

# An In-scattering Transport Correction by the Neutron Leakage Conservation Method and Its Application to the DeCART Multigroup Library

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## 1. Introduction

Modern method of characteristics (MOC) whole-core transport codes provide several options to deal with anisotropic scattering effects. As a superior option, explicit treatment using high-order ( $\geq P2$ ) scattering data is possible in most MOC codes. However, eigenvalue calculation with high-order scattering gives more accurate solutions than the isotropic (P0) calculation yet it requires twice the computing time. Moreover, since the high-order scattering option has not been sufficiently validated, it may lead to unexpected errors in a reactor core design and analysis.

The typical option is implicit treatment using transport-corrected P0 (TCP0) scattering cross sections, which approximates the effects of linear anisotropy by the transport correction [1]. The out-scattering assumption has been widely used to obtain the TCP0 scattering matrix, in which the diagonal terms of the P0 scattering matrix are subtracted by the total P1 scattering cross sections. However, the P1-corrected P0 scattering matrix may include negative value in the diagonal components, which causes negative flux and results in convergence error. Another issue associated with out-scattering correction shows a significant global power tilt for whole-core problems, including reflectors. Based on these issues, a proper transport correction is needed to (1) ensure reasonable neutron leakage as high-order scattering is considered and (2) to guarantee no negative flux.

There have been many approaches to in-scattering transport corrections, such as the method that computes group diffusion coefficients by solving the P1 moment equation in a one-dimensional (1D) geometry (implemented in nTRACER [2]) and the method using P1 moment weighting from STREAM [3]. Recently, Kim [4] investigated the neutron leakage conservation (NLC) method [5] to fix the out-scattering approximation for hydrogen for the MPACT multigroup library. However, no in-scattering transport correction is available in DeCART [6]. The objective of this study is to generate the in-scattering TCP0 cross sections by using the NLC method, and then to examine its effectiveness by using the DeCART2D [7] code with the 47-group library. If this method is successful, then an accurate, efficient reactor core design and analysis may be possible.

## 2. Methods and Results

### 2.1 Conventional Transport Correction Methods

There are two methods to generate the transport cross sections ( $\Sigma_{tr,g}$ ) and the TCP0 scattering matrix ( $\Sigma_{s,0,g \rightarrow g'}^{tr}$ ). The out-scattering transport correction, the most commonly used method, can be expressed as follows:

$$\Sigma_{tr,g}^{out} = \Sigma_{t,g} - \Sigma_{s,1,g}, \quad (1)$$

$$\Sigma_{s,0,g \rightarrow g'}^{tr,out} = \Sigma_{s,0,g \rightarrow g'} - \Sigma_{s,1,g}, \quad (2)$$

where  $\Sigma_{t,g}$  and  $\Sigma_{s,1,g}$  are total and P1 scattering cross sections, respectively.

In Eqs. (1) and (2), it is approximated that the scattering into a group of neutrons from higher energy groups is roughly balanced by the scattering out to lower energy groups. Due to this assumption, it has been reported that the out-scattering correction significantly overestimates the neutron leakage, resulting in highly underestimated eigenvalues for problems with large neutron leakage. Therefore, a more rigorous method or high-order scattering model should be used to obtain accurate results.

The in-scattering transport correction, the most rigorous method, can be written as follows:

$$\Sigma_{tr,g}^{in} = \Sigma_{t,g} - \frac{\sum_{g'=1}^G \Sigma_{s,1,g' \rightarrow g} \phi_{1,g'}}{\phi_{1,g}}, \quad (3)$$

$$\Sigma_{s,0,g \rightarrow g'}^{tr,in} = \Sigma_{s,0,g \rightarrow g'} - \frac{\sum_{g'=1}^G \Sigma_{s,1,g' \rightarrow g} \phi_{1,g'}}{\phi_{1,g}}. \quad (4)$$

Eqs. (3) and (4) contains the high-order flux moment that should be calculated. However, it is not straightforward to obtain this high order solution, and further analyses are essential.

