Validation of COMSOL Multiphysics® for PWR Power Distribution via 3D IAEA PWR Benchmark Problem

Abdelfattah Y. Soliman
Department of Nuclear Engineering, King Abdulaziz University
Corresponding author: P.O.BOX. 80204 Jeddah 21589, Saudi Arabia
ausoliman@kau.edu.sa

Abstract: Design of the Pressurized Water Reactors (PWRs) involves extensive calculations to verify the reactor safety criteria such as power peaking factor during the reactor lifetime. Coupling of neutronic calculations, thermal hydraulic calculations and other reactor phenomena requires a multiphysics software to model the different reactor equations and solve it simultaneously without the need to use different computer codes. COMSOL multiphysics can solve the multi-group neutron diffusion equation using the finite element method. The power distribution from the output can be used for further thermal hydraulic calculations. The main purpose of the 3D IAEA light water reactor benchmark problem is to benchmark computer codes by calculating the core multiplication factor, flux and power distributions using the two group neutron diffusion method. A three dimensional model was constructed using COMSOL multiphysics to solve the two group neutron diffusion equations for the 3D IAEA PWR benchmark problem with adaptive mesh refinement option. Reactor effective multiplication factor "K_{eff}", flux distributions and power distributions were calculated and compared to the results of VENURE code. Calculations give a difference of 31 pcm in the K_{eff} and almost 2% in calculating the average assembly power distribution compared to VENURE code.

Keywords: Core calculations, finite element, COMSOL

1 Introduction

Accurate and robust simulation of the different reactor phenomena require an integration of multiphysics such as neurotics, reactor dynamics, thermal hydraulics, stress analysis and computational fluid dynamics. CMOSOL multiphysics provides a promising tool to integrate these multiphysics in the reactor steady state and transient state. Simulation of the High Flux Isotope Reactor (HFIR) core thermal hydraulics was developed using COMSOL multiphysics to facilitate the conversion from high enriched fuel (HEF) to low enriched fuel (LEF) [1,2]. Methodologies have been developed to extend HFIR two-dimensional (2D) analysis to 3D models in a timely manner [3]. The space-time simulations using multi-group diffusion equation was performed for HFIR to investigate the dynamic behavior of the reactor [4, 5]. COMSOL was benchmarked against experimental results for research reactors core calculations [6, 7]. Single channel Multi-Physics Model was investigated for lead-cooled ELSY reactor and show reasonable capabilities for steady state and transient conditions [8]. Deformation behavior of a CANDU 37-element bundle was successfully benchmarked using COMSOL to calculate elastic stresses and strains [9].

Validating the code capabilities requires benchmarking the code for different physics problems in 2D and 3D models. Due to geometrical complexity and solution time, the reactor core calculations are divided into two levels. The first level is the lattice calculation, these calculations is performed to prepare the groups constants for the multi-group neutron diffusion equation for each region in the core. The lattice calculations is done by solving the steady state transport equations. The second level is the homogenized core calculations, these calculations is performed to calculate the neutron flux and power distributions by solving the multi-group diffusion equation. This paper documents the use the commercial finite element multiphysics software package COMSOL 5.2 on a three dimensions benchmark problem for light water reactor.

2 Model description

The three dimensional light water reactor LWR problem, also known as 3D IAEA benchmark problem, is defined by B. Micheelsen (RISØ) in 1971 [10]. The main purpose of the benchmark problem is to calculate the K_{eff} and the power distribution using two group diffusion method. The two-group neutron diffusion equations for fast and thermal fluxes in the multiplying regions, noted by subscript 1 and 2 respectively, are shown in equations 1 and 2. For the non-multiplying regions the source term of equation 1 will be zero. The eigenvalue of the problem is the reactor multiplication factor which balance the left side of equation

1 that represent leakage and absorption and (or) removal from the fast group with the right hand side, which represent the source term. It is assumed that all fission neutrons are born as fast neutrons and the source term for the thermal group is the down-scattered neutrons from the fast group. It's also assumed that there is no up-scattering from the thermal group to the fast group.

