

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

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01

Introduction

Introduction

Cylindrical NeUtronic Simulator (CYNUS)

- Neutronics code based on Coarse Mesh Finite Difference Method
- 3D Neutron diffusion equation decomposition into three 1D equations via transverse integration
- Two-node approach applied to Source Expansion Nodal Method and Nodal Expansion Method, for high accuracy neutron current (Yoon & Joo, 2008)
- Robust and reliable solutions without computationally expensive fine mesh discretization`
- Coordinate system well-suited for Molten Salt Reactor calculations

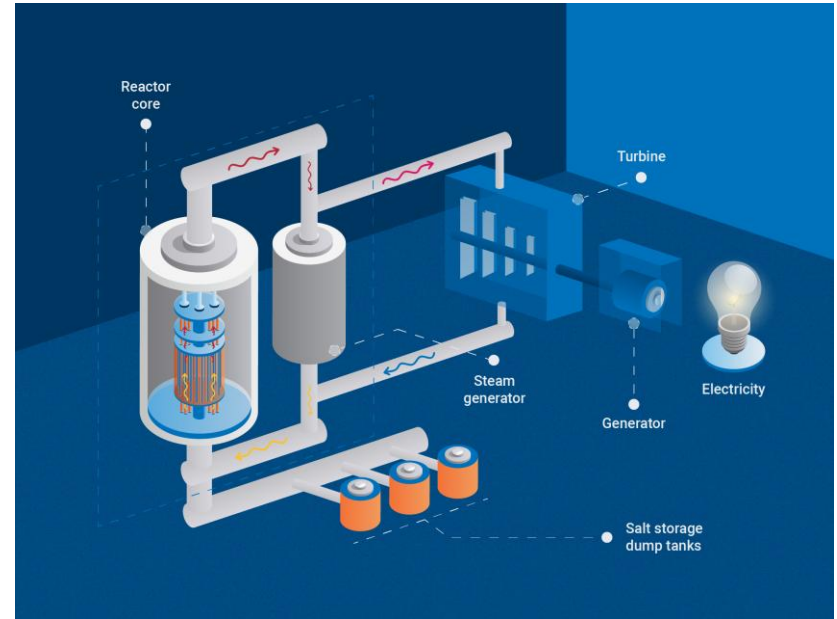


Fig. 1. Molten Salt Reactor conceptual diagram (1)

(1) - <https://www.iaea.org/newscenter/news/what-are-molten-salt-reactors>

Introduction

Research Gap and Challenges

Cylindrical geometry introduces numerical challenges absent in Cartesian coordinate system

- Coordinate singularity at $r=0$
- Jacobian affecting integrals over volume
- Complicated Laplace operator

Significant academic effort has been dedicated to cylindrical nodal methods. However, no single approach has proven fully satisfactory across all three coordinate direction (Bandini, 1990; Cho & Lee, 2008; Ougouag & Terry, 2002; Wang et al., 2010; Wen et al., 2023)

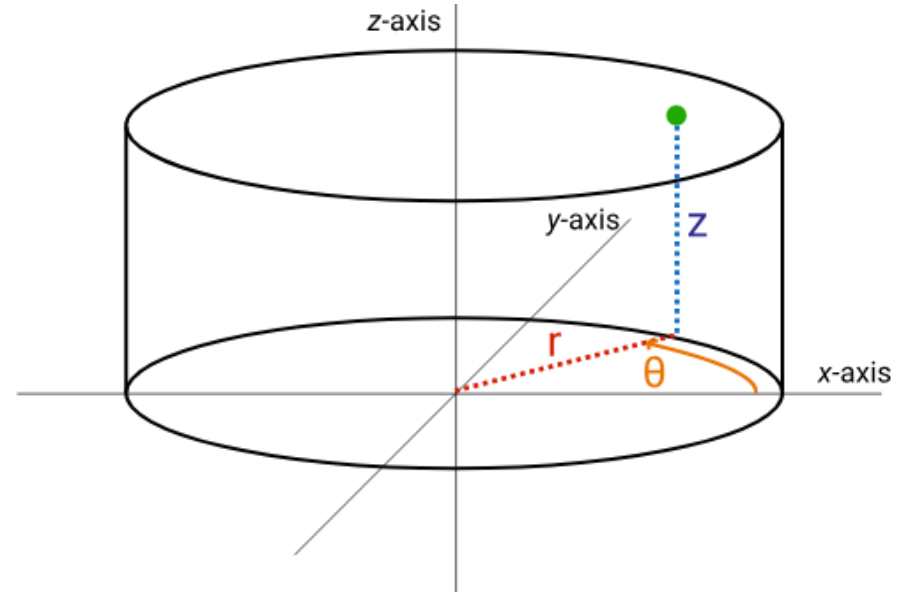


Fig. 2. Cylindrical coordinate system (2)

