Generation of Cross Section Library for Lattice Physics Code, AEGIS

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Abstract

This paper describes generation of cross section library (AELIB) for lattice physics code, AEGIS. Furthermore, an issue of the NJOY code that has considerable impact on multi-group scattering matrix in thermal energy range is pointed out and its solution is provided.

KEYWORDS: AEGIS, AELIB, NJOY, XMAS, Ultra fine energy group, ENDF/B-VI, ENDF/B-VII, JENDL3.3

1. Introduction

AELIB is a dedicated cross section library for the lattice physics code, AEGIS. [1]-[4] The present paper is devoted to describe various aspects of AELIB, including cross section processing, post-processing and a related topic that is identified through generation and validation of AELIB.

Accuracy of a lattice physics code is mainly dominated by a neutron flux solver and a cross section set. Recent advances in a neutron flux solver, especially incorporation and improvement of the method of characteristics (MOC) in lattice physics calculations, significantly reduce prediction uncertainty of the spatial and energy distribution of neutrons in an assembly. Therefore, accuracy of the cross section library of the lattice physics codes are becoming crucial.

The major lattice physics codes used in the production calculations have their own cross section libraries. Since generation of a cross section library requires many resources (both manpower and computational capability), improvement of the cross section library is a considerable work. Especially, modification (extension) of library, e.g. improvement of resonance parameter representation, would be troublesome since cross section processing modules in lattice physics codes generally depends on their particular cross section library formats.

The above discussion suggests that architecture of the cross section library is important. Since AELIB is designed from scratch, various considerations from the view point of accuracy, extensibility, versatility and maintainability are taken into account.

Major features of AELIB are summarized as follows:

· 172 XMAS energy group structure [5],[6]
· Major heavy nuclides are come from latest releases of evaluated nuclear data files, i.e. ENDF/B-VII(beta0)[7], ENDF/B-VI(R8) or JENDL3.3
· Minor heavy nuclides are come from
· Other nuclides (e.g., moderator or structural material, burnable absorber) are mainly come from ENDF/B-VI(R8)

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· Number of heavy nuclides: 43
· Number of fission product nuclides: 193
· Number of other nuclides: 194
· Applicable to both U-Pu and Th-U cycles analysis
· Applicable to various burnable absorber chain, i.e., Cd-In, Eu-Gd, Gd-Tb, Er-Tm and Hf
· Thermal cut-off energy: 4.0eV
·Maximum order of anisotropic scattering: P3
·Temperature and self-shielding correction tables have dependency not only on one-dimensional cross sections (e.g. σt, σa) but also on scattering matrix.
·Incorporation of (n,2n), (n, 3n), (n, 4n) and other similar reactions
·Index library system, which has independent cross section file for each nuclide, is adopted
·Ultra fine energy group cross sections (32,000 groups) is prepared for continuous energy deterministic spectrum calculation in resolved energy range.

A cross section library for a lattice physics code should handle large amount of cross section data. Though storage restriction was severe in decade years ago, current computer has large hard-drive with order of dozens or hundreds giga-bytes. Therefore, restriction on computer storage is significantly relaxed. One of the primary decision in the cross section library generation is the number of nuclides included. In common lattice physics calculation, number of nuclides greatly depends on the design of burnup chain that handles fission product and heavy nuclides. Detailed modeling of heavy and fission product nuclides is desirable for accurate calculation. In particular, detailed treatment of fission product nuclides is desirable to eliminate the presence of "pseudo fission product" nuclide(s). From this view point, 193 fission product nuclides are processed and stored in AELIB. The 193 nuclides almost cover fission products that have evaluated nuclear data file such as ENDF or JENDL.[8] Number of nuclides for heavy isotopes is also important from the view point of calculation accuracy and versatility. For example, ^{232}Th and ^{233}U is necessary for Th-U cycle analyses, which is recently paid more attention due to its higher non-proliferation nature. Higher minor actinides, e.g., Am or Cm, is important for transmutation and MOX fuel analyses. Currently, 43 heavy nuclides from ^{230}Th to ^{253}Cf are prepared in AELIB. Detailed treatment of fission product and heavy nuclides is also important from the viewpoint of source term (e.g., gamma or neutron source) intensity calculations. The source term analysis is becoming more important for the high burnup and MOX fuels.

