

Simulation of the egyptian 2nd testing research reactor (ETRR-2) experimental benchmark in aid of verification and validation of the OSCAR-4 system

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Abstract.

This paper investigates the applicability of the current OSCAR-4 code system to simulate the ETRR-2 reactor. Various modelling approaches are applied to this benchmark, in order to quantify the capability of neutronic modelling in OSCAR-4. In particular, the modelling of the control rod calibration experiments poses challenges to the traditional deterministic calculational path and alternatives are investigated to address these shortcomings. Results indicate that an improved homogenization approach directly impacts on the accuracy of the full core diffusion solution.

1. Background and motivation

The reliable and safe operation of a nuclear reactor highly depends upon the ability to accurately predict the neutron flux distribution, which is required to determine quantities such as power distributions, effective multiplication factor (k_{eff}), control rod worths, shutdown margins and isotopic depletion rates – quantities required throughout the reactor operation [5]. As a means of predicting the above mentioned quantities and safety limits during reactor operation, computational reactor codes become invaluable. Safety being the key issue, it is of importance to perform safety analysis of research reactors through validating reactor codes against experimental data. Recently, the IAEA (International Atomic Energy Agency) published a set of experimental benchmarks, including neutronics and thermal-hydraulic benchmarks for, amongst others, the ETRR-2 reactor [3]. Previously, such an expansive, collated set of results had only been published for power reactors, which limited the benchmark tests for research reactors to code-to-code comparison.

For the purpose of this work, ETRR-2 was of particular interest, since some of its core components are similar in design as compared to the SAFARI-1 reactor (South African Fundamental Atomic Research Installation) operated by Necsa. Therefore, ETRR-2 was chosen as a test case to strengthen the validation basis for calculating research reactors with the OSCAR-4 (Overall System for the Calculation of Reactors, generation 4) code system. OSCAR-4 is currently utilized to simulate the SAFARI-1 reactor [6] at Necsa. OSCAR-4 is a nodal diffusion based code which is used to perform day-to-day reactor calculations in support of the SAFARI-1

reactor. As a means of improving the capabilities of OSCAR-4, there is a need to solve more benchmark problems in aid of verification and validation of the code system for research reactor applications. Verification means the precision of the code is tested against other standard codes for reactor analysis, whilst validation is comparing the accuracy of the code against experimental data.

OSCAR-4 is a deterministic code system, and its standard calculational path introduces a number of typical approximations in the modelling of the physical phenomena present during the operation of a reactor. As a result of these approximations within the code system, certain modeling scenarios, particularly in regions near strongly absorbing materials (such as control rods) pose challenges to these standard methods and careful adaptations should be considered. Deterministic code systems are typically used for reactor operation support calculations as their computer simulation time is significantly lower than Monte Carlo based full core solvers. Hence, the main focus of this study is on the modelling approach of the ETRR-2 control rods, and then in particular on how to establish or propose a better model to simulate control rod worth experiments. From the experimental benchmarks published for ETRR-2 [3], Core SU-29 was chosen as the base core configuration for simulating the proposed experiments.

A full core OSCAR-4 model was built and tested for its precision using a more accurate Monte-Carlo based code (SERPENT [4]), as a reference model. Furthermore, using a newly developed link between OSCAR-4 and SERPENT, the existing calculational path can be modified or improved by generating cross sections from SERPENT. As a way of resolving the challenge, associated with modelling the ETRR-2 control rods, a modified OSCAR-4 model was built using cross sections generated from SERPENT for selected core components. These models were compared with experimentally measured data and the results will be discussed. The SERPENT code is thus used both as full-core reference solver, and cross section generation tool.

2. Theoretical background and OSCAR-4 overview

In order to determine the neutron flux distribution in a reactor core, the neutron transport equation must be solved, which describes the movement, distribution and interaction of neutrons with matter. In typical reactor simulation tools, calculations are performed based on steady-state conditions, assuming that the system evolves slowly with time in such a way that the time-independent solution of the neutron transport equation can be used to predict the required quantities during reactor operation.