(2) - <https://brilliant.org/wiki/cylindrical-coordinates/>

02

CMFD Scheme

CMFD Scheme

- Coarse Mesh Finite Difference Method work as regular Finite Difference Method for few iterations
- Nodal Expansion Method of choice approximates neutron flux across the node as a function, which is used to analytically determine high quality neutron current
- Accurate neutron current values between nodes are incorporated into FDM part of scheme

$$\hat{D}^k = \frac{J_{FDM}^k - J_{NEM}^k}{\bar{\phi}^k + \bar{\phi}^{k+1}}$$

- In the CMFD scheme neutron current is established via modified FDM formula

$$J^k = -\tilde{D}^k(\bar{\phi}^k - \bar{\phi}^{k+1}) - \hat{D}^k(\bar{\phi}^k + \bar{\phi}^{k+1})$$

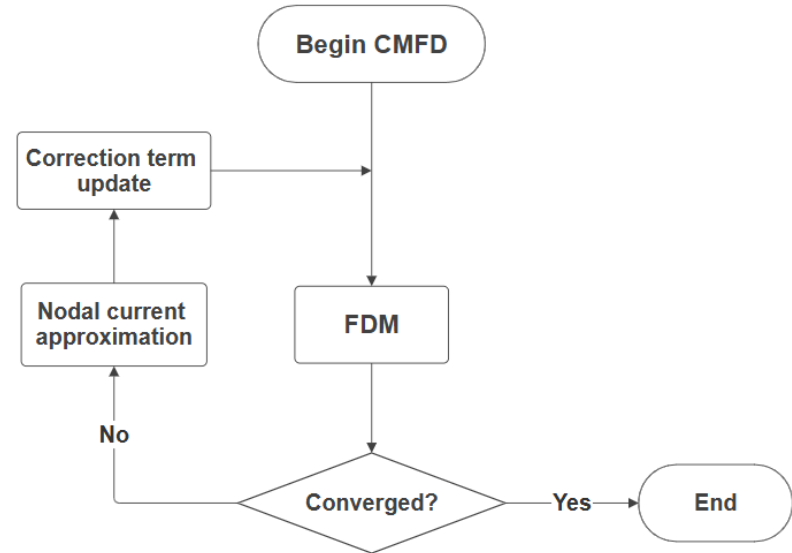


Fig. 3. CMFD flowchart

Steady-state 3D Neutron Diffusion Equation

$$\nabla \cdot \vec{J}_g(r, \theta, z) + \Sigma_{tg} \phi_g(r, \theta, z) = \frac{\chi_g}{k_{eff}} \sum_{g'=1}^G v \Sigma_{fg'} \phi_{g'}(r, \theta, z) + \sum_{g'=1}^G \Sigma_{sg' \rightarrow g} \phi_{g'}(r, \theta, z)$$



Three 1D Transverse Integrated Neutron Diffusion Equations

$$-\frac{4D_g}{h_u^2} \cdot \frac{d^2}{d\xi_u^2} \bar{\phi}_{gu}(\xi_u) + \Sigma_{tg} \bar{\phi}_{gu}(\xi_u) = \frac{\chi_g}{k_{eff}} \sum_{g'=1}^G v \Sigma_{fg'} \bar{\phi}_{g'u}(\xi_u) + \sum_{g'=1}^G \Sigma_{sg' \rightarrow g} \bar{\phi}_{g'u}(\xi_u) - L(\xi_u)$$
$$-D_g \cdot \frac{d^2}{dr^2} \bar{\phi}_{gr}(r) + \Sigma_{tg} \bar{\phi}_{gt}(r) = \frac{\chi_g}{k_{eff}} \sum_{g'=1}^G v \Sigma_{fg'} \bar{\phi}_{g'r}(r) + \sum_{g'=1}^G \Sigma_{sg' \rightarrow g} \bar{\phi}_{g'r}(r) - L(r)$$

Where independent variables have been normalized

$\xi_u = \frac{2u}{h_u}$ and $\xi_u \in \langle -1; 1 \rangle$ for $u = \theta, z$

CMFD Scheme

- Transverse neutron leakage is result of transverse integration

$$L_{gr}^k(\xi_r) = \frac{1}{\Delta z_k} \cdot (J_{gz+}^k(\xi_r) - J_{gz-}^k(\xi_r)) + \frac{1}{r_k \Delta \theta_k} \cdot (J_{g\theta+}^k(\xi_r) - J_{g\theta-}^k(\xi_r))$$

