Analysis and quantification of modelling errors introduced in the deterministic calculational path applied to a 2-node problem

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Abstract. The objective of this work is to analyse and quantify modelling errors introduced by simplifications made in the deterministic calculational path as applied to nuclear reactor simulation. These simplifications are introduced in order to make a model practically solvable with a diffusion code, and they are classified as follows: spatial homogenization, energy (spectral) condensation, diffusion approximation and environmental dependency. In this work, a two-node model consisting of a SAFARI-1 reactor fuel assembly next to a water node is modelled because it is a typically encountered configuration and fairly sensitive to spatial and spectral approximations. The analysis and quantification of modelling errors introduced in the calculational path were performed. Errors introduced by the four approximations in the calculational path are quantified by investigating the effective multiplication factor (k-eff) as well as calculational time as an integral measure of difference between two models. All calculations were performed with the neutron transport codes NEWT, the Monte Carlo Serpent and the diffusion code MGRAC. The results indicate that for the fuel-water model, environmental dependency and the diffusion approximation are the largest contributors to the total calculational error.

Keywords: condensation, homogenization, diffusion, environmental error

1. Introduction

For the development of computer codes that accurately predict the flux distribution in nuclear reactors, modelling error analysis is necessary. The majority of publications on the modelling error analysis [3][4][5] focused on power reactors. Not much work has been published on modelling error analysis for research reactor (such as material testing reactors (MTRs)) simulation. This work forms part of a bigger study focused on improving the errors made in modelling MTRs. As a first step in this larger study, modelling error analysis is done on a 2-node problem. In future work, the approach defined will be applied to a full-core MTR model. This paper is arranged as follows: Section 2 discusses the theoretical background and calculational path. Section 3 provides a layout of the research methodology and the codes used. Section 4 discusses the results and the final section discusses concluding remarks for this work.

2. Theoretical background and calculational path

In order to predict neutron flux distribution in the reactor core, neutronics modelling of the reactor is performed by solving the neutron transport equation. The neutron transport equation describes the motion and interaction of neutrons with nuclei in a nuclear reactor [2] and is given by:

$$\frac{1}{\nu}\frac{\partial\phi}{\partial t}(\bar{r},\hat{\Omega},E,t)+\hat{\Omega}\cdot\bar{\nabla}\phi(\bar{r},\hat{\Omega},E,t)+\Sigma_t\phi(\bar{r},\hat{\Omega},E,t) = \int_{4\pi}d\hat{\Omega}'\int_0^{\infty}dE'\Sigma_s(\hat{\Omega}'\rightarrow\hat{\Omega},E'\rightarrow E)\phi(\bar{r},\hat{\Omega}',E',t)+s(\bar{r},\hat{\Omega},E,t). \quad (1)$$

Equation (1) has 7 independent variables, position $\bar{r}(x,y,z)$, angular $\Omega(\theta,\phi)$, energy (E) and time (t) variables. The dependent variable is the angular neutron flux $\phi(\bar{r},\hat{\Omega},E,t)$. All terms on the left hand side of the equal sign are neutron loss terms and terms on the right hand side are neutron gain terms. Σ_t and Σ_s are total and scattering macroscopic cross-sections of the system being modelled, and they are measured in cm^{-1}. The source term $s(\bar{r},\hat{\Omega},E,t)$ includes external neutron sources and neutrons from fission, and is thus dependent on the neutron flux. Typically, for day-to-day reactor calculations, a deterministic approach is used to solve this equation because of its computational efficiency compared to other approaches such as the stochastic approach. The deterministic approach involves discretizing the variables of the neutron transport equation to a set of discrete equations that are numerically solvable [2] and is applied to reactor analysis calculations via a two step process.