### 2.2 Neutron Leakage Conservation (NLC) Method

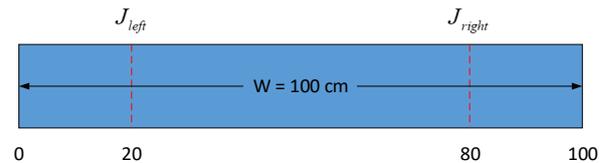


Fig. 1. Slab geometry for the NLC method.

The main idea of the NLC method is to obtain the group diffusion coefficients that provide the same

neutron leakage as that obtained in the high-order scattering transport calculation, as follows:

$$\Omega \cdot \nabla \Phi_g(\Omega) = -D_g \nabla^2 \phi_g. \quad (5)$$

With an infinite bare slab model filled with a homogeneous medium (shown in Figure 1), the flux solution to this problem has a cosine distribution. Then, the net leakage rate at specified surfaces can be obtained from the high-order scattering transport calculation in terms of neutron currents as follows:

$$J_g^{right} - J_g^{left} = \int_{left}^{right} dx D_g B^2 \phi_g(x) = D_g B^2 \hat{\phi}_g, \quad (6)$$

where  $B^2$  is the buckling given as

$$B^2 = B_{geom}^2 = \left( \frac{\pi}{W} \right)^2. \quad (7)$$

When performing the multigroup transport calculation with high-order scattering, one must verify whether the group-wise bucklings are constant, independent of the energy group.

Based on Eq. (6), if the buckling, net currents, and flux are known, then the diffusion coefficients can be determined to preserve the net leakage rate of the transport solution if diffusion theory is valid. Therefore, the group diffusion coefficients and transport cross sections can be obtained as follows:

$$D_g = \frac{J_g^{right} - J_g^{left}}{B^2 \hat{\phi}_g}, \quad (8)$$

$$\Sigma_{tr,g} = \frac{1}{3D_g}. \quad (9)$$

Finally, transport correction factors, defined as the ratio of transport-to-total cross sections, can be obtained as follows:

$$f_{tr,g} \equiv \frac{\Sigma_{tr,g}}{\Sigma_{t,g}}. \quad (10)$$

This problem involves solving the neutron transport equation to compute diffusion coefficients that reproduce the spatial flux distribution. Here, diffusion coefficients are chosen to preserve leakage and therefore the shape of the scalar flux distribution. This can also be accomplished by employing either continuous energy Monte Carlo or multigroup deterministic transport calculations.

### 2.3 Generation of Transport Correction Factors

The NLC method is applied to fix the out-scattering approximation for a conventional light-water reactor, for which it is assumed that most of the anisotropic scattering occurs in hydrogen bound to water. This assumption is made because the average cosine of the scattering angle from elastic collisions with hydrogen is 2/3. As the atomic weight increases, this forward-peaked scattering becomes more isotropic. Therefore, a hydrogen-only problem will be used to generate transport correction factors.

Transport correction factors for hydrogen have been generated by using a 1D multigroup MOC solver. The ENDF/B-VII.1-based 47-group cross sections required for the MOC calculation, including the high-order scattering data, were generated by using GREDIT [8], one of the key programs comprising the KAERI library generation code system. The computational model is as follows:

- The size of the slab with vacuum boundary is 100 cm. As shown in Figure 1, neutron currents are edited at two red dotted positions, where transport edge effects at vacuum boundaries are not present.
- Hydrogen is placed throughout the slab at a particle number density of 0.478 atoms/barn/cm.
- Temperatures are 293.6, 350, 400, 450, 500, 550, 600, 650, and 800 K.
- The external source is the Watt fission spectrum with buckled cosine spatial distribution.