- Zero order approximation for radial direction NEM
- Second order approximation based on neighboring nodes for SENM

$$L_{gr}^k(\xi_r) = \bar{L} + l_1 P_1(\xi_r) + l_2 P_2(\xi_r)$$

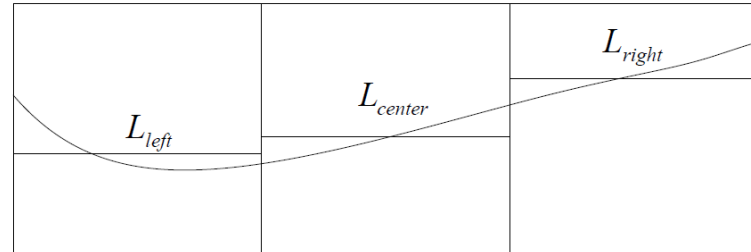


Fig. 4. Second order transverse leakage

CMFD Scheme

Laplace operator for:

- *Cartesian coordinate system*

$$\nabla^2 \phi(x, y, z) = \frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} + \frac{\partial^2 \phi}{\partial z^2}$$

- *Cylindrical coordinate system*

$$\nabla^2 \phi(x, y, z) = \frac{1}{r} \cdot \frac{\partial}{\partial r} \left(r \cdot \frac{\partial \phi}{\partial r} \right) + \frac{1}{r^2} \cdot \frac{\partial^2 \phi}{\partial \theta^2} + \frac{\partial^2 \phi}{\partial z^2}$$

- Constant radius approximation has been established for azimuthal direction (Wang et al., 2010)

$$\nabla^2 \phi(\theta) = \frac{1}{r^2} \cdot \frac{\partial^2 \phi}{\partial \theta^2} \cong \frac{1}{C_k^2} \cdot \frac{\partial^2 \phi}{\partial \theta^2}$$
$$C_k^2 = \frac{r_k \Delta r_k}{\ln \left(r_k + \frac{1}{2} \Delta r_k \right) - \left(r_k - \frac{1}{2} \Delta r_k \right)}$$

CMFD Scheme

01

Axial direction

Laplace operator formulation for this direction is the same as in Cartesian coordinate system, so Two-node **Source Expansion Nodal Method** is applied directly

02

Azimuthal direction

After the constant radius approximation Two-node **Source Expansion Nodal Method** is also applicable for this direction

03

Radial direction

Because there is no reliable way to transform r-direction diffusion term to form that would suitable for SENM, regular Two-node **Nodal Expansion Method** is applied

03

Radial Equations Derivation

Radial Equations Derivation

- Neutron flux in the radial direction is approximated as a second order polynomial

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

- Basis functions are given by (Komlev & Suslov, 1995)

$$P_0^k(r) = 1$$

$$P_1^k(r) = 6 \frac{r - r_k}{\Delta r_k} - \frac{\Delta r_k}{2r_k}$$

$$P_2^k(r) = 12 \left(\frac{r - r_k}{\Delta r_k} \right)^2 - 1$$

Radial Equations Derivation

- Two-node approach results in 6 unknown coefficients for each surface, that are not located at boundary
- That implies the need to establish conditions that will serve as base for coefficient determination
- First two conditions apply for both left and right node

- Average neutron flux conservation
- Nodal balance equation satisfaction
- Neutron flux and neutron current

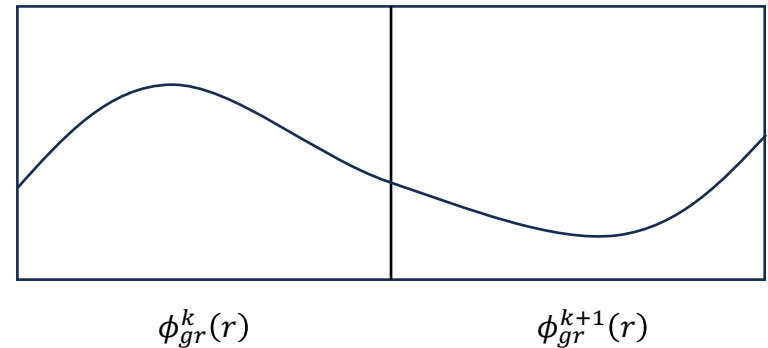


Fig. 5. Two-node NEM neutron flux approximation

Radial Equations Derivation

Average neutron flux conservation

Selected basis functions share property 0th order coefficient of flux function approximation is equal to average flux value at given node

$$\frac{1}{r_k \Delta r_k} \int_{r_k - \frac{\Delta r_k}{2}}^{r_k + \frac{\Delta r_k}{2}} \phi_{gr}^k(r) r dr = \bar{\phi}_{gr}^k$$

$$a_{gr0}^k = \bar{\phi}_{gr}^k$$

Neutron flux and neutron current continuity

Given conditions are satisfied by imposing two equations and separating unknown coefficients