A reactor core is discretized into nodes (assemblies). In the 2-step deterministic approach; the first step, a 2D steady state transport calculation is performed for each detailed assembly (node) type. The transport solution is used to produce energy collapsed, and spatially homogenized assembly parameters. During the homogenization and energy group condensation process the node-averaged parameters are conserved. The energy collapsed and homogenized parameters will be used in the second step by the full core diffusion solver. The homogenized group-collapsed parameters are generated in an approximated environment instead of the true physical conditions of the assembly in the reactor or full-core calculation. The four simplifications introduced in the deterministic calculational path are discussed in more detail in the following three subsections.

2.1. Energy group condensation and spatial homogenization

The simplifications made in the energy and geometric representation in the node involve performing a fine-group (100s) heterogeneous transport calculation. The transport solution (group heterogeneous neutron flux) is used to collapse the number of energy groups to few-group (less than 10) and homogenize the geometry over the node so that, each node has a constant set of few-group homogenized parameters that preserve the transport solution in an average sense. For few-group homogenized node to be equivalent to the fine-group heterogeneous node, the node-averaged reaction rates and surface transport leakages must be preserved. Therefore, for the homogeneous model to preserve the same average parameters calculated by heterogeneous model, the homogeneous cross-sections ($\tilde{\Sigma}^i_{\alpha,g}$) per group (where α is the type of nuclear reaction) must satisfy the following condition.

$$\int_{V_i}\int_{E_g}^{E_{g-1}}\tilde{\Sigma}^i_{\alpha,g}(\bar{r},E)\tilde{\phi}(\bar{r},E)d\bar{r}dE=\int_{V_i}\int_{E_g}^{E_{g-1}}\Sigma^i_{\alpha,g}(\bar{r},E)\phi(\bar{r},E)d\bar{r}dE. \quad (2)$$

However, because we do not have the few-group homogeneous flux ($\tilde{\phi}$) to accurately preserve heterogeneous solution, the few-group homogeneous cross-sections are calculated with approximated neutron flux before being used in the diffusion full core calculation, and this contributes to the spectral and spatial homogenization errors.

2.2. The diffusion approximation

The diffusion equation is a simplified form of the neutron transport equation. The main simplification of the diffusion theory is that, it eliminates the need to solve for angular flux as in most transport approximations. The derivation of the diffusion equation uses various approximations, one of them being Fick's law (Equation 3 which relates neutron current ($\bar{J}$) to neutron flux (ϕ) [2].

$$\bar{J}(\bar{r},t) = -D(\bar{r})\bar{\nabla}\phi(\bar{r},t). \tag{3}$$

$$\frac{1}{\nu}\frac{\partial\phi}{\partial t} - \bar{\nabla}\cdot D(\bar{r})\bar{\nabla}\phi + \Sigma_a(\bar{r})\phi(\bar{r},t) = S(\bar{r},t). \tag{4}$$

Equation (4) is the single group diffusion equation, and is valid when: there is an isotropic neutron source and scattering, angular flux distribution is linearly anisotropic and current density varies slowly with time. Here, D is called diffusion coefficient, and S is the source term. In both Equations (3 and 4) the energy variable has been suppressed for clarity.

2.3. Environmental dependency

Macroscopic cross-sections are generated in an environment that is not an exact match to the environment where the assembly will be used in the core calculation. For example, fuel cross-sections are typically generated in an infinite fuel environment (i.e. a fuel element with reflective boundary conditions), but in a reactor core, fuel elements are surrounded by fuel of, potentially different burn-up history and composition or even non-fuel elements (such as control rods or reflectors). By using cross-sections from an infinite environment for the fuel elements in a different core environment (i.e using approximate boundary conditions), an environmental error is introduced in the model. Not only fuel cross-sections suffer from environmental errors but also other cross-sections (control rods, reflectors, moderator, etc.) may suffer the same environmental errors.

The spectral, homogenization, and diffusion approximation errors are typically addressed by using equivalence theory (ET). ET is able to mitigate these errors by reproducing the node-integrated properties (reaction rates and leakage rates) of the known heterogeneous solution by introducing discontinuity factors in the homogenization procedure [3]. However, ET cannot address environmental error.

