

# **APPLICATION OF COUPLED MONTE CARLO AND BURN-UP METHOD FOR DETAILED NEUTRONIC ANALYSIS FOR THE FRJ-2 RESEARCH REACTOR ON HIGH PERFORMANCE COMPUTERS**

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## **ABSTRACT**

Using the high capability and performance of the MPP computer systems CRAY T3E-1200 and IBM-p690, a coupled Monte Carlo and burn-up code was applied for neutronic analysis, optimum core management and reactor utilisation of the 20 MW FRJ-2 Reactor at Research Centre of Juelich, Germany. The Monte Carlo (program MCNP4C3) model consists of a detailed geometrical description of the reactor core and surroundings with 11 250 fuel material cells for which the individual power density burn-up was calculated. The fuel elements, absorber arms and beam tubes were highly segmented. The calculations were based mainly on the JEF-2.2 nuclear data evaluation. The accuracy of the model was verified by the simulation of criticality experiments and many comparisons with the measured distribution of average and local n-flux. The reactivity value of each individual core configuration at any burn-up step could be predicted within 2 standard deviation. The local flux was determined with a deviation of less than 5 %. In addition to the routine application for fuel management, the method was applied to determine the n-flux and fission power in the fuel tubes as well as to study the burn-up behaviour of the absorber blades with regard to the change of effectiveness and lifetime.

*Key Words:* Research Reactor, Monte Carlo, Burn-up, Neutronics

## **1 INTRODUCTION**

For the optimum fuel utilization and safe operation of the research reactor FRJ-2 [1] at the research center Juelich, the fuel management and reloading is supported by both experimental and theoretical methods. During refueling of the core and before start of operation the estimated excess and shutdown reactivity is checked by the inverse kinetic method. This method cannot be seen as very accurate since space-time effects due to the change in flux shape after the movement of the six so-called coarse control arms cannot be taken into account. Especially the shutdown reactivity of four of the six control arms with the lowest effectiveness must be determined under the assumption that the control arm with the highest reactivity effect drops out of the core. Therefore, to overcome the short comings of the measuring method and to reduce the

experimental effort, a theoretical method was established to get accurate reactivity balances for operational and accidental control arm movements and for the optimization of the fuel management.

The theoretical model for the determination of reactivity effects and power distribution must take into account the very complex core, control arm and beam tube geometry as well as the 3D burn-up distribution. Since the geometrical complexity does not allow a detailed description with orthogonal mesh nets, a deterministic transport method, e.g. the  $S_N$  method is not applicable without strong simplifications. Therefore, the Monte Carlo method was used for all calculations. One of the most appropriated Monte Carlo codes for these calculation is the MCNP code developed by LANL [2]. This code is based on pointwise cross sections in energy space and is suitable to account for the complex neutron interaction in fuel and  $D_2O$  moderator for a very detailed geometry. MCNP (version 4C3) was used, therefore for all transport calculations. To account for burn-up effects MCNP was coupled to a burn-up module solving the equations for nuclide building, decay and change by nuclear reactions during and after irradiation. To get a detailed information of the burn up distribution every fuel element was subdivided into several radial, azimuthal and axial sections. This led to a large number of material zones for the core (>10.000). To get sufficient statistical accuracy for the Monte Carlo calculation, a fast computer must be available to get results – especially for the calculation of a complete irradiation cycle needs a large amount of computing time. At the Research Center Juelich, in the past, the MPP high performance computer CRAY-T3E-1200 was available. Since 2003 this computer was replaced by a IBM p690 with 1200 processors. The use of MPP computers is necessary since one irradiation cycle is only about 25 days so that the preparing of the necessary documents for the next cycle must be performed in a comparable short time. The large number of zones with different fuel materials – every fuel zone contains mixing tables up to 105 nuclides – requires an efficient method for the calculation of the one-group cross sections for the relevant nuclear reactions for the depletion calculation since for both the CRAY T3E and p690 the available memory is limited and the amount of communication overhead increases with number of zones, number of nuclides and number of tallies. The present paper describes the details of the calculational scheme and the validation of the methods used for the FRJ-2 fuel management.