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

$$J_{gr+}^k = J_{gr-}^{k+1}$$

Radial Equations Derivation

Neutron flux continuity at the common surface

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

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

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

Radial Equations Derivation

Neutron current continuity at the common surface

$$J_{gr+}^k = J_{gr-}^{k+1}$$

$$-D_{gr}^k \cdot \phi_{gr}^{k'} \left(r_k + \frac{\Delta r_k}{2} \right) = -D_{gr}^{k+1} \cdot \phi_{gr}^{k+1'} \left(r_{k+1} - \frac{\Delta r_{k+1}}{2} \right)$$

$$-D_{gr}^k \cdot \left(a_{gr1}^k \cdot \frac{6}{\Delta r_k} + a_{gr2}^k \cdot \frac{12}{\Delta r_k} \right) = -D_{gr}^{k+1} \cdot \left(a_{gr1}^{k+1} \cdot \frac{6}{\Delta r_{k+1}} - a_{gr2}^{k+1} \cdot \frac{12}{\Delta r_{k+1}} \right)$$

$$a_{gr1}^k \cdot \frac{-6D_{gr}^k}{\Delta r_k} + a_{gr2}^k \cdot \frac{-12D_{gr}^k}{\Delta r_k} + a_{gr1}^{k+1} \cdot \frac{6D_{gr}^{k+1}}{\Delta r_{k+1}} - a_{gr2}^{k+1} \cdot \frac{12D_{gr}^{k+1}}{\Delta r_{k+1}} = 0$$

Radial Equations Derivation

Nodal balance equation for both nodes

$$Q_{gr}^k = \frac{\chi_g^k}{k_{eff}} \sum_{g'=1}^G \nu \Sigma_{fg'}^k \bar{\phi}_{g'} + \sum_{g'=1}^G \Sigma_{sg' \rightarrow g}^k \bar{\phi}_{g'}$$

$$L_{gr}^k = \frac{J_{gz+}^k \left(z_k + \frac{\Delta z_k}{2} \right) - J_{gz-}^k \left(z_k - \frac{\Delta z_k}{2} \right)}{\Delta z_k} + \frac{J_{g\theta+}^k \left(\theta_k + \frac{\Delta \theta_k}{2} \right) - J_{g\theta-}^k \left(\theta_k - \frac{\Delta \theta_k}{2} \right)}{r_k \Delta \theta_k}$$

$$\frac{J_{gr+}^k \left(r_k + \frac{\Delta r_k}{2} \right) - J_{gr-}^k \left(r_k - \frac{\Delta r_k}{2} \right)}{r_k \Delta r_k} + \bar{\phi}_{gr}^k \Sigma_g^k = Q_{gr}^k - L_{gr}^k$$

Radial Equations Derivation

Nodal balance equation for both nodes

$$\frac{-D_{gr}^k \cdot \left[\phi_{gr}^{k'} \left(r_k + \frac{\Delta r_k}{2} \right) \cdot \left(r_k + \frac{\Delta r_k}{2} \right) - \phi_{gr}^{k'} \left(r_k - \frac{\Delta r_k}{2} \right) \cdot \left(r_k - \frac{\Delta r_k}{2} \right) \right]}{r_k \Delta r_k} + \bar{\phi}_{gr}^k \Sigma_g^k = Q_{gr}^k - L_{gr}^k$$

$$\frac{-D_{gr}^k \cdot \left[\left(\frac{6a_{gr1}^k}{\Delta r_k} + \frac{12a_{gr2}^k}{\Delta r_k} \right) \cdot \left(r_k + \frac{\Delta r_k}{2} \right) - \left(\frac{6a_{gr1}^k}{\Delta r_k} - \frac{12a_{gr2}^k}{\Delta r_k} \right) \cdot \left(r_k - \frac{\Delta r_k}{2} \right) \right]}{r_k \Delta r_k} + \bar{\phi}_{gr}^k \Sigma_g^k = Q_{gr}^k - L_{gr}^k$$

$$-D_{gr}^k \cdot \frac{a_{gr1}^k \cdot 6 + a_{gr2}^k \cdot \frac{24r_k}{\Delta r_k}}{r_k \Delta r_k} + \bar{\phi}_{gr}^k \Sigma_g^k = Q_{gr}^k - L_{gr}^k$$

$$a_{gr1}^k \frac{-6D_{gr}^k}{r_k \Delta r_k} + a_{gr2}^k \frac{-24D_{gr}^k}{\Delta r_k^2} = Q_{gr}^k - L_{gr}^k - \bar{\phi}_{gr}^k \Sigma_g^k$$

