide demands on accurate cross sections.

The three-dimensional (3D) whole-core high-fidelity transport calculation has been being studied worldwide. The emphasis of the 3D whole-core transport researches has been placed on the spatial discretization and parallel computations. Recently, it has been recognized that the error caused by transport calculation has been significantly reduced with the development of advanced transport calculation methodologies, and the evaluated nuclear data and the processing methods have become the main error sources (Pusa, 2012, Zu et al., 2016). In the researches on Monte Carlo based 3D transport calculation, accurate nuclear data processing methods aiming to avoid the error introduced by the temperature interpolation of cross sections have been systematically studied (Forget et al., 2014; Walsh et al., 2017; Ducru et al., 2017; Liu and Yuan et al., 2016; Liu et al., 2018). While in the aspect of deterministic whole-core transport calculations, the generation of multi-group cross sections has not been given much concern, and the conventional processing methods are still being used in the preparation of multi-group cross sections. Some problems such as the resonance elastic scattering (Ouisloumen and Sanchez, 1991; Lee et al., 2009; Ouisloumen et al., 2015) of heavy isotopes have not been well solved in the widely used nuclear data processing codes.

Moreover, the current evaluated nuclear data files released by different countries commonly apply the ENDF-6 format (Trkov...
et al., 2012) to store the data. Recently, this format has been considered to be changed by the Generalized Nuclear Data (GND) format (Mattoon et al., 2012). The basic techniques of processing evaluated nuclear data should be widely researched, only thus can more nuclear data processing codes be developed to validate each other.

For the above motivations, NECP-Atlas is developed. At the time when the present paper is prepared, NECP-Atlas can process the widely used ENDF-6 format evaluations, including: ENDF/B-VII.1, ENDF/B-VI.0, CENDL-3.1, JEFF-3.2 and JENDL-4.0. The ACE and WIMS-D format libraries can be produced. NECP-Atlas has also been connected with a newly developed 3D whole-code high-fidelity transport code NECP-X (Chen et al., 2018), and it can provide all the data needed by NECP-X to perform transport calculations. Besides, some new functions which are not included in NECP-Atlas, such as the treatment of resonance elastic scattering kernel and the generation of multi-band parameters in unresolved resonance region (URR).

This paper is organized as follows. Section 2 overviews the development of NECP-Atlas. The methods used in the current version of NECP-Atlas are briefly described in Section 3. The verification of NECP-Atlas is shown in Section 4. Some conclusions are given in the last section.

2. Overview of NECP-Atlas

NECP-Atlas is developed as a platform to produce accurate cross sections for different application aspects. In order to test different nuclear data processing methods conveniently, NECP-Atlas is written in standard Fortran 2008 with object-oriented method, and different processing functions are encapsulated in different modules. The names and processing functions of the modules implemented into NECP-Atlas are given in Table 1. In NECP-Atlas, the data transferred among different modules is realized in memory, and each module can also output PENDF or GENDF format files used in NJOY code (MacFarlane et al., 2016), so that the modules from the two codes can be combined to process the nuclear data or compared with each other.

Modern software engineering practices are utilized in the development of NECP-Atlas. The Git system is chosen as the version control tool, and the CMock tools including CMock and CTest are used to accomplish cross-platform compilation. NECP-Atlas has been successfully compiled with Gfortran, Intel compilers with various platforms including several Linux distributions and Windows. As a part of CMock tools, CTest is used for the unit testing and regression testing of NECP-Atlas. Unit testing is adopted to guarantee that each module in NECP-Atlas can produce accurate results after modified, and is performed automatically once the modified modules are pushed to the server. In the unit testing, the results such as cross sections or angular distributions generated by NECP-Atlas are compared with the reference results based on the same inputs. At a fixed time, regression testing is executed as scheduled. In the regression testing, NECP-Atlas is invoked to process different evaluations and generate WIMS-D and ACE format libraries. Then, DRAGON5 (Hebert, 2013) is used to calculate benchmarks from the WIMS-D Library Update Project (WLUP) (IAEA) with WIMS-D libraries, and MCNP (Briesmeister, 2000) is used to calculate benchmarks from the International Handbook of Evaluated Criticality Safety Benchmark Experiments (ICSBEP) (OECD-NEA, 2006) with ACE libraries. The WLUP benchmarks are listed in Section 4.2, and they are calculated every year. The ICSBEP benchmarks are listed in Section 4.3, and they are calculated at weekend, because MCNP calculations are time-consuming. The results of effective multiplication factors from DRAGON5 and MCNP are compared with the reference values to ensure the robustness and accuracy of NECP-Atlas. In the regression testing, CTest submits results of NECP-Atlas to a CDash dashboard system. Through the CDash pages, the state of NECP-Atlas such as configuration, building and test errors can be displayed.