## 2 DESCRIPTION OF THE FRJ-2

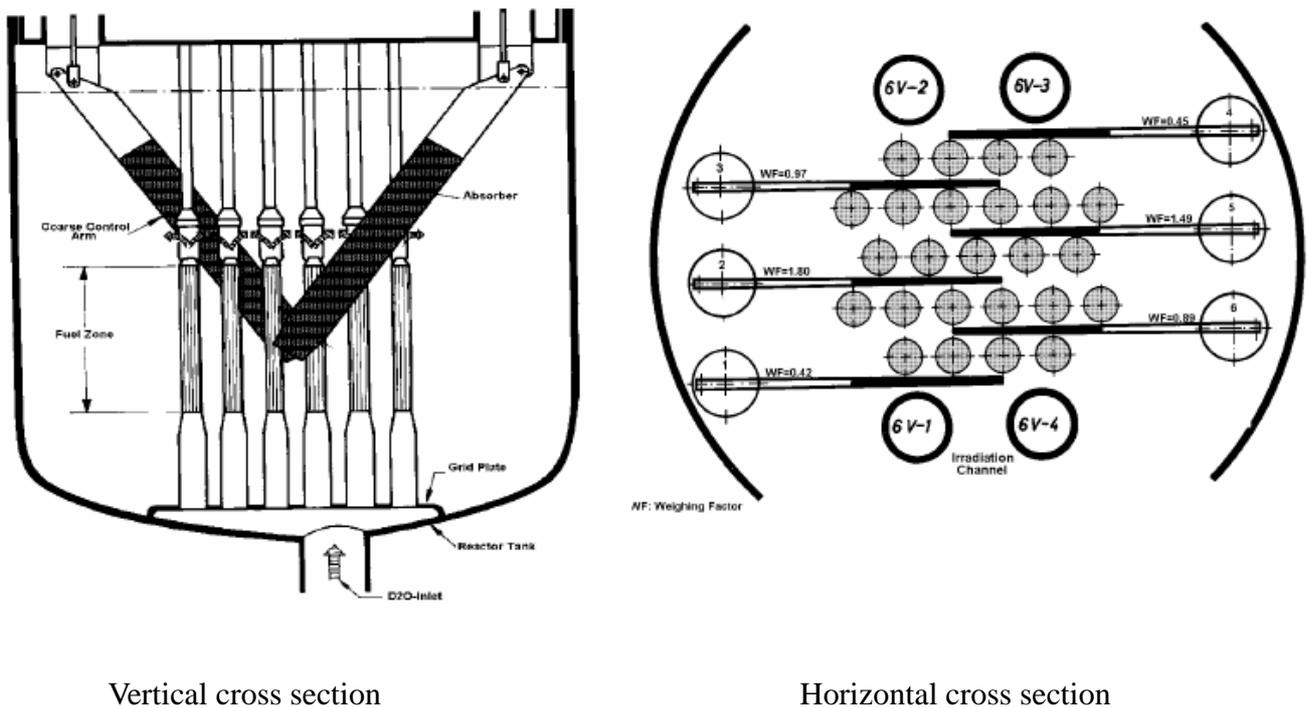
The FRJ-2 is a DIDO-class tank-type research reactor cooled and moderated by heavy water. The core consists of 25 so-called tubular MTR fuel elements arranged in five rows of 4, 6, 5, 6 and 4 fuel elements (see Fig. 1). It is located within an aluminum tank of 2 m in diameter and 3.2 m in height. The tank is surrounded by a graphite reflector of 0.6 m thickness enclosed within a double-wall steel tank.

The active part of the tubular fuel elements is formed by four concentric tubes having a wall thickness of 1.5 mm and a length of 0.63 m. The tubes consist of fuel meat clad with pure aluminum and are inset into a shroud tube of 103 mm diameter. The fuel meat contains  $UAlx$  in an aluminum-matrix with an U-235 enrichment of 80 %. The annular water gap between the tubes has a width of about 3 mm leaving a central hole of 50 mm diameter filled with a thimble

for irradiation purposes. The reactor is equipped with two independent and diverse shutdown systems, the coarse control arms (CCAs) and the rapid shutdown rods (RSRs). In case of request, the six CCAs are released from their electromagnets and drop into the shutdown position by gravity, whereas the three RSRs are shot in by their pneumatic actuators. The CCAs are lowered and raised manually around a pivot in order to control power levels during normal operation, whereas the RSRs are permanently in their upper position. The shutdown position of the CCAs is at an angle of  $56^\circ$  against the horizontal line. In this position, they have the highest worth. In case of a failure of the holding mechanism of one CCA, the sword would swing out of the core causing high amount on reactivity insertion.

Thirty horizontal tubes penetrate through the concrete shielding and the graphite reflector. Eight of these beam tubes and one through tube lead into the maximum or near maximum thermal neutron flux of  $2 \cdot 10^{14} \text{ cm}^2 \text{ s}^{-1}$ . These tubes are almost exclusively used for neutron scattering experiments as far as spatial conditions permit. In addition, there are more than thirty vertical tubes, some of them containing facilities used for special (fuel and structural material) and standard (isotope production and neutron activation analysis) irradiation.

