Incorporation of Collision Probability Method in STREAM to Consider Non-uniform Material Composition in Fuel Subregions

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1. Introduction

The resonance self-shielding method in neutron transport code STREAM [1] has been enhanced by incorporating a collision probability method to consider non-uniform material composition in fuel subregions.

STREAM uses a pin-based slowing-down method (PSM) which solves pointwise energy slowing-down problems with sub-divided fuel pellet, and shows a great performance in calculating effective cross-section (XS). Various issues in the conventional resonance treatment methods (*i.e.*, approximations on resonance scattering source, resonance interference effect [2], and intrapellet self-shielding effect) were successfully resolved by PSM [3].

PSM assumes that a fuel rod has a uniform material composition and temperature even though PSM calculates spatially dependent effective XSs of fuel subregions. When the depletion calculation or thermal/hydraulic (T/H) coupling are performed with sub-divided material meshes, each subregion has its own material condition depending on position. It was reported that the treatment of distributed temperature is important to calculate an accurate fuel temperature coefficient (FTC) [4]. In order to avoid the approximation in PSM, the collision probability method (CPM) [5] has been incorporated as a calculation option.

Light water reactor (LWR) pin-cell problems with non-uniform temperature profiles are analyzed to demonstrate accuracies of the original and modified PSM methods. Furthermore, calculation efficiency of the method is studied.

2. Methods

PSM was derived to solve pointwise energy slowingdown equations written as following lethargy form.

$$\begin{cases} \phi_{i}(u) = \sum_{j \in F} \frac{P_{ij}(u)}{\Sigma_{t,j}(u)} Q_{s,j}(u) + \frac{P_{iM}(u)}{\Sigma_{p,M}} Q_{s,M}(u) \\ \phi_{M}(u) = \sum_{i \in F} \frac{P_{Mi}(u)}{\Sigma_{t,i}(u)} Q_{s,i}(u) + \frac{P_{MM}(u)}{\Sigma_{p,M}} Q_{s,M}(u) \end{cases}, (1)$$

where *u* is the index of pointwise energy; *F* and *M* are the indexes of fuel and pseudo moderator, respectively; *i* and *j* are the indexes of fuel subregions; ϕ is the flux; Q_s is the elastic scattering source; P_{ij} is the collision

probability from *i* to *j* of fuel rod in lattice; Σ_t is the total XS; and $\Sigma_{p,M}$ is the potential XS.

Once the collision probabilities are known, Eq. (1) is solved with a fixed source at high energy. After the pointwise energy flux is calculated, the multi-group effective XS is evaluated through energy condensation.

In original PSM, the collision probabilities are calculated through two-step strategy as follow. First, the collision probability of isolated fuel pin, $P_{ij}^{iso}(\Sigma_{t,F}^*)$, is tabulated as a function of total XS of fuel before solving the slowing-down equation. Here, $\Sigma_{t,F}^*$ is the total XS used in the tabulation. CPM or method of characteristic (MOC) transport solver can be used to generate the table. In the second step, a shadowing effect correction factor is applied to correct the shielding effect from neighboring fuel pin and structure material as follows:

$$P_{ij}(\Sigma_{t,F}(u)) = P_{ij}^{iso}(\Sigma_{t,F}(u)) \frac{1 - \eta(\Sigma_{t,F}(u)) \left\{ 1 - \sum_{j \in F} P_{ij}^{iso}(\Sigma_{t,F}(u)) \right\}}{\sum_{j \in F} P_{ij}^{iso}(\Sigma_{t,F}(u))} , (2)$$

where the shadowing effect correction factor, η , is defined as a ratio of escape probabilities of fuel rod in lattice to those of isolated fuel rod.

The two-step strategy in original PSM enables to avoid a direct evaluation of collision probability for a large geometry (*i.e.*, fuel assembly or core) which requires significant computing resources. In addition, simple interpolation is performed to get P_{ij}^{iso} for a given energy point because P_{ij}^{iso} is tabulated as a function of total XS before solving the slowing-down equation. Therefore, quite efficient evaluation of the collision probability is possible by using the two-step strategy.

PSM assumes that all subregions of a fuel rod have an identical material composition. In other words, the pointwise energy total XS is same in all subregions of fuel such as $\sum_{t,F} (u) = \sum_{t,i} (u)$. The assumption is needed to generate $P_{ij}^{iso}(\Sigma_{t,F}^*)$ table. If the material composition depends on subregions, one of the following methods should be used to calculate collision probability.

1) Use of average total XS as $\sum_{t,F} (u) \approx \overline{\Sigma}_{t,F}(u)$. 2) Use of CPM to calculate P_{ij}^{iso} .