More information is available online at: atlas.xjtu.edu.cn.

3. Methods used in NECP-Atlas

3.1. Reconstruction and linearization

In resolved resonance region (RRR), the resonance parameters are given for reconstructing the cross section values on a fixed energy grid. To obtain the energy dependent cross sections, the resonance contribution is firstly calculated with resonance parameters and corresponding formulae. Then the resonance contribution is added to a smooth part also given in the evaluations. In ENDF-6 format evaluations, the smooth cross sections are given in File 3 (Trkov et al., 2012). Therefore, one important procedure in nuclear data processing codes is to reconstruct the cross sections in RRR. NECP-Atlas can treat resonance parameters of the following formats: Single-Level Breit-Wigner, Multi-Level Breit-Wigner, Reich-Moore and R-Matrix Limited.

In URR, the evaluations provide mean values of resonance spacing, resonance partial width and their statistical distribution functions. The distribution function of the resonance spacing is the Wigner distribution, and the distribution function for the partial width is chi-square distribution for various numbers of degrees of freedom. The energy dependent cross sections in URR can not be constructed as RRR, in the reconstruction process, the infinitely diluted cross sections are computed using the average values and statistical distribution functions of resonance parameters. In NJOY, the energy points, where the average parameters are provided in an evaluation, are chosen for the reconstruction, and the cross sections at other energies are obtained by linear interpolation. In NECP-Atlas, more energy points can be added among the original ones, and the cross sections at these energies are calculated using the unresolved resonance parameters which are obtained by linear interpolation. The interval of energy points can be controlled by the users.

In principle, the cross sections at an energy point can be uniquely defined by the interpolation laws or resonance formulae, but it is a convention to convert the cross sections from their original nonlinear-tabulated form to linear interpolation form. The purpose of this treatment is to ensure the consistency of sum cross sections (such as total cross section) with the summation of its partial cross sections; and to prepare linearized data for the following processing procedures (such as Doppler broadening). The conventional interval-halving technique is adopted for linearization in NECP-Atlas, and several convergence criteria are adopted to ensure the precision and efficiency for linearization.

<table>
<thead>
<tr>
<th>Table 1</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Names of modules</strong></td>
</tr>
<tr>
<td>Recon_calc</td>
</tr>
<tr>
<td>Broad_calc</td>
</tr>
<tr>
<td>Ures_calc</td>
</tr>
<tr>
<td>Table_calc</td>
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<tr>
<td>MBand_calc</td>
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<tr>
<td>RESK_calc</td>
</tr>
<tr>
<td>Therm_calc</td>
</tr>
<tr>
<td>Group_calc</td>
</tr>
<tr>
<td>WIMS_outp</td>
</tr>
<tr>
<td>ACE_outp</td>
</tr>
<tr>
<td>NECPX_outp</td>
</tr>
</tbody>
</table>
3.2. Doppler broadening

In the evaluations, the nuclear data is stored as the function of relative kinetic energy between the incident neutron and target nucleus, which means that the neutron energy in evaluations is measured in the relative frame of reference. Before transport calculation, the neutron energy should be transformed from the relative to laboratory frame of reference, because the Boltzmann equation is expressed in the latter. At 0 K, the target nuclei in a medium are stationary, so the neutron energies in the two frames of reference are identical. While in the real medium at a temperature, the target nuclei are moving about in a random manner with a distribution of velocity, therefore, neutrons with the same kinetic energy in laboratory frame of reference will have different relative kinetic energies when the target moves in different velocities. Therefore, an effective cross section in laboratory frame of reference is defined to preserve the average reaction rate in relative frame of reference. This is known as Doppler broadening. Besides, the velocity distribution of target nuclei is dependent on the temperature, so that the effective cross section varies with the medium temperature.

