HIGH PRECISION NEUTRONIC CALCULATIONS FOR TRANSIENT SIMULATIONS FOR FRM II

C. Reiter, H. Breitkreutz, A. Röhrmoser, W. Petry

Forschungs-Neutronenquelle Heinz Maier-Leibnitz (FRM II), Technische Universität München Lichtenbergstraße 1, 85748 Garching bei München, Germany

A. Seubert

Gesellschaft für Anlagen- und Reaktorsicherheit (GRS) gGmbH Boltzmannstraße 14, 85748 Garching bei München, Germany

ABSTRACT

A new high density fuel element consisting of an alloy of uranium and molybdenum (UMo) is being developed for the conversion of FRM II's compact core from high enriched uranium towards lower enriched uranium. Required slight changes of the core geometry demand both neutronical and thermo-hydraulical re-calculations. This is achieved by coupled calculations of the neutronic TORT-TD code and the thermo-hydraulic ATHLET code for transient calculations. Starting from the well proven full MCNP6 model of FRM II, a substitutional MCNP6 model was developed and validated. Based on the MCNP6 vertical stack model, a geometrically equivalent Serpent 2 model was created. With the validated Serpent 2 model the multi group cross sections needed for TORT-TD can be calculated. In the next step, the vertical stack model was translated into an r- ϕ -z geometry for TORT-TD. It is shown, that the developed system consisting of data processing tools and new models leads to matching results between Monte Carlo and deterministic codes. With that system of models and postprocessing tools, high precision neutronic calculations can easily be embedded in transient calculations for FRM II.

1. Introduction

The Forschungs-Neutronenquelle Heinz Maier-Leibnitz (FRM II) is Germany's most powerful neutron source and has the highest flux-to-power ratio world-wide. With a thermal power of only 20 MW, the compact core provides an undisturbed maximum thermal neutron flux of $8.0 \cdot 10^{14}$ n/(s cm²). To support the global non-proliferation efforts, FRM II is actively working towards the conversion of its compact fuel element to a uranium enrichment which is significantly lower than its current enrichment of 93%. Changes in fuel type and core geometry require a re-evaluation of both the neutronic and thermal-hydraulic behavior of the FRM II's compact core, in normal operation as well as in off-normal transients.

A coupling of the neutronic code TORT-TD [6] and the thermal-hydraulic system code ATHLET [7] will be used for transient evaluation. This paper is focused on the efforts made in the neutronic calculations. As with most standard deterministic neutronic codes, TORT-TD is not capable of directly modeling the unique geometry of the FRM II core. Therefore, as a first step, a reliable emulation of the geometry must be found.

2. Explanation of the underlying model

Starting from the well proven full MCNP6 [5] model of FRM II [2], a simplified MCNP6 model uses a vertical stack of plates instead of involutes [1, 3]. The total core material inventory and the general assembly design are retained. Also, it correctly preserves the core key parameters like fresh core excess reactivity, thermal and fast neutron flux and power

deposition in the core. Details of this model as well as a comparison between both models are discussed in [1].



Figure 1: Top view of the involute MCNP6 model (left). Side view of the substitutional vertical stack MCNP6 model (right).

3. Calculation of the multi-group cross sections

Based on the MCNP6 vertical stack model, a geometrically equivalent Serpent 2 [4] model was created. This model is constructed in a way that allows for a simple generation of multigroup cross sections for almost every single part of the core. Comparison of the results obtained with MCNP6 and Serpent 2 shows a perfect match for fresh core excess reactivity and thermal neutron flux. This is also discussed in [1].



Figure 2: Relative deviation in percent of the fast neutron flux in the involute model calculated with MCNP and the vertical stack model calculated with Serpent 2.

The results of both codes for the fast neutron flux also match within a statistical uncertainty of $\pm 2\%$ for the zones of interest (see Figure 2). Obviously, with increasing distance to the fuel zone and increasing moderation the fast neutron flux decreases.





Comparison of the fission rates in the fuel zone shows well matching results with minor statistical fluctuations as depicted in Figure 3. Except the fuel zone near the hafnium absorber, the power depositions match within $\pm 2\%$.

The fully validated Serpent model is used as the basis for the calculation of multi-group cross sections for TORT-TD. With the data from this model, the deterministic calculations can be performed.

4. Deterministic calculations

As first step, the vertical stack model has been translated in an r- ϕ -z geometry for TORT-TD. The first calculations have been performed with a very detailed mesh, so it consists in total of 442224 cells, with 333 nodes in r-direction, 4 nodes in ϕ -direction and 332 in z-direction. Serpent 2 can calculate multi-group cross sections for universes. Therefore, the Serpent 2 model has been set up in the way that every single cell is defined in a corresponding universe. With a transition matrix and self-written post processing tools, the nodes of the TORT-TD mesh are linked to the corresponding cross sections.

In order to reduce the total number of mesh cells, the virtual disks of the vertical stack model are not explicitly modeled, but rather implemented as homogenized materials with position-dependent cross sections to respect local flux changes.