Below is the time-independent neutron transport equation [1] and each symbol has its standard meaning in reactor physics.

$$\Omega \cdot \nabla \Phi(\mathbf{r}, E, \Omega) + \Sigma_t(\mathbf{r}, E, \Omega) \Phi(\mathbf{r}, E, \Omega) = \int dE' \int d\Omega' \Sigma_s(\mathbf{r}, E' \rightarrow E, \Omega' \rightarrow \Omega) \Phi(\mathbf{r}, E', \Omega') + \frac{\chi(E)}{4\pi} \int dE' \int d\Omega' \nu \Sigma_f(\mathbf{r}, E') \Phi(\mathbf{r}, E', \Omega') \quad (1)$$

Equation (1) is derived based on mechanisms which are responsible for neutron production and neutron loss. The ratio between these two mechanisms determines the value of k_{eff} . For a reactor operating at a critical state, the value of k_{eff} is one. Equation (1) is often written in the form of an eigenvalue problem, where k_{eff} is the eigenvalue to be calculated. The first term describes the net leakages, the second term describes the removal of neutrons due to absorption or scattering. The third term describes the gain of neutrons due to in-scattering from all other energy E' and angles Ω' and the last term is the source term. There exist two classes of transport solution methods to calculate the neutron flux distribution for reactor analysis. These methods are classified as Stochastic and Deterministic.

The scale of the problem is often too large to solve (1) directly with all six independent variables: position $\vec{r} = (x, y, z)$, energy E and direction $\Omega = (\theta, \phi)$. Deterministic based methods solve (1) by discretizing each independent variable to form a set of algebraic equations that can be solved numerically [1]. The most commonly-employed approach approximates the solution of (1) by solving the multi-group neutron diffusion equation below:

$$-\nabla D_g^n \nabla \Phi_g^n(\mathbf{r}) + \Sigma_{t,g}^n \Phi_g^n(\mathbf{r}) = \sum_{g'=1}^G \Sigma_{g' \rightarrow g}^n \Phi_{g'}^n(\mathbf{r}) + \chi_g \sum_{g'=1}^G \nu \Sigma_{f,g'}^n \Phi_{g'}^n(\mathbf{r}) \quad (2)$$

Here (2) is written in discretized form for n nodes, assuming constant cross sections per mesh (core components can be treated as nodes).

In neutron diffusion theory, the angular flux distribution is assumed to be at most linearly anisotropic[1]. In this regard, the flux distribution is expanded over the angle up to the first order term. The theory also assumes that the neutron current density changes slowly with time and that the neutron sources are isotropic. For a given core component or mesh, 2D detailed neutron transport calculations (solving (1)) in fine energy group structure are performed, to obtain the heterogeneous flux shape. The flux shape is then used as a weighting factor, to produce accurate flux-volume weighted cross sections and equivalence parameters (this technique is collectively known as spatial homogenization and energy group condensation)[2]. These equivalence parameters must be defined in such a way that component-average reaction rates and surface-averaged net leakages are preserved when the multi-group diffusion equation is solved[5]. The success or failure of this approach is often found in the quality of the 2D transport solution, as well as the relevance of the boundary conditions used to perform such calculations. Applying (2) to perform full core simulations in 3D does not necessarily weaken the solution, since cross sections and associated equivalence parameters act as correction factors in regions where diffusion approximation falls apart.

In this work we apply the OSCAR-4, which is the current version of the OSCAR code system. To generate flux-volume weighted cross sections and equivalence parameters, a collision probability transport code, HEADE, is used to solve a 2D fine-group problem for a given core component. HEADE is based on a low-order response matrix formalism, applying isotropic partial current boundary conditions on internal boundaries. As such it is quite applicable to the modelling of fuel elements (since fission dominate components have near-isotropic angular flux distributions). However, due to its approximations, HEADE is not necessarily suited to components such as control rods and/or reflectors. As an alternative to HEADE, SERPENT is used as a 2D transport code, to improve the quality of the transport solution needed to generate cross sections and required parameters. These cross sections are then tabulated against state parameters (such as Fuel Temperature, Burn-up, Moderator density, etc) for later use. This is a once-off process and the results for all core components are linked into a single run-time cross-section library. The linked cross sections and associated parameters are then passed to the global diffusion solver, Multi-Group Reactor Analysis Code (MGRAC). MGRAC uses the Multi-Group Analytic Nodal Method (MANM)[8], to solve the multi-group diffusion equations for a 3D full core model.

3. Experiments and model description

ETRR-2 is a 22 Mega-Watt pool-type research reactor. It is fuelled with low enriched uranium (19.7 %), cooled, moderated with light water and reflected by beryllium. In this paper we focus on the ETRR-2 benchmark experiments, in particular the control rod worth or calibration experiments. To perform these experiments, a reactor core is adjusted to be critical at low power to avoid feedback effects. The reactor is made super-critical by extracting the rod to

be calibrated by a certain distance and the period method is used to measure the reactivity. The core configuration is again adjusted to be critical by inserting one of the rods not being calibrated into the core, to compensate for the change in reactivity. These steps are repeated until the calibrated rod is fully extracted from the core. In this regard, a typical outcome of such an experiment, and associated calculation, is the differential rod worth curve for each calibrated rod. Additionally, the so-called control rod s-curve, used to characterise the absorbing capability of the rod as a function of extraction position, may be produced.