The Doppler broadening equation is established by preserving the average reaction rate in the relative frame of reference and assuming that the speed distribution of target nuclei is a Maxwellian distribution and the angular distribution is isotropic for a given speed. In NECP-Atlas, the Kernel Broadening method (Cullen, 2010; Romano and Trumbull, 2015) is adopted to solve the Doppler broadening equation. This method is originally implemented in the SIGMA1 code (Cullen and Weisbin, 1976), and now is used in most major cross section processing codes, such as NJOY and AMPX. In this method, the cross sections at 0 K or any lower temperature are firstly represented as a series of linear-tabulated points. Except for this treatment of the cross sections, the Doppler broadening equation is solved exactly without any further approximations.

3.3. Processing of nuclear data in URR

As mentioned above, in the URR, we cannot get accurate energy dependent cross sections. In NECP-Atlas, there are three different processing methods for the nuclear data in URR.

Firstly, the effective self-shielded cross sections of different energy regions are calculated at various dilution conditions, which are used by deterministic transport codes. In NECP-Atlas, similar method with the UNRESR module in NJOY (MacFarlane et al., 2016) is used to calculate the effective cross sections. Like the reconstruction of infinitely diluted cross sections mentioned above, NECP-Atlas adds some energy points among the original ones given in evaluations, and the cross sections at these energies are calculated using the unresolved resonance parameters obtained by linear interpolation.

Secondly, the probability table used by Monte Carlo transport codes are calculated based on the unresolved resonance parameters. In NECP-Atlas, the ladder sampling method (Levitt, 1972) is used to generate the probability table. In this method, for each spin sequence, a set of resonance energies in an energy range are sampled according to the spacing distribution function, and then the resonance cross section contributions at these energies are calculated using resonance parameters obtained by sampling the resonance partial widths. The above process is repeated for each spin sequence. A resonance ladder is obtained by accumulating the cross sections in all spin sequences, and the probability table contributed from the resonance ladder is calculated. Enough ladders should be processed to guarantee the accuracy of the probability table. NJOY also adopts this method in PURR module to produce the probability table. In NECP-Atlas, some techniques are used to improve the calculation efficiency. In NJOY, after a resonance ladder is obtained, the sampled energy points are sorted according to the values of total cross sections, and then the total cross sections are gone through and determined how many values hit each probability bin. Due to the sorting, the calculation efficiency is improved. In NECP-Atlas, the quick sorting algorithm is adopted instead of the bubble sorting algorithm used in the NJOY code.

Thirdly, a method called multi-band method similar with the URR-PACK (Cullen and Trkov, 2016) is also implemented into NECP-Atlas. In the above described probability table method, the cross sections are usually divided into 20 bands; while in the multi-band method, only two band data are provided and they can produce statistically identical effective multiplication factor results to 20 band data. We take the total cross section as an example to explain how to calculate the multi-band data. The generation method for the other types of cross sections can be found in Cullen and Trkov (2016). Three self-shielded cross sections are defined as:

\[ \langle \Sigma_0 \rangle = \frac{\sum P \Sigma_i}{\sum P} \]
\[ \langle \Sigma_1 \rangle = \frac{\sum P_i \Sigma_i}{\sum P_i} \]
\[ \langle \Sigma_2 \rangle = \frac{\sum P_i \Sigma_i^2}{\sum P_i \Sigma_i} \]

where \( \Sigma_i \) and \( P_i \) is the band cross section and band weight of the \( i \)-th band, respectively. The effective self-shielded cross sections (\( \langle \Sigma_0 \rangle \)), (\( \langle \Sigma_1 \rangle \)) and (\( \langle \Sigma_2 \rangle \)) can be pre-calculated using the probability table data gotten from the above ladder sampling method. Next, if two-band data, including the band cross sections \( \Sigma_1, \Sigma_2 \) and band weights \( P_1, P_2 \), are calculated, the four known parameters should make the right hand sides of Eqs. (1)–(3) equal to the pre-calculated values. Besides, the band weights should be normalized as:

\[ P_1 + P_2 = 1 \]

The four known parameters are finally solved by the above four equations.

3.4. Generation of thermal scattering cross section

In the thermal energy region, the wavelengths of neutrons approach the size of molecules and the spacing of crystalline lattices. The target velocity will alter both the scattering cross sections and the secondary energy and angle distributions of scattered neutrons. The evaluations provide the thermal scattering law data of several bound molecules, such as hydrogen in water, graphite and beryllium. Different types of thermal scattering law can be processing by NECP-Atlas, e.g. coherent elastic scattering, incoherent elastic scattering and incoherent inelastic scattering. For the materials without thermal scattering law data, the free gas model is adopted to consider the effect of target thermal agitation on the secondary energy and angle distributions. The basic calculation methods are similar with the THERMR in NJOY.

