Development of a Direction-Specific Nodal Diffusion Solver for Cylindrical Geometry

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1. Introduction

Accurate prediction of the core power distribution is a central objective in reactor physics, as it directly underpins fuel integrity assessment, core design optimization, and safety margin evaluation. This requirement has intensified in the context of Generation IV reactor development, where Molten Salt Reactors (MSRs) have attracted considerable attention owing to their inherent safety features, high thermal efficiency, and potential for closed fuel cycle operation. As MSR development programs continue to advance globally, the establishment of a reliable and efficient neutronics calculation framework tailored to MSR-specific characteristics has become an increasingly pressing need.

A comprehensive neutronics framework for MSR analysis ultimately requires a tightly integrated two-step calculation system coupling a high-fidelity Monte Carlo code with a deterministic multigroup diffusion code. In such a scheme, the Monte Carlo solver generates homogenized few-group cross sections and equivalence parameters — most critically the discontinuity factors from generalized equivalence theory — which are then passed to the diffusion solver for efficient whole-core calculations. Realizing this framework demands progress along several parallel lines: development of a multigroup diffusion code suited to the cylindrical geometry native to MSR cores, proper implementation of equivalence theory to preserve transport-level accuracy, and extension of Monte Carlo tally capabilities to generate the required homogenized constants. The present work addresses the most foundational of these components — the development of the diffusion solver — as a robust and independently validated diffusion code must first be established before the broader coupling infrastructure can be meaningfully built upon it.

The cylindrical geometry (r, θ, z) introduces numerical challenges absent in the Cartesian case. In the radial direction, non-uniform cell face areas and the coordinate singularity at r = 0 require special treatment of polynomial basis functions. In the azimuthal direction, the $1/r^2$ factor in the diffusion operator prevents a rigorous one-dimensional transverse-integrated equation from being derived in closed form. These challenges have motivated sustained research into cylindrical nodal methods (Bandini, 1990; Cho & Lee, 2008; Ougouag & Terry, 2002; Wang et al., 2010; Wen et al., 2023) yet no single approach has proven fully satisfactory across all three coordinate directions simultaneously.

Recognizing that r, θ, and z present mathematically distinct challenges, the proposed code CYNUS (CYlindrical NeUtronic Simulator) adopts a direction-specific nodal strategy. The Source Expansion Nodal Method (SENM) is applied in the θ- and z-directions where the governing equations are amenable to standard polynomial expansion, while a two-node Coarse Mesh Finite Difference (CMFD) formulation is used in the r-direction to handle geometric singularities robustly. Global convergence is then driven by the CMFD framework, which exploits discontinuity factors supplied by the nodal solver to preserve accuracy on coarse meshes. This paper presents the theoretical foundation of CYNUS, with emphasis on the two-node CMFD formulation in the radial direction and the SENM solutions in the θ- and z-directions, alongside preliminary numerical results compared against established reference solutions. This work constitutes the first step toward a fully integrated Monte Carlo/diffusion calculation system for MSR neutronics analysis.

2. Numerical Method

2.1 Solution of CMFD two-node equations in r-direction

Approach taken for solving neutron diffusion equation in radial direction for cylindrical geometry was two-node second order Coarse Mesh Finite Difference Method (CMFD). Instead of assuming one neutron flux value for given node, as in usual FDM it is approximated to be a polynomial function given as (2.1).

$$\phi_{gr}^{k}(r) = \sum_{i=0}^{2} a_i p_i \tag{2.1}$$

Where a_i are coefficients obtained by solving equations that satisfy: neutron flux continuity (2.2), neutron current density continuity (2.3), nodal balance equations (2.4) and average flux preservations (2.5), where last two are applied for two nodes.

$$\phi_{gr+}^{k} = \phi_{gr-}^{k+1} \tag{2.2}$$

$$J_{gr+}^{k} = J_{gr-}^{k+1} \tag{2.3}$$

$$\frac{J^k_{gr+}\left(r_k+\frac{\Delta r_k}{2}\right)-J^k_{gr-}\left(r_k-\frac{\Delta r_k}{2}\right)}{r_k\Delta r_k}+ \\ +\bar{\phi}^k_{gr}\Sigma^k_g=Q^k_{gr}-L^k_{gr} \tag{2.4}$$

$$\frac{1}{r_k\Delta r_k}\int_{r_k-\frac{\Delta r_k}{2}}^{r_k+\frac{\Delta r_k}{2}}\phi^k_{gr}(r)\,dr=\bar{\phi}^k_{gr} \tag{2.5}$$

