

## Calculation Models of AEGIS/SCOPE2, a Core Calculation System of Next Generation

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### Abstract

This paper provides calculation models of AEGIS/SCOPE2, a core calculation system of next generation. This paper especially focuses on the resonance calculation method of the AEGIS code, which has not been published yet. In the AEGIS code, effective cross sections in resonance region are generated from ultra-fine-group calculations utilizing tabulated collision probabilities for square pin-cells. In addition, the SPH method in the energy domain is used to preserve reaction rates in the energy-collapsed multi-group calculations. The validity of the resonance calculation method of the AEGIS code is verified through the comparison with the continuous energy Monte-Carlo calculation in pin-cell geometry.

**KEYWORDS:** *AEGIS, MOC, Resonance, Ultra-fine-group, Collision probability, SPH method*

### 1. Introduction

The evolution of the fuel assemblies brings the highly spatial heterogeneity of neutronics properties in the commercial LWRs. Furthermore, the concept of advanced fuel assemblies of Generation-IV reactors are more complicated [1] and their neutronics properties will be more heterogeneous. In order to accurately compute such highly heterogeneous cores, AEGIS/SCOPE2, a core calculation system of next generation, is being developed by NEL and NFI in cooperation with Nagoya University.

The AEGIS code [2] is a two-dimensional (2-D) multi-group lattice physics code based on the method of characteristics. [3] The effective cross sections are generated by ultra-fine-group calculation. The SCOPE2 code is a core analysis code based on multi-group pin-by-pin nodal SP3 transport theory. [4] Although the load of pin-by-pin transport calculation in three-dimensional full core geometry is considerably heavy, the SCOPE2 code achieves practical calculation time by the use of efficient numerical algorithms and parallel computing. In the AEGIS/SCOPE2 system, the AEGIS code generates pin-wise multi-group cross sections. The SCOPE2 code takes over them and carries out core calculations.

The overview of the AEGIS/SCOPE2 system is described in Sec. 2. In Sec.3, the resonance calculation method in the AEGIS code, which has not been published yet, is described in details.

