International Journal of Integrated Sciences & Technology (IJIST)
http://www.cuet.ac.bd/IJIST/index.html

International Journal of Integrated Sciences & Technology **4** S (2022) 40-44

Modeling and Validation of IAEA 3D PWR Benchmark Problem Using COMSOL Multiphysics Code

Ariful Islam, R. Nushrat, T.A. Rahim and A.S. Mollah*

[1] Department of Nuclear Science and Engineering, Military Institute of Science and Technology (MIST), Dhaka-1216, Bangladesh.

ABSTRACT

Akey difficulty in nuclear reactor analysis is to provide a wide description of nuclear systems through the coupling of neutronics and thermal-hydraulics. COMSOL Multiphysics software provides an advanced tool to integrate user-defined physics modules to analyze reactors at steady and transient state by mathematics module. To validate the capability of solving different nuclear reactor phenomena e.g., neutron flux distribution and effective multiplication factor (k_{eff}) in COMSOL software, it's worth solving a benchmark problem. A classic 3D IAEA benchmark problem is selected to for estimation of effective multiplication factor, neutron flux, radial, and axial power distributions in the core using the neutron diffusion equation. The 3D model was developed with SolidWorks and afterwards imported into COMSOL to solve two-group neutron diffusion equations. To avoid the peculiarities that commonly occur when solving the neutron diffusion equation with unstructured grids, an adaptive meshing approach was utilized. The effective multiplication factor, thermal and fast neutron flux profiles, as well as power distributions were calculated and compared with the results of another standard PARCS code. There is good agreement between the COMSOL and PARCS code results. The value of k_{eff} is 1.02799 which shows a smaller difference of 0.11% compared to reference value from PARCS code. The results presented in this paper are primarily intended as a demonstration of the neutronics behavior of this benchmark problem with COMSOL multiphysics software. Based on the present study, it is evident that the COMSOL software could be used for neutronics analysis for nuclear reactor like PWR. VVER etc.

Keywords: CFD, COMSOL Multiphysics, k_{eff}, PWR, Solid Works.

1. Introduction

Recent advancements in computer science have led to an increased capability to solve complicated nuclear reactor problems. Neutronics behavior in different reactor models should be analyzed through the coupling of Multiphysics problems[1] by different techniques to solve reactor problems and code must be validated through benchmark experimental data. The Boltzmann neutron transport equation depicts how neutrons interact with matter and represents a neutron balance that exists at all points in space and time. The neutron diffusion equation is a simplified version of the Boltzmann neutron transport equation, which asserts that neutron current is proportional to neutron flux gradient. An IAEA 3D PWR, defined by B. Micheelsen [2] in 1971 and later published in 1977 by the computational benchmark problems committee of the mathematics and computation division of the American Nuclear Society, the problem has been chosen in recent years as the standard benchmark problem for validating advanced neutronics and thermal-hydraulics codes and nuclear data libraries. COMSOL[3-5] is a powerful computational software to model and predict different physical phenomena with diversified engineering applications. Because of its powerful mesh creation, coupling phenomenon capabilities, solution function, and extensive post-process operation, it has a high potential for use in neutronics calculation [5, 6]. From the literature survey, it is found that there have been quite a number of researches related to reactor simulation with COMSOL Multiphysics software as computational fluid dynamics (CFD) purpose. But to the best of the authors' knowledge, the prospect of using COMSOL software for obtaining solely the neutronics behavior of the nuclear reactor might not have been studied earlier. In this paper, COMSOL Multiphysics has been adopted for validation with detailed specifications from the IAEA 3D benchmark problem for neutronics analysis. The IAEA 3D benchmark problem defines two-group cross-sections in the steady-state beginning of the cycle (BOC) for two different fuel assemblies and reflector regions. Power distribution, fast and thermal neutron flux is calculated by solving two group diffusion equations by commercial finite element method based software COMSOL-5.4. With detailed specifications and high-quality experimental data from the IAEA Technical Report Series, a full-core, three-dimensional model is created in this study.

