COMPARISON BETWEEN COMSOL AND RFSP-IST FOR A 2-D BENCHMARK PROBLEM

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Abstract

RFSP-IST (Reactor Fuelling Simulation Program) is a computer code used for the full-core neutronics design and analysis of CANDU® reactors. RFSP-IST calculates the static flux and power distributions in the core by solving the neutron diffusion equation in two energy groups. For validation purposes, results from RFSP-IST are often compared with those from other codes. This paper documents the comparison with the commercial finite element multiphysics software package COMSOL on a two-dimensional benchmark problem. Normalized bundle powers from RFSP-IST compared favourably with those from COMSOL, with the largest difference being 0.3%.

1. Introduction

RFSP-IST [1] is a computer code for the full-core neutronics design and analysis of CANDU reactors. RFSP-IST calculates the static flux and power distributions in the core by solving the neutron diffusion equation in two energy groups. This paper documents the comparison of RFSP-IST with the commercial finite element multiphysics software package COMSOL [2] on a two-dimensional benchmark problem.

The benchmarking model, shown in Figure 1, consists of an 8 x 8 lattice array of cells containing fuel surrounded by a 1-lattice pitch wide reflector region. The width of the lattice is 24 cm.

The mathematical problem being solved on the 2D surface is the two-group neutron diffusion equation.

$$-D_1\nabla^2\phi_1 + \Sigma_{R1}\phi_1 = \frac{1}{k}\left[\nu\Sigma_{f1}\phi_1 + \nu\Sigma_{f2}\phi_2\right] + \Sigma_{s21}\phi_2 \quad (1)$$

$$-D_2\nabla^2\phi_2 + \Sigma_{R2}\phi_2 = \Sigma_{s12}\phi_1 \quad (2)$$

where the removal cross sections are defined as

$$\Sigma_{R1} = \Sigma_{a1} + \Sigma_{s12} \quad (3)$$

$$\Sigma_{R2} = \Sigma_{a2} + \Sigma_{s21} \quad (4)$$

In the equations, numerical indices 1 and 2 designate fast and thermal neutrons or groups one and two respectively. The subscript 12 designates scatter from group 1 to 2 (downscatter) and 21 designates scatter from group 2 to 1 (upscatter) and the diffusion coefficient, $D = 1/(3\Sigma_{tr})$.

The right side of equations (1) and (2) are the production terms for each group, which are a result of fission or scatter from one group to another. It is assumed that all fission neutrons are born as fast neutrons. The only production term for thermal neutrons is via downscatter from group 1. The left side of equations (1) and (2) are the loss terms for each group, which occur as a result of leakage, absorption and scatter from one group to another.

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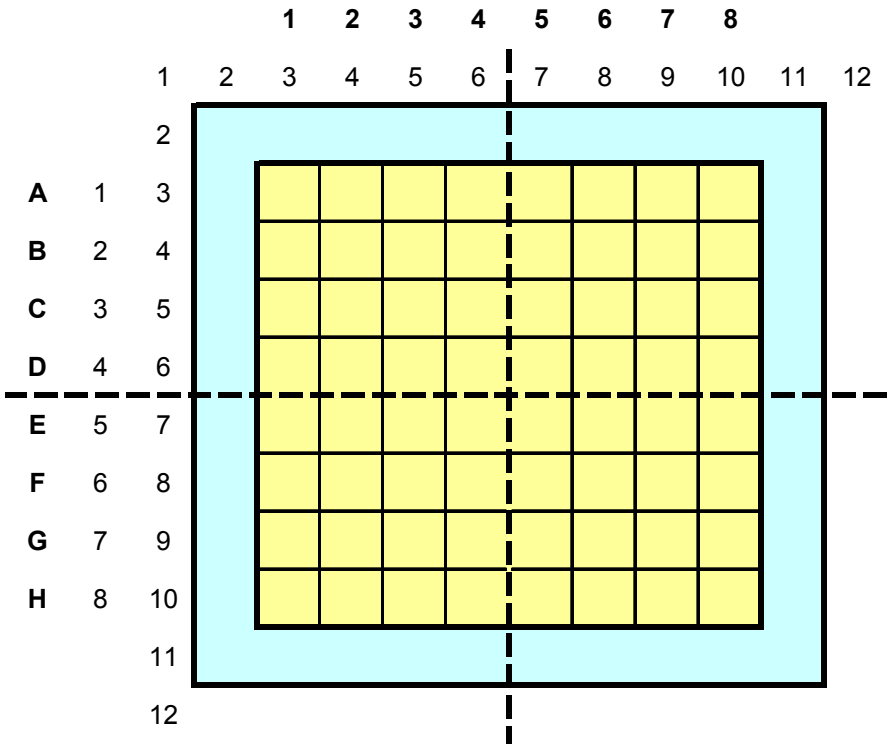


Figure 1 – The 2D 10 x 10 Mini-Core Benchmarking Model

2. Creating the COMSOL Model

The model as it appears in the COMSOL Graphical User Interface (GUI) is shown in Figure 2. Creating geometries is easy using drawing features found in most Computer Aided Design (CAD) packages. Among the tools is an array replication button, which was used to draw the fuel lattice. The GUI can be used to create complex 1D, 2D and 3D geometries. Geometries created with standard CAD packages can also be imported into COMSOL.