Number of library energy groups has major impact on the calculation accuracy. Though various energy structure has been developed, the 172 XMAS energy group structure is adopted in AEGIS. The XMAS energy group structure has been mainly optimized for LWR analysis, it is main application area of the AEGIS code. Recently, Hfaiedh and Santamarina proposed the SHEM structure of 281 energy groups.[9] The SHEM energy group structure is mainly intended to reduce error of resonance calculations. Since AEGIS utilizes more fine energy group structure for resonance calculation, the SHEM energy group structure was not adopted from the viewpoint of computational efficiency.

Treatment of effective resonance cross section is one of the major topics in lattice physics calculation. Various approaches can be adopted, e.g., the equivalence theory, subgroup and fine energy group treatment. In the AEGIS code, "continuous energy" spectrum calculation is carried out with the ultra-fine energy group structure (32,000 groups, from approximately 10keV-0.1eV). By adopting this approach, accurate estimation of effective resonance cross section can be carried out. Furthermore, resonance overlapping effect can be directly taken into account by the ultra-fine energy group calculations. Though cross section data for the ultra-fine energy group structure is considerably large, *all* nuclides (over 400 nuclides) in

AELIB have their own ultra-fine energy group cross sections. Consequently, resonance overlapping effect can be accurately taken into account not only among heavy nuclides but also among heavy and fission product nuclides. For unresolved resonance region, the equivalence theory with the NR approximation is applied. Unlike the WIMS-type library, AELIB does not have the particular energy range of "resonance energy region". It means that the self-shielding table is prepared for all energy range. Therefore, accurate resonance treatment can be carried out mainly for light nuclides, whose resonance energy region is higher than heavy nuclides.

Many current lattice physics codes approximate the anisotropic scattering through the transport corrected P0 cross sections. Though the transport corrected cross section performs well for UO2 fuels, its accuracy degrades in MOX fuels. Recent study on anisotropic scattering reveals that the transport correction may have a few hundreds pcm discrepancy in reactivity prediction. Anisotropic scattering up to P3 component would be necessary for accurate analysis of MOX fuels.[10] Therefore, more than 20 nuclides, which are mainly moderator and structural materials, have anisotropic scattering data up to P3 in AELIB. Note that self-shielding and temperature dependent tables are prepared not only for one dimensional cross section (e.g. σ_t, σ_a, σ_f) but also for scattering matrix including anisotropic scattering.

Since nuclear data library is continuously updated taking into account recent measurement and theoretical predictions, utilization of latest revision of nuclear data file is important. From this viewpoint, data for the major heavy nuclides in AELIB are generated from the latest nuclear data files, i.e., ENDF/B-VII (beta0), ENDF/B-VI(R8) and JENDL3.3. Since improved resonance parameter is adopted for ^{238}U of ENDF/B-VII(beta0), negative reactivity bias of ENDF/B-VI(R8) generally found in thermal reactor analyses is expected to be resolved. [11]

The choice of the thermal cut-off energy has considerable impact on calculation accuracy especially in MOX fuels. In AELIB, 4eV is chosen as the thermal cut-off energy; it is sufficient for LWR analyses including MOX fuels.

Many lattice physics codes have an integrated cross section library that contains all cross section data in it. However, the authors believe that the integrated cross section library has difficulties from the viewpoint of maintainability and extensibility. Therefore, AELIB adopts the index library system, in which a nuclide has independent cross section data file. An index (directory) file is used to manage many cross section data file. This approach is used in MCNP and MVP.[12],[13]

In the following sections, detail discussion on generation of AELIB will be provided.

2. Generation of Cross Section Library for AEGIS (AELIB)

2.1 Overview

Cross section sets in AELIB are generated by the following procedures:

(1)Generation of multi-group cross section set by NJOY [14]

(2)Post-processing of NJOY results to generate AELIB

Since total number of nuclides in AELIB is large (over 400 nuclides), its generation is a considerable task. Manual executions of NJOY and related post-processings are not desirable from the viewpoint of workload and quality control. Actually, more than 1500 NJOY executions are necessary to make AELIB, i.e., more than one thousand NJOY input data should be prepared with adequate quality control. Therefore, an automated processing system is developed and used to generate AELIB as will be described in the latter section.

2.2 Processing by NJOY

The NJOY code is a de-facto processing system of nuclear data file that are developed and maintained by LANL. Though various versions of NJOY have been released, NJOY(99.67) with dedicated patch for JENDL 3.3 is utilized throughout generation of AELIB.

