### Radiological Characterization and Decommissioning of Research and Power Reactors – 15602

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### **INTRODUCTION**

The production of the detailed activity and dose rate atlases (ADAs) is one of the indispensable measures in the decommissioning process of nuclear reactors which allows to determine the radiation field for optimal radiation protection as well as to quantify and characterize nuclear waste for disposal. High-detailed simulation models capable of performing neutron and radiation transport calculations at different levels of precision and details are applied for this purpose. Within the framework of the research project "*Decommissioning of Research and Power Reactors*", funded by the German Federal Ministry of Education and Research (BMBF), and implemented by the Institute of Nuclear Engineering and Technology Transfer (NET) -RWTH Aachen, sophisticated simulation tools are developed. The enhances capability of these tools for the generation of the activity and dose rate distribution are tested and demonstrated on the shutdown German research reactor *FRJ-2*. To achieve the project goal different computational steps were required:

- 1. Development of a calculational *CAD*-based model for Monte Carlo neutron and gamma transport simulation using converter tool McCad
- 2. Design of the neutron source which reproduce the neutron distribution leaving the core
- 3. Enhancement of the simulation performance by using the hybrid deterministic Monte Carlo variance reduction methods
- 4. Calculation of N-flux distribution in the entire geometry
- 5. Development of couple codes between MCNP5 and the activation code ORIGEN2.2

This paper describes the main significant project milestones.

## The FRJ-2 Research Reactor

The FRJ-2 is a heavy water cooled and moderated DIDO-type research reactor which has been operated for 44 years and was shut down on May 2nd 2006. The core consisted of 25 fuel elements, which were disassembled with other structures in an earlier stage of the decommissioning process. Each fuel elements consisted of five tubes; four fuel tubes which were contained within an aluminum cladding and one outermost aluminum tube [1].

The core was located within an aluminum tank; this is surrounded by a graphite reflector which rests within a double-walled steel tank. This steel tank is then surrounded by a biological shield which was constructed from different kinds of heavy concrete. The reactor is equipped with two diverse and independent shutdown systems: the coarse control arms (CCAs) and the rapid shutdown rods (RSRs). There are several channels for irradiation purposes passing through the reflector.

The reactor reached its first criticality in November 1962 with a thermal power of 10 MW as a material testing reactor. Over the course of 10 years, its power was increased to 23  $MW_{th}$  with a thermal neutron flux of 2.5 \*  $10^{14}$  [1/cm<sup>2</sup> s] until operations ceased in 2006. Thus, the FRJ-2 operated with an average thermal power of 20 MW<sub>th</sub> for approximately 19.6 years [1].

## **Model Development for the Simulation**

The production of the detailed activity and dose rate atlases is associated with the precise modeling of the outer core structures for subsequent neutron and gamma transport simulations. The existing CAD model of the reactor, which was developed at the Research Centre Jülich, reflects the high accuracy of the geometry model however, it is not applicable for neutron and gamma transport calculation. On the other hand, developing an MCNP geometry model in this level of complexity is not practical and, furthermore, doesn't promise to save the entire accuracy of the originally geometry model. For this reason the CAD model of the reactor is converted into the MCNP syntax [9] by employing the CAD-converter tool McCad (version 0.3.0). This converter tool has been developed at the Karlsruhe Institute for Technology (KIT) and processes CAD-model in the STEP format (Standard for the Exchange of Product). This tool is limited to some specific volumetric solids and cannot handle bodies generated by some function e.g., spline functions. However, only three parts of the entire model were defined by spline functions which could be removed because of insignificant volumes and low influence on the neutron or gamma transport calculations. Different steps of the conversion proses with McCad are:

- 1. Decomposition of the components of the CAD-input
- 2. Producing a voxel model for overlapping and collision test
- 3. Generation of solid MCNP cells and discretizing the empty spaces as void cells
- 4. linking the material definitions and number which are saved in an external file

After the first conversion the user needs to run an MCNP calculation to check the geometry for errors. In case of "Lost particles" which are a consequent of the geometry errors subsequent corrections in the MCNP input are required. After a correction step, by manually excluding the corresponding material cells, a unique cell configuration comes out with no undefined and interrupted space. The cross sectional plots of the CAD-model (left) and the converted MCNP model are shown in the next figure.