And the p^k_i are given base functions expressed as following (2.6-8) per (Komlev & Suslov, 1995).

$$p^k_0(r)=1 \tag{2.6}$$

$$p^k_1(r)=6\frac{r-r_k}{\Delta r_k}-\frac{\Delta r_k}{2r_k} \tag{2.7}$$

$$p^k_2(r)=12\left(\frac{r-r_k}{\Delta r_k}\right)^2-1 \tag{2.8}$$

Because equation (2.5) can be simplified to (2.9), basing on properties of the base functions (2.6-8)

$$a^k_{gr0}=\bar{\phi}^k_{gr} \tag{2.9}$$

After inputting function (2.1) to the equations (2.2-5), following conditions are obtained (2.10-12).

$$a^k_{gr1}\left(-3-\frac{\Delta r_k}{2r_k}\right)+2a^k_{gr2}+a^{k+1}_{gr1}\left(3+\frac{\Delta r_{k+1}}{2r_{k+1}}\right)- \\ -2a^{k+1}_{gr2}=\bar{\phi}^k_{gr}-\bar{\phi}^{k+1}_{gr} \tag{2.10}$$

$$a^k_{gr1}\frac{-6D^k_g}{\Delta r_k}+a^k_{gr2}\frac{-12D^k_g}{\Delta r_k}+a^{k+1}_{gr1}\frac{6D^{k+1}_g}{\Delta r_{k+1}}+ \\ +a^{k+1}_{gr2}\frac{-12D^{k+1}_g}{\Delta r_{k+1}}=0 \tag{2.11}$$

$$a^k_{gr1}\frac{-6D^k_g}{r_k\Delta r_k}+a^k_{gr2}\frac{-24D^k_g}{\Delta r^2_k}=Q^k_{gr}-L^k_{gr} \tag{2.12}$$

Which than can be expressed as the set of equation (2.13).

$$\begin{bmatrix} -3-\frac{\Delta r_k}{2r_k} & 2 & 3+\frac{\Delta r_{k+1}}{2r_{k+1}} & -2 \\ \frac{-6D^k_g}{\Delta r_k} & \frac{-12D^k_g}{\Delta r_k} & \frac{6D^{k+1}_g}{\Delta r_{k+1}} & \frac{-12D^{k+1}_g}{\Delta r_{k+1}} \\ \frac{-6D^k_g}{r_k\Delta r_k} & \frac{-24D^k_g}{\Delta r^2_k} & 0 & 0 \\ 0 & 0 & \frac{-6D^{k+1}_g}{r_{k+1}\Delta r_{k+1}} & \frac{-24D^{k+1}_g}{\Delta r^2_{k+1}} \end{bmatrix}\cdot \\ \cdot\begin{bmatrix} a^k_{gr1} \\ a^k_{gr2} \\ a^{k+1}_{gr1} \\ a^{k+1}_{gr2} \end{bmatrix}=\begin{bmatrix} \bar{\phi}^k_{gr}-\bar{\phi}^{k+1}_{gr} \\ 0 \\ Q^k_{gr}-L^k_{gr}-\bar{\phi}^k_{gr}\Sigma^k_g \\ Q^{k+1}_{gr}-L^{k+1}_{gr}-\bar{\phi}^{k+1}_{gr}\Sigma^{k+1}_g \end{bmatrix} \tag{2.13}$$

After establishing values of coefficients a^k_{gri} on basis the function (2.1), new corrected neutron current density is obtained (2.14), and correction factor for harmonic diffusion coefficient (2.15) is being introduced that is applied for future iterations of FDM calculation (2.16).