The next step to solving a problem with COMSOL is to choose from a set of physics equations that describe the problem. Though in this case a single physics equation is used, the PDE Coefficient Form Eigenvalue, that is not necessarily always the case. A particular problem may require the use of more than one set of physics equations, hence the term multiphysics.

The equation solved by the PDE Coefficient Form Eigenvalue mode is of the form

$$\nabla \cdot (-c\nabla\phi - \alpha\phi + \gamma) + a\phi + \beta \cdot \nabla\phi = d_a \lambda\phi - e_a \lambda^2 \phi \qquad (5)$$

where the nomenclature is as follows:

ϕ - dependent variable (flux)

c - Diffusion coefficient (D_1, D_2)

a - Absorption coefficient (Σ_{R1}, Σ_{R2})

d_a - Damping/Mass coefficient

λ - Eigenvalue, where 0 is the assumed linearization point for the eigenvalue

e_a - Mass coefficient = 0 (not used)

α - Conservative flux convection coefficient = 0 (not used)

β - Convection coefficient = 0 (not used)

γ - Conservative flux source term = 0 (not used)

Two instances of the PDE Coefficient Form Eigenvalue mode are required, one for thermal neutrons and another for fast neutrons.

Figure 3 shows the window to import physics modes. The mode is selected from a categorized dropdown list and is added to the model by clicking the Add button.

In the benchmarking model there are 2 distinct domain types, the reflector and the fuel as shown in Fig. 1. As a result, Equation (5) will have four distinct sets of values for each of the coefficients. Two sets of values are required for each group since each energy group requires one set for the fuel region and another for the reflector region.