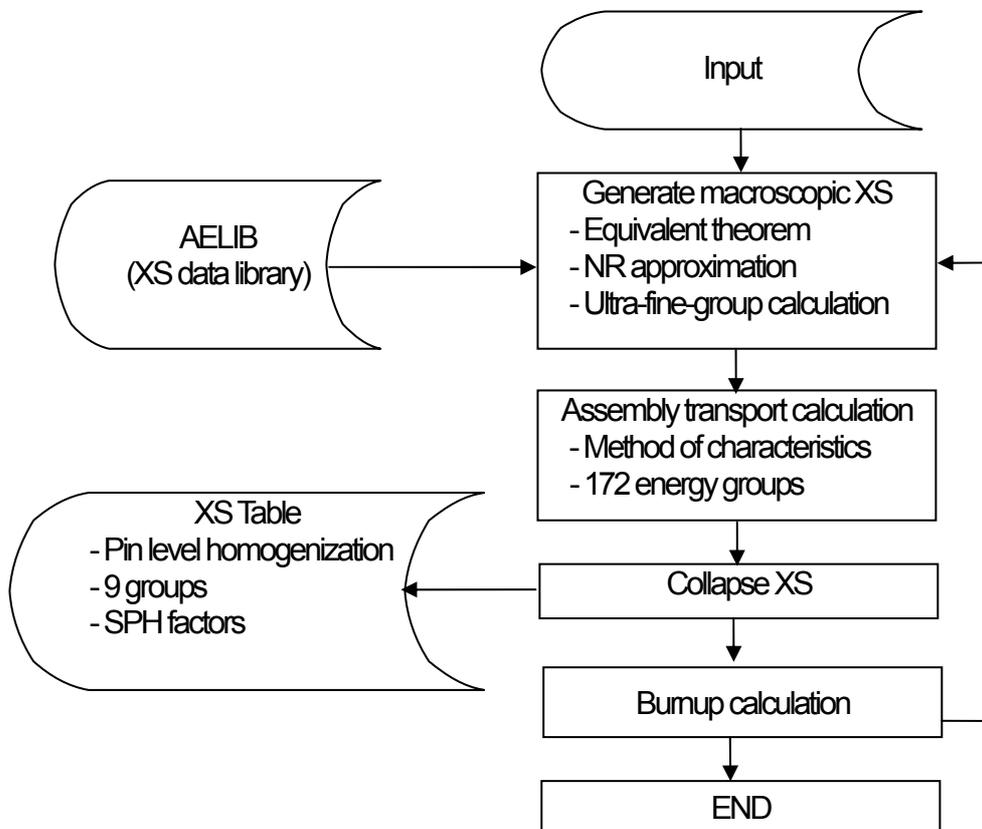
## 2. Overview of AEGIS/SCOPE2

### 2.1 AEGIS code

Fig.1 shows the calculation flow of the AEGIS code. The AEGIS code has a dedicated cross section library named AELIB,[5] which is based on a multi-group cross section set generated by the NJOY code. [6] The major features of AELIB are as follows:

1. 172 XMAS energy group structure[7]
2. Number of heavy nuclides: 43
3. Number of fission product nuclides: 193
4. Number of other nuclides: 194
5. Data are come from ENDF/B-VI(R8). For some major nuclides, the data based on ENDF/B-VII(bata0) or JENDL3.3 are available.
6. Maximum order of anisotropic scattering: P3
7. Temperature and self-shielding correlation table not only for one-dimensional cross section set (e.g.,  $\sigma_t$ ,  $\sigma_a$ ) but also for scattering matrix.

**Figure 1:** Calculation flowchart of the AEGIS code



The effective cross sections for the unresolved energy region are evaluated by the equivalent theorem and the NR approximation. For the resolved energy region, effective cross sections are evaluated by ultra-fine-group (32000 groups) calculations. For each fuel type in a fuel assembly, Ultra-fine-group calculations are carried out three times, i.e., with large, medium, small moderator regions. Effective cross sections are interpolated from these results by the position dependent Dancoff factor of each fuel pin. The ultra-fine-group calculation method is described in the next section.

Using these effective cross sections, 172-group transport calculations in fuel assembly geometry are carried out. In these transport calculations, the AEGIS code can reduce computation time by utilizing various symmetry of target geometry, e.g., half, quarter, octant symmetry.

After 172 groups transport calculations, the AEGIS code collapses the cross sections into 9 energy groups in each pin-cell region and generates SPH factors for core calculations by the SCOPE2 code.

## 2.2 SCOPE2 code

Fig.2 shows the calculation flow of the SCOPE2 code. The SCOPE2 code uses a tabulated cross section library which is prepared from the results of the AEGIS calculation. The main features of the SCOPE2 code are as follows:

### Neutronics/thermal hydraulic models

1. 9 energy groups (variable)
2. Complete 3-dimensional pin-by-pin calculation (SP3 nodal transport theory)
3. Reduction of space homogenization errors with the SPH method
4. 1-group acceleration based on generalized coarse mesh rebalance (GCMR)
5. Macroscopic or Microscopic burnup model can be selected
6. Reconstruction of cross sections from tabulation using a variety of indexes.
7. Intra-node burnup distribution
8. Quarter assembly-wise closed channel model or Thermal mixing model between sub-channels