The average moderator temperature at nominal power of 23 MW is about  $55^\circ\text{C}$ . The average cycle length is about 20 Full Power days, depending on reload strategy.



**Fig. 1: Arrangement of fuel elements and coarse control arms (at low position) inside the reactor tank**

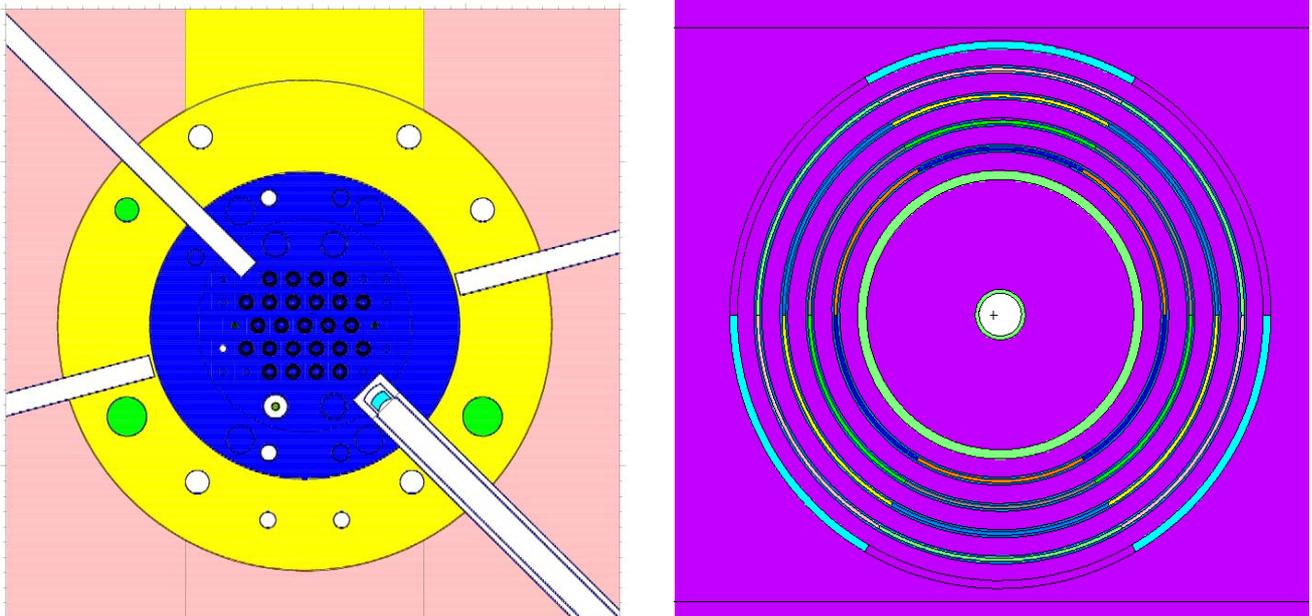
### 3 CALCULATIONAL MODEL OF THE FRJ-2

#### 3.1 The MCNP model

The complex structure of the reactor requires a geometrical description by general geometrical objects as realized in the Monte Carlo code MCNP. The fuel elements and the control arms could be described in detail by this method as well as the beam tubes, reflectors and other structures like the cold source. Especially, the subdivision of a fuel assembly into 6x5x15 burn-up zones required a large number of cells with different burn-up dependent material compositions which could not be efficiently described by the repeated structure option of MCNP. Therefore, a program was written to generate all necessary input cards for the fuel element description. The position of the 25 fuel elements in the core and their horizontal cross section shows Fig. 2 for the MCNP model. In Fig. 3 a vertical cross section of the MCNP model is shown.

The D<sub>2</sub>O tank was represented by a cylinder with an outer diameter of 2.00 m. The lower region of the core down to the bottom of the tank accommodating the grid plate, unfueled ends and nozzle of the fuel elements, the aluminum structures and corresponding D<sub>2</sub>O were modeled in detail. In the whole geometric model the cell boundaries were specified by 1st and 2nd degree surfaces with appropriate transformation in accordance with the position of the cells in the model.

The rapid absorber rods were located in the periphery of the core and modeled in the form of a hollow cylinder with a wall thickness of 4 mm. The fine control rod was modeled in the same detail and placed in the D<sub>2</sub>O region. The beam tubes of varying diameter and length were modeled in detail and integrated in the corresponding position of the entire model in accordance with the design and construction documents.