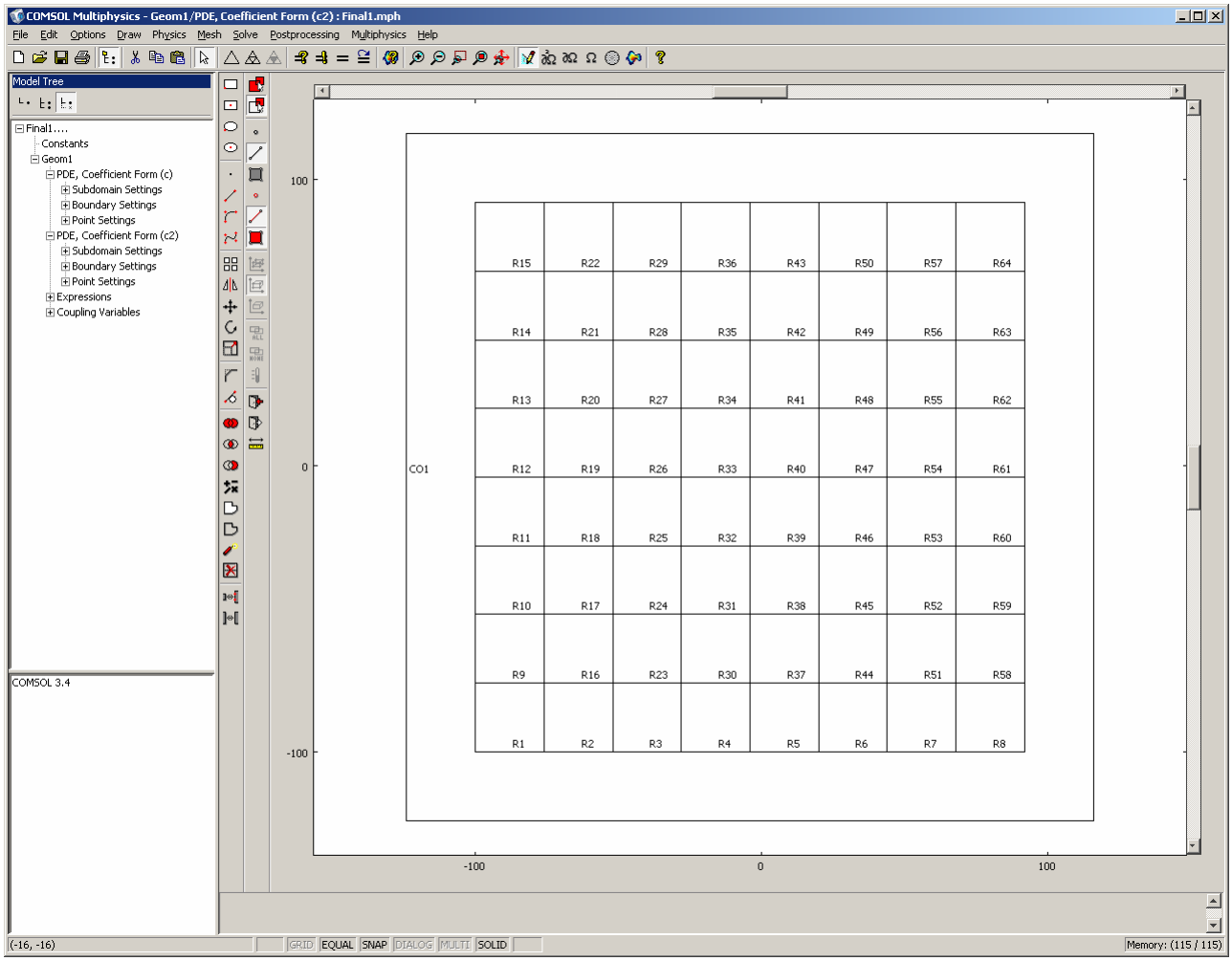


Figure 2 – COMSOL Geometry Drawing Interface

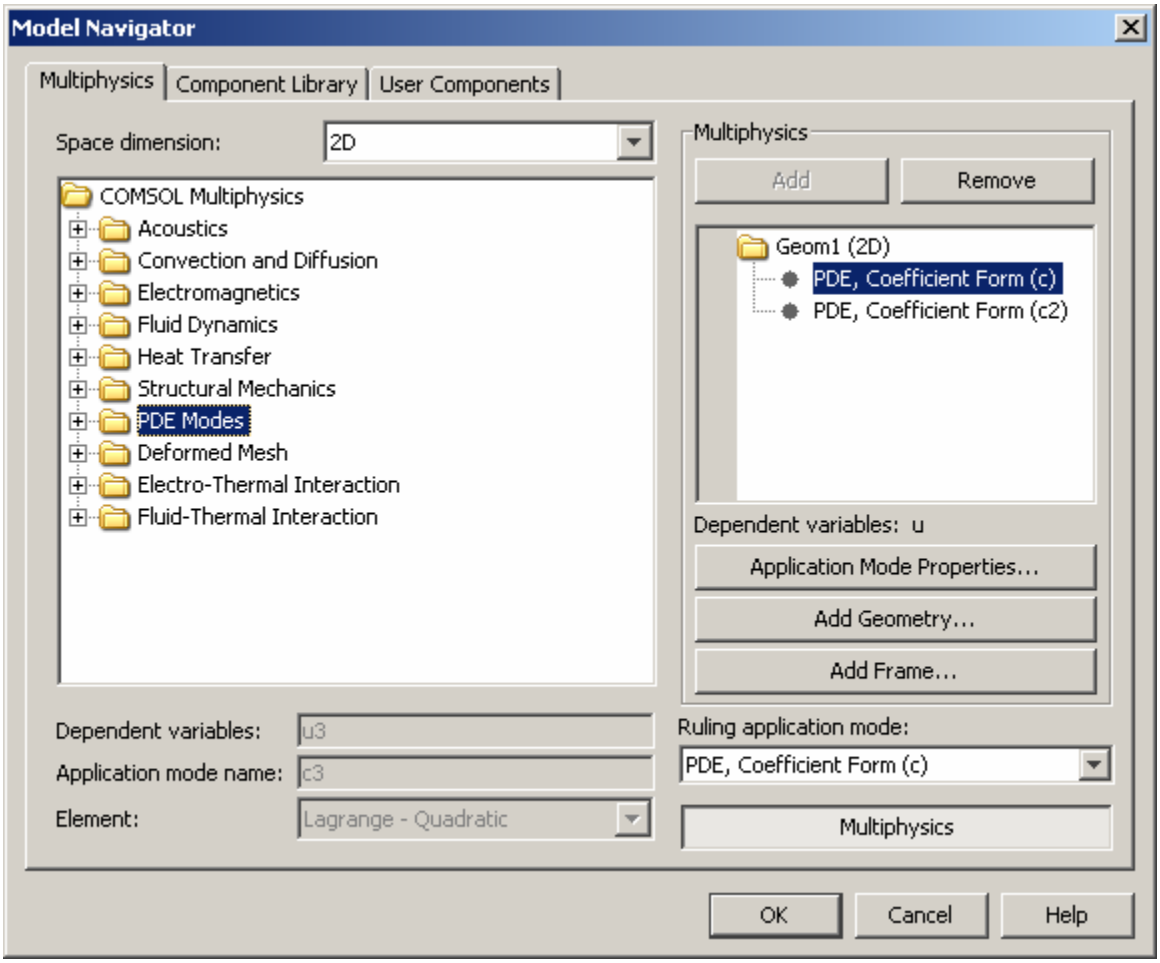


Figure 3 – Multiphysics Mode Selection Window

The last step in building this model is the selection of appropriate boundary conditions. Continuity boundary conditions, the default for inner surfaces, were applied to all fuel cells and inner reflector regions. For the four outer reflector surfaces, the transport theory vacuum boundary condition was applied, namely that the flux is assumed to drop linearly outside the external reflector boundary and vanish at a distance of $0.7104\lambda_{tr}$.