Radial Equations Derivation

Two-node Neutron flux coefficient matrix

$$\begin{bmatrix}
 3 - \frac{\Delta r_k}{2r_k} & 2 & 3 + \frac{\Delta r_{k+1}}{2r_{k+1}} & -2 \\
 \frac{-6D_g^k}{\Delta r_k} & \frac{-12D_g^k}{\Delta r_k} & \frac{6D_g^{k+1}}{\Delta r_{k+1}} & \frac{-12D_g^{k+1}}{\Delta r_{k+1}} \\
 \frac{-6D_g^k}{r_k \Delta r_k} & \frac{-24D_g^k}{\Delta r_k^2} & 0 & 0 \\
 0 & 0 & \frac{-6D_g^{k+1}}{r_{k+1} \Delta r_{k+1}} & \frac{-24D_g^{k+1}}{\Delta r_{k+1}^2}
 \end{bmatrix} \cdot \begin{bmatrix} a_{gr1}^k \\ a_{gr2}^k \\ a_{gr1}^{k+1} \\ a_{gr2}^{k+1} \end{bmatrix} = \begin{bmatrix} \bar{\phi}_{gr}^{k+1} - \bar{\phi}_{gr}^k \\ 0 \\ Q_{gr}^k - L_{gr}^k - \bar{\phi}_{gr}^k \Sigma_g^k \\ Q_{gr}^{k+1} - L_{gr}^{k+1} - \bar{\phi}_{gr}^{k+1} \Sigma_g^{k+1} \end{bmatrix}$$

Radial Equations Derivation

Outside boundary condition radial surfaces

- One-node NEM approach
- Need to establish 3 unknown coefficients
- Average flux conservation and nodal balance equation satisfaction conditions are passed
- New albedo boundary condition-based equation to be satisfied

$$J_{gr}^k \left(r_k + \frac{\Delta r_k}{2} \right) = \phi_{gr}^k \left(r_k + \frac{\Delta r_k}{2} \right) \cdot \alpha_k$$

$$-D_g^k \cdot \phi_{gr}^k \left(r_k + \frac{\Delta r_k}{2} \right) = \alpha_k \cdot \phi_{gr}^k \left(r_k + \frac{\Delta r_k}{2} \right)$$

$$-D_g^k \left(a_{gr1}^k \cdot \frac{6}{\Delta r_k} + a_{gr2}^k \cdot \frac{12}{\Delta r_k} \right) = \alpha_k \cdot \left[\bar{\phi}_{gr}^k + a_{gr1}^k \cdot \left(3 - \frac{\Delta r_k}{2r_k} \right) + a_{gr2}^k \cdot 2 \right]$$

$$a_{gr1}^k \cdot \left(\frac{\Delta r_k \cdot \alpha_k}{2r_k} - 3\alpha_k - \frac{6D_g^k}{\Delta r_k} \right) + a_{gr2}^k \cdot \left(-\frac{12D_g^k}{\Delta r_k} - 2\alpha_k \right) = \alpha_k \cdot \bar{\phi}_{gr}^k$$

Radial Equations Derivation

One-node boundary Neutron flux coefficient matrix

$$\begin{bmatrix} \frac{-6D_g^k}{r_k \Delta r_k} & \frac{-24D_g^k}{\Delta r_k^2} \\ \frac{\alpha_k \Delta r_k}{2r_k} - 3\alpha_k - \frac{6D_g^k}{\Delta r_k} & -2\alpha_k - \frac{12D_g^k}{\Delta r_k} \end{bmatrix} \cdot \begin{bmatrix} a_{gr1}^k \\ a_{gr2}^k \end{bmatrix} = \begin{bmatrix} Q_{gr}^k - L_{gr}^k - \bar{\phi}_{gr}^k \Sigma_g^k \\ \alpha_k \bar{\phi}_{gr}^k \end{bmatrix}$$

04

Results and Discussion

Results and Discussion

- CYNUS code has been validated with IAEA 3D “cylindricalized” PWR problem, provided by (Prinsloo & Tomašević, 2008)
- Considering symmetrical properties of the reactor volume calculations have been applied for one-eighth of the whole geometry. Reflective boundary condition has been applied in azimuthal direction
- Reference effective multiplication factor

$$k_{\text{eff}} = 1,03353$$

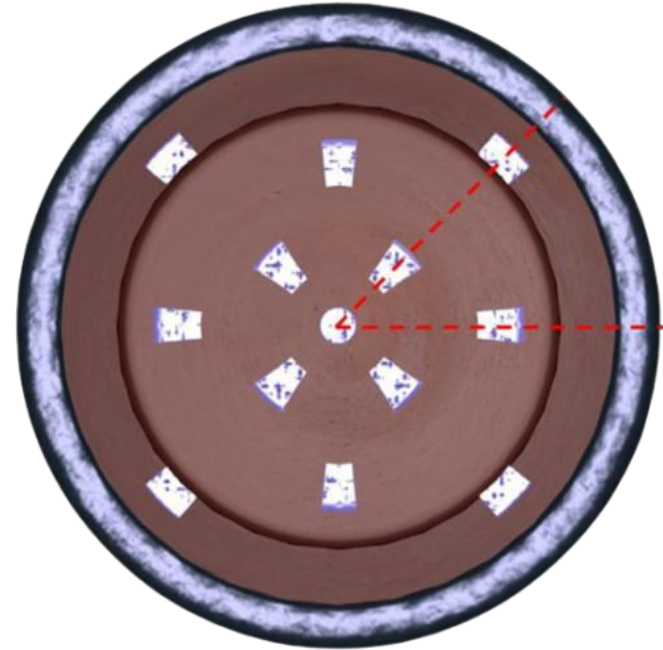


Fig. 6. IAEA 3D “cylindricalized” PWR problem top view
(Prinsloo & Tomašević, 2008)