Corresponding author:
E-mail: mosattar54@gmail.com
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2 Model Description

An IAEA 3-dimensional PWR problem is chosen as a benchmark problem in this paper for the validation of COMSOL software. The core loading pattern is shown in Fig. 1 and axial core configuration is shown in Fig. 2 and the corresponding two group cross sections are given in Table 1. In the full core, there are 177 fuel assemblies including 9 fully rodded fuel assemblies and 4 partially rodded fuel assemblies composing the core with 125 fuel assemblies across the core major axis. The radial assembly width is 20 cm and the active core height is 340 cm. The core contains 64 reflector assemblies at the bottom and top of the core and the height of the reflector region is 20 cm.

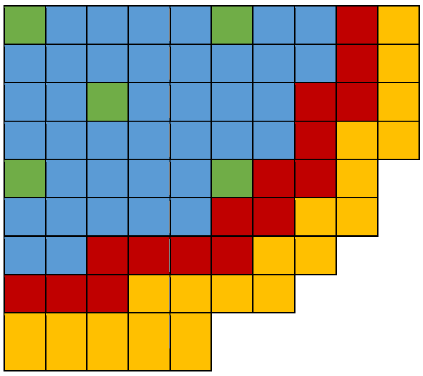

Fig. 1: Radial core configuration of IAEA 3-D benchmark problem

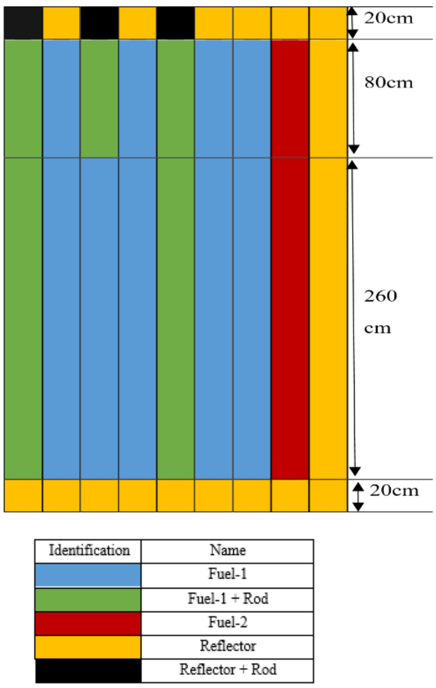

Fig. 2: Axial core configuration of IAEA 3-D benchmark problem.

Table 1: Two neutron groups constant data for the IAEA 3D PWR benchmark problem

FA Name	D_1	D_2	Σ_{a2}	Σ_{a2}	$\vartheta\Sigma_{f1}$	$\vartheta\Sigma_{f2}$	$\Sigma_{1\to2}$
Fuel-1	1.5	0.4	0.01	0.085	0	0.135	0.02
Fuel-1+Rod	1.5	0.4	0.01	0.13	0	0.135	0.02
Fuel-2	1.5	0.4	0.01	0.08	0	0.135	0.02
Reflector	2.0	0.3	0	0.01	0	0	0.04
Reflector + Rod	2.0	0.33	0	0.055	0	0	0.04

3. Theory and Methodology

Only the stationary two-group neutron diffusion equation is considered in this study. Fast and thermal neutron flux in the multiplying region is indicated by subscripts 1 and 2 respectively. Down scattered neutrons from the fast group are considered as a source term for thermal group, a further assumption is made by taking zero up-scattered effect from fast to the thermal group and all neutrons are born as fast neutrons.

$$-D_1\nabla^2\emptyset_1 + (\Sigma_{a1} + \Sigma_{1\to2})\emptyset_1 = \frac{1}{k}(\vartheta\Sigma_{f1}\emptyset_1 + \vartheta\Sigma_{f2}\emptyset_2) \ \ldots\ldots\ldots\ldots (1)$$

$$-D_2\nabla^2\emptyset_2 + \Sigma_{a2}\emptyset_2 = \Sigma_{1\to2}\emptyset_1 \ \ldots\ldots\ldots\ldots\ldots\ldots (2)$$

$\emptyset_1$ and $\emptyset_2$ are the fast and thermal neutron flux respectively, k is the eigenvalue of this problem also known as effective multiplication factor which balances the left side of the equation, represent leakage and absorption, with the right-hand side equation, represent source term. D is the diffusion coefficient and Σ_f is the macroscopic fission cross-section. The benchmark model consists of five different regions given in Table 1 with cross-section data for fast and thermal groups respectively. Three boundary conditions are applied as symmetry boundary conditions (BC), vacuum BCs and continuity BCs.