Since COMSOL boundary conditions are applied to surfaces, the extrapolation length was reformulated as a surface boundary condition. Figure 4 illustrates the vanishing flux boundary condition in 1-D.

$$\left.\frac{d\phi}{dx}\right|_{x1} = \frac{\phi(x2)-\phi(x1)}{x2-x1} = \frac{-\phi(x1)}{x2} \qquad (6)$$

$$\left.\frac{d\phi}{dx}\right|_{x1} = \frac{-\phi(x1)}{x2} = \frac{-\phi(x1)}{0.7104*\lambda_{tr,g}} = \frac{-\phi(x1)}{2.1312*D_g} \qquad (7)$$

Rearranging, the expression for the boundary condition becomes

$$\phi(x1) = -2.1312*D_g*\left.\frac{d\phi}{dx}\right|_{x1} \qquad (8)$$

Generalizing to a multidimensional surface

$$\phi_b = -2.1312*D_g*\nabla\phi\big|_b \quad , \qquad (9)$$

where the subscript “b” designates the reflector vacuum boundary and D_g is the diffusion coefficient in the reflector for neutrons belonging to energy group g.

A sample boundary condition entry window is shown in Figure 5, where the COMSOL Dirichlet boundary condition option has been used. A Dirichlet boundary condition is of the form $h\phi = r$ where h is a weight that normally equals 1. In this particular problem, $r = -2.312 * Dg * \nabla\phi|_b$.

The next step is to generate a mesh for the model as shown in Figure 6. In this particular case, not much effort was involved, as two mesh refinements with default settings mapped the surface adequately. Mesh statistics are displayed in Figure 7.

The last step is to choose a solver. For this problem, the Direct (PARDISO) solver was chosen as it is a highly efficient solver for symmetric systems and often uses less memory than other solvers.

3. Analysis

Data used in the analysis was extracted from an RFSP-IST output file, which contained cross sections for a range of fuel irradiations. Cubic spline interpolation using MATLAB [3] was used to extract cross sections corresponding to an irradiation of 0.5 n/kb, the irradiation analyzed by RFSP-IST. The cross-sections are listed in Tables 1 and 2. The thermal and epithermal properties of the fuel and reflector

were calculated with the multicell methodology in WIMS-AECL/RFSP [4], which allows an accurate treatment of neutronic heterogeneity.