Figure 1: Front Cross sectional plots of the CAD-model of the out core structures (left) and the converted MCNP model (right)

## Neutron Surface Source Model for MCNP Simulations

The existing MCNP core model of the FRJ-2 is a complex 3-dimensional full scale model with a high level of geometric precision which contains: the reactor core; coarse control arms (CCAs), core structures, beam tubes, the graphite reflector, and the biological shield. The core region consisting of 25 fuel elements and is modeled as a cylinder containing a square lattice with an array of cells representing the individual fuel elements. Each cell in the lattice contains a detailed model of each fuel element comprising the internal thimble, 4 circular fuel tubes and the borated outer shroud tube. Each individual cell is divided into 15 axial and 35 radial and azimuthal material zones (Fig. 2).



Figure 2: full scale MCNP model of the reactor core used for reactor physics simulations

The material zones containing fuel are segmented in detail in the axial, radial and azimuthal direction leading to 11250 geometrical cells containing material composition according to the existing fuel burnup state. The Idea of this project was replacing the reactor with an equivalent source definition on the core surface. This source definition should be directed outwardly and has to reproduce the correct position, angle and energy distribution of the neutrons leaving the core. These distributions have to be recorded in a preceding criticality calculation. The implementation of this idea is depicted in figure 2. In order to obtain a coarse position distribution the tallies on the cylindrical surface were divided into six segments: bottom area, lower  $D_2O$  cylinder barrel, fuel cylinder barrel, upper  $D_2O$  cylinder barrel (2 segments), and top area. Each tally segment is then subdivided into six sectors of 30° aperture angle which are defined with respect to a reference vector in z-direction and describe sections of a cone around the reference vector situated perpendicular or parallel on the segmented tally surface [4].

#### Calculation of N-flux Distribution in the Entire Geometry

The use of Monte Carlo method for the complex reactor system has, however, some numerical and statistically based limitations resulting from the attenuation of the neutron field at large distances and deep penetrations. For this purpose and to improve the computational efficiency, variance reduction (VR) methods are widely used within MCNP which allow to reduce the statistical errors by sampling more particle histories in the regions of interest [2, 3].

The variance of the MCNP calculations is mainly influenced by the number of particles tracked in different material and geometrical zones of the whole model and depends on the sampling method

applied [6]. A particularly important issue is the simulation efficiency as well as the precision of the flux distribution that is achieved by the application of different variance reduction techniques. The common variance reduction techniques encompass a wide range of statistical methods which allow to modify the random-walk process in such a way that the neutron histories with the lowest contributions on the results are scored more frequently. This is achieved by adjusting the corresponding weights to assure preserving the statistical validity of the simulation by appropriate biasing of the scores.

The Application of the basic VR methods to the CAD-based MCNP model of the FRJ-2 leads to results with high statistical uncertainties, mainly in structures with a large distance from the core area (s. Fig. 3). Despite the high CPU time and large number of particle histories in many parts of the entire reactor model very low or no particle sampling and neutron track density is achieved. This is a consequence of limited particle sampling in these regions resulting in a high level of variance. Increasing the number of particle histories would directly contribute to the numerical and statistical precision. Nevertheless, this does not improve the statistics efficiently, as a reduction of the simulation error and uncertainty from 10% to 1% requires 100 times more particle histories and simulation time respectively.



Figure 3: CAD-based MCNP model of FRJ-2 (left), N-Flux distribution via MCNP VR methods (right)

To overcome inherent statistical limitations in high performance Monte-Carlo simulation, FW-CADIS [7] is applied. This improves the particle sampling and scoring by generation and application of properly distributed particle weights and importances. This method is based on the forward and adjoint flux calculation using the deterministic method for neutron transport simulations [8]. Deterministic methods provide the approximate solution of the forward as well as adjoint transport equation using the method of discrete coordinates (SN-approximation). For this aim the code package SCALE6 consisting of different tools, subroutines and flux solvers for forward and adjoint calculations was used.

The final MCNP simulation based on the converted outer core model combined with the designed surface source and optimized weight window parameters from MAVRIC sequence of SCALE6 was performed. Accordingly, the utilization of adjoint driven technique (FW-CADIS) leads to a significant improvement of the simulation performance in terms of statistical certainties in the whole geometrical model. Figures 4 and 5 show the 3-D visualization of the neutron flux and the corresponding relative errors. Accordingly the relative uncertainty in the majority of the geometry is below 0.002, indicating a high level of reliability and precision. However, there are still some small regions where the

statistical error is higher than 0.1. This is due to the strong shielding effect and results in lower neutron flux that could be improved by a longer simulation time.