For outside boundaries, there is no incoming current as showing in eq^n (3)

$$j_g^{in} = 0 \ \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (3)$$

Reflective boundaries without net current as shown in eq^n (4)

$$\frac{\partial\emptyset_g}{\partial n} = \frac{0.4692}{D_g}\emptyset_g \ \ldots\ldots\ldots\ldots (4)$$

Simplified of above equation for using in COMSOL is eq^n (5)

$$\emptyset_{g|boundary} = -2.1312 D_g \nabla\emptyset_{g|boundary} \ \ldots\ldots\ldots\ldots (5)$$

Simplified neutron diffusion equation is in non-linear form which is non-symmetric matrix. This problem can easily solve in eigenvalue mode.

$$-\lambda.\ \emptyset_1 - D_1\nabla^2\emptyset_1 + (\Sigma_{a1} + \Sigma_{1\to2})\ \emptyset_1 = (\vartheta\Sigma_{f1}\emptyset_1 + \vartheta\Sigma_{f2}\emptyset_2) \ldots\ldots\ldots. (6)$$

$$-\lambda.\ \emptyset_2 - D_2\nabla^2\emptyset_2 + \Sigma_{a2}\emptyset_2 = \Sigma_{1\to2}\emptyset_1 \ldots\ldots\ldots\ldots\ldots (7)$$

Simplified neutron diffusion equation in COMSOL is in following form-

$$-\lambda d_a u + \nabla.(-d_g\nabla u) + \textstyle\sum_r u = \sum_{f,\,g} \ldots\ldots\ldots (8)$$

Symmetry Neuman boundary condition is included in COMSOL software in the form of

$$(-D\nabla\emptyset_g) = 0 \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots. (9)$$

Dirichlet boundary condition is the value of variable at a certain point. Dirichlet boundary condition in reflective region where flux is vanished at extrapolated distance.

$$hu = r \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots. (10)$$

The final condition is the continuity condition as shown in Equations 11 and 12.

$$n.\ ((c\nabla u - \alpha u + \gamma)_1 - (c\nabla u - \alpha u + \gamma)_2) + qu = g \ldots\ldots\ldots. (11)$$

$$n.\ ((D\nabla\emptyset)_1 - (D\nabla\emptyset)_2) = 0 \ldots\ldots\ldots\ldots (12)$$

K_{eff} value is calculated by following equation-

$$\begin{aligned} k_{eff} &= [\iiint \Sigma_f^1\emptyset^1 dv + \iiint \Sigma_f^2\emptyset^2 dv]^{R1} \\ &+ [\iiint \Sigma_f^1\emptyset^1 dv + \iiint \Sigma_f^2\emptyset^2 dv]^{R2} \\ &+ [\iiint \Sigma_f^1\emptyset^1 dv + \iiint \Sigma_f^2\emptyset^2 dv]^{R3} \\ &+ [\iiint \Sigma_f^1\emptyset^1 dv + \iiint \Sigma_f^2\emptyset^2 dv]^{R4} \\ &+ [\iiint \Sigma_f^1\emptyset^1 dv + \iiint \Sigma_f^2\emptyset^2 dv]^{R5} \\ &- P_0 \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots. (4.13) \end{aligned}$$

Here, R_1=Fuel 1

R_2= Fuel 1+ Rod

R_3=Fuel 2

R_4=Reflector

R_5= Reflector + Rod

Graphical User Interface of mesh in IAEA 3D PWR for one-quarter is given in following Figure (3).