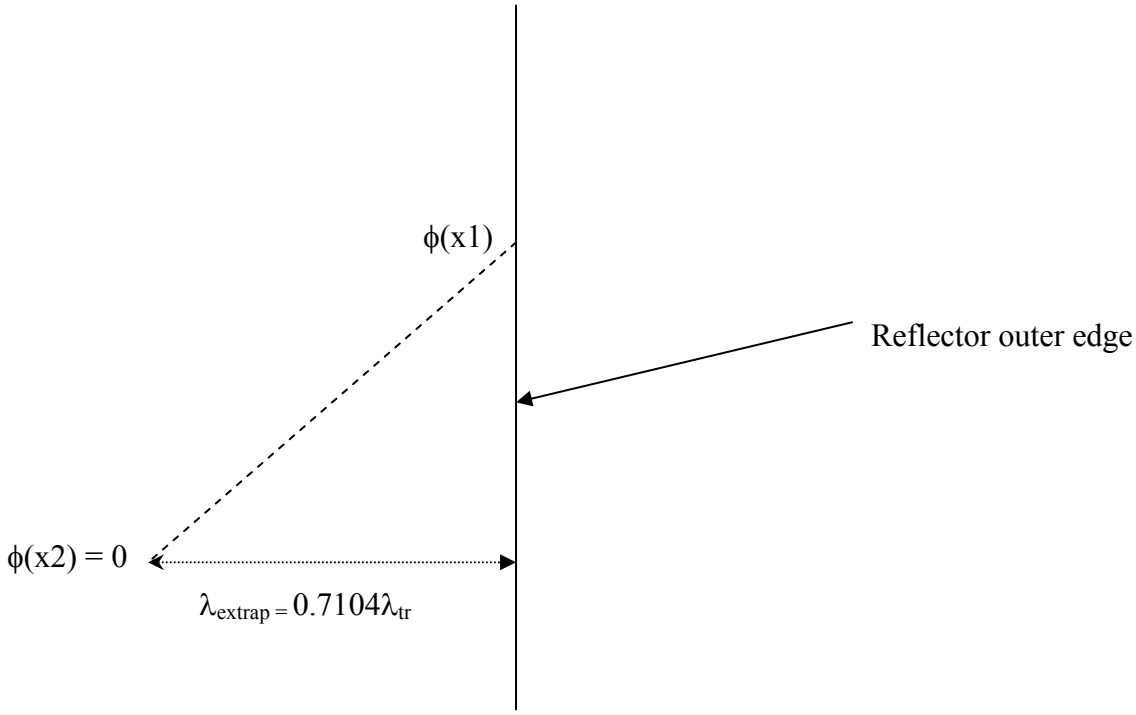


Figure 4 – Vanishing Flux Boundary Condition

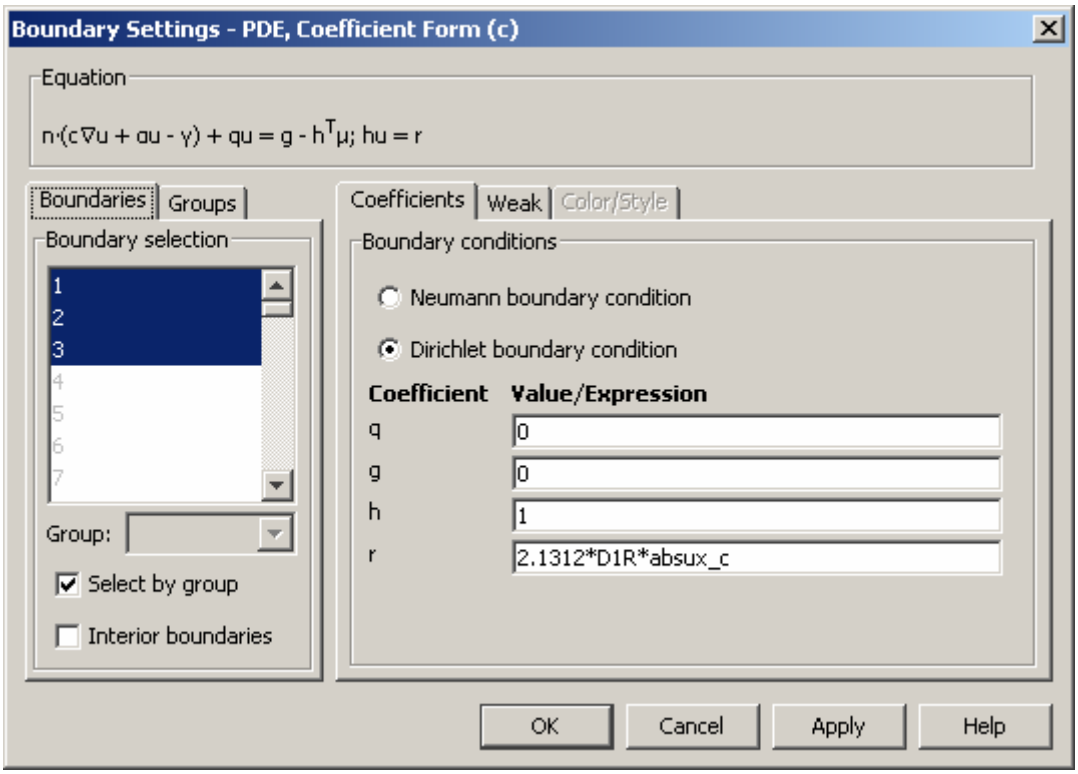


Figure 5 – Boundary Settings for Fast Neutrons in Reflector Region

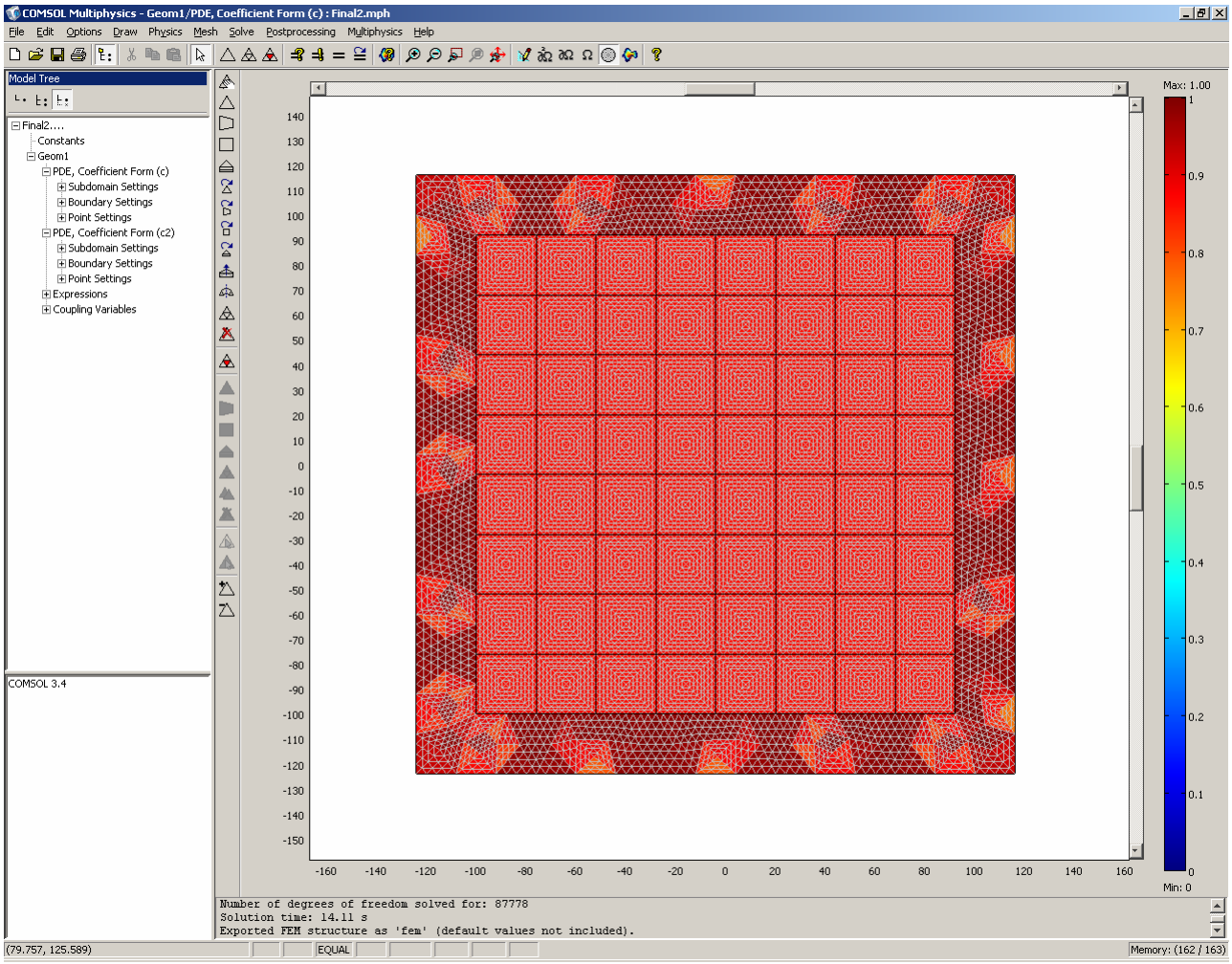


Figure 6 – Mesh Used in COMSOL Model

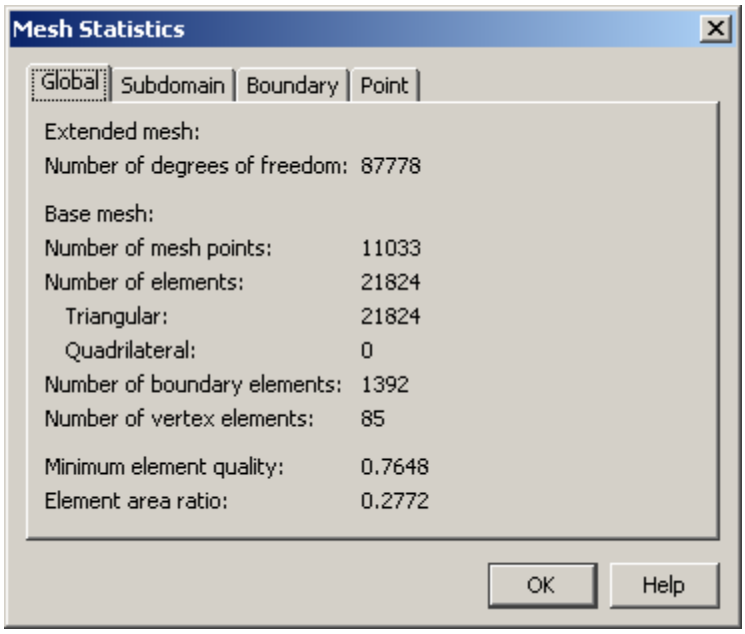


Figure 7 – Mesh Statistics for COMSOL Model

Parameter	Value
Σ_{tr1}	0.21010 cm^{-1}
Σ_{tr2}	0.33443 cm^{-1}
Σ_{a1}	0.0026253 cm^{-1}
Σ_{a2}	0.0076474 cm^{-1}
Σ_{s12}	0.0087518 cm^{-1}
Σ_{s21}	0.00015315 cm^{-1}
$\kappa\Sigma_{f1}$	0.065321 energy·cm^{-1}
$\kappa\Sigma_{f2}$	0.51197 energy·cm^{-1}
$\nu\Sigma_{f1}$	0.001288 cm^{-1}
$\nu\Sigma_{f2}$	0.0097323 cm^{-1}

Table 1 – Cross-Sections Used in COMSOL Model for Fuel

Parameter	Value
Σ_{tr1}	0.2584679 cm^{-1}
Σ_{tr2}	0.3951946 cm^{-1}
Σ_{a1}	6.4×10^{-6} cm^{-1}
Σ_{a2}	6.93×10^{-5} cm^{-1}
Σ_{s12}	0.0122234 cm^{-1}
Σ_{s21}	5.3×10^{-5} cm^{-1}

Table 2 – Cross-Sections Used in COMSOL Model for Reflector

Normalized bundle powers in the centre core region from COMSOL were compared with those from RFSP-IST. The COMSOL normalized bundle power was obtained by using subdomain integration coupling variables to calculate the following

$$\frac{\iint_{bundle}(\kappa\Sigma_{f1}\phi_1 + \kappa\Sigma_{f2}\phi_2)}{\iint_{\text{core centre}}(\kappa\Sigma_{f1}\phi_1 + \kappa\Sigma_{f2}\phi_2)}, \qquad (10)$$

where core centre denotes the fuel area bounded by bundles, shown in Fig. 1, that are not in contact with the reflector; namely those in columns 2 through 7 and rows B through G.