The following modules are used to generate AELIB: MODER, RECONR, BROADR, UNRESR, THERMR, GROUPR and MATXSR. Several modules are available to output multi-group cross section set in the NJOY code. For example, the WIMSR module is frequently used in the LWR analysis. Though the WIMSR module gives a very compact multi-group cross section set, it also has some restrictions to reduce size of the cross section set:

· Energy range is classified into three, i.e., fast, resonance and thermal. In the fast energy range (typically > 10keV), dependences on background cross section and temperature are not taken into account. For thermal energy range (typically < 4eV), dependence on background cross section is not considered, i.e., no (or fixed) self-shielding effect is taken into account. The present restriction is not adequate for nuclides that have resonance in fast or thermal energy range.
· Anisotropic scattering cross section up to P1 component is treated.
· Self-shielding table is prepared only for one-dimensional cross section, e.g. σ_t, σ_a and σ_s. No self-shielding table is generated for scattering matrix; fixed background cross section is assumed in the NJOY processing.

The above limitations are fairly appropriate for current LWR analyses, but have potential impact in analyses of advanced LWR. For example, higher order anisotropic scattering have considerable effect on MOX fuel analysis in which anisotropy of neutron flux is significantly larger than current UO2 fuels. Therefore, the MATXSR module was applied to output cross sections for AELIB since the MATXSR format does not have the above limitations.

In GROUPR module of NJOY, the narrow resonance (NR) approximation or spectrum calculation based on slowing-down equation can be used to compute effective cross section. Though computation time of the NR approximation is short, its accuracy is generally inferior to that of the spectrum calculator. Therefore, the spectrum calculator is used throughout the generation of AELIB. Note that several input data for the GROUPR module of NJOY should be carefully chosen. For example, maximum number of computed flux points (NFLMAX) should be large enough to cover detailed energy representation of resonance region for heavy nuclides in latest nuclear data evaluation. When the choice of NFLMAX is too small, the NR approximation is automatically used even for the part of resolved energy range.

During the processing and generation of AELIB, an issue of NJOY, which is related to the accuracy of scattering matrix in thermal energy range, was found. This topic will be discussed in the latter section.

2.3 Generation of AELIB

Since MATXSR in NJOY is a general purpose module, it provides cross sections for individual reactions. On the other hand, the AEGIS code requires conventional one- and two-dimensional cross sections typically used in the transport code, i.e. σ_t, σ_a, σ_f, σ_c, σ_{n2n}, $\nu\sigma_f$, χ and σ_s. Therefore, a post-processing code is developed to convert the MATXSR format to AELIB.

In MATXSR, various absorption reaction is independently treated, e.g. (n,γ), (n,f), (n, p), (n, d), (n, t), (n, α). These reactions are summed up to obtain σ_a. Since fission matrix is given in MATXSR, the following equations are used to obtain ν (neutron production per fission) and χ (fission spectrum) values:[14]

$$\nu_g = \sum_{g'} \sigma_{fg\to g'} / \sigma_{fg} \tag{1}$$

$$\nu_g^{SS} = \nu_g + \nu_g^D \tag{2}$$

where,

ν_g : number of prompt neutrons generated by a fission,

$\sigma_{fg\to g'}$: fission matrix,

σ_{fg} : total fission cross section,

ν_g^{SS} : total number of neutrons generated by a fission,

ν_g^{D} : number of delayed neutrons generated by a fission.

$$\chi_g^{SS} = \frac{\sum_{g'} \sigma_{fg'\to g}\phi_{g'} + \chi_g^D \sum_{g'} \nu_{g'}^D \sigma_{fg'}\phi_{g'}}{\sum_{g}\sum_{g'} \sigma_{fg'\to g}\phi_{g'} + \sum_{g'} \nu_{g'}^D \sigma_{fg'}\phi_{g'}} \tag{3}$$

$$\chi_g^D = \sum_i \chi_{ig}^D \tag{4}$$

where,

χ_g^{SS} : fission spectrum (including prompt and delayed neutrons),

χ_g^{D} : fission spectrum of delayed neutrons,

χ_{ig}^{D} : fission spectrum of delayed neutrons of *i*-th group,

ϕ_g : scaler (total) neutron flux.

For scattering cross section, elastic and inelastic scattering cross sections are summed up. Note that break-up reactions are also taken into account.