$$-D_1\nabla^2\varphi_1 + (\Sigma_{a1} + \Sigma_{1\to2})\varphi_1 = \frac{1}{k}.\nu\Sigma_{f2}\varphi_2 \quad (1)$$

$$-D_2\nabla^2\varphi_2 + \Sigma_{a2}\varphi_2 = \Sigma_{1\to2}\varphi_1 \quad (2)$$

The benchmark model consists of five regions as shown in figures 1 and 2, the group constants of each region are shown in table 1. The core consist of three types of fuel elements fuel 1, 2 and fuel 2 plus control rod. The 3D model represent one-eighth of the reactor core as shown in figures 1 and 2. Four control rods are completely or partially inserted in the entire reactor core, these rod is presented in the one-eighth core model, as shown in figure 2.

Two boundary condition are applied, the external boundaries and the symmetry boundaries. For external boundaries there is no incoming current as shown in equation 3.

$$J_g^{in} = 0 \quad (3)$$

Equations 4 and 5 are deduced from equation 3, where n is the outward directed normal to the surface. The symmetry boundaries is reflective boundaries with no net current as shown in equation 6.

$$\frac{\partial\varphi_g}{\partial n} = -\frac{0.4692}{D_g}.\varphi_g \quad (4)$$

$$\varphi_g\big|_{boundary} = -2.1312.D_g.\nabla\varphi_g\big|_{boundary} \quad (5)$$

$$\frac{\partial\varphi_g}{\partial n} = 0 \quad (6)$$

PDE Coefficient mode is chosen from COMSOL physics to write the equations of each region in the eigenvalue mode. The form of the equation in the eigenvalue mode is shown in equation 7.

$$\nabla.(-c\nabla u - \propto u + \gamma) + au + \beta.\nabla u = d_a(\lambda - \lambda_o)u - e_a(\lambda - \lambda_o)^2u + f \quad (7)$$

The nomenclature of equation 7 is transformed to the diffusion equation so that "u" is the dependent variable that represent the flux φ, "c" represent the diffusion coefficient D, "a" represent the removal cross section, "f" represent the source term of equations 1 and 2, "λ" represent the eigenvalue where 0 is assumed linearization, "d_a "is the damping coefficient its value is 1, "α" is the conservative flux convection coefficient, "β"is convection coefficient and "γ" is the conservative flux source term. The values of α, β, and γ are set zero because it is not used in equation 1 and 2. Equations 1 and 2 are rearranged to follow equation 7 format. Equations 8 and 9 represent equations 1 and 2 respectively after the rearrangement.

$$-D_1\nabla^2\varphi_1 + (\Sigma_{a1} + \Sigma_{1\to2})\varphi_1 = \lambda\varphi_1 + \frac{1}{k}.\nu\Sigma_{f2}\varphi_2 \quad (8)$$

$$-D_2\nabla^2\varphi_2 + \Sigma_{a2}\varphi_2 = \lambda\varphi_2 + \Sigma_{1\to2}\varphi_1 \quad (9)$$

The boundary conditions is introduced to COMSOL model for each region as follows:
Symmetry: Neumann boundary condition is written in the form of equations 10 or 11 to represent equation 6. This boundary condition shows that divergence of the gradient of the neutron flux is equal to zero at the boundary.

$$n.(-c\nabla u - \propto u + \gamma) + qu = g \quad (10)$$

$$n.(-D\nabla\varphi) = 0 \quad (11)$$

Vacuum: Dirichlet boundary condition is applied to external surfaces and equation 5 is written in the form of equation 12.

$$hu = r \quad (12)$$

Continuity: Neumann boundary condition is applied at the surfaces between different regions, as shown in equations 13 1nd 14.