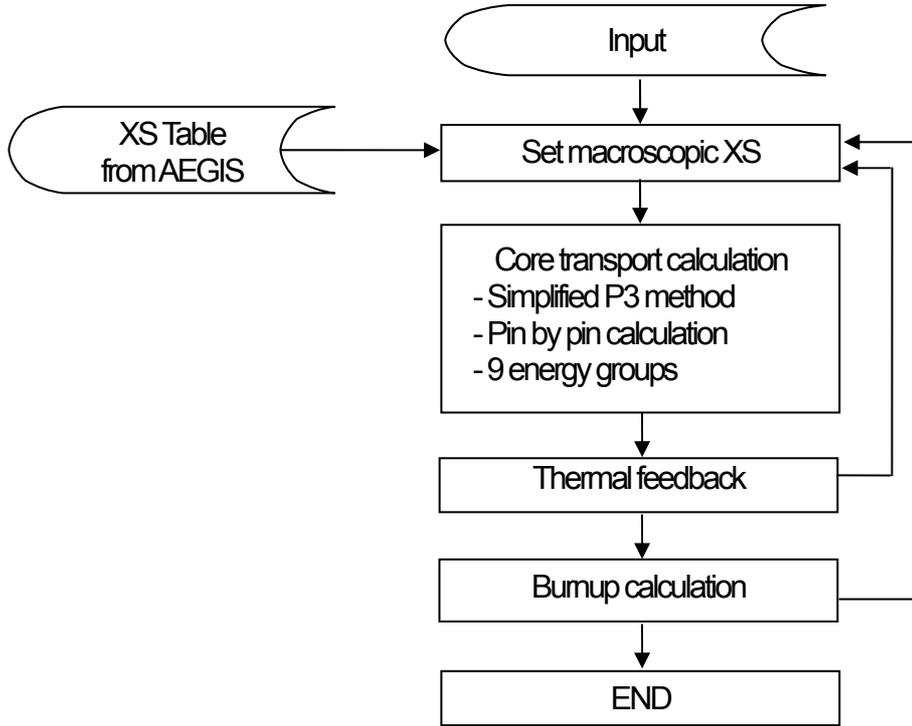
### Computing model

1. Red/Black iterative solver with a fine-grain parallel mode
2. 2D domain decomposition for distribution of work load to processors
3. Identical solution with serial execution regardless the number of processors
4. Efficient handling of restart files with parallel I/O mechanism

The SCOPE2 code is designed and implemented for the use in reload core design; it must give the solution within reasonable computing time. In order to accomplish the requirements, a number of acceleration techniques are adopted including parallel computing. Data structure in SCOPE2 that is carefully derived helped us implement parallel algorithm very efficiently with the help of a template library in the C++ language.

Parallel computing is established based on the MPI (Message Passing Interface), a de-facto standard specification for message passing mechanism. SCOPE2 runs on any parallel environments where a MPI implementation is available such as Linux-powered PCs or parallel super computers. Typical computing time for a set of depletion calculation of a commercial PWR is a few hours using 24 processors or more. Since the scalability of SCOPE2 is quite good, the less computation time is expected with more processors at least up to a hundred processors.

**Figure 2:** Calculation flowchart of the SCOPE2 code



### 3. Resonance calculation of AEGIS

In the AEGIS code, the neutron spectrum calculation in ultra-fine energy group structure is adopted to calculate effective resonance cross sections. In order to realize practical calculation time and accuracy, various methods are examined. Consequently, the tabulated collision probability method for square pin-cell geometry is selected to estimate spatial flux distribution. Furthermore, in order to eliminate errors due to energy collapse of cross sections, the reactivity equivalence approach using the SPH factor is used. [8] The SPH method has been traditionally used to mitigate spatial homogenization errors. However, the SPH factor is also valid to mitigate errors caused by energy collapse of cross sections.

#### 3.1 Ultra-fine-group calculation

The spectrum calculation of the AEGIS code utilizes the following slowing-down equations to calculate the scattering neutron source in each flat flux region.

$$Q_h = \sum_{k=1}^{h-1} \sum_{g=1}^{h-1} \int_{E_h}^{E_{h-1}} f(E) \frac{dE}{(1 - \alpha_k) E_g} \Sigma_S^{k,g} \psi^g \quad (1)$$

$$f(E) = \begin{cases} 1 & : \alpha_k E_g < E < E_g \\ 0 & : E < \alpha_k E_g \end{cases}, \quad \alpha_k = ((A_k - 1)/(A_k + 1))^2 \quad (2)$$