3.5. Treatment of resonance elastic scattering

In the epithermal energy regions, it’s customary to neglect the motion of the target nuclei, and the classical asymptotic transfer kernel is used to calculate the secondary energy distribution of scattered neutrons. In this situation, neutrons always lose energy after colliding with the target. For the light nuclei, this assumption is valid, however, it is not the case for the heavy nuclei (Ouisloumen and Sanchez, 1991). After a neutron collides with...
the heavy nuclei in the epithermal energy region, it has a probability of gaining energy. Moreover, the heavy isotopes have resonance elastic scattering cross sections, which significantly increases the probability of gaining energy. Therefore, both the elastic scattering cross sections and transfer kernel should be Doppler broadened to incorporate the thermal agitation of target nuclei and the resonance elastic scattering. The Doppler broadening of elastic scattering cross sections is performed in the Doppler broadening module described in Section 3.2.

In NECP-Atlas, a new resonance elastic scattering kernel (RESK) processing module is developed to exactly Doppler broaden the transfer kernel to the desired temperature. In this module, the scattering kernels up to any Legendre order is exactly calculated for a series of incident neutron energies, and a precious interpolation method is developed to get the secondary energy and angle distributions at other incident energies. The details of RESK processing method used in NECP-Atlas will be introduced in another paper of the authors, because the present paper is intended to overview the main characteristics of NECP-Atlas.

3.6. Generation of multi-group cross section

The multi-group cross sections used in the deterministic transport calculation are generated by condensing the point-wise cross sections. The calculation of weighting spectrum is a crucial part affecting the accuracy of multi-group cross sections.

There are two energy spectrum calculation methods to take into account the self-shielding effect in NECP-Atlas. The Bondarenko model similar with that used in GROUPR module of NJOY is adopted to calculate effective cross sections in the energy regions where the resonance is narrow. For the RRR, a new point-wise neutron slowing-down spectrum calculation method is developed based on RESK, which can take into account the effect of neutron upscattering on the energy spectrum. The multi-group cross sections (such as fission and absorption cross sections) or resonance integral (RI) calculated using this spectrum are more accurate than those calculated using the conventional asymptotic scattering kernel. The details of the method will be described together with the RESK in another paper of the authors mentioned above.

### Table 2

<table>
<thead>
<tr>
<th>Enrichment (wt%)</th>
<th>Asymptotic k&lt;sub&gt;eff&lt;/sub&gt;</th>
<th>k&lt;sub&gt;eff&lt;/sub&gt; (pcm)</th>
<th>( \delta k_{\text{eff}} )</th>
<th>( \rho ) (pcm)</th>
<th>( \delta \rho / \rho (%) )</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>HZP</td>
<td>HFP</td>
<td>HZP</td>
<td>HFP</td>
<td>Asymptotic</td>
</tr>
<tr>
<td>0.71</td>
<td>0.66656</td>
<td>0.66076</td>
<td>−25</td>
<td>−85</td>
<td>−4.39</td>
</tr>
<tr>
<td>1.60</td>
<td>0.96140</td>
<td>0.95291</td>
<td>−35</td>
<td>−122</td>
<td>−3.09</td>
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<tr>
<td>2.40</td>
<td>1.09918</td>
<td>1.08953</td>
<td>−39</td>
<td>−137</td>
<td>−2.69</td>
</tr>
<tr>
<td>3.10</td>
<td>1.17679</td>
<td>1.16653</td>
<td>−40</td>
<td>−144</td>
<td>−2.29</td>
</tr>
<tr>
<td>3.90</td>
<td>1.23902</td>
<td>1.22831</td>
<td>−41</td>
<td>−148</td>
<td>−2.35</td>
</tr>
<tr>
<td>4.50</td>
<td>1.27416</td>
<td>1.26321</td>
<td>−40</td>
<td>−150</td>
<td>−2.27</td>
</tr>
<tr>
<td>5.00</td>
<td>1.29831</td>
<td>1.28719</td>
<td>−41</td>
<td>−150</td>
<td>−2.22</td>
</tr>
</tbody>
</table>