$$n.((c\nabla u - \propto u + \gamma)_1 - (c\nabla u - \propto u + \gamma)_2) + qu = g \quad (13)$$

$$n.((D\nabla\varphi)_1 - (D\nabla\varphi)_2) = 0 \quad (14)$$

Table 1. Group constants for different reactor regions

Region	D1	D2	$\Sigma_{1\to2}$	Σ_{a1}	Σ_{a2}	$\nu\Sigma_{f2}$	Material
1	1.5	0.4	0.02	0.01	0.080	0.135	Fuel 1
2	1.5	0.4	0.02	0.01	0.085	0.135	Fuel 2
3	1.5	0.4	0.02	0.01	0.130	0.135	Fuel 2 + Rod
4	2	0.3	0.04	0.00	0.010	0.000	Reflector
5	3	0.3	0.04	0.00	0.055	0.000	Reflector + Rod

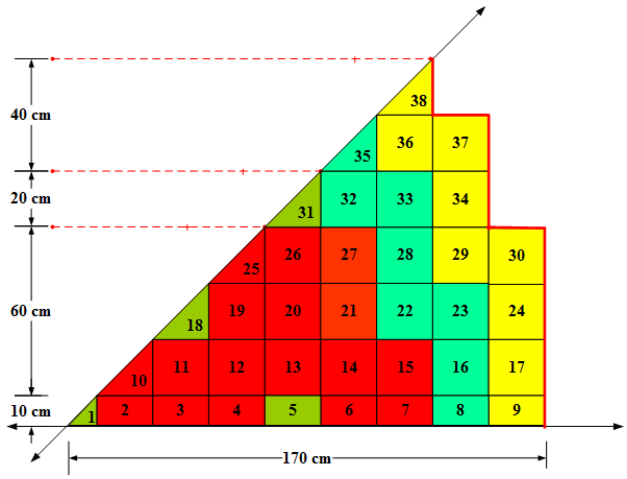

Figure 1. Horizontal Cross Section of 3D IAEA PWR benchmark problem

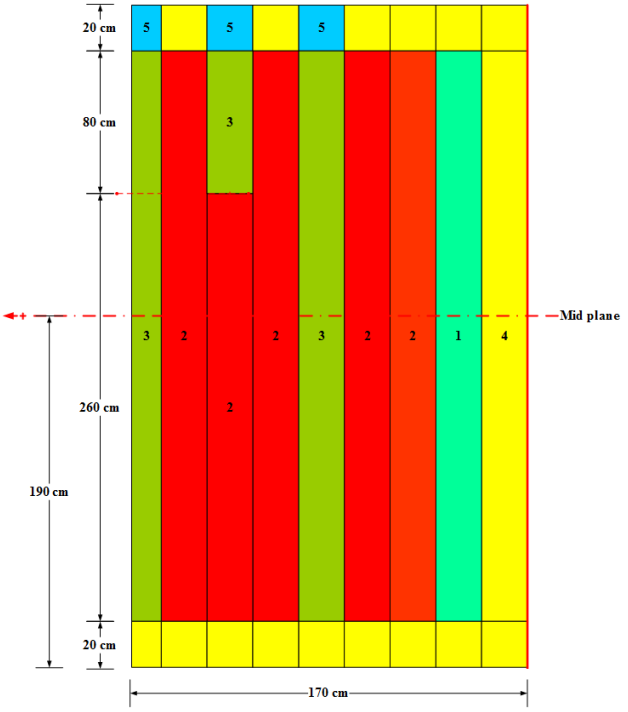

Figure 2. Vertical Cross Section of 3D IAEA PWR benchmark problem, y=0

Adaptive mesh refinement option is used to increase the accuracy of the solution in a reasonable time without the need to construct a small one size mesh everywhere. In the regions of large errors COMSOL construct finer meshes to reduce the error. While in the fixed mesh size codes the user should take this small mesh size everywhere which increase the total number of meshes in the model and then the run time. Figure 6 shows the COMSOL created mesh structure for 1/8 of the core.