$Q_h$  : Scattering source of group  $h$        $\Sigma_S^{k,g}$  : Scattering cross section of isotope  $k$ , group  $g$

$\psi_g$  :Neutron flux of group  $g$                        $E_g$  :Lower energy boundary of group  $g$   
 $A_k$  :Mass number of isotope  $k$

Elastic scattering in resonance energy region is assumed in Eq. (1). Neutron flux distribution in each ultra-fine-group is calculated by assuming slowing-down neutron in each region as a fixed source. In the AEGIS code, several options to evaluate spatial flux distribution are available:

- Option 1 : MOC. It is enable to treat not only isotropic but also anisotropic scattering by expanding the scattering source by spherical harmonics. However, it should be noted that the scattering angle and the loss of neutron energy are calculated separately, i.e., the correlation between a scattering angle and a loss of neutron energy is ignored.
- Option 2 : The collision probability method utilizing cylindrical approximation and white boundary condition. Collision probabilities are directly computed in each energy group.
- Option 3 : The tabulated collision probability method. Collision probabilities are computed in square pin-cell geometry by the ray tracing method. Since it takes considerable computation time, the tables of collision probabilities are generated before the ultra-fine-group calculation. It takes several seconds.

The accuracy and computation time of above mentioned options were compared in pin-cell geometry. The fuels are UO<sub>2</sub> (<sup>235</sup>U=5.0%) and MOX (10%Pu<sup>total</sup>). The results are shown in Table 1. Table 1 summarizes the relative differences of effective cross sections between each option and the continuous energy Monte-Carlo code, MVP. [9] The same cross section library (ENDF/B-VI(R8)) was used in both AEGIS and MVP codes. The statistical error of the effective cross section obtained by the MVP calculations is less than 0.05%. The energy groups in Table 1 (i.e., 69, 75, 80 and 88) include a giant resonance peak of <sup>238</sup>U in their energy ranges.

**Table 1:** Comparison of macroscopic absorption cross section and calculation time

Gr.	Energy (eV)		Difference of $\Sigma_a$ obtained by MVP (%)									
			UO2				MOX					
			MOC (P3)	MOC (P0)	C.P. (Cylindrical)	Tabulated C.P. (Square)	MOC (P3)	MOC (P0)	C.P. (Cylindrical)	Tabulated C.P. (Square)		
	Upper	Lower										
69	67.90	55.60	0.3	0.3	1.3	0.1	0.2	0.2	1.0	0.1		
75	37.27	33.72	0.5	0.5	1.5	0.5	1.2	1.1	2.5	1.0		
80	22.60	19.45	1.1	1.1	2.4	1.0	1.1	1.0	2.2	1.0		
88	7.52	6.16	0.3	0.2	1.6	0.2	0.2	0.2	1.5	0.1		
	Calculation time		9 hours	9 hours	1 min.	1 min.	9 hours	9 hours	1 min.	1 min.		

We can obtain the following observations from the results:

1. Comparing the results of MOC(P3) with that of MOC(P0), the effect of the anisotropic scattering is not very large. The isotropic scattering approximation is enough valid to estimate effective cross section in resonance region. However, it should be noted that the present P3 calculation is approximation as mentioned above. If we can exactly treat anisotropic scattering, the difference between MOC(P3) and MVP may be smaller.
2. The difference of collision probability using cylindrical approximation is larger than other methods. On the other hand, the accuracy of the tabulated collision probability

method is equivalent to MOC. Exact treatment of geometry is important in resonance calculation.

3. In the viewpoint of calculation time, both of the collision probability methods are superior to MOC.
4. The tabulated collision probability method is best among these methods in the viewpoint of both accuracy and calculation time.

In the case of the tabulated collision probability method, the bottleneck of computation time is the scattering source calculation, especially scattering by hydrogen. In order to further reduce the calculation time, an approximated treatment of scattering source in moderator regions and the grouping of scattering nuclides were examined. The details are described in the following section.