In this study, the following modeling options were used:

- No. of meshes: 20,000 (mesh size=0.005 cm)
- No. of polar angles per 90°: 8 (S16)
- Anisotropic scattering order: 3 (P3)

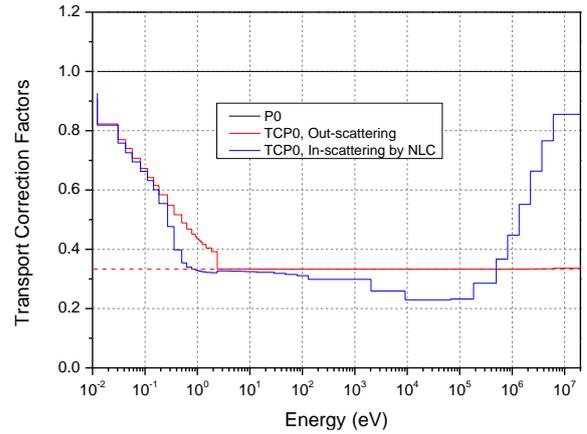


Fig. 2. Transport correction factors for hydrogen.

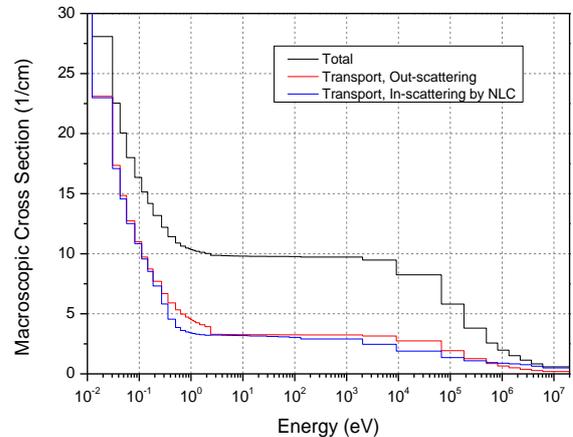


Fig. 3. Total and transport cross sections for hydrogen.

Figure 2 shows the transport correction factors for hydrogen plotted as a function of energy group. The top horizontal black solid line represents pure isotropic scattering: hence the ratio is unity at all energy groups. The other horizontal red dotted line represents the out-scattering assumption from Eq. (1). For hydrogen, assuming negligible absorption, the transport correction factors should be 1/3. When the transport cross section is 1/3 of the total cross section, then the out-scattering approximation is valid. However, for most of the energy groups, the curves differ, so this hydrogen correction is needed.

Figure 3 is a plot of the group transport cross sections. In addition to the two transport cross section curves, the total cross sections are shown. There is a large deviation between total and transport cross sections, which means there is a significant amount of anisotropic scattering. Although the transport cross section curves are close, there is deviation present in certain regions.

#### 2.4 Modification of DeCART 47-group Library

The ENDF/B-VII.1-based 47-group library used for the SMART [9] core design and analysis has been modified to consider the transport correction factors for hydrogen. In Eq. (11), the in-scattering-based transport cross sections can be easily obtained by multiplying the total cross sections by the transport correction factors. The in-scattering TCP0 scattering matrix can be adjusted as shown in Eq. (12).

$$\sigma_{tr,g}^{NLC} = \sigma_{t,0,g} f_{tr,g}, \quad (11)$$

$$\sigma_{s,0,g \rightarrow g}^{tr,NLC} = \sigma_{s,0,g \rightarrow g} - \sigma_{t,0,g} (1 - f_{tr,g}). \quad (12)$$

where the superscript *NLC* represents the in-scattering correction by the NLC method.

#### 2.5 1D Core Problem

Benchmark calculations were performed for a simple 1D core problem as proposed by Seoul National University to compare assembly power distribution for anisotropic scattering options. In this calculation, a problem-specified ray tracking option (4 polar angles for 90°, 16 azimuthal angles for 90°, and a ray-spacing of 0.05 cm) was used. Table I gives the DeCART2D solutions with various scattering treatment options. The difference in multiplication factor is not significant, whereas the difference in the assembly power is meaningful. In particular, the out-scattering-based TCP0 remarkably underestimates the peripheral assembly power, whereas the high-order ( $\geq P2$ ) calculation slightly overestimates it. On the other hand, the in-scattering-based TCP0 shows a very good agreement compared to other options. Of course, P1 gives the best match, but it seems to be due to coincidence.