In the first method, the total XSs of fuel subregions are spatially homogenized with flux-volume weighting.

The homogenization is a simple calculation so that it does not require noticeable computation burden. However, the resulting collision probability has error because of the constant pointwise energy XS assumption. In the second method, CPM can be directly used in the evaluation of P_{ij}^{iso} . CPM for the cylindrical geometry is well-established [5]. If CPM is used, an exact P_{ii}^{iso} can be calculated. However, computing time would increase because the collision probability is calculated for all energy points by using CPM solver. Furthermore, if the number of fuel subregions increases, the time elapsed in solving CPM matrix equation increases proportionally to the square of the number of regions. Using P_{ii}^{iso} calculated by CPM, the collision probability of fuel in lattice is written as follows:

$$P_{ij}(u) = \hat{P}_{ij}^{iso}(u) \frac{1 - \eta(\overline{\Sigma}_{t,F}(u)) \left\{ 1 - \sum_{j \in F} \hat{P}_{ij}^{iso}(u) \right\}}{\sum_{j \in F} \hat{P}_{ij}^{iso}(u)} , \quad (3)$$

where \hat{P}_{ij}^{iso} is the collision probability of isolated pin calculated by CPM.

 \hat{P}_{ij}^{iso} is calculated by CPM for all energy points. The shadowing correction factor depends on total XS of entire fuel pellet so that the average total XS is still used in the evaluation.







Fig. 2. Temperature distributions of pin-cell problems with non-uniform temperature profile.

There is no difference in applying the method to the non-uniform temperature and non-uniform composition cases because the issue is related to the spatial distribution of pointwise energy total XS. For this reason only non-uniform temperature problem is studied in the following numerical test.

3. Numerical Test

OPR1000 pin-cell problems which have different temperature profiles are analyzed to demonstrate accuracy of proposed methods. The pin-cell problems compose of 3 % enriched UO_2 fuel, gap, zirconium cladding and H₂O coolant. There are two sets of problems, *i.e.*, pin-cells with uniform and non-uniform temperature profiles. Pin-cells have different temperatures depending on their power level as show in Fig. 1 and Fig. 2. For each power level, average fuel temperatures of pin-cells with uniform and non-uniform profiles are identical. More detailed specification of the problems is well described in reference [4].

The transport code STREAM is used in the numerical test. PSM has been implemented in STREAM and the code uses 72 energy group structure for the transport calculation. Two calculation options are used in the numerical tests, i.e., PSM with and without CPM. PSM without CPM uses the average total XS in computing collision probability while PSM with CPM uses Eq. (3) as described in the previous section. Strict MOC ray conditions (i.e., 32 azimuthal angles and 3 polar angles for the octant of solid angle with 0.01 cm ray spacing) and the P₃ high order scattering model are used in the test to minimize errors caused from MOC transport analysis. The reference solution was generated by the Monte Carlo code MCNP6 [6]. For consistent comparison, STREAM uses the resonance upscattering correction which is to fit the upscattering model of MCNP6 [3].

Table I: k_{eff} results for pin-cell with uniform temperature

Douvor	k_{eff} ; and k_{eff} difference			
lovel (%)	MCNP6	PSM	PSM	
level (70)	(Reference)	w/o CPM	w/ CPM	
50	1.31920	1.31869	1.31872	
	± 0.00003	(-51)*	(-48)	
75	1.31678	1.31605	1.31609	
	± 0.00003	(-73)	(-69)	
100	1.31394	1.31330	1.31333	
	± 0.00003	(-64)	(-61)	
105	1.31117	1.31051	1.31055	
125	± 0.00003	(-66)	(-62)	
150	1.30843	1.30785 (-58)	1.30789	
150	± 0.00003		(-54)	
175	1.30602	1.30529	1.30533	
	± 0.00003	(-73)	(-69)	
200	1.30322	1.30235	1.30239	
	± 0.00003	(-87)	(-83)	

Difference of k_{eff} compared to MCNP6 result (unit: pcm).

Doutor	k_{eff} ; and k_{eff} difference			
Fower	MCNP6	PSM	PSM	
1evel (%)	(Reference)	w/o CPM	w/ CPM	
50	1.31954	1.31872	1.31893	
30	± 0.00003	(-82)	(-61)	
75	1.31694	1.31609	1.31645	
75	± 0.00003	(-85)	(-49)	
100	1.31446	1.31333	1.31384	
	± 0.00003	(-113)	(-62)	
125	1.31179	1.31055	1.31128	
123	± 0.00003	(-124)	(-51)	
150	1.30915	1.30789	1.30864	
150	± 0.00003	(-126)	(-51)	
175	1.30661	1.30533	1.30597	
	± 0.00003	(-128)	(-64)	
200	1.30383	1.30239	1.30321	
200	± 0.00003	(-144)	(-62)	

Table II: k_{eff} results for pin-cell with non-uniform temperature



Fig. 3. Reactivity of pin-cell with uniform temperature.