3. Methodology

The four simplifications introduced in the deterministic calculational path are investigated for a 2-node model consisting of fuel assembly next to a water node as shown in Figure 1. Reflective boundary conditions were applied to all outer sides.

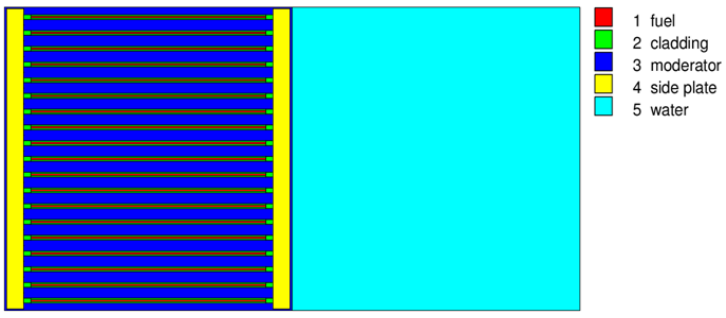

Figure 1. Heterogeneous 2-node model.

Three codes were used in this work, namely NEWT, MGRAC and Serpent. NEWT is part of the SCALE code system, MGRAC is part of the OSCAR-4 code system, and Serpent is a Monte Carlo code system. NEWT (NEW Transport code) is a 2D discrete ordinate transport code [8]. MGRAC (Multi-group Reactor Analysis Code) is a 3D nodal diffusion code [1][6] and Serpent uses Monte Carlo stochastic approach to reactor modelling [9].

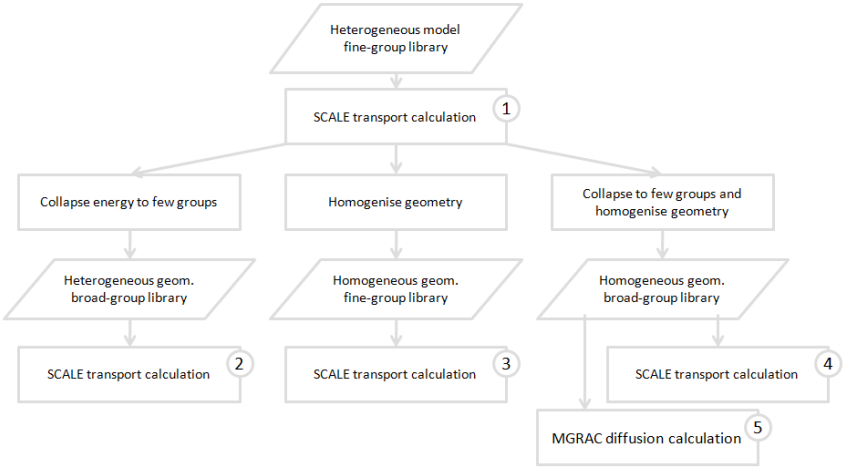

Figure 2. Flow diagram of breakdown of errors in the calculational path.

The first three simplifications can be quantified in a step-wise procedure as described in Figure 2. The NEWT and MGRAC codes are used in this part of the study. In Figure 2, calculation (1) is the reference transport calculation with a fine-group (238 groups) cross-section library and heterogeneous geometry. Calculation (5) is the few-group homogenized diffusion calculation after all simplifications have been made to the model. The errors induced by condensation, homogenization, and the diffusion approximation are determined by comparing the results of the five calculations marked in Figure 2. Table 1 is a summary of the breakdown of errors introduced in the calculational path. Only NEWT and MGRAC were used for this part of the study.