Results and Discussion

	10	20	25	20	25	20	15	15	25
0.0982	0.7405	1.2896	1.3790	1.3882	1.2318	0.8773	0.3733	0.4089	
0.0982				1.3828	1.2343	0.9585	0.7011	0.5210	
0.2454		1.2934	1.4073	1.3518	1.2116	1.0509	0.9146	0.6741	
0.2454		1.2959	1.4009	1.2475	1.0196	1.0090	0.9674	0.7387	
0.0982		1.2965	1.3932	1.1481	0.5651	0.9006	0.9452	0.7353	

Reflector
 Fuel with control
 Fuel 2
 Fuel 1

*Fig. 7. Reference relative assembly averaged power [-]
 (Prinsloo & Tomašević, 2008)*

Results and Discussion

0.6694	1.3969	1.4679	1.4597	1.2760	0.8972	0.3476	0.3419
			1.4535	1.2740	0.9607	0.6721	0.4384
	1.3993	1.5008	1.4171	1.2450	1.0385	0.8740	0.5756
	1.4015	1.5015	1.3145	1.0383	0.9834	0.9159	0.6285
	1.4019	1.4998	1.2359	0.5535	0.8822	0.8998	0.6244
-9.597	8.323	6.444	5.153	3.587	2.267	-6.896	-16.394
			5.113	3.214	0.230	-4.142	-15.861
	8.187	6.647	4.833	2.756	-1.185	-4.438	-14.613
	8.151	7.182	5.369	1.837	-2.536	-5.321	-14.924
	8.131	7.649	7.647	-2.046	-2.045	-4.799	-15.086

Figure 8. Relative assembly averaged power [-] and power errors [%] for CYNUS all direction NEM/SENM solution

CYNUS code solution with derived radial direction NEM, along with azimuthal and axial direction SENM

- $\Delta k_{\text{eff}} = 13\text{pcm}$
- $R^2 = 0,9686$
- $\text{RMSE} = 0,1443$

Results and Discussion

CYNUS code solution only with azimuthal and axial directions SENM

- $\Delta k_{\text{eff}} = 281\text{pcm}$
- $R^2 = 0,9845$
- $\text{RMSE} = 0,1041$

0.6105	1.2914	1.3411	1.3502	1.2140	0.9102	0.3368	0.4169	
			1.3450	1.2133	0.9602	0.6963	0.4985	
	1.2922	1.3771	1.3181	1.1789	1.0418	0.9643	0.6470	
	1.2929	1.3850	1.2500	0.9576	1.0441	1.0654	0.7342	
	1.2930	1.3840	1.2050	0.4896	0.9994	1.0632	0.7423	
-17.551	0.143	-2.746	-2.738	-1.448	3.753	-9.785	1.954	
			-2.734	-1.705	0.174	-0.680	-4.328	
	-0.090	-2.148	-2.491	-2.701	-0.863	5.429	-4.025	
	-0.233	-1.138	0.199	-6.085	3.475	10.129	-0.605	
	-0.269	-0.663	4.959	-13.361	10.975	12.483	0.947	

Figure 9. Relative assembly averaged power [-] and power errors [%] for CYNUS azimuthal and axial directions SENM