\( \delta k_{\text{eff}} \) is the k<sub>eff</sub> calculated using RESK minus that calculated using asymptotic kernel.

\[ \delta k_{\text{eff}} = k_{\text{eff}}^{\text{RESK}} - k_{\text{eff}}^{\text{asym}} \]

\[ \delta \rho / \rho = (\rho_{\text{RESK}} - \rho_{\text{asym}})/\rho_{\text{asym}} \]

### Table 3

<table>
<thead>
<tr>
<th>Enrichment (wt%)</th>
<th>Asymptotic k&lt;sub&gt;eff&lt;/sub&gt;</th>
<th>k&lt;sub&gt;eff&lt;/sub&gt; (pcm)</th>
<th>( \delta k_{\text{eff}} )</th>
<th>( \rho ) (pcm)</th>
<th>( \delta \rho / \rho (%) )</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>HZP</td>
<td>HFP</td>
<td>HZP</td>
<td>HFP</td>
<td>Asymptotic</td>
</tr>
<tr>
<td>0.71</td>
<td>0.66580</td>
<td>0.66000</td>
<td>−26</td>
<td>−72</td>
<td>−4.40</td>
</tr>
<tr>
<td>1.60</td>
<td>0.96107</td>
<td>0.95293</td>
<td>−45</td>
<td>−114</td>
<td>−2.96</td>
</tr>
<tr>
<td>2.40</td>
<td>1.09928</td>
<td>1.09021</td>
<td>−53</td>
<td>−131</td>
<td>−2.52</td>
</tr>
<tr>
<td>3.10</td>
<td>1.17727</td>
<td>1.16774</td>
<td>−57</td>
<td>−139</td>
<td>−2.31</td>
</tr>
<tr>
<td>3.90</td>
<td>1.23992</td>
<td>1.23006</td>
<td>−60</td>
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<td>4.50</td>
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<td>1.26531</td>
<td>−61</td>
<td>−148</td>
<td>−2.07</td>
</tr>
<tr>
<td>5.00</td>
<td>1.29964</td>
<td>1.28952</td>
<td>−62</td>
<td>−149</td>
<td>−2.01</td>
</tr>
</tbody>
</table>

NECP-Atlas can also realize the continuous-energy slowing-down spectrum calculation for 1D heterogeneous geometry, which is designed to generate the heterogeneous RI table, because previous researches have indicated that the heterogeneous RI table provides more accurate effective self-shielded cross sections than the conventional homogeneous RI table (Liu and Martin, 2016; Hong and Kim, 2011).

3.7. Transformation into different formats

The point-wise and multi-group cross sections obtained by the above processing procedures should be transformed into a specific format, before used by transport codes. At the present time, the point-wise cross sections and multi-group cross sections can be respectively transformed into ACE library and WIMS-D library by NECP-Atlas.

Besides, the NECP-Atlas is developed as a platform to research more accurate nuclear data processing methods. It has been connected with a new 3D whole-core high-fidelity transport code called NECP-X. NECP-Atlas can provide all the cross sections needed by NECP-X.

4. Verification of NECP-Atlas

4.1. Verification of the RESK processing method

The RESK processing is a new function in NECP-Atlas. Besides, an accurate continuous-energy slowing-down spectrum calculation method is developed based on the RESK to consider the impact of neutron upscattering on the multi-group cross sections. The performances of these methods are tested on UO<sub>2</sub> fuel Mosteller Doppler-effect benchmarks (Mosteller, 2006). Two different WIMS-D format libraries are generated by NECP-Atlas. In one library, the group-to-group scattering matrix, multi-group cross sections and RI are calculated using the conventional asymptotic scattering kernel; in another library, they are calculated using the RESK. The energy group structure is WIMS-D 69 group structure. DRAGON5 code is used to calculate the effective multiplication factors and fuel temperature coefficients (FTC) at Hot Zero
Power (HZP) condition (600 K) and Hot Full Power (HFP) condition (900 K). The FTC is calculated as follows (Lee et al., 2009):

\[
\rho = \left( \frac{1}{k_{\text{HFP}}^{\text{eff}}} - \frac{1}{k_{\text{HZP}}^{\text{eff}}} \right) \frac{1 \times 10^5}{\text{K}} \quad (\text{pcm/K})
\]

(5)

where FTC is denoted as \(\rho\), \(k_{\text{HZP}}^{\text{eff}}\) and \(k_{\text{HFP}}^{\text{eff}}\) are the effective multiplication factors at HZP and HFP, respectively; \(\Delta k\) is the variation of reactivity when the fuel temperature varies by 1 K, where a pcm (per cent mille) is one one-thousandth of a percent. The unit pcm/K means the variation of reactivity when the fuel temperature varies by 1 K, where a pcm (per cent mille) is one one-thousandth of a percent, i.e. \(10^{-5}\) K.