#### 2.6 2D Core Problem

To confirm an improvement in radial power tilt for a two-dimensional (2D) core geometry, the VERA benchmark [10] has been solved. For this purpose, the problem #5-2D—including complex effects such as high neutron leakage at the core periphery and neutron flux suppression from inserting control rods—was chosen. In this calculation, a default ray tracking option (3 polar angles for 90°, 8 azimuthal angles for 90°, and a ray-spacing of 0.02 cm) was used. Figure 4 shows the comparison of reactivity differences for several scattering treatment options. One can clearly observe that the in-scattering-based TCP0 is the most accurate compared to others, even when control rods are present. Figure 5 shows the comparison of assembly-wise powers for unrodded and B<sub>4</sub>C rodded cases. Like the results for 1D core problem, the out-scattering-based TCP0 underestimates the assembly power at the core periphery, and the error in the interior of the core is quite large. However, the in-scattering-based TCP0 introduces negligible power tilt similar to that obtained when employing P2.

Table I: DeCART2D solutions for 1D core problem

McCARD Reference								
Normalized Assembly Power								keff
0.9211	1.4287	0.8886	1.3276	0.7932	1.1329	0.6353	0.8332	1.08077
Center				Edge				
DeCART2D, TCP0, Out-scattering								
0.9406	1.4622	0.9029	1.3448	0.7926	1.1195	0.6133	0.7945	Norm. P
1.95	3.35	1.43	1.72	-0.06	-1.34	-2.20	-3.87	Abs.Err.[%]
2.11	2.34	1.61	1.29	-0.08	-1.18	-3.46	-4.64	Rel.Err.[%]
Abs. Err. [%]	RMS	2.35	Max.	3.87	keff		1.07582	
Rel. Err. [%]	RMS	2.56	Max.	4.64	$\Delta p$ [pcm]	-426		
Computing Time [min.] = 92 (1.00)								
DeCART2D, TCP0, In-scattering								
0.9167	1.4287	0.8845	1.3284	0.7903	1.1350	0.6339	0.8410	Norm. P
-0.44	0.00	-0.41	0.08	-0.29	0.21	-0.14	0.78	Abs.Err.[%]
-0.48	0.00	-0.46	0.06	-0.37	0.18	-0.22	0.94	Rel.Err.[%]
Abs. Err. [%]	RMS	0.39	Max.	0.78	keff		1.07649	
Rel. Err. [%]	RMS	0.45	Max.	0.94	$\Delta p$ [pcm]	-368		
Computing Time [min.] = 92 (1.00)								
DeCART2D, P1								
0.9234	1.4316	0.8904	1.3292	0.7937	1.1317	0.6334	0.8288	Norm. P
0.23	0.29	0.18	0.16	0.05	-0.12	-0.19	-0.44	Abs.Err.[%]
0.25	0.20	0.20	0.12	0.06	-0.11	-0.29	-0.52	Rel.Err.[%]
Abs. Err. [%]	RMS	0.24	Max.	0.44	keff		1.07645	
Rel. Err. [%]	RMS	0.27	Max.	0.52	$\Delta p$ [pcm]	-371		
Computing Time [min.] = 116 (1.26)								
DeCART2D, P2								
0.9151	1.4244	0.8836	1.3262	0.7910	1.1363	0.6373	0.8443	Norm. P
-0.60	-0.43	-0.50	-0.14	-0.22	0.34	0.20	1.11	Abs.Err.[%]
-0.65	-0.30	-0.56	-0.11	-0.28	0.30	0.32	1.34	Rel.Err.[%]
Abs. Err. [%]	RMS	0.55	Max.	1.11	keff		1.07691	
Rel. Err. [%]	RMS	0.62	Max.	1.34	$\Delta p$ [pcm]	-332		
Computing Time [min.] = 136 (1.48)								
DeCART2D, P3								
0.9156	1.4248	0.8840	1.3263	0.7912	1.1360	0.6371	0.8435	Norm. P
-0.55	-0.39	-0.46	-0.13	-0.20	0.31	0.18	1.03	Abs.Err.[%]
-0.60	-0.27	-0.52	-0.10	-0.25	0.27	0.29	1.24	Rel.Err.[%]
Abs. Err. [%]	RMS	0.51	Max.	1.03	keff		1.07685	
Rel. Err. [%]	RMS	0.57	Max.	1.24	$\Delta p$ [pcm]	-337		
Computing Time [min.] = 149 (1.62)								