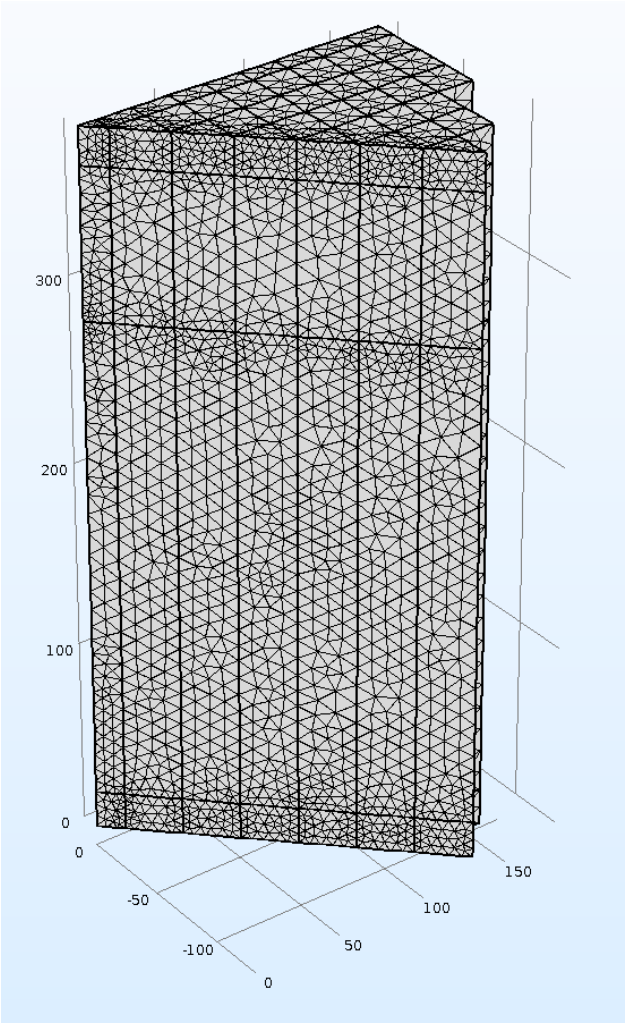

Figure 3. 3D Mesh structure by generated by COMSOL.

3 Results and discussions

COMSOL was used to model the 3D IAEA PWR benchmark problem. Thermal and fast fluxes at the core mid-plane are shown in figures 4 and 5. The calculated K_{eff} using COMSOL 5.2 using PDE mode is 1.02934. This value is compared to the VENTURE code result which is 1.02903 [8] .The difference between the COMSOL result and VENTURE code is 31 pcm. The average power distribution has been compared to the reference results. Figure 6 shows a comparison between the calculated power distribution using COMSOL and the reference value calculated by VENTURE. The maximum percentage difference found to be almost 2%. Thermal and fast flux at the mid-plane (y=0, z=190) are shown in figure 7.

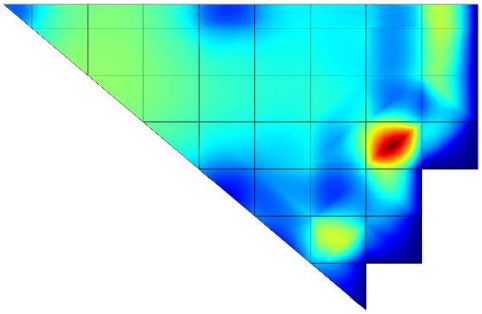

Figure 4. Thermal flux distribution at the core mid-plane (z=190)

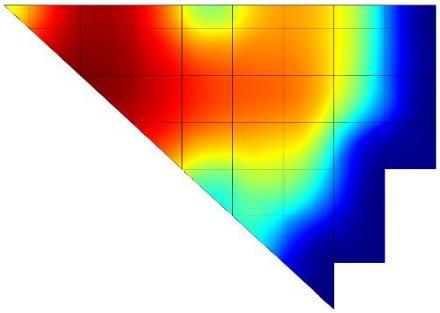

Figure 5. Fast flux distribution at the core mid-plane (z=190)