In the AEGIS code, effective cross sections in the resonance region can be calculated in two different methods. The first one is a conventional approach based on the equivalence theory and the narrow resonance (NR) approximation. This method is always applied to the unresolved energy range. Since the equivalence theory may cause considerable error in the effective cross section evaluation, the alternative method can be utilized in the AEGIS code. In the second method, ultra-fine (point-wise) energy group spectrum calculation is carried out in heterogeneous geometry, e.g. pincell, then the effective cross section is generated using the fine energy spectrum. Furthermore, errors due to energy collapsing (point-wise to 172 XMAS group structure) is mitigated by reactivity equivalence approach using the SPH method.[4]

AELIB has cross section data that is necessary to perform ultra-fine energy group calculations. The ultra-fine energy group cross sections are generated by fitting the results of the BROADR module to a union energy grid that has about 32,000 energy points. Number of energy grid points is chosen based on some sensitivity calculations and energy range from 10keV to 0.1eV are divided in detail. Major one-dimensional cross sections including elastic scattering are edited for all nuclides in AELIB.

2.4 Automated AELIB generation system

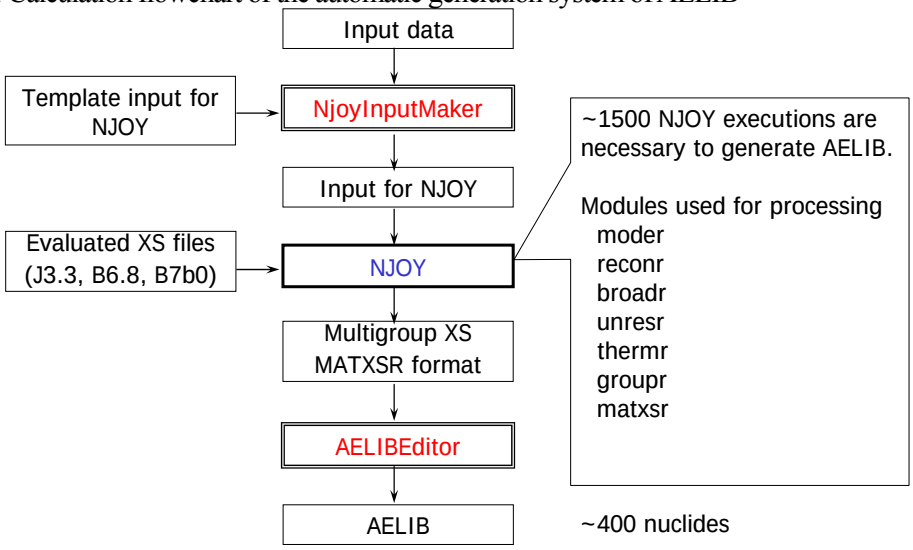
More than 400 nuclides are processed to generate AELIB. Therefore, an AELIB generation system, which automatically generates NJOY inputs and manages successive post processing using minimum user input, was developed and used to generate AELIB. Calculation flowchart of the system is shown in Fig.1. The `NjoyInputMaker` code generates input data of NJOY by using small user input that contains the following information:

· Nuclide identification name in AELIB
· Upper energy boundary of resolved energy range
· Potential scattering cross section
· Order of anisotropic scattering

· Temperature points
· Background cross sections

Not only the input data of NJOY, but also the execution shell is automatically generated by `NjoyInputMaker`. The NJOY code is executed using the automatically generated shell. A calculation result of NJOY is dumped into a file of the MATXS format. The `AELIBEditor` code performs post-processing of the NJOY results as shown in the previous section and generates AELIB, which is a binary file of a particular format. Note that the `AELIBEditor` code can generate AELIB not only from the NJOY result, but also from input data. For example, some of the fission product nuclides which have short half life are defined as a "dummy" nuclide with zero cross section, i.e. only decay is considered for these nuclides. In such a case, zero cross section is given from input file. Since an ideal nuclide that has particular multigroup cross section can be defined, a multi-group benchmark calculation, in which given cross section is used, can be easily analyzed. Note that approximately two CPU days are necessary to generate whole set of AELIB using a common PC.