The aim of this work then is to quantify the improvement provided on this benchmark by addressing two particular shortcomings identified in the standard deterministic calculational path as applied in OSCAR-4. These are:

- The shortcomings in HEADE to calculate the reference transport solution for non-fuel components;
- The impact of utilizing, for non-fuel components, explicit component environments as boundary conditions for cross-section generation, as opposed to the standard approach of typical generic, mini-core environments.

To facilitate this investigation, three models were built to simulate rod worth experiments. Their description is summarized in the following table:

Table 1. Models

Model	Description
Reference (SERPENT)	Full core 3D heterogeneous Monte-Carlo calculations with SERPENT.
Standard OSCAR-4	HEADE-based cross sections were generated in 6 energy groups (e.g Fuel, reflectors, control rods and water box). For fuel components, cross sections are generated from an infinite environment with reflective boundary conditions, and for non-fuel components, cross sections are generated from a mini-core environment with fuel acting as a driver zone.
Modified OSCAR-4	For the selected non-fuel components, cross sections were generated in 6 energy groups from SERPENT. environment. A full-core 2D SERPENT model was utilized to generate cross-sections, with the 2D model representing a case where all control rods are inserted. Fuel element cross-sections were generated using HEADE, utilizing the standard model.

A note is needed here. The construction of the modified OSCAR-4 model, described in table 1 above, has particular significance with regard to practical reactor core calculations. The usage of infinite (or reflective) boundary conditions for the cross-section generation models of fuel elements is quite typical, and in actual fact preferable, as compared to utilizing their explicit environments (given their respective core locations). In other words, one generic environment for all fuel is often a more practical option than unique cross-sections per fuel element, particularly since fuel elements are move around and shuffled throughout the core during their lifetimes. Non-fuel elements however, do not generally move around the core structure from cycle to cycle and as such more detailed environmental conditions may be utilized during the cross-section generation process for such components. For this reason both the Standard and Modified OSCAR-4 models utilize infinite environment for fuel elements, but differ with respect to both the code (HEADE vs SERPENT) and environmental accuracy (approximate 2D vs full-core 2D), respectively.

4. Results and discussion

Table 2. Results

	k_{eff} rods in	k_{eff} rods out	Critical k_{eff}	Max power error	Rod 5 total worth (\$)	Rod 6 total worth (\$)
Reference (SERPENT)	0.86311	1.02542	1.00294 ± 38.8 pcm	–	2.89	1.03
Standard OSCAR-4	0.86489	1.03160	1.01254 ± 128 pcm	4.94%	3.28	0.95
Modified OSCAR-4	0.85560	1.02028	0.99850 ± 50 pcm	2.73%	3.06	1.05
Experimental value	N/A	N/A	1.000	N/A	2.17	0.86

Table 2 provides an overview of the primary performance of each of the three models considered. In particular, we compare the two OSCAR-4 models (Standard and Modified) with the reference SERPENT results. We compare the models to one-another with respect to k_{eff} for the all rods in and out cases, as well as for maximum assembly power errors (here for the rods in case). Furthermore, we compare all three models to experimental values for criticality prediction and control rod worth experiments (for rods 5 and 6). Note that a large number of critical cases were analysed and as such results are given in terms of average predicted k_{eff} and standard deviation.

In particular we notice that both OSCAR-4 models predict the k_{eff} of the all rods in and out cases to around 500 pcm of the reference SERPENT result, but that the maximum power error is noticeably improved for the Modified OSCAR-4 model. This indicates that the Modified model captures the local effects within the reactor core to a greater degree of accuracy. This is expected, since the HEADE code may not correctly capture the sharp gradients which occur at the interface between, for example, fuel and control elements, during cross-section generation, whereas the Monte Carlo based SERPENT code should resolve these regions accurately.

With respect to the experimental comparisons, we notice that the estimation of criticality ($k_{eff} = 1$) by the two OSCAR-4 models once again show a marked improvement for the case of the Modified OSCAR-4 model. The critical estimation improves from $k_{eff}=1.01254$ (error of 1254 pcm) to 0.99850 (error of 150 pcm). The standard deviation for the modified model is also significantly lower. The comparisons with the two control rod calibration experiments show a more complicated behaviour. The predicted total control rod worth of the Modified OSCAR-4 model is closer to the SERPENT result for both the rod 5 and rod 6 calibration experiments, as compared to the Standard OSCAR-4 model. However, all models overestimate the total control rod worth of both rods 5 and 6 as compared to their respective experimental values of 2.17\$ and 0.86\$. Although this could indicate some bias in all the models, it is also possible that some normalisation, such as β_{eff} or prompt neutron lifetime, used to convert doubling times into reactivity values, may not have been reported correctly by the benchmark supplier. Further investigation into this issue revealed that other institutions who have calculated this experiment noted similar concerns, while calculating similar control rod worth values as given here [7].