Results and Discussion

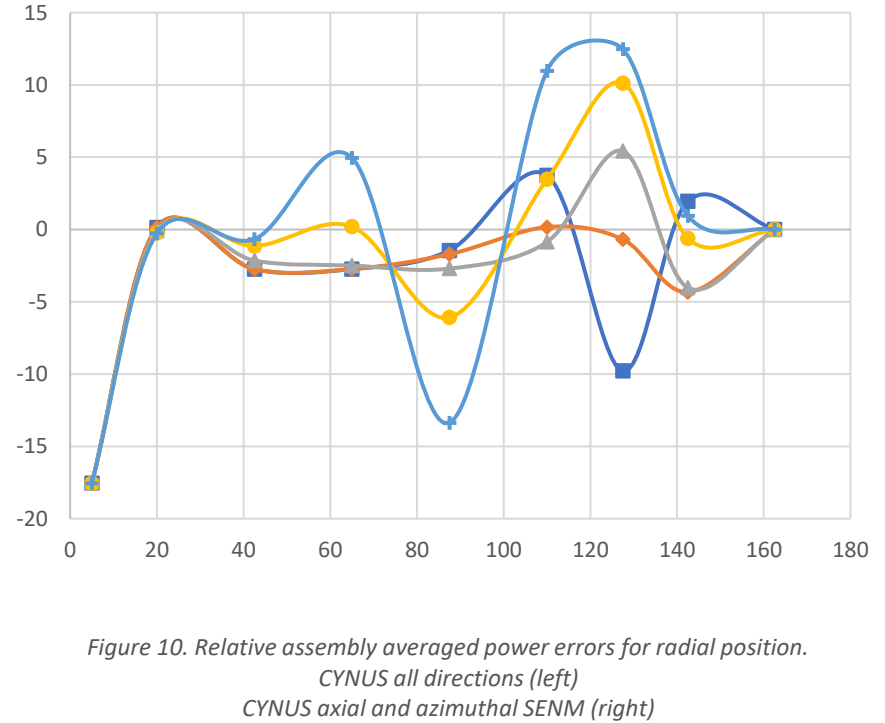
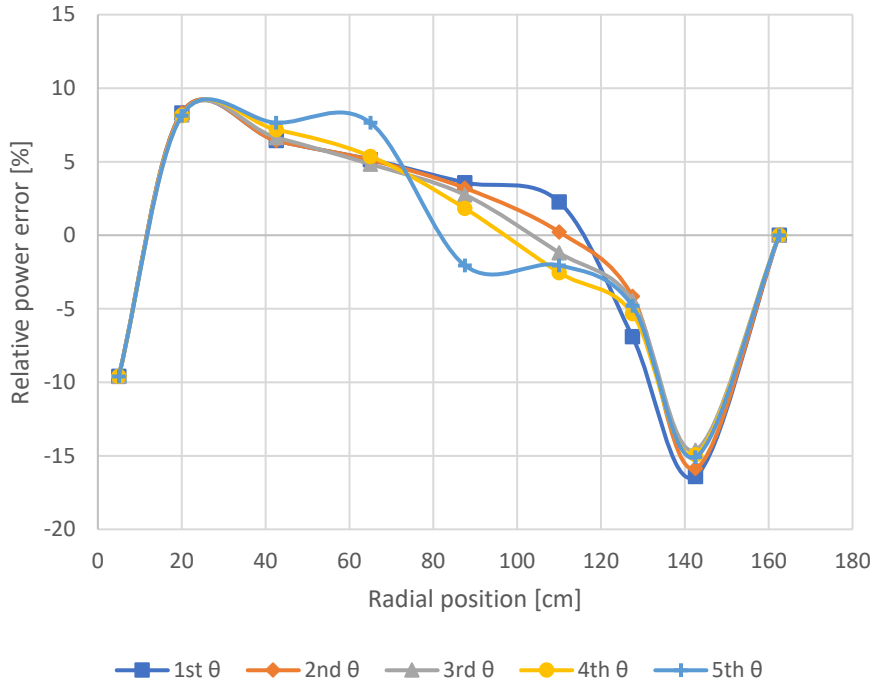


Figure 10. Relative assembly averaged power errors for radial position.
CYNUS all directions (left)
CYNUS axial and azimuthal SENM (right)

Results and Discussion

0.7472	1.3014	1.3915	1.3757	1.2211	0.8694	0.3766	0.4110
			1.3703	1.2449	0.9499	0.7074	0.5184
	1.3051	1.3946	1.3640	1.2010	1.0415	0.9064	0.6708
	1.2842	1.4135	1.2363	1.0105	0.9999	0.9587	0.7350
	1.3082	1.3807	1.1583	0.5601	0.9087	0.9537	0.7316
0.905	0.915	0.906	-0.900	-0.869	-0.900	0.884	0.514
			-0.904	0.859	-0.897	0.899	-0.499
	0.905	-0.902	0.903	-0.875	-0.894	-0.897	-0.490
	-0.903	0.899	-0.898	-0.893	-0.902	-0.899	-0.501
	0.902	-0.897	0.888	-0.885	0.899	0.899	-0.503

Figure 11. Relative assembly averaged power [-] and power errors [%] for CYNUS azimuthal and axial directions SENM and radial direction FMDM

CYNUS code solution including radial direction fine mesh discretization, along with azimuthal and axial direction SENM

- $\Delta k_{\text{eff}} = 24\text{pcm}$
- $R^2 = 0,9997$
- $\text{RMSE} = 0,0199$