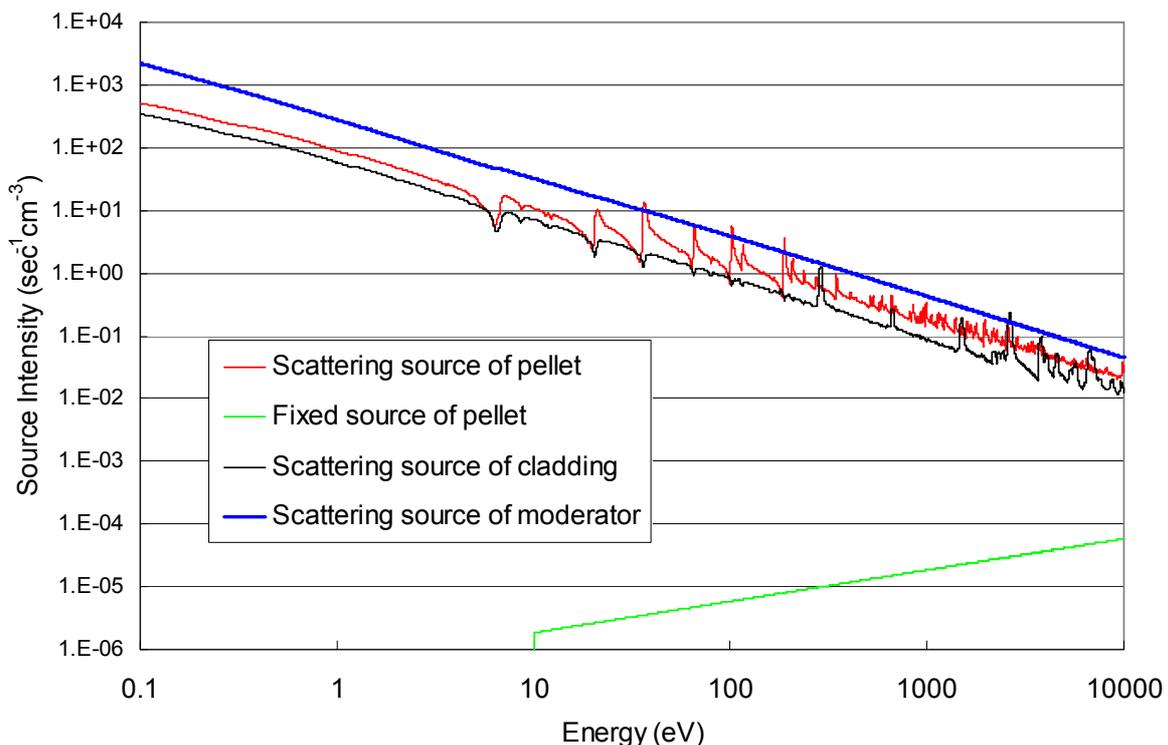
### 3.2 Approximations for high speed calculation

In the AEGIS code, two options are prepared to reduce the computation time of the scattering source calculation. One is 'Moderator scattering source approximation', and another is 'Grouping of scattering nuclides'.

#### 3.2.1 Moderator scattering source approximation

In the scattering source calculation, moderator regions are most time-consuming since it contains hydrogen. Therefore, it is possible to reduce computation time by approximately treating the scattering source of moderator. Fig. 3 shows scattering neutron sources and the fixed source of the above mentioned UO2 pin-cell problem. We can obtain the following observations from Fig. 3:

**Figure 3:** Neutron source intensity



1. In the moderator region, the effect of resonance absorptions in the fuel region is small. Therefore, the shape of scattering source in the moderator region is almost the well-known 1/E shape.
2. In resonance energy region (less than 10 keV), the fixed source in the fuel region is smaller than a hundredth of the scattering sources.

Based on the above observation, the following approximations are used in this option.