Normalized bundle powers in rows C and D were compared with those from RFSP-IST. They are listed in Tables 3 and 4 and depicted graphically in Figures 8 and 9. The corresponding percentage difference, (COMSOL/{RFSP-IST} - 1)*100, are listed in Tables 5 and 6.

4. Discussion and Conclusion

Tables 3-6 and Figures 8 and 9 show that there is good agreement between COMSOL and RFSP-IST for the 2-D benchmarking problem. The user-friendly interface and advanced capabilities make COMSOL a powerful tool for multi-group diffusion theory analysis and because it solves the eigenvalue problem it can also be used for neutron flux modal analysis

Acknowledgements
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5. References

[1] B. Rouben, “RFSP-IST, The Industry Standard Tool Computer Program for CANDU Reactor Core Design and Analysis”, Proceedings of the 13th Pacific Basin Nuclear Conference, Shenzhen, China, 2002 October 21-25.

[2] COMSOL: COMSOL, Inc., 1 New England Executive Park Suite 350, Burlington, MA 01803, Version 3.4.

[3] MATLAB: The MathWorks Inc., 3 Apple Hill Drive, Natick, MA 01760-2098, Version 7.6.

[4] W. Shen, “Development of a Multicell Methodology to Account for Heterogeneous Core Effects in the Core-Analysis Diffusion Code”. Proceeding of The International Conference on the Advances in Nuclear Analysis and Simulation, PHYSOR-2006, Vancouver, Canada, 2006 September 10-14.

Channel	COMSOL	RFSP-IST
2	2.409E-02	2.414E-02
3	2.944E-02	2.941E-02
4	3.226E-02	3.219E-02
5	3.226E-02	3.219E-02
6	2.944E-02	2.941E-02
7	2.409E-02	2.415E-02

Table 3 – Normalized Bundle Powers for COMSOL – Row C

Channel	COMSOL	RFSP-IST
2	2.641E-02	2.643E-02
3	3.226E-02	3.219E-02
4	3.535E-02	3.523E-02
5	3.535E-02	3.523E-02
6	3.226E-02	3.219E-02
7	2.641E-02	2.644E-02

