Status of Deterministic Transport Code Development at UNIST

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1. Introduction

Deterministic transport code has been developed at UNIST. The code uses the method of characteristics (MOC) for neutron transport analysis. The MOC can provide accurate numerical solutions when accurate multi-group cross section library is given. In this work, nuclear library generation process and implemented resonance treatment method are presented. The code can cover PWR and VHTR system. NJOY code system [2] and RMET21 [3] are used to generate self-shielded cross section and resonance parameter. Equivalence theory [1] is adopted in the code as a resonance treatment method. Additionally, Doubly-heterogeneous (DH) self-shielding method [4] is implemented in the code to consider double heterogeneity of fuel in VHTR. At the end of this work, case test results are presented for both PWR and VHTR system.

2. Library generation

The nuclear data processing code, NJOY, was used to process the ENDF/B-VII.0 data for generating multi-group cross section libraries. Two types of libraries are used depending on reactor type. For generating VHTR library, MCNP [5] is used to calculate spectrum for typical VHTR pin cell and then the spectrum is used as weighting function to generate cross section. The number of background cross section is determined by the type of isotope.

RMET21 has been used to generate Intermediate Resonance (IR) parameter λ. The IR parameter table has been generated for U238 which is dominant isotope in view of resonance for thermal reactors. In the IR parameter table, there are 13 groups × 10 isotopes parameters. The IR parameters are interpolated by mass for not listed isotopes in the table.

3. Resonance treatment

The equivalence theory and IR approximation [1] have been used as resonance treatment method. Resonance integral is written by

$$RI_a = \int \sigma_a(E)\left[(1-\tilde{P}_{FF}) + \frac{\lambda\Sigma_p}{\Sigma_t(E)}\tilde{P}_{FF}\right]\frac{dE}{E}, \quad (1)$$

where Σ_p and Σ_t are potential and total cross section of fuel. σ_a is absorption cross section and $\tilde{P}_{FF}$ is fuel-to-fuel collision probability which is

$$\tilde{p}_{FF} = \sum_{n=1}^{N}\frac{\beta_n\Sigma_t}{\Sigma_t + \alpha_n\Sigma_e}, \quad (2)$$

where Σ_e is escape cross section which takes into account the heterogeneity of the medium. *N* denotes the number of rational expression terms. The constants α_n and β_n denotes the *n*-th rational coefficients. α_n and β_n are derived by the Dancoff factor and fuel escape probability expression for isolated pin such as Wigner's one-term and Carlvik's two-term approximation [1].

3.1. Gray resonance treatment method

The gray resonance treatment method [6] has been implemented to minimize the rational approximation error in the gray region which is between black and white limit. The MOC module is used to calculate fuel-to-fuel collision probability $\tilde{P}_{FF}^{MOC}$ of fixed source problem for several values of optical length *x* which is fuel total cross section divided by escape cross section. From this work, a set of $(x_i, \tilde{P}_{FF}^{MOC}(x_i))$ is generated. The least square fitting is applied to this set to minimize the residual error $\|\Delta\tilde{P}_{FF}\|^2$ in Eq. (3).

$$\left\|\Delta\tilde{p}_{FF}\right\|^2 = \sum_{i=1}^{m}\left[\tilde{p}_{FF}^{\mathrm{MOC}}(x_i) - \sum_{n=1}^{N}\frac{\beta_n x_i}{x_i+\alpha_n}\right]^2, \quad (3)$$

where *m* denotes the number of values of optical length calculated by MOC module. A new $\tilde{P}_{FF}$ approximation can be calculated from this least square fitting calculation.

3.2. Doubly-heterogeneous self-shielding method

The DH method is implemented to treat resonance self-shielding in VHTR system in which the fuel compact consists of small fuel kernel in a graphite sleeve. The method first homogenizes material in the fuel compact region using an analytical approximation for the disadvantage factor based on equivalence theory. The disadvantage factor accounts for spatial self-shielding of the resonance flux within the fuel kernel. DH effects are accounted by using a modified definition of background cross section, which includes geometry parameters and cross sections for the both fuel kernel and fuel compact region.

4. Test Results

4.1. PWR pin cell problem

PWR pin cell models were designed to verify PWR library and implemented resonance treatment method. Table I indicates model geometry. The pin cell is composed of three regions: UO2 fuel, natural Zirconium for cladding and light water for coolant. Table II summarizes the test case results for k_{eff}. The tests were performed for three kinds of geometry and enrichment. The code in UNIST expects k_{eff} with the average error of 174pcm compared to the results of McCARD [7].

Table I: Model Geometry

Type	Radius (cm)		Pin pitch(cm)
	Fuel	Cladding	Coolant
Geometry A	0.4900	0.5500	1.4700
Geometry B	0.4125	0.4760	1.2800
Geometry C	0.3931	0.4580	1.2621

Table II: Test results of k_{eff} and relative error

Case	Geometry Type	Enrichment [wt%]	k_{eff} and error	
			McCARD	UNIST
1	Geometry A	3.9%	1.39163 ±0.00008	1.38987 (-176)
2	Geometry A	2.4%	1.29659 ±0.00008	1.29461 (-198)
3	Geometry A	1.6%	1.19282 ±0.00007	1.19080 (-202)
4	Geometry B	3.9%	1.39558 ±0.00008	1.39411 (-147)
5	Geometry B	2.4%	1.29831 ±0.00007	1.29663 (-168)
6	Geometry B	1.6%	1.19180 ±0.00008	1.19021 (-159)
7	Geometry C	3.9%	1.41021 ±0.00008	1.40846 (-175)
8	Geometry C	2.4%	1.30936 ±0.00008	1.30767 (-169)
9	Geometry C	1.6%	1.19937 ±0.00007	1.19764 (-173)
Average error [pcm]				-174

4.2. VHTR pin cell problem

Simplified VHTR pin cell model were designed as shown in the Fig. 1. Fuel compact consists of fuel kernels and graphite sleeve. Outside of fuel compact, graphite and helium are used as moderator and coolant respectively. Single Heterogeneity (SH) model is designed by homogenizing materials in fuel compact region to verify DH effects on k_{eff}.

Table III indicates test results for both SH and DH models compared to results of MCNP. The values of k_{eff} for SH cases are predicted within ~200pcm error compared to MCNP results for the SH cases. The DH effects increase the value of k_{eff} about 3000~5000pcm. The values of k_{eff} are predicted within ~400pcm error compared to MCNP results for the DH cases.

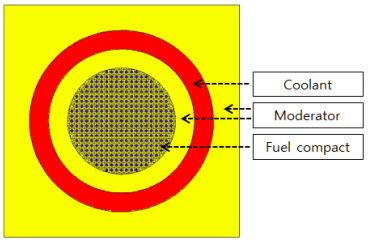

Fig. 1. VHTR simplified unit cell model.

Table III: Test results of k_{eff} and relative error

Fuel volume in compact	k_{eff} and error			
	Single Heterogeneity		Double Heterogeneity	
	MCNP	UNIST	MCNP	UNIST
6.07%	1.39081 ±0.00020	1.39208 (+127)	1.44050 ±0.00020	1.44448 (+398)
9.33% (base case)	1.30063 ±0.00007	1.30221 (+158)	1.34446 ±0.00007	1.34535 (+394)
13.00%	1.22387 ±0.00020	1.22585 (+198)	1.26205 ±0.00020	1.26099 (-106)

5. Conclusions

The library generation process and resonance treatment method in the deterministic transport code in UNIST has been summarized. The code shows reasonable results of k_{eff} compared to Monte Carlo results for pin cell problems.

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