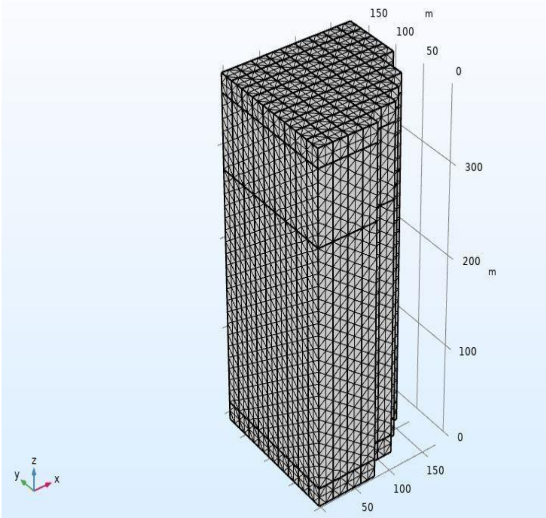

Fig. 3: 3D mesh generated by COMSOL Multiphysics software

4. Results and discussion

The result is compared with PARCS[6], a code that solves the time-dependent two-group neutron diffusion equation using the analytic nodal method, for validating the COMSOL code. Along with the PARCS code, many more codes such as MCNP, SuperMC [7] etc. have been used to estimate the multiplication factor of the same reactor. The value of k_{eff} obtained by using COMSOL Multiphysics software for extremely fine meshes per assembly is 1.02799. The reference value of k_{eff} = 1.029096 which is calculated by PARCS code and error is 0.11%.

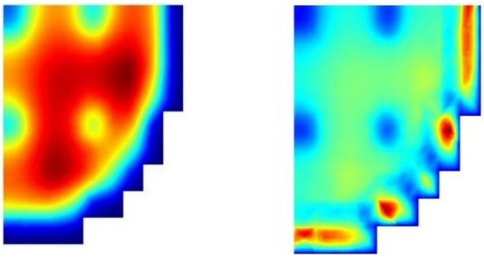

Fig. 4: 2D plot of fast (left) and thermal (right) neutron flux at z = 150 cm

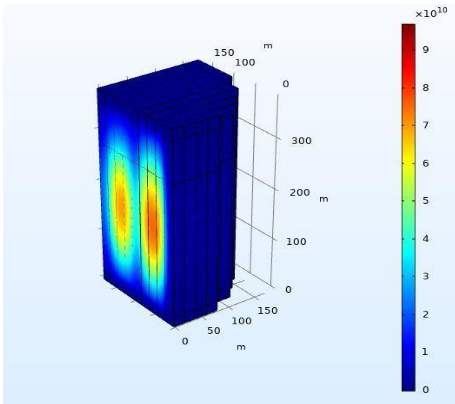

Fig. 5: 3D plot of fast neutron flux

Three-dimensional neutron flux distribution in the whole rector core is shown in Figs. 4 and 5 respectively. In Y-Z plane 50 slice plots are taken to plot neutron flux distribution quite density in whole core. The largest flux of fast neutrons occurs in the midsection of the core. Thermal neutron flux in the central plane is fairly steady (no abrupt changes or peak values of flux) except in the radial direction in the reflector region. Not all reflector periphery sides show this perturbation, only a certain location gives peak value of thermal flux distribution. Line graph of fast and thermal neutron flux from Figs. 6 and 7 respectively show detailed information how these values change. It's worth noting that thermal flux peaks on the inner side of the core. Both thermal and fast neutron flux create a hump at the middle point, although not in the same quantity. Fast neutron flux value changes at a large amount because of partially rodded fuel assembly at mid plane.

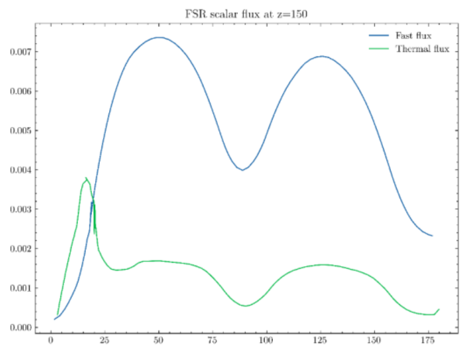

Fig. 6: Fast and thermal neutron flux at YZ plane

Power at axial layer number is normalized over whole core. At middle point in axial direction power is maximum. Power distribution curve is Cosine-shape which is in good agreement with our theoretical concept. Power is decreasing at axial direction.