RMS: Root Mean Square

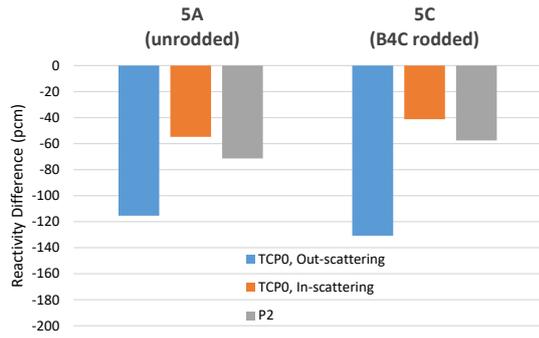


Fig. 4. Reactivity difference for 2D core problems.

	1.0055	0.9307	1.0170	0.9961	1.1248	1.0519	1.0668	0.7767
	3.02	3.15	2.41	1.83	0.58	-0.10	-1.16	-0.76
	-1.39	-0.97	-1.24	-0.61	-0.76	0.02	0.04	1.12
	-2.11	-1.78	-1.82	-1.10	-0.86	0.08	0.52	1.60
		0.9995	0.9048	1.0829	1.0554	1.1556	1.0480	0.8881
		2.76	2.53	1.39	0.68	-0.54	-0.84	-0.82
		-1.33	-0.75	-1.00	-0.31	-0.37	0.68	1.13
		-1.99	-1.41	-1.33	-0.51	-0.16	0.99	1.60
			1.0569	1.0366	1.1704	1.1418	1.0859	0.7887
			1.74	1.21	0.03	-0.60	-1.53	-1.01
			-1.06	-0.46	-0.62	0.11	0.13	1.18
			-1.49	-0.82	-0.61	0.22	0.65	1.57
Time [min.]			1.1646	1.0989	1.1518	1.0395	0.6486	
155 (1.00)			0.27	-0.17	-1.13	-1.11	-0.94	
160 (1.03)			-0.70	-0.03	-0.13	0.82	1.05	
248 (1.60)			-0.80	-0.09	0.12	1.06	1.31	
RMS Max.				1.3154	0.9132	0.9447		
1.43	3.15			-0.62	-1.04	-0.92		
0.82	1.39			0.07	0.49	0.95		
1.14	2.11			0.07	0.55	1.04		
KENO-VI Reference					0.9243	0.6321		
DeCART2D, TCP0, Out-scattering (Rel. % Err.)					-0.91	-0.52		
DeCART2D, TCP0, In-scattering (Rel. % Err.)					0.91	1.27		
DeCART2D, P2 (Rel. % Err.)					0.82	1.25		

(a) 5A (unrodded)

	0.3987	0.7247	0.9200	0.8059	0.5068	1.0222	1.3106	1.0293
	5.87	4.93	3.72	3.46	2.23	-0.36	-2.07	-1.87
	-1.13	-1.23	-1.50	-0.83	-0.22	0.09	0.08	1.11
	-3.41	-2.88	-2.73	-2.03	-1.38	0.19	0.91	2.04
		0.8674	0.8484	0.9833	0.9267	1.2244	1.2934	1.1766
		4.21	3.60	2.51	1.35	-0.84	-1.72	-1.87
		-1.57	-1.05	-1.20	-0.39	-0.34	0.68	1.09
		-2.86	-2.17	-1.97	-0.94	0.01	1.38	2.03
			1.0347	1.0077	1.1616	1.2514	1.3291	1.0254
			2.54	1.96	0.43	-0.89	-2.26	-1.94
			-1.35	-0.70	-0.76	0.03	0.09	1.11
			-2.07	-1.35	-0.97	0.29	0.98	1.96
Time [min.]			1.0645	0.9295	1.1493	1.2003	0.8115	
152 (1.00)			1.32	0.83	-0.97	-1.56	-1.68	
154 (1.01)			-0.94	-0.23	-0.19	0.75	0.99	
236 (1.55)			-1.40	-0.70	0.06	1.24	1.63	
RMS Max.				0.5589	0.7727	0.9989		
2.38	5.87			1.27	-0.36	-0.97		
0.88	1.57			0.47	0.48	0.84		
1.64	3.41			-0.57	0.26	0.94		
KENO-VI Reference					0.8453	0.6401		
DeCART2D, TCP0, Out-scattering (Rel. % Err.)					-0.30	-0.31		
DeCART2D, TCP0, In-scattering (Rel. % Err.)					0.93	1.16		
DeCART2D, P2 (Rel. % Err.)					0.69	1.12		