Figure 1: Calculation flowchart of the automatic generation system of AELIB



3. Improvement of Scattering Matrix in Thermal Energy Range

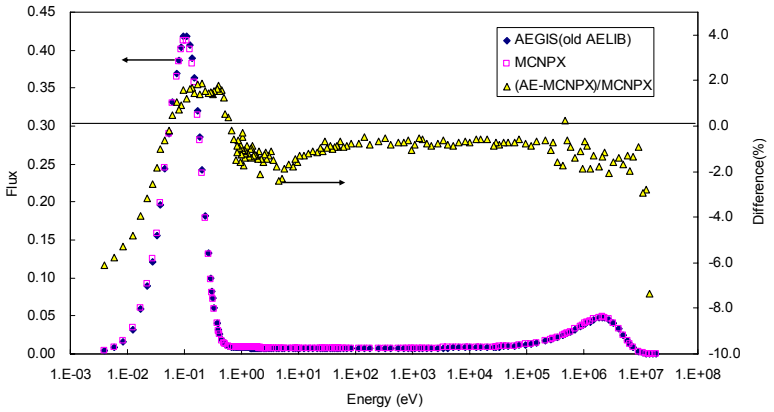
3.1 Discrepancy of Neutron Spectrum in Thermal Energy Range

After the completion of the AELIB generation, various verification calculations are carried out in order to confirm the validity of the newly generated AELIB. The verification calculations in primary stage were mainly carried out by comparison with the continuous-energy Monte-Carlo code, MCNPX(2.5.0). [15] Since point-wise cross section library for the MCNPX code can be generated by NJOY, it was quite useful to check validity of AELIB.

Throughout preliminary comparisons, considerable difference in neutron spectrum in thermal energy range was observed between MCNPX and AEGIS. Further investigation about this issue clarifies that this discrepancy can be found in very simple problem. Figure 2 shows comparison of neutron flux in a homogeneous system of H (free-gas) and ^{235}U (H/U=10^8) at 600K. A systematic bias is observed in thermal energy region.

Since ^{235}U is highly diluted, ^{235}U has very small impact on neutron flux in thermal energy range. Therefore, root cause of the observed discrepancy was presumed to be cross section of H (free-gas) in AELIB.

Figure 2: Difference of neutron spectrum in H+^{235}U homogeneous system (old AELIB)



3.2 Accuracy in Scattering Matrix of NJOY in Thermal Energy Range

Further investigation on this issue clarified that the above difference comes from scattering matrix of H (free gas) in the thermal energy range, which is obtained by NJOY. Namely, the post-processing code for AELIB did not contribute the above difference. Difference of scattering matrix between AELIB (NJOY) and analytical value in 172 XMAS energy group is shown in Fig.3. Note that analytical value of the scattering matrix is obtained through analytical expression (error function, ERF) of energy transfer function on H (free gas):

$$\sigma(E \to E') = \frac{\sigma}{E}\exp\left(\frac{E-E'}{kT}\right)erf\left(\sqrt{\frac{E}{kT}}\right) \qquad \text{(up-scattering, i.e. } E' > E\text{)} \qquad (5)$$

$$\sigma(E \to E') = \frac{\sigma}{E}erf\left(\sqrt{\frac{E'}{kT}}\right) \qquad \text{(down-scattering, i.e., } E' < E\text{)} \qquad (6)$$

where, *erf* is the error function.

Figure 3 clearly shows that scattering matrix obtained by NJOY (i.e. AELIB) has considerable error. By reducing the difference, discrepancy on neutron spectrum in thermal energy range will be reduced.

3.3 Improvement of NJOY

In the GROUPR module of NJOY, a special scheme is adopted for interpolation of scattering matrix in the thermal energy range. Since interpolation error was the main cause of the above difference, more detailed energy grid is implemented in the THERMR modules of NJOY. The original implementation, 59 energy grid points (egrid) are used to cover thermal energy range (<5.1eV) in the THERMR module. Through several preliminary calculations, the number of energy grid points was increased from 59 to 349. Note that each original energy grid is subdivided into six energy grids assuming constant lethargy width. For example, the lowest energy grid, whose energy range is from 1.0×10^{-5} to 1.78×10^{-5}eV, is subdivided into 1.0×10^{-5}, 1.10×10^{-5}, 1.21×10^{-5}, 1.33×10^{-5}, 1.47×10^{-5}, 1.62×10^{-5}, 1.78×10^{-5} eV.

Figure 4 indicates that improvement of the accuracy of scattering matrix by the subdivision of incident energy grid. Difference of scattering matrix of H in AELIB becomes smaller when the finer (revised) incident energy grid is used.