1. Scattering sources in the moderator region are not calculated, but given as the fixed source whose shape is 1/E.
2. Fixed sources in the pellet region are not given.

### 3.2.2 Grouping of scattering nuclides

In the scattering source calculation using Eq.(1), all nuclides in a region are considered. Therefore, it takes more computation time for the pellet which includes many fission products. In this option, scattering nuclides are grouped into the following four groups and Eq. (1) is estimated for these four groups.

1.  $^1\text{H}$ .
2.  $^{16}\text{O}$ .
3. Nuclides whose atomic numbers are smaller than 90, except  $^1\text{H}$  and  $^{16}\text{O}$ .
4. Nuclides whose atomic numbers are larger than or equal to 90.

### 3.2.3 Verification

These approximations are verified for the same pin-cell problem in the previous section. The verified items are the same as the previous section (Table.1). The results shows in Table.2

**Table 2:** Comparison of macroscopic absorption cross section and calculation time

Gr.	Energy (eV)		Difference of $\Sigma_a$ obtained by MVP (%)			
			UO2		MOX	
	Upper	Lower	Moderator scattering source approximation + Grouping of scattering nuclides		Moderator scattering source approximation + Grouping of scattering nuclides	
			Off	On	Off	On
69	67.90	55.60	0.1	-0.2	0.1	-0.3
75	37.27	33.72	0.5	-0.4	1.0	0.1
80	22.60	19.45	1.0	1.1	1.0	0.7
88	7.52	6.16	0.2	1.1	0.1	1.0
Calculation time			1 min.	3 sec.	1 min.	3 sec.

By utilizing these approximations, it is possible to reduce the computation time without large aggravation of the accuracy.

### 3.3 SPH method

Consider collapsing of multi-group cross sections into one-group cross sections. In a homogeneous infinite system, the multi-group reaction rates before the collapsing are preserved in the calculation using the one-group cross-section generated by simple flux-volume-weighted collapsing. However, in the multi-region system, it is unable to preserve the reaction rates by the simple flux-volume-weighted collapsing.

In order to preserve the reaction rates of ultra-fine-group calculation in the subsequent calculation, The SPH method is utilized in the AEGIS code. SPH factors are computed by the iterative calculation using collapsed cross sections.

The validity of the SPH method was verified against the above mentioned pin-cell geometry. Table 3 shows the differences of the effective multiplication factors between AEGIS and MVP. In the AEGIS calculation, the following three cross section sets are used:

- Case 1: Cross section sets obtained by equivalence theory and NR approximation;
- Case 2: For the resolved resonance region, cross sections obtained by ultra-fine-group calculations are used. For the unresolved resonance region, the same as Case 1;
- Case 3: The same cross section sets as Case 2 and SPH factors are used for resolved resonance region.

**Table 3:** Comparison of k-infinity

Case	Method	Difference of k-inf from MVP (%Δk/k)	
		UO2	MOX
1	Equivalence theory	-1.14	-0.93
2	Equivalence theory + Ultra-fine-group calculation	-0.56	-0.27
3	Equivalence theory + Ultra-fine-group calculation + SPH factor	-0.13	0

It should be noted that the moderator scattering source approximation and grouping of scattering nuclides are applied for ultra-fine-group calculations in Case 2 and 3.

By utilizing the SPH factor, the agreement of the k-infinity values between AEGIS and MVP is improved.

### 4. Conclusion

The theoretical models of the core calculation system of next generation, AEGIS/SCOPE2, are provided, especially, the resonance treatment in the AEGIS code is explained in detail.

For the ultra-fine-group calculation to generate effective cross sections, the tabulated collision probability method in square pin-cell geometry is adopted in the AEGIS code. In addition, the SPH method is used to preserve reaction rates in the energy-collapsed multi-group calculations.

Through the comparison with continuous-energy Monte-Carlo calculation in pin-cell geometry, the validity of the resonance treatment in AEGIS is verified.

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