Results and Discussion

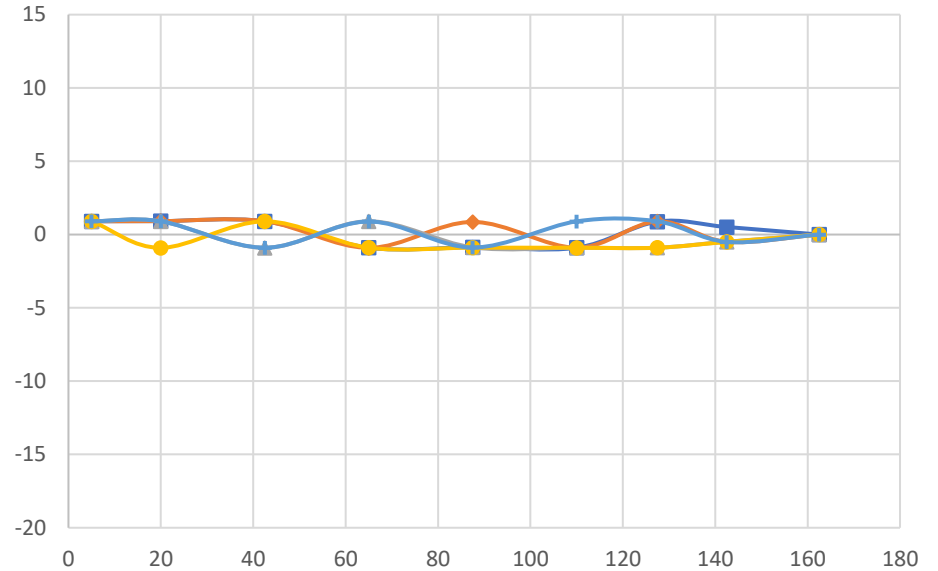
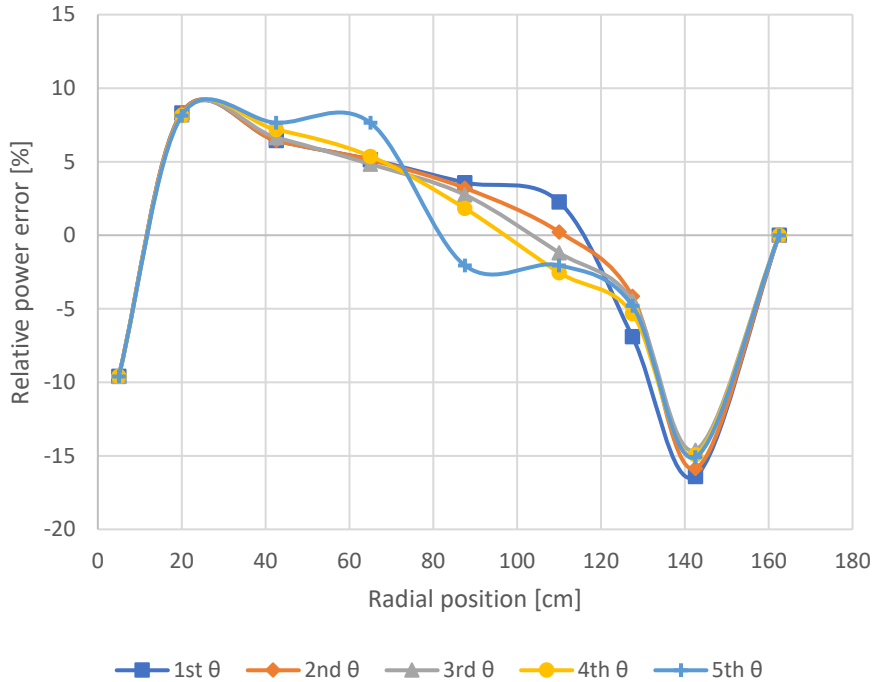


Figure 12. Relative assembly averaged power errors for radial position
CYNUS all directions (left)
CYNUS azimuthal and axial SENM and radial FMDM (right)

Results and Discussion

Table 1. Summary of key parameters.

Solver's version	Eigenvalue		Eigenvector	
	$k_{\text{eff}} [-]$	$\Delta k_{\text{eff}} [\text{pcm}]$	$R^2 [-]$	RMSE [-]
Reference	1,03353	N/A	N/A	N/A
CYNUS all direction NEM/SENM	1,03366	13	0,9686	0,1443
CYNUS azimuthal and axial SENM	1,03634	281	0,9845	0,1041
CYNUS azimuthal and axial SENM + radial fine mesh	1,03379	24	0,9997	0,0199

05

Conclusions

Conclusions

1

Current radial direction NEM performance is not satisfactory due to significant error in obtained eigenvector

2

Second order approximation of flux in radial direction is too low for robust CMFD application in cylindrical coordinate system

3

CYNUS azimuthal (with constant radius approximation) and axial direction SENM are providing accurate solutions in comparison to reference values

4

Future work: Fourth order flux approximation and second order transverse leakage expansion. Two additional conditions for flux coefficients determination based on Galerkin's Weighted Residual Method

06

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Questions & Discussion

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