# Implementation of Pin-based Pointwise Energy Slowing-down Method into DeCART

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#### 1. Introduction

DeCART [1] uses the pre-generated multi-group cross section library by KAERI library processing system [2] based on two resonance treatment methods, the direct resonance integral table method [3] and the subgroup method. The library processing system was, however, originally developed and optimized for the light water reactor (LWR). It is not simple to generate a multi-group library for very high temperature reactors (VHTR) with the system considering the characteristics of VHTR fuels such as high fuel temperature, various packing fraction, double heterogeneity, and high burnup. Especially, it is known from prior experiences that the keff error on a VHTR fuel by DeCART rapidly increases at the high burnup and the main cause of the error is the inaccuracy of the multi-group library. Thus, in order to overcome the difficulties, we applied the pin-based pointwise energy slowing-down method (PSM) [4] performing the resonance treatment on a specific problem on-the-fly.

In this study, we implemented the PSM into DeCART and the verification calculation results were presented.

#### 2. Methods and Results

The simple review of the PSM was described in section 2.1 and the procedure of PSM/DeCART was summarized in the next section. Lastly, calculation results on two typical reactors, LWR and VHTR, were compared to McCARD results.

### 2.1 Review of PSM

Basically, the PSM solve the slowing down equation for all energy points with the collision probability (CP) as follows:

$$\Sigma_{t,i} \phi_i V_i = \sum_{j \in F} P_{ji} V_j Q_{s,j} + P_{Mi,g} V_M Q_{s,M} , \quad (1)$$

where, *i* and *j* are fuel sub-region indexes and *M* is a moderator region index.  $P_{ij}$  is the CP which a neutron born at a sub-region *i* has its first collision at sub-region *j*. In addition,  $V_i$  is the volume of the sub-region *i* and  $Q_{s,j}$  is the slowing down scattering source of the sub-

region *j*. At first, the PSM should generate collision probability tables using the method of characteristics (MOC). The CP calculation consists of two sub-parts for an isolated fuel pin and a lattice fuel pin. For the CP of an isolated fuel pin, the fuel region is divided into about 15 sub-region and fixed source problems are solved by MOC for every fuel sub-region and about 200 levels of total cross section range of interest as follows:

$$\Omega \cdot \nabla \psi(r, \Omega) + \Sigma_{t,i}^{T}(r)\psi(r, \Omega) = \frac{1}{4\pi} \delta_{i}(r), (1)$$
$$P_{ij}^{iso}(\Sigma_{t,i}^{T}) = \frac{\Sigma_{t,j}^{T} \phi_{j} V_{j}}{V_{i}}, \qquad (2)$$

where,  $\Sigma_{t,i}^{T}$  is a total cross section in sub-region *i* with 200 levels from 10<sup>-3</sup> to 10<sup>4</sup> cm<sup>-1</sup>.  $P_{ij}^{iso}$  is the CP in the isolated fuel pin.

The CP for a lattice pin can be obtained from the CP of the isolated pin and the shadowing effect factor. The factor can be calculated using the Carlvik's two-term rational approximation and Dancoff factor by the enhanced neutron current method. The Dancoff factor is obtained by solving the fixed source problem with MOC as follows:

$$\Omega \cdot \nabla \psi(r, \Omega) + (\Sigma_a(r) + \Sigma_p(r))\psi(r, \Omega) = \frac{1}{4\pi} \Sigma_p(r), (3)$$

$$D = \lim_{\Sigma_{t,F} \to \infty} \frac{1 - P_{F,F}}{1 - P_{F,F}^{iso}} \approx \frac{(\Sigma_{a,F} + \Sigma_{p,F})\phi_F - \Sigma_{p,F}}{\Sigma_{e,F}} \bigg|_{\Sigma_{a,F} \to \infty}.$$
 (4)

where,  $P_{F,F}^{iso}$  is the CP from the fuel region to the fuel region in the isolated system and  $P_{F,F}$  is the CP in the lattice system. In addition,  $\Sigma_{p,F}$  is the potential cross section of the fuel region and  $\Sigma_{e,F}$  is the escape cross section of the fuel region which is defined by the inverse of the average chord length ( $\Sigma_e = 1/\bar{l}$ ).