Nevertheless, the accuracy of the Modified OSCAR-4 model as compared to the full-core SERPENT solution again shows a noticeable improvement. In particular for rod 5, we notice that the Modified model improves the total rod worth estimate by more than 20 cents. To illustrate this in more detail,

Figure 1 shows the control rod 5 calibration curves for the reference SERPENT model, the

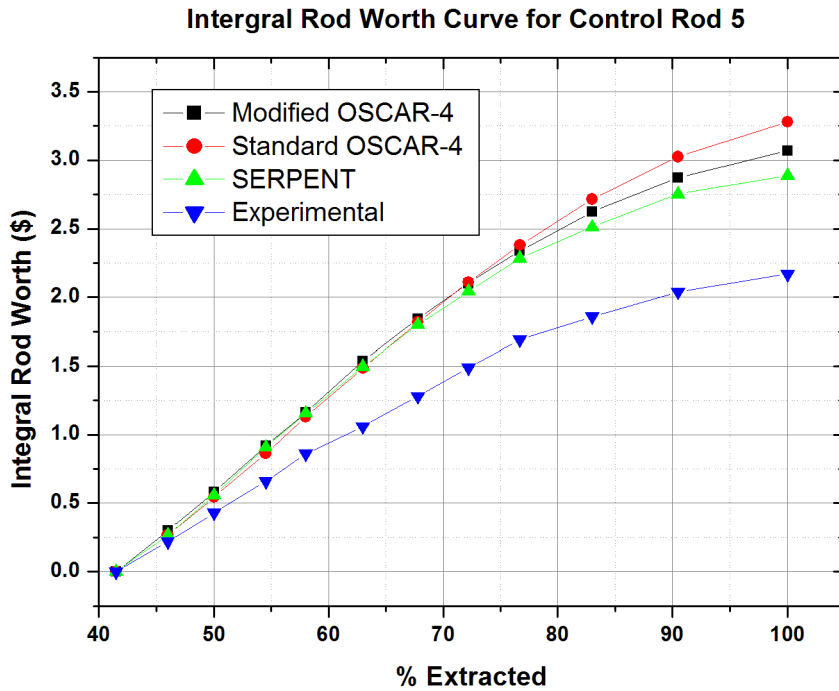


Figure 1. Integral rod worth curve for control rod 5 calibration

Standard OSCAR-4 model and the Modified OSCAR-4 model as well as the experimental results. Here it is once again clear that the Modified model improves upon the Standard model, but also that some general offset exists between all the models and the experimental curve. As noted before, further investigation into the experimental procedure is needed to resolve this.

5. Conclusions

From the results presented above, it can be seen that the Modified OSCAR-4 model shows improvement in most of the calculated parameters, with the exception of the k_{eff} value for the case with all rods in the core. Furthermore, the Modified model shows a more stable prediction of k_{eff} values for critical reactor configurations. This shows that the improved transport solution in the non-fuel elements (specifically the control rods), and hence improved cross sections and equivalence parameters, impact greatly on the accuracy of the full core diffusion model, as expected. In the case of ETRR-2, these improvements are required to predict the reactor state to an acceptable degree of accuracy.

An important result to note, is the fact that the use of fuel cross sections and equivalence parameters, generated from an infinite lattice environment, yields acceptable results. This is important from an operational point of view, as position dependent parameters need not be generated for fuel elements. During reactor operation, the core configuration changes from cycle to cycle, meaning fuel elements are not bound to a specific position as the non-fuel elements are. If position dependent parameters were required for fuel elements as well, it would be required to generate these parameters for each new core configuration, making the current approach not feasible.

Finally, the good agreement between the Modified OSCAR-4 model and SERPENT reference results, makes the ETRR-2 benchmark (core SU-29) a good case to be added to the verification

set of the OSCAR-4 system. This shows that the current OSCAR-4 system, with the link to SERPENT, is capable of simulating ETRR-2 with comparable precision, for the chosen parameters, to a full -core Monte Carlo transport simulation. As far as validation is concerned, further investigation into the experimental results is required to determine the accuracy of the models. This can be done by simulating different core configurations and their associated experiments with both the Modified model as well as SERPENT, and again comparing the results with the supplied experimental results.

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