Table 4 – Normalized Bundle Powers for COMSOL – Row D

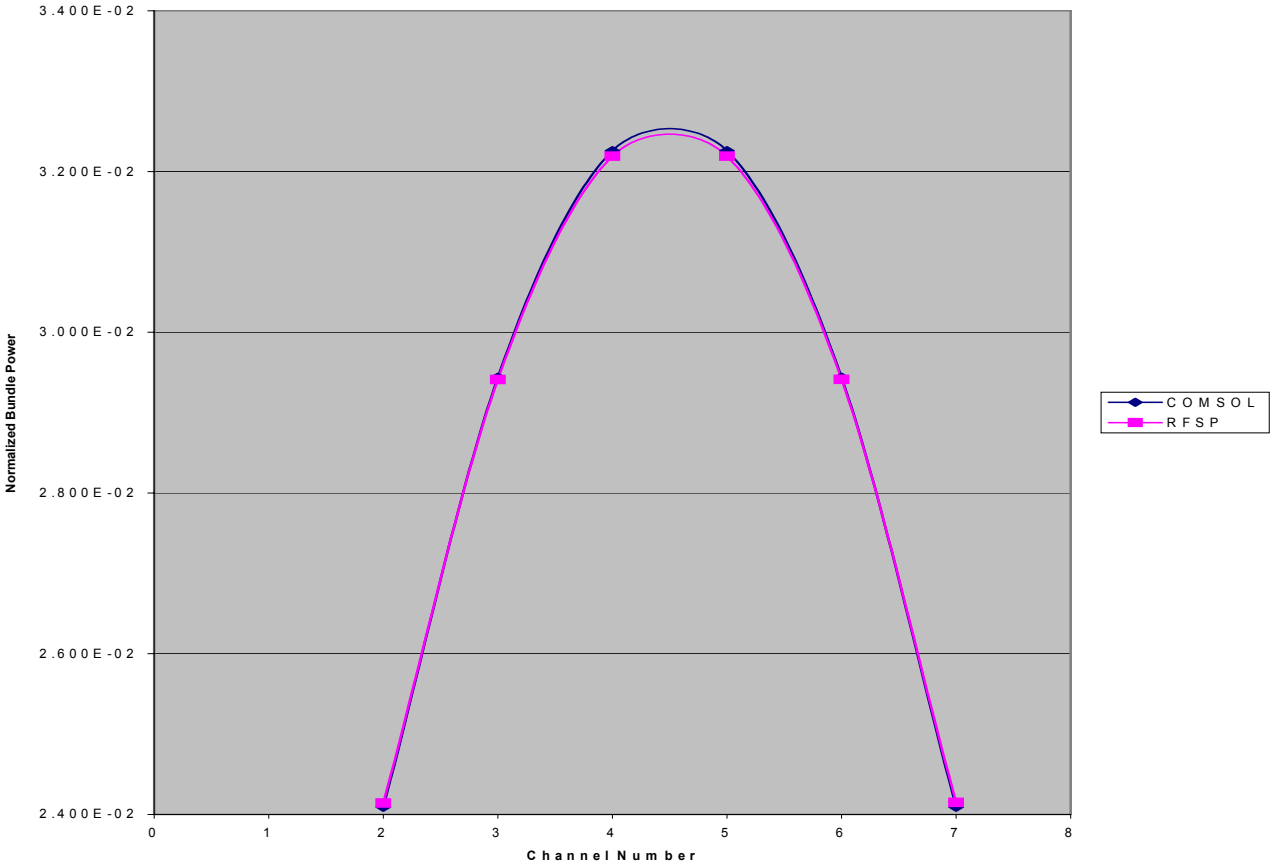


Figure 8 – Normalized Bundle Powers Along Row C in Benchmark Model

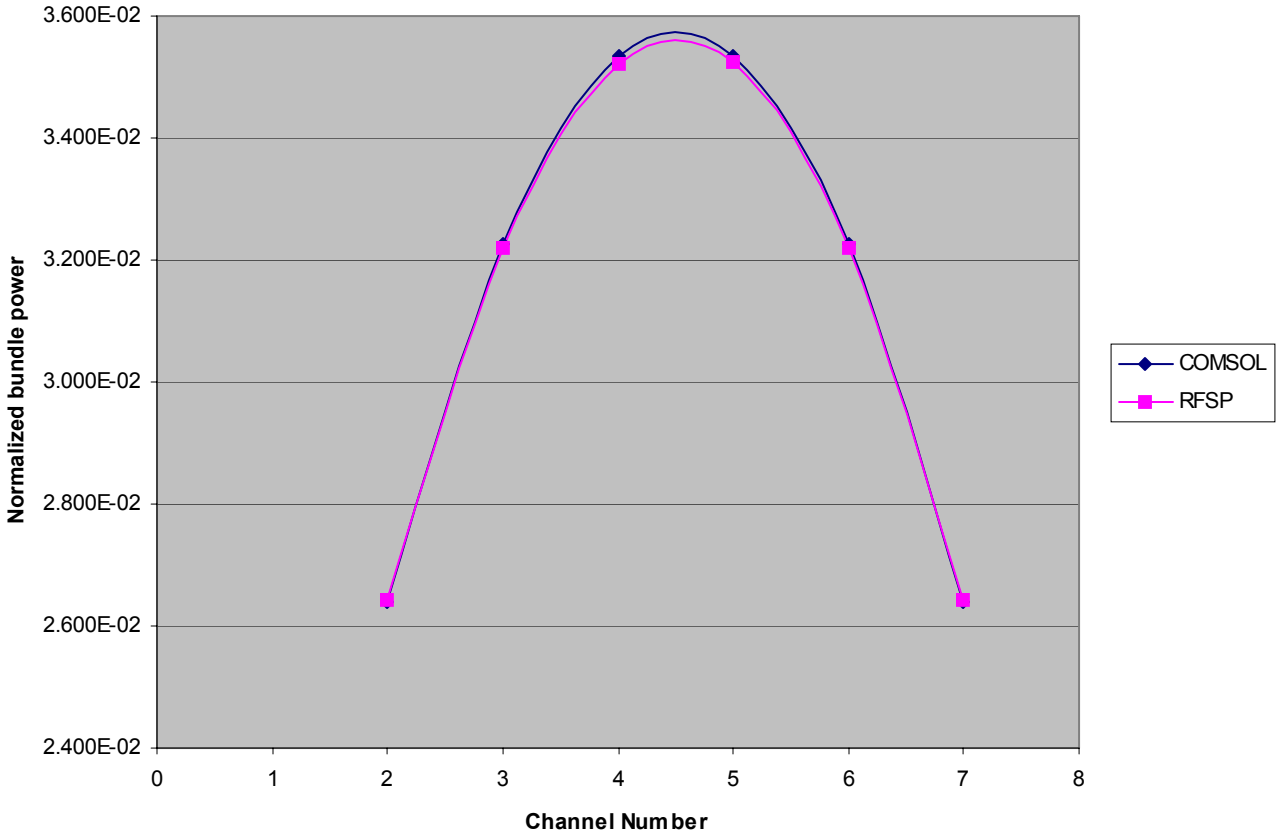


Figure 9 - Normalized Bundle Powers Along Row D in Benchmark Model

Channel	Difference (%)
2	-0.2
3	0.1
4	0.2
5	0.2
6	0.1
7	-0.2

Table 5 – Difference Between COMSOL and RFSP-IST – Row C

Channel	Difference (%)
2	-0.1
3	0.2
4	0.3
5	0.3
6	0.2
7	-0.1

Table 6 – Difference Between COMSOL and RFSP-IST – Row D