						0	
					0.6536 0.6666 1.9887	0	0
Ref. Cal. % error				0.4906 0.4946 0.8175	0.7186 0.7254 0.9476	0.6717 0.6827 1.6399	0
			1.1495 1.1545 0.4348	0.9583 0.9652 0.7233	0.9358 0.9430 0.7703	0.9203 0.9324 1.3154	0	0
		1.3174 1.3246 0.5451	1.2705 1.2777 0.5643	1.1615 1.1687 0.6184	1.0931 1.1004 0.6645	1.0260 1.0329 0.6696	0.7770 0.7849 1.0176	0
	1.3404 1.3453 0.3670	1.3732 1.3784 0.3778	1.2408 1.2476 0.5489	1.0410 1.0469 0.5691	1.0500 1.0577 0.7291	0.9920 1.0023 1.0335	0.8000 0.8116 1.4461	0
0.7220 0.7231 0.1589	1.2652 1.2675 0.1805	1.3317 1.3348 0.2304	1.1315 1.1361 0.4078	0.6057 0.6101 0.7199	0.9450 0.9522 0.7627	0.9700 0.9810 1.1361	0.8089 0.8218 1.5917	0

Figure 6. Average assembly power distribution compered to reference values [10].

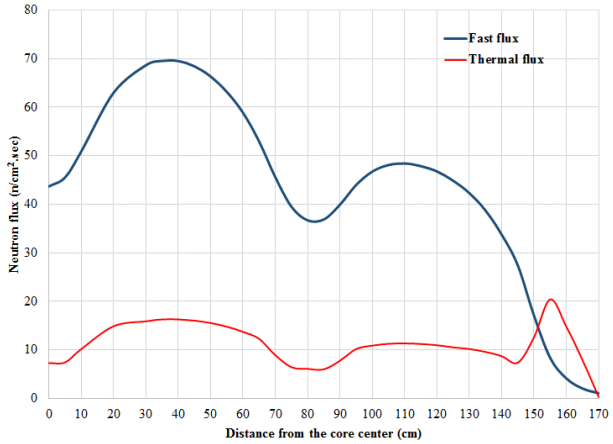

Figure 7. Flux along the x-axis at the core mid-plane (y=0, z=190).

The full reactor core is simulated by removing the symmetry conditions to represent the full core instead of 1/8 of the reactor core. Figures 8 and 9 show the thermal and fast flux distributions respectively for the full reactor core.