Fig. 4. Reactivity of pin-cell with non-uniform temperature.

Fable III: FTC results for pin-cell probl	ems
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Tomporatura	FTC (pcm/K); and FTC difference			
remperature	MCNP6	PSM	PSM	
prome	(Reference)	w/o CPM	w/ CPM	
Uniform	-1.896	-1.925	-1.924	
		(-1.49 %)	(-1.43 %)	
Non-	1.940	-1.924	-1.857	
uniform	-1.849	(-4.04 %)	(-0.42 %)	

The multiplication factor results for pin-cell problems with uniform temperature profile are shown in Table I. For all power levels, two PSM options give quite accurate multiplication factors with less than 100 pcm difference.

Theoretically, PSM with and without CPM should give an identical result because material conditions of fuel subregions, *i.e.*, temperature distribution, are constant in the fuel pellet. However, there are few pcms differences (< ~4 pcm) between PSM with and without CPM. The differences are caused by the interpolation error of collision probability into $P_{ij}^{iso}(\Sigma_{t,F}^{*})$ table. This difference is negligible in terms of practical use.

In Table II, k_{eff} results for pin-cell problems with nonuniform temperature profile are compared. PSM without CPM shows less than 100 pcm difference for low power problems. However, there is a slight bias in the multiplication factor as the power level increases. As the power level increases, the variation of temperatures becomes larger as shown in Fig. 2. Therefore, it can be said that higher power problem is more difficult to get an accurate result using PSM without CPM because the model uses pellet-averaged total XS in computing P_{ii}^{iso} . PSM without CPM give more underestimated results as the power increases. However, the model still gives reasonable results with an order of 100 pcm differences. On the other hand, PSM with CPM shows consistent results for all power levels. The differences in the multiplication factor are -62 ~ -49 pcms. There is no noticeable bias. Therefore it can be said that replacing the method to calculate P_{ii}^{iso} is effective to consider the non-uniformly distributed material conditions.

Fig. 3 and Fig. 4 show the reactivity versus average temperature of fuel pellet. The reactivity results of each method are fitted with a linear function. The slope of the linear function represents the FTC. The FTCs are summarized and compared in Table III. PSM without CPM shows -1.49 % and -4.04 % differences in the FTC for uniform and non-uniform temperature problems, respectively. PSM without CPM also have a slight bias in the FTC calculation. On the other hand, PSM with CPM shows accurate and consistent results which have -1.43 % and -0.42 % differences. PSM with CPM is also effective to calculate accurate FTC.



Fig. 5. Elapsed time in 17x17 FA analysis.

The calculation efficiency of the method is also important for practical use. A 17x17 FA problem, which is frequently used in a reactor design, is analyzed with two PSM options for the efficiency test because the elapsed time for the pin-cell problem is quite short so that it does not represent realistic situation. In the test, following calculation options are used: 12 azimuthal angles and 3 polar angles for the octant of solid angle with 0.05 cm ray spacing, 8 azimuthal sectors in pin-cell, 3 radial subregions in coolant, octant symmetric modeling, and transport-corrected P₀ model [7]. The test is performed with the different number of radial subregions in fuel pellet. The result is shown in Fig. 5. As described in the previous section, PSM with CPM takes a longer time to calculate the collision probability. If the number of subregions are small, the difference between PSM with and without CPM is not much. As the number of subregions increases, PSM with CPM take much longer time than the original PSM. The elapsed time for CPM is proportional to square of the number of regions. Although less than 10 fuel subregions are usually used in the practical calculation (e.g., ~ 3 for UO₂ fuel and ~ 10 for gadolinia), it is needed to enhance the calculation efficiency. This point would be one of future works.

3. Conclusions

The resonance treatment method, PSM, used in the transport code STREAM has been enhanced to accurately consider a non-uniform material condition. The method incorporates CPM in computing collision probability of isolated fuel pin. From numerical tests with pin-cell problems, STREAM with the method showed very accurate multiplication factor and FTC results less than 83 pcm and 1.43 % differences from the references, respectively. The original PSM showed larger differences than the proposed method but still has a high accuracy. From the computing time test with an assembly problem, it was noticed that PSM with the CPM took a long time if the large number of subregions were modeled. The work to enhance efficiency of the method will be performed in the future.

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