The impact of resonance elastic scattering kernel on effective multiplication factors and the FTC is given in Table 2. It can be seen that taking into account the resonance elastic scattering makes the values of effective multiplication factors more negative, and the values are reduced by about 150 pcm for HFP cases with high enrichments; and the RESK makes the FTC more negative by about 10%. The reason for the decrease of the effective multiplication factor and FTC is that the neutron upscattering effect makes more neutrons be absorbed by U-238. The differences of effective multiplication factor and FTC between two scattering kernels obtained by the work (Ouisloumen et al., 2015) are summarized in Table 3 for comparison. It can be seen that the differences of effective multiplication factor are comparable with those listed in Table 2. But for the FTC and its relative difference, the results listed in the two tables have larger bias. This is caused by the neutronics calculation codes. But the FTC values are consistently more negative in an order of 10%.

### 4.2. Verification of NECP-Atlas with WLUP benchmarks

The WLUP benchmarks are used to test the accuracy of NECP-Atlas. The calculated benchmarks are summarized in Table 4. In these problems, 64 nuclides are involved including 6 light nuclides, 48 nuclides appearing in cladding and 10 actinides. NECP-Atlas and NJOY2016 are respectively adopted to process different evaluations, and generate WIMS-D format libraries. The energy group structure is WIMS-D 69 group structure. DRAGON5 code is used to calculate the benchmarks.

In the generation of the libraries, the following modules in NECP-Atlas are used: Recon_calc, Broad_calc, Unres_calc, Therm_calc, Group_calc and WIMS_outp. The differences of results calculated using the libraries generated by NECP-Atlas and NJOY2016 are shown in Fig. 1. It can be seen that the results calculated using libraries from NECP-Atlas agree well with those calculated using libraries from NJOY2016. For all the cases, the absolute values of the difference are less than 40 pcm.

### 4.3. Verification of NECP-Atlas with ICSBEP benchmarks

32 ICSBEP benchmarks are calculated using ACE format libraries prepared by NECP-Atlas and NJOY2016. The calculated benchmarks are listed in Table 5. There are 59 nuclides involved in the calculations. The modules of Recon_calc, Broad_calc, Table_calc, 

![Graph showing difference between NECP-Atlas and NJOY2016 tested against WLUP benchmarks.](image)

**Fig. 1.** Difference between NECP-Atlas and NJOY2016 tested against WLUP benchmarks.
Therm_calc and ACE_outp in NECP-Atlas are tested. MCNP is adopted to perform transport calculations. Fig. 2 shows the difference between the two codes. The absolute value of the largest difference between the two codes is 26 pcm. In MCNP calculations, 50 thousand particles per batch, 2000 batches and 400 inactive batches are set to reduce the stochastic uncertainty. The stochastic uncertainties for all benchmarks are less than ±8 pcm.

Besides, in the above calculations, the probability table method is used to generate the ACE libraries. We also used the multi-band method to generate an ACE library based on ENDF/B-VII.0. The results of ICSBEP benchmarks calculated with the libraries respectively generated by multi-band method and probability table method are compared in Fig. 3. The absolute value of the largest difference between the two methods is 46 pcm.

4.4. Verification of the cross sections of fission product and actinide nuclides

In the above WLUP and ICSBEP benchmarks, tens of moderator, structure and actinide nuclides are tested. When the nuclear fuel is burnt in the reactor, there are hundreds of fission product and actinide nuclides born in the fuel. Therefore, the cross sections of these isotopes have been tested through burnup problems.