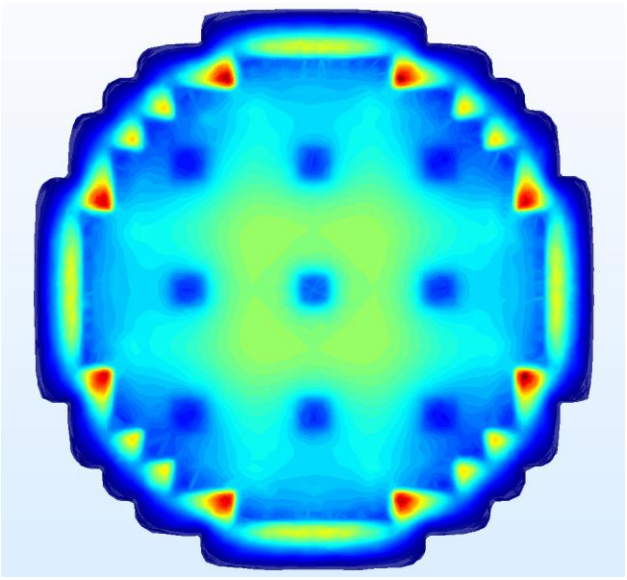

Figure 8. Thermal flux distribution in the full reactor core

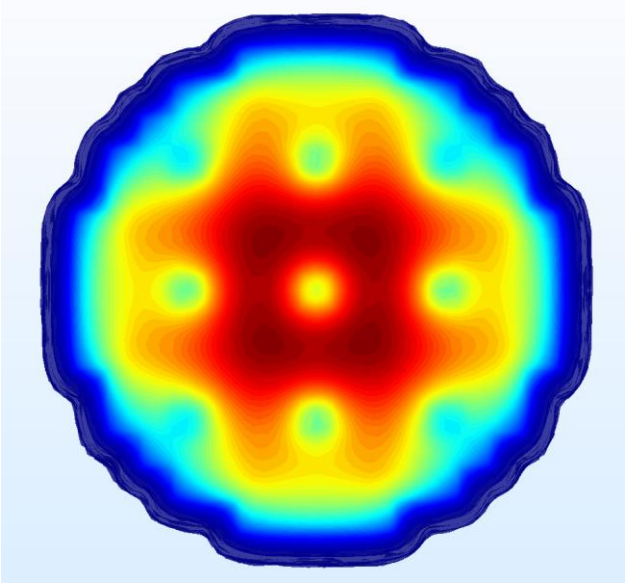

Figure 9. Fast flux distribution in the full reactor core

Conclusions

The 3D IAEA PWR benchmark problem was modeled using COMSOL 5.2. The model solves the two group neutron diffusion equation using the finite element method. There is a good agreement between the results from COMSOL and VENTURE code for the 3D IAEA PWR benchmark problem. The value of K_{eff} is 1.02934, which shows a smaller difference of 3% compared to VENTURE code. The maximum percentage difference between COMSOL and VENTURE code, in calculating the power distribution, is 2%.

References

1. Freels , J. D.; . Bodey ,I. T; Arimilli ,R. V. ; Lowe†,K. T. : Two-Dimensional Thermal Hydraulic Analysis and Benchmark in Support of HFIR LEU conversion using COMSOL. Oak Ridge National Laboratory, September 2010. (http://info.ornl.gov/sites/publications/Files/Pub23015.pdf)
2. Tschaepe, L.; Ruggles ,A. E.; Freels , J. D ; Primm, R. T. :Evaluation of HFIR LEU Fuel Using the COMSOL Multiphysics Platform. Oak Ridge National Laboratory, March 2009. (https://wiki.ornl.gov/sites/publications/Files/Pub13011.pdf)
3. Freels , J. D.; . Bodey ,I. T; Arimilli ,R. V; Curtis, F. G.; Ekici ,K. ; Jain, P. K. :Preliminary multiphysics analyses of HFIR LEU fuel conversion using COMSOL. Oak Ridge National Laboratory, June 2011.
4. Chandler, D.; Maldonado, G. I.; Primm, R.T.; Freels , J.D.: Neutronics modeling of the High Flux Isotope Reactor using COMSOL. Annals of Nuclear Energy 38 (2011) 2594–2605.
5. Chandler, D.: Spatially-Dependent Reactor Kinetics and Supporting Physics Validation Studies at the High Flux Isotope Reactor. Doctoral Dissertations, University of Tennessee, Knoxville, 2011.
6. Ned Xoubi ; Abdelfattah Y. Soliman,"Neutronic calculations of the IAEA 10 MW MTR benchmark reactor via finite element method using COMSOL multiphysics code", Annals of Nuclear Energy, Volume 109, November 2017, Pages 277-283.
7. Ned Xoubi ; Abdelfattah Y. Soliman," Neutronic modeling and calculations of the ETRR-2 MTR reactor using COMSOL multiphysics code", Annals of Nuclear Energy, Volume 109, November 2017, Pages 667-674
8. Aufiero, M.; Cammi, A.; Fiorina, C.; Luzzi,L.: Development of a single-channel multi-physics model for lead fast reactors. 20th international conference of nuclear energy for new Europe, Bovec, Slovenia, 2011.
9. Bell ,J.S.; . Lewis, B.J.: CANDU fuel bundle deformation modelling with COMSOL multiphysics. Nuclear Engineering and Design 250 (2012) 134– 141.
10. Argon Code Center, Benchmark Problem Book, Report ANL-7416 (Suppl. 2). Argonne National Laboratory, Argonne, IL, 1977.