Figure 3: Difference of scattering matrix of H (from group 95, 3.30-2.77eV) between AELIB (AE) and analytical value obtained by the error function (ERF)

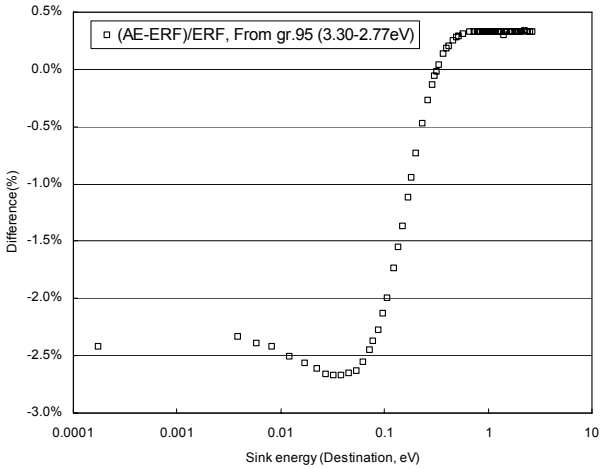
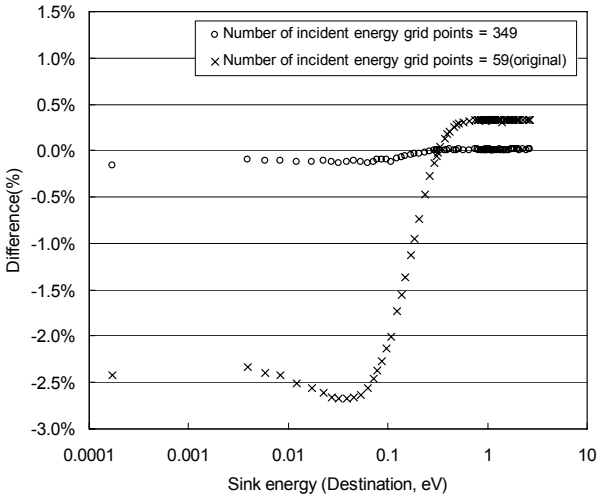


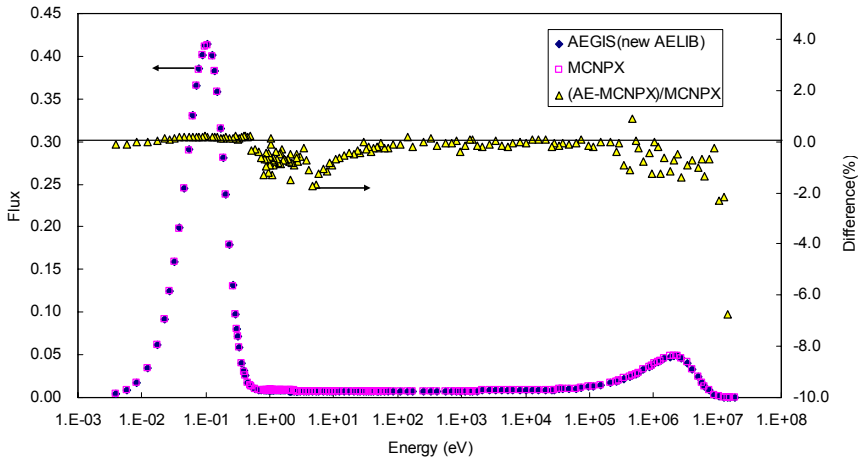
Figure 4: Difference of scattering matrix of H (from group 95, 3.30-2.77eV) between AELIB and analytical value obtained by the error function (ERF)



Comparison of neutron spectrum between AEGIS using the modified AELIB and MCNPX are shown in Fig.5. From Fig.5, discrepancy between the two codes are reduced and both codes show good agreement.

The above modification is incorporated into the production version of AELIB.

Figure 5: Comparison of neutron spectrum in H+^{235}U homogeneous system (modified AELIB)



4. Concluding Remarks

In this paper, AELIB, which is a cross section library of the lattice physics code, AEGIS, is described in detail. Design concept of AELIB is accuracy, extensibility, versatility and maintainability. These concepts are realized through detailed treatment of heavy and fission product nuclides, utilization of ultra-fine energy group calculations for effective resonance cross section, the index library system and so on.

For cross section processing, the NJOY code is adopted. Since large number of NJOY executions and post-processing of the NJOY results are necessary, a dedicated system to generate AELIB has been newly developed.

Through the verification calculations of AELIB, an issue of the thermal scattering cross section generated by the NJOY code was identified. This issue is resolved by utilization of finer incident energy grid (egrid) that is hardwired in the NJOY code. By implementing the present modification, difference of neutron spectra between AEGIS and MCNPX code becomes small.

More detailed verification results of the AEGIS code with AELIB is presented in the companion paper.[16]

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