From the Carlvik's two-term rational approximation, the fuel escape probability for the isolated and lattice system,  $\overline{P}_{e,F}^{iso}$  and  $\overline{P}_{e,F}$ , can be calculated and the shadowing effect factor for the fuel region can be obtained as the following equation.

$$\eta_F = \frac{\overline{P}_{e,F}}{\overline{P}_{e,F}^{iso}}.$$
(5)

Thus, the CP inside the fuel sub-region is expressed as follows:

$$P_{ij} = P_{ij}^{iso} \frac{1 - P_{e,i}}{1 - P_{e,i}^{iso}},$$
(6)

where,

$$P_{e,i} = P_{iM} \approx \eta_F(u) P_{e,i}^{iso} , \qquad (7)$$

$$P_{e,i}^{iso} = P_{iM}^{iso} \approx 1 - \sum_{j \in F} P_{ij}^{iso}(\Sigma_{t,F}^T), \qquad (8)$$

and  $P_{iM}^{iso}$  and  $P_{iM}$  are the CP from the fuel region to the non-fuel region in the isolated and lattice system, respectively. Also, the CP from the non-fuel region can be readily obtained from the above equations.

Finally, the flux at an energy point of the slowing down equation, Eq.(1), can be calculated as the following equation.

$$\phi_i = \sum_j \frac{P_{ij}}{\sum_{t,j}} Q_{s,j} \,. \tag{9}$$

The further information for the PSM can be found in the reference [4].

# 2.2 Procedure of PSM/DeCART

Prior to solve the neutron transport equation, DeCART should obtain background cross sections and subgroup parameters by solving a heterogeneous fixed source problem with MOC and determines the effective cross section for a uniform cross section region. However, the PSM/DeCART directly reads pointwise cross sections processed by NJOY and calculates the effective cross sections with the pointwise spectrum. Thus, PSM modules replace the modules for generating the subgroup parameter in the original DeCART.

Fig.1 shows the flowchart for the resonance treatment of the PSM/DeCART.



Fig. 1. Flowchart for the Resonance Treatment of PSM/DeCART

## 2.3 Verification Results

For evaluating the performance of the PSM/DeCART, two typical fuel pins, LWR and VHTR, were set up. In case of VHTR fuel, the fuel compact region was homogenized. Table I shows the number densities for two pin types. The code used the pointwise cross sections processed from ENDF/B-VII.1 in the resonance energy region and the existing 190g cross section library in the other energy region.

Table I: Number Densities for the pin problems

Region	LWR Pin		VHTR Pin	
Fuel	<sup>235</sup> U	9.3947E-04	<sup>235</sup> U	1.5765E-04
Region	<sup>238</sup> U	2.2262E-02	<sup>238</sup> U	8.4864E-04
	<sup>16</sup> O	4.6422E-02	<sup>16</sup> O	1.5094E-03
			Graphite	6.9958E-02
			<sup>28</sup> Si	2.8459E-03
			<sup>29</sup> Si	1.4410E-04
			<sup>30</sup> Si	9.5657E-05
Moderator	$^{1}\mathrm{H}$	4.680460E-02	Graphite	9.2756E-02
	<sup>16</sup> O	2.340570E-02		

Table II shows the comparisons between the  $k_{inf}$  by McCARD and PSM/DeCART for the LWR fuel pin problem. The difference between two codes is under 100 pcm at every burnup points. It can be seen that they are in a very good agreement.

Table III shows the comparisons between the  $k_{inf}$  by McCARD and PSM/DeCART for the VHTR fuel pin problem. The difference at low burnup is slightly larger than the LWR case, about 100 pcm, and is around 200 pcm at high burnup. It is shown that two codes agree well with each other in the VHTR case, as well.