(b) 5C (B<sub>4</sub>C rodded)

Fig. 5. Normalized assembly radial power difference (%) for 2D core problems.

### 3. Conclusions

The in-scattering-based TCP0 cross sections were generated by using the NLC method and were implemented to the DeCART 47-group library. As demonstrated by the benchmark calculations, the in-scattering correction for hydrogen can improve the significant error of using the out-scattering-based TCP0. This approach would be especially helpful in obtaining very accurate results when performing TCP0 calculations for whole-core problems with a reflector, such as the generation of reflector cross sections for typical reactor core design and analysis. However, despite using the NLC method, negative flux issues that appear in the TCP0 calculations still remain.

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### REFERENCES

- [1] R.J.J. Stamm'ler, M.J. Abbate, *Methods of Steady-State Reactor Physics in Nuclear Design*, Academic Press, London, 1983.
- [2] M. Ryu, Y. S. Jung, C. H. Lim, H. G. Joo, Incorporation of Anisotropic Scattering in nTRACER, *Trans. Kor. Nucl. Soc. Autumn Mtg.*, Pyeongchang, Korea, Oct. 30-31, 2014.
- [3] S. Y. Choi, K. S. Smith, H. Kim, T. Tak, D. Lee, On the Diffusion Coefficient Calculation in Two-step Light Water Reactor Core Analysis, *J. Nucl. Sci. Tech.*, vol. 54, no. 6, pp. 705-715, 2017.
- [4] K. S. Kim, M. L. Williams, D. Wiarda, K. T. Clarno, Development of the Multigroup Cross Section Library for the CASL Neutronics Simulator MPACT: Method and procedure, *Ann. Nucl. Energy*, vol. 133, pp. 46-58, 2019.
- [5] B. R. Herman, B. Forget, K. Smith, B. N. Aviles, Improved Diffusion Coefficients Generated from Monte Carlo Codes, *Proc. M&C 2013*, Sun Valley, Idaho, May 5-9, 2013.
- [6] J. Y. Cho, H. G. Joo, K. S. Kim, S. Q. Zee, Cell Based CMFD Formulation for Acceleration of Whole-core Method of Characteristics Calculations, *Nucl. Eng. Tech.*, vol. 34, no. 3, pp. 250-258, 2002.
- [7] J. Y. Cho, et al., DeCART2D v1.0 Methodology Manual, KAERI/TR-5283/2013, Dec. 2013.
- [8] H. J. Park, K. S. Kim, S. G. Hong, J. S. Song, An Improved DeCART Library Generation Procedure with Explicit Resonance Interference Using Continuous Energy Monte Carlo Calculation, *Ann. Nucl. Energy*, vol. 105, pp. 95-105, 2017.
- [9] J. S. Song, S. Y. Park, K. K. Kim, H. R. Kim, "The Daily Load Follow Capability of the SMART Reactor Core without the Soluble Boron Change in the Primary Coolant," *Proc. PBNC 2010*, Cancun, Mexico, Oct. 24-30, 2010.
- [10] A. T. Godfrey, VERA Core Physics Benchmark Progression Problem Specifications, CASL-U-2012-0131-004, Revision 4, Aug. 29, 2014.