$$J^k_{gr\,CMFD}=-D^k_g\cdot\nabla\phi^k_{gr}(r) \tag{2.14}$$

$$\widehat{D}^k_g=\frac{J^k_{gr\,FDM}-J^k_{gr\,CMFD}}{\bar{\phi}^k_{gr}+\bar{\phi}^{k+1}_{gr}} \tag{2.15}$$

$$J^k_{gr}=-\widetilde{D}^k_g\left(\bar{\phi}^k_{gr}-\bar{\phi}^{k+1}_{gr}\right)-\widehat{D}^k_g\left(\bar{\phi}^k_{gr}+\bar{\phi}^{k+1}_{gr}\right) \tag{2.16}$$

However, approach for boundary nodes is modified as they are lacking one neighboring cell. In this instance the additional second neutron flux function is being disregarded. Equations that are to be satisfied are than nodal balance equation (2.4), average flux preservation (2.5) and albedo boundary condition (2.17).

$$J^k_{gr}=\phi^k_{gr}(r)\cdot\alpha_k \tag{2.17}$$

Equation (2.17) after substitutions is than given as (2.18), for the outer layer nodes.

$$a^k_{gr1}\left(\frac{\alpha_k\Delta r_k}{2r_k}-3\alpha_k-\frac{6D^k_g}{\Delta r_k}\right)+ \\ +a^k_{gr2}\left(-2\alpha_k-\frac{12D^k_g}{\Delta r_k}\right)=\alpha_k\bar{\phi}^k_{gr} \tag{2.18}$$

Then new set of equations (2.19) is given for the boundary node.

$$\begin{bmatrix} \frac{-6D^k_g}{r_k\Delta r_k} & \frac{-24D^k_g}{\Delta r^2_k} \\ \frac{\alpha_k\Delta r_k}{2r_k}-3\alpha_k-\frac{6D^k_g}{\Delta r_k} & -2\alpha_k-\frac{12D^k_g}{\Delta r_k} \end{bmatrix}\cdot \\ \cdot\begin{bmatrix} a^k_{gr1} \\ a^k_{gr2} \end{bmatrix}=\begin{bmatrix} Q^k_{gr}-L^k_{gr}-\bar{\phi}^k_{gr}\Sigma^k_g \\ \alpha_k\bar{\phi}^k_{gr} \end{bmatrix} \tag{2.19}$$

2.2 Solution of SENM for θ-direction

Source Expansion Nodal Method has been introduced for solving the neutron diffusion equation in angular direction. In this purpose constant approximation method (2.20-21) was used to simplify the weighting factor r present in the 1D transverse integrated equation in θ-direction per (Wang et al., 2010).

$$-D_g^k \frac{1}{C_k^2}\frac{d^2}{d\theta^2}\phi_{g\theta}^k(\theta) + \Sigma_g^k \phi_{g\theta}^k(\theta) = Q_{g\theta}^k - L_{g\theta}^k \quad (2.20)$$

$$C_k^2 \approx \frac{r_k \Delta r_k}{\ln\left(\left(r_k + \frac{\Delta r_k}{2}\right)\left(r_k - \frac{\Delta r_k}{2}\right)\right)} \quad (2.21)$$

Afterwards regular SEMN is being applied as per. Where source term is approximated with use of Legendre polynomials.

2.3 Solution of SENM for z-direction

Handling the z-direction 1D transverse integrated equation is the easiest one because the Laplace operator appearing in the leakage term gives off the same results as in the Cartesian coordinate system. Therefore, algorithm of calculations is the same as given per (Yoon & Joo, 2008).

3. Numerical Result

To verify the CYNUS code, the "Cylindrized" version of the three-dimensional IAEA PWR benchmark problem proposed by (Prinsloo & Tomašević, 2008)is employed as a preliminary test case. This benchmark adapts the original IAEA 3D PWR problem to cylindrical (r, θ, z) geometry while preserving the nature of the flux gradients in the problem. Reflective boundary conditions are applied on the azimuthal surfaces, and vacuum boundary conditions are applied on the outer radial, top, and bottom axial surfaces.

Figures 1-3 present the reference and CYNUS solutions for the problem along with the nodal relative assembly averaged power errors. The maximum 0.915% and appears near to the center of the given "cylindralized" LWR problem. Presented figures are established in the r, z plane.