The TCWU08 problem in Marleau et al. (2018) is calculated, which is a homogeneous cell problem consisting of U-235 and H-1. NECP-Atlas and NJOY2016 are respectively adopted to generate WIMS-D format libraries, and there are 62 fission product nuclides and 23 actinide nuclides included in each library. The burnup chain is directly from the WLUP project (IAEA). The burnup calculation is carried out by DRAGON5. In the burnup calculation, the cell is burnt in the reactor for the 1000 days. The power is 60.0 kW/kg. Fig. 4 shows the values of effective multiplication factors at different time calculated using libraries prepared by NECP-Atlas and NJOY2016 based on various evaluations. The differences of effective multiplication factors calculated based on ENDF/B-VII.1 are displayed in Fig. 5. It can be seen that NECP-Atlas agrees well with NJOY2016 during the whole life, and the largest difference is about 7 pcm. Table 6 gives the relative differences of number densities of some isotopes calculated using the two libraries. It can be seen that the difference between NECP-Atlas and NJOY2016 is very small.
Moreover, VERA core physics benchmark (Godfrey, 2014) Problem #1B: 2D HZP BOC Pin Cell problem is calculated by a code package coupling Monte Carlo transport calculation and burnup calculation, to test the accuracy of ACE libraries for fission products and actinides. There are 279 nuclides involved in the calculations, and the nuclides are listed in Table 7. Figs. 6–10 compare the burnup calculation results between NECP-Atlas and NJOY2016. It can be seen that for ENDF/B-VII.1, ENDF/B-VII.0, CENDL-3.1, JEFF-3.2

Table 6  
Difference of number densities of TCWU08 benchmark based on ENDF/B-VII.1.

<table>
<thead>
<tr>
<th>Burnup (MWd/kgU)</th>
<th>NECP-Atlas</th>
<th>NJOY2016</th>
<th>Relative Difference (pcm)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>U-235</td>
<td>U-238</td>
<td>Pu-239</td>
</tr>
<tr>
<td>3</td>
<td>9.959E-01</td>
<td>8.688E-10</td>
<td>6.613E-13</td>
</tr>
<tr>
<td>12</td>
<td>9.836E-01</td>
<td>1.858E-01</td>
<td>1.701E-10</td>
</tr>
<tr>
<td>24</td>
<td>9.671E-01</td>
<td>7.879E-08</td>
<td>2.680E-09</td>
</tr>
<tr>
<td>42</td>
<td>9.425E-01</td>
<td>2.495E-07</td>
<td>2.502E-08</td>
</tr>
<tr>
<td>60</td>
<td>9.178E-01</td>
<td>5.190E-07</td>
<td>1.043E-07</td>
</tr>
<tr>
<td></td>
<td>I-135</td>
<td>Xe-135</td>
<td>Sm-149</td>
</tr>
<tr>
<td></td>
<td>I-135</td>
<td>Xe-135</td>
<td>Sm-149</td>
</tr>
<tr>
<td></td>
<td>I-135</td>
<td>Xe-135</td>
<td>Sm-149</td>
</tr>
<tr>
<td></td>
<td>I-135</td>
<td>Xe-135</td>
<td>Sm-149</td>
</tr>
</tbody>
</table>

Table 7  
Nuclides involved in VEAR-1B burnup calculations.

<table>
<thead>
<tr>
<th>Material types</th>
<th>Nuclides</th>
</tr>
</thead>
<tbody>
<tr>
<td>Moderator</td>
<td>H-1, O-16, B-10, B-11</td>
</tr>
<tr>
<td>Gap</td>
<td>H-4</td>
</tr>
</tbody>
</table>
and JENDL-4.0, the absolute value of the largest difference between NECP-Atlas and NJOY2016 is less than 40 pcm. In Monte Carlo transport calculations, 100 thousand particles per batch, 500 batches and 100 inactive batches are set to reduce the stochastic uncertainty. At each burnup step, the stochastic uncertainty is kept less than ±10 pcm.

5. Conclusions

A new nuclear data processing code called NECP-Atlas has been developed to study more accurate nuclear data processing methods. The code can process the widely used evaluated nuclear data files: ENDF/B-VII.1, ENDF/B-VII.0, CENDL-3.1, JEFF-3.2 and JENDL-4.0, and generate WIMS-D and ACE format library. Besides, some new processing methods have been implemented into the code such as the functions to treat the resonance elastic scattering cross sections and to generate multi-band parameters in unresolved resonance region. This paper describes the methods used in NECP-Atlas and its verification. The numerical results show that NECP-Atlas has comparable accuracy with NJOY2016. NECP-Atlas is competent to provide cross sections for deterministic and Monte Carlo transport calculations.

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References