The TORT-TD calculations were performed with a quadrature order of 4, cross sections to the first legendre order and 30 energy groups with the following energy intervals in MeV:

Group 1	Group 2	Group 3	Group 4	Group 5	Group 6
4.00	3.00	1.85	1.353	9.00E-1	1.00E-1
Group 7	Group 8	Group 9	Group 10	Group 11	Group 12
3.00E-3	1.00E-4	3.00E-5	1.00E-5	3.00E-6	1.77E-6
Group 13	Group 14	Group 15	Group 16	Group 17	Group 18
1.00E-6	0.625E-6	0.5125E-6	0.40E-6	3.375E-7	0.275E-6
Group 19	Group 20	Group 21	Group 22	Group 23	Group 24
0.15E-6	1.00E-7	5.00E-8	3.00E-8	1.00E-8	6.50E-9
Group 25	Group 26	Group 27	Group 28	Group 29	Group 30
3.00E-9	2.50E-9	2.00E-9	1.00E-9	1.00E-10	0

Table 1: Lower boundaries of the used energy groups in MeV.

With this system of models and post-processing tools, deterministic calculations with TORT-TD can be performed next and the steady state results can be compared with the Monte Carlo method. As listed in Table 2 all three codes deliver matching multiplication factors.

Table 2: Calculated multiplication factors calculated with the three used codes.

Code	MCNP 6	Serpent 2	TORT-TD
Multiplication Factor	0.99794 ± 0.00029	0.99832 ± 0.00031	0.99700

This model also allows for the high detailed calculations of fluxes and power deposition distribution (see Figure 4).



Figure 4: Calculated power deposition in a fuel plate (MW/I) calculated with TORT-TD (left). Thermal neutron flux in 10¹⁴ n/(cm² s) calculated with TORT-TD (right).

For verification, the thermal neutron flux of the original MCNP model is compared with the result obtained with TORT-TD. The fluxes of the lowest eight related energy groups up to 3.00E-8 MeV are then summed up and then compared with MCNP calculations, where the same energy groups have been applied.



Figure 5: Relative deviation in percent of the thermal neutron flux in the involute model calculated with MCNP and the vertical stack model calculated with TORT-TD.

In Figure 5, the relative deviation of the thermal fluxes is shown. The resolution of the used quadrature order S4 is not high enough to reproduce the highly directed neutron fluxes at the edges of the fuel zone. That leads to the in Figure 5 noticeable "ray effects" starting at the edges of the fuel zone. The thermal fluxes match within \pm 5%, even though TORT-TD over estimates the thermal flux systematical near the fuel plates. For transient calculations the power deposition is far more crucial than the thermal neutron flux inside the heavy water moderation tank. As long as the power deviations match perfectly, the observed over estimation of TORT-TD is acceptable.

The relative deviation is strongly related to the energy group, as shown in Figure 6. Inside the hafnium absorber, TORT-TD over estimates the flux by more than 10%, which is due to the different calculation approach. The used hafnium absorber is not very thick. While the Monte Carlo approach will cut mostly the total neutron flux within that short range, the discrete ordinates is too inert to follow a high flux gradient on such a small distance. This leads to the observable over estimation of TORT-TD inside the hafnium absorber. For the important zone inside the heavy water moderator tank, where the emergency shutdown rods are located, the thermal fluxes match within $\pm 5\%$.



Figure 6: Relative deviation in percent of the thermal neutron flux of the third energy group (from 1.00E-9 to 2.00E-9 MeV) in the involute model calculated with MCNP and the vertical stack model calculated with TORT-TD (left). Relative deviation in percent of the thermal neutron flux of the fifth energy group (from 2.50E-9 to 3.00E-9 in MeV) in the involute model calculated with MCNP and the vertical stack model calculated with TORT-TD (right).

Last the calculated power deposition distribution will be compared, i.e. the given TORT-TD mesh is compared to an equivalent MCNP6 mesh tally TMESH type 3. As shown in Figure 7 (a), the power deposition is systematically shifted by roughly 18%. This is because TORT-TD transports no secondary particles and calculates a distribution for the power deposition only in cells where fission occurs. So, no power is calculated outside of the fuel zone, in contrary to MCNP where significant power is deposited outside of the fuel.

To correct this behavior, the integral power thus MCNP deposits in the fuel zone is compared with the integral power used by TORT-TD. A possible correction must be independent of the

used number of mesh tally cells. For a fine mesh tally which covers the complete fuel zone, an averaged deviation of 17.9% has been calculated. In comparison to that result, the total power, deposited in the fuel zone calculated with just one cell, leads to an over estimation of TORT-TD of 18.1%. With that information, a systematic shift between both codes of 17.7% can be explained. The final result which has been corrected for this systematic shift is illustrated in Figure 7 (b) and shows results matching within $\pm 3\%$ for the power deposition.



Figure 7: Non shifted relative deviation in percent of the power deposition in the involute model calculated with MCNP and the vertical stack model calculated with TORT-TD (left). Shifted relative deviation in percent of the power deposition in the involute model calculated with MCNP and the vertical stack model calculated with TORT-TD (reght).

5. Summary

With this system of models and post-processing tools, high detailed deterministic neutronic calculations can easily be embedded in transient calculations for FRM II. With Serpent 2 model, multi-group cross-sections for different fuel variants can be created and then used in TORT-TD for the coupling into transient simulations. In the next steps, optimization regarding performance will be performed and the control rod movement will be implemented. In the final step, coupled transient calculations with ATHLET will be performed and the results will be compared to previous results from FRM II design calculations and measured data.

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