Table 1 presents the k-eff obtained by CYNUS for the Prinsloo LWR benchmark problem in comparison with the reference solution. CYNUS yields a k-eff of 1.03379, which is in good agreement with the reference value provided by (Prinsloo & Tomašević, 2008).

Table 1. k-eff comparison

Code	k-eff	Error (pcm)
Reference (Prinsloo and Tomasevic, 2008)	1.03353	–
CYNUS (present)	1.03379	24pcm

The k-eff result demonstrates the basic capability of CYNUS to solve the neutron diffusion equation in three-dimensional cylindrical geometry. A more comprehensive validation, including nodal power distribution and assembly-averaged flux comparisons against the reference solutions of (Prinsloo & Tomašević, 2008), is currently in progress and will be reported, also. In particular, the accuracy of the direction-specific nodal strategy — SENM in the θ- and z-directions and two-node CMFD in the r-direction — will be assessed through detailed spatial distribution comparisons.

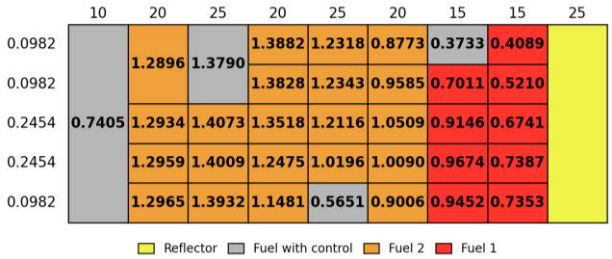

Fig. 1. Reference relative assembly averaged power for the "cylindralized" LWR problem. (Prinsloo & Tomašević, 2008)

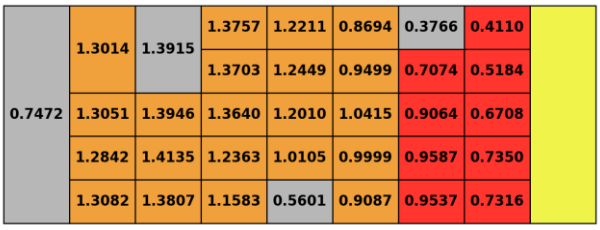

Fig. 2. CYNUS relative assembly averaged power for the "cylindralized" LWR problem.

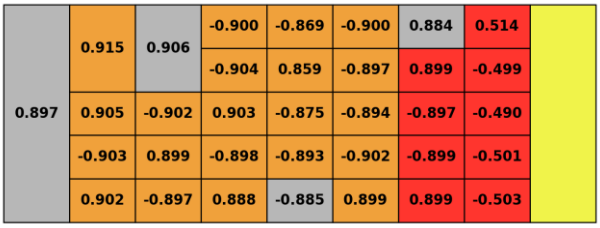

Fig. 3. CYNUS nodal relative assembly averaged power errors for the "cylindralized" LWR problem.

3. Conclusions

This paper presented the theoretical foundation and preliminary results of CYNUS, a multigroup neutron diffusion code under development for three-dimensional cylindrical geometry. The development of CYNUS constitutes the first step toward a fully integrated Monte Carlo/diffusion two-step calculation framework for Molten Salt Reactor (MSR) neutronics analysis, in which the diffusion solver plays a central role in efficient whole-core power distribution calculations.

To address the distinct mathematical characteristics of each coordinate direction in cylindrical geometry, CYNUS adopts a direction-specific nodal strategy. The two-node SENM is applied in the θ- and z-directions, where the transverse-integrated diffusion equations reduce to a standard form amenable to polynomial expansion. In the r-direction, where the non-uniform cell face areas and the coordinate singularity at r = 0 pose significant numerical difficulties, a two-node NEM with quadratic expansion of 1D flux is employed to ensure geometric robustness. Global convergence of the neutron flux and eigenvalue is achieved through the CMFD

As a preliminary verification, the "Cylindrized" version of the three-dimensional IAEA PWR benchmark problem proposed by Prinsloo and Tomasevic (2008) was solved using CYNUS. The code yielded a k-eff of 1.03379, which is in good agreement with the reference solution, demonstrating the basic correctness of the implemented numerical methods.

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