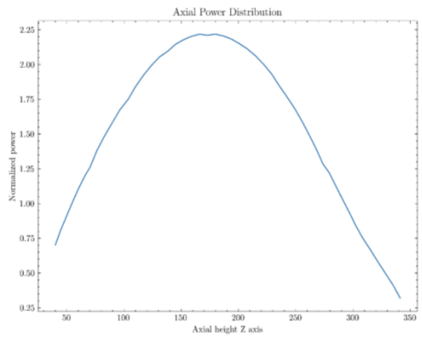

Fig. 7: Axial power distribution

Because thermal flux peaks in the radial direction, assembly power in that assembly is unusually large compared to the reference value[6]. Near high absorber material containing assemblies, a higher flux and power gradient is observed. Fig. 8 depicts the assembly power distribution for one-quarter geometry of IAEA 3D PWR core calculated by COMSOL Multiphysics software. The results of assembly power distribution are given in Fig. 8. The maximum assembly power difference is 35% which is still considered large in the PWR benchmark problems. Further mesh refinement is not completed due to the memory limitation. Overall, the comparisons between COMSOL's predictions and the reference PARCS values are in good agreement. This study demonstrates the ability of COMSOL software to predict the simulation of the IAEA 3-D PWR benchmark problem accurately. The COMSOL software could be used for simulation of different nuclear power reactors to evaluate the neutronics parameters.

0.72 0.87 -20.8%	1.27 1.4462 -13.39%	1.42 1.781 -25.42%	1.18 1.6452 -20.98%	0.61 0.6452 -11.48%	0.95 1.033 -8.74%	0.96 0.99 -3.125%	0.78 0.85 -8.97%
1.27 1.4436 -13.67%	1.39 1.7432 -25.41%	1.42 1.10925 -21.88%	1.29 1.0058 22.03%	1.07 1.03099 3.65%	1.05 1.0048 4.3%	0.98 0.98 0%	0.76 0.87 -14.47%
1.42 1.7801 -25.35%	1.42 2.01 -41.5%	1.36 0.99 29.41%	1.31 1.07 18.32%	1.18 1.0086 14.5%	1.08 1.28 1.805%	1.00 1.0185 -1.85%	0.72 1.75 -43%
1.19 1.5312 -28.67%	1.29 1.9945 -35.02%	1.31 1.01 22.9%	1.18 1.002 15.08%	0.97 1.03 -6.19%	0.92 .09878 -6.52%	0.87 1.0243 -17.74%	
0.61 0.4876 20.06%	1.07 0.81 24.3%	1.18 1.01 14.4%	0.97 1.028 -5.98%	0.48 0.7122 4.9%	0.7 0.84 -08.7%	0.62 0.805 -29.35%	
0.95 1.0309 -8.5%	1.05 0.9946 5.71%	1.08 1.00 8%	0.92 0.9895 -6.52%	0.7 1.05 50%	0.6 1.07 -6.78%		

0.96 0.99 -3.125%	0.98 0.9843 0.1%	1.00 1.023 -2.3%	0.87 1.039 -19.42%	0.62 0.867 39.4%
0.77 0.8593 -11.6%	0.76 0.8802 -15.8%	0.72 0.8766 -21.11%		

Reference value (PARCS code)
Calculated value (COMSOL)
Difference (%)

Fig. 8: Power distribution in quarter core compared with reference value

5. Conclusions

The IAEA 3D reactor is one of the most commonly benchmark problems used in computational simulations in the area of reactor physics, in general to evaluate the performance of neutronics calculation methods. The 3D PWR IAEA benchmark problem was modeled using COMSOL 5.4 in the .mphbin file. Adaptive mesh refinement is taken care of for accurate solutions. Normalized power is in good agreement with reference PARCS and CITVAP [8] code except for the assembly in the radial direction, which is close to the reflector side. Thermal and Fast neutron flux in one-quarter geometry also is in good agreement with our reference solution. The value of k_{eff} is found to be 1.02799, which shows a smaller difference of 0.11% with PARCS code (k_{eff} =1.029096). Power distribution is scaled throughout the entire geometry. The flux value in the reflector region has a substantial disparity, which impacts the normalized power distribution. The theoretical concept is also well validated by the cosine shape power distribution in each assembly. Further works are in progress for utilizing the COMSOL software for neutronics simulation of VVER-1200 reactor to be commissioned at Rooppur along with other codes such as MCNP, SuperMC and WIMSD5B for the nuclear safety evaluation of nuclear systems.

Acknowledgements

We are thankful to the Department of Nuclear Science and Engineering, MIST for the arrangement of workshop on COMSOL Multiphysics in 2018 to complete this research.

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