Table 1. Breakdown of error in calculational path

Compare calculations	Quantity to investigate
1 and 2	Spectral error
1 and 3	Homogenization error
2 and 4	Homogenization error in few-group
4 and 5	Diffusion approximation error in few-group
1 and 5	Total simplification error in calculational path

To investigate environmental error, the Serpent code was used to generate fuel and water cross-sections in the correct environment (fuel next to water) and continuous in energy (from which the reference k-eff is taken) and also to generate fuel cross-sections in the approximated environment (infinite fuel environment). The cross-sections generated by Serpent were used in MGRAC diffusion solver to calculate the k-eff in few-group (6 groups). Two MGRAC calculations were

set up; one with no environmental error (fuel and water cross-sections from 2-node Serpent, exact same environment) and one with environmental error where the cross sections were taken from an infinite fuel calculation in Serpent and placed in the 2-node model in the MGRAC. The comparison was made between k-eff calculated in the correct environment and k-eff calculated in the approximate environment for 6 groups. Serpent was used here because the functionality exists to generate nodal equivalence parameters for MGRAC (including discontinuity factors) from the Serpent calculation, but not from SCALE calculation. The generated equivalence parameters were used to resolve the first three errors and only the environmental error need to be studied further and corrected.

4. Results and discussion

The k-eff is a measure of the reactivity of a model and serves as an integral parameter to describe a model. The error will be described as the difference in k-eff (Δk) is measured in pcm (per cent mille) and calculated as: $\Delta k = \frac{k_1 - k_2}{k_1 \times k_2} \times 10^5$ where $\Delta k > 500$pcm is considered large.
The heterogenous transport calculation in 238 energy groups yields the reference reactivity k-eff = 1.17073 in 4118 seconds.

Table 2. Breakdown of errors introduced by simplifications in the 2-node problem

	2-groups	4-groups	6-groups	238-groups
Spectral error (pcm)	3267	819	63	N.A
Homogen. error (pcm)	-214	-141	-81	-22
Diffusion error (pcm)	-6525	-5084	-4094	N.A
Total error (pcm)	-3472	-4406	-4113	N.A

Table 3. Calculational time

	2-groups	4-groups	6-groups	238-groups
Spectral (second)	37	50	60	4118
Homogen.(second)	8	9	17	1313

Table 3 shows the time each calculation took to complete. In Table 2, the spectral error introduced by energy group condensation increases as the number of groups decreases. The reactivity increases with energy group collapsing because physical processes (nuclear reactions) are under represented in the group structures.
Homogenization induces somewhat smaller errors compared to the larger spectral errors observed. Unlike energy condensation, homogenization reduces reactivity, and this error increases as the number of groups decreases. It can be observed that, the 2-group case gives the largest error in reactivity of 214 pcm.
A large error in reactivity is introduced when using a diffusion solver instead of a transport solver. The 6-groups case, yields a reactivity of 4000 pcm lower than the transport calculation. The error increases to just above 6000 pcm as the energy groups are further collapsed. All three simplifictions reduce the calculational time significantly when applied to a 2-node problem.
In Table 4, environmental error was investigated in 6-groups only. Notice that the continuous energy, heterogeneous Serpent calculation and the 6-group homogenized diffusion calculation are equivalent (within some statistical margin) because ET was used in the cross-section generation.

Table 4. Environmental dependency effect in 6 energy groups

Codes	k_{eff}correct env.	k_{eff}Approx. env.	Δk (pcm)
Serpent	1.17050	-	N.A
MGRAC	1.17047	1.16051	733

This shows that ET can mitigate the error of the first 3 simplifications if the cross-sections are used in the exact same environment as that in which they were generated. We see that even though an error of about 4000 pcm has been negated by the use of ET, we are left with an environmental error of 733 pcm.

5. Conclusion

All four simplifications introduced in the deterministic calculational path were investigated for a two node fuel-water problem. From the results presented above, it can be seen that the diffusion approximation and environmental dependency are major contributors to the total error in the deterministic calculational path for a fuel-water model. However, the first 3 simplifications are mitigated through the use of equivalence theory by introducing equivalent nodal parameters to preserve not only node-averaged reaction rates but also the node-leakages. The equivalence theory only addresses the first 3 errors and not the environmental, therefore, the environmental error mitigation is still an area of active research. The findings can be used to develop models that can address environmental and diffusion approximation errors. Future work will look at modelling error analysis and quantification for other configurations (fuel-absorber, fuel-reflector, etc.) found in SAFARI-1 and go to the full core calculations.

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