Figure 4: 3D distribution of the neutron flux over the entire geometry



Figure 5: 3D distribution of the relative errors over the entire geometry

## **Activity Calculation**

One of the main tasks in this project is the development of a software package that couples the computer code *MCNP* with the activation code *ORIGEN2*. These tools are able to control the activation analysis with *ORIGEN* to provide activation data in the form of two or three-dimensional

atlases. Furthermore, they are capable to combine the *ORIGEN* results for a new *MCNP* gamma source definition file for the determination of the gamma dose distribution. The following program modules are already developed: *GenXS* generates cross-sectional data for the burnup and depletion program *ORIGEN2*. *PTRACMapper* uses the output of the *MCNP-PTRAC* runs to create a map of *MCNP*-geometry cells from the defined mesh-structure. *ACTivAid* uses the mapping from the program *PTRACMapper*, the cross-section libraries from *GenXS*, material composition defined in an *MCNP* input, and an *MCNP* neutron-*mesh-tally* and calculates the nuclide activity for each mesh element and each component by the program *ORIGEN2*. Finally an activity atlas is created for later 3D visualization. The activity distribution of C-14 in the entire model is shown in the next figure.



Figure 6: Activity distribution of C-14 [Bq/g]

In order to validate the accuracy, of the simulation, results are subjected to a plausibility check. For this reason, a drill test has been applied which was realized in the scope of cooperation with research center Juelich. For the same position, and isotopes the simulation results have been analyzed. In the same drill position the simulated activity of Ba-133 and Eu-152 deviates only slightly from the measured value and of Co-60 by 20%.

# SUMMARY AND CONCLUSION

For the decommissioning of nuclear facilities in Germany, activity and dose rate atlases (ADAs) are required to create and manage a decommissioning plan and optimize the radiation protection measures. Additionally, detailed ADAs can contribute to minimize radiation exposure of the staff involved in the dismantling and disposing activities. Finally, ADAs have the potential to efficiently reduce the cost for decommissioning as nuclear wastes can be characterized and quantified in detail which allows to minimize the total waste volume. In regard to the demand for highly detailed ADAs, an elaborate automated simulation tool was developed.

Using the example of the FRJ-2, a detailed MCNP model for Monte-Carlo neutron and gamma transport calculations based on a full scale out-core CAD-model was generated. However, to improve the simulation efficiency and convergence performance of the MCNP runs, the CAD-model was partly modified by lumping together the parts of minor physical effect. After the CAD-MCNP conversion

with McCad and the corrections of the residual errors in the MCNP geometry definitions, the model was completed by manually adding the source definition, material compositions, and physics cards to the final MCNP input. In this way, the convenient features of the CAD environment could be utilized for the modeling of complex structures and the generation of an MCNP-model for subsequent Monte-Carlo-based neutron and gamma transport simulations at a high level of precision [9].

On the basis of KCODE simulations with the full scale MCNP model of the core, the energy and angular distribution of neutrons crossing the core cylinder surface are recorded. The obtained results are implemented in an SDEF source definition which is position-, direction-, and energy-dependent. According to the simulations run for validation, the source definition on the core cylinder surface correctly reproduces the distribution of neutrons in a full scale KCODE-calculation, after certain manual adjustments of the emission probability functions. The benefit of such a sophisticated source definition is a significant gain in performance of the simulations compared to full scale core criticality calculations. Therefore, the statistical quality of neutron and radiation transport simulations in complex geometry models can be enhanced for similar computation time [4].

To cope with the inadequacies of the MCNP code for the simulation of a large and complex system like FRJ-2, the FW-CADIS method [5] was embedded in the MCNP simulation runs to optimise particle sampling and weighting. The MAVRIC sequence of the SCALE6 program package, capable of generating importance maps, was applied for this purpose. The application resulted in a significant increase in efficiency and performance of the whole simulation method and in optimised utilization of the computer resources. As a result, the distribution of the neutron flux in the entire reactor structures – as a basis for the generation of the detailed activity atlas was produced with a low level of variance and a high level of spatial, numerical and statistical precision.

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