Table II: Comparison of kinf for LWR Fuel Pin Problem

EFPD	Burnup	McCARD	DCM/DaCADT	Diff.
(day)	(GWd/MTU)	(o~10pcm)	r SM/DeCART	(D-M)
0.00	0.00	1.40672	1.40607	-0.00066
6.25	0.21	1.35904	1.35839	-0.00065
12.50	0.43	1.3532	1.35247	-0.00073
25.00	0.86	1.34536	1.34486	-0.00050
50.00	1.72	1.33368	1.33329	-0.00039
100.00	3.43	1.31056	1.31003	-0.00053
150.00	5.14	1.28712	1.28658	-0.00054
200.00	6.86	1.26469	1.26416	-0.00053
250.00	8.57	1.24371	1.24312	-0.00059
300.00	10.29	1.22414	1.22341	-0.00073
350.00	12.00	1.20577	1.20487	-0.00090
400.00	13.72	1.18815	1.18734	-0.00081
450.00	15.43	1.17151	1.17063	-0.00088
500.00	17.15	1.15543	1.15461	-0.00082
562.50	19.29	1.13653	1.13579	-0.00074
625.00	21.43	1.11799	1.11735	-0.00064
687.50	23.58	1.10013	1.09950	-0.00063
750.00	25.72	1.08285	1.08216	-0.00069
812.50	27.86	1.06592	1.06526	-0.00066
875.00	30.01	1.04926	1.04876	-0.00050
937.50	32.15	1.0331	1.03263	-0.00047
1000.00	34.29	1.01731	1.01686	-0.00045
1062.50	36.44	1.00155	1.00144	-0.00011
1125.00	38.58	0.98683	0.98638	-0.00045
1187.50	40.72	0.97200	0.97167	-0.00033
1250.00	42.87	0.95792	0.95735	-0.00057

EFPD	Burnup	McCARD	DSM/DoCAPT	Diff.
(day)	(GWd/MTU)	(o~15pcm)	I SIVI/DECART	(D-M)
0.00	0.00	1.35104	1.35202	0.00098
6.25	0.48	1.31299	1.31365	0.00066
12.50	0.96	1.30764	1.30877	0.00113
25.00	1.92	1.30026	1.30117	0.00091
50.00	3.85	1.28838	1.28941	0.00103
100.00	7.70	1.26712	1.26819	0.00107
150.00	11.55	1.24523	1.24669	0.00146
200.00	15.40	1.22367	1.22524	0.00157
250.00	19.24	1.20249	1.20435	0.00186
300.00	23.09	1.18247	1.18434	0.00187
350.00	26.94	1.16358	1.16535	0.00177
400.00	30.79	1.14558	1.14745	0.00187
450.00	34.64	1.1287	1.13063	0.00193
500.00	38.49	1.11292	1.11484	0.00192
562.50	43.30	1.09459	1.09647	0.00188
625.00	48.11	1.07757	1.07942	0.00185
687.50	52.92	1.06177	1.06363	0.00186
750.00	57.73	1.04694	1.04894	0.00200
812.50	62.54	1.03315	1.03522	0.00207
875.00	67.35	1.02026	1.02236	0.00210
937.50	72.16	1.00824	1.01026	0.00202
1000.00	76.97	0.99695	0.99882	0.00187
1062.50	81.78	0.98582	0.98798	0.00216
1125.00	86.60	0.97552	0.97765	0.00213
1187.50	91.41	0.96576	0.96779	0.00203
1250.00	96.22	0.95621	0.95834	0.00213

Table III: Comparison of *k*<sub>inf</sub> for VHTR Fuel Pin Problem

#### **3.** Conclusions

In this study, the pin-based pointwise energy slowing-down method was implemented into DeCART for performing the resonance treatment on a specific problem on-the-fly and the verification calculation results for two typical fuel pin, LWR and VHTR, were presented.

Two verification results show that the difference with the reference is around 100 pcm at low burnup and increases to around 200 pcm at high burnup. It can be seen that they are in a good agreement.

For practical use, the PSM/DeCART needs to be optimized to increase calculation efficiency. In addition, it is required to study for applying the PSM to a TRISO fuel of a VHTR.

# ACKNOWLEDGMENTS

This work was supported by the National Research Foundation of Korea (NRF) grant funded by the Korea government(MSIP) (No.2017M2A8A1014757).

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