**Fig. 2: MCNP model of core and fuel assembly of the FRJ-2 at Juelich: Horizontal cross section**

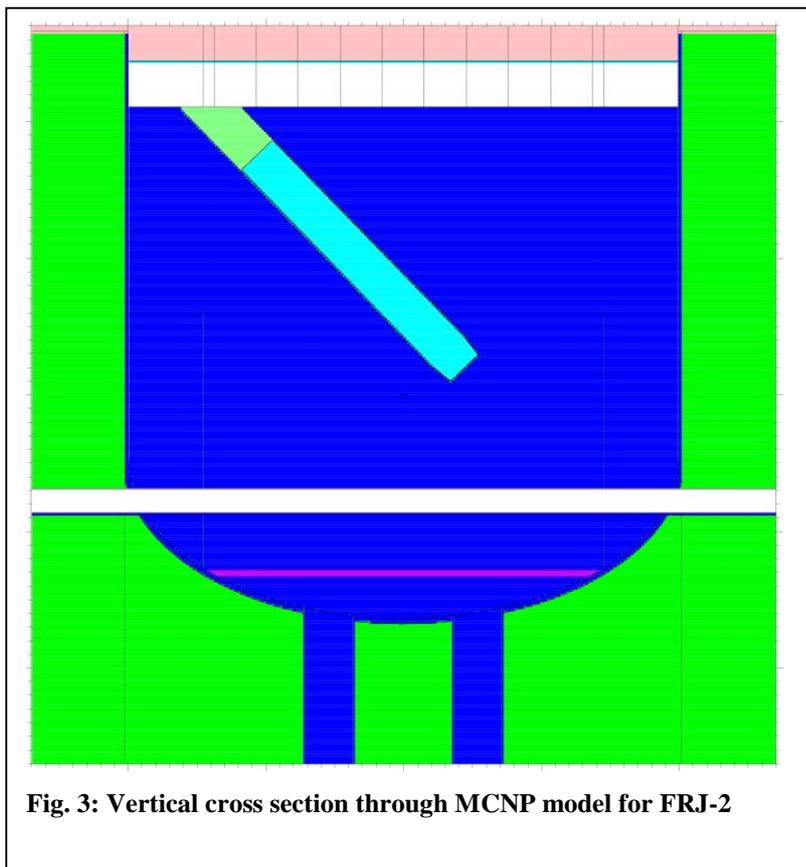


Fig. 3: Vertical cross section through MCNP model for FRJ-2

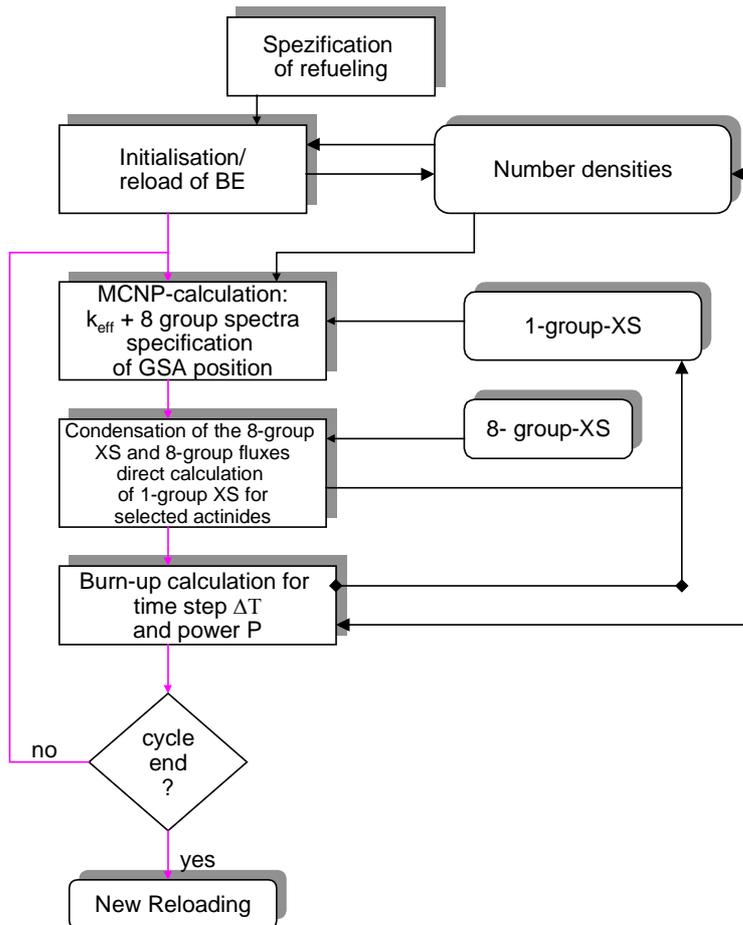
The coarse control arms were also subdivided into burn-up zones to evaluate the burn-up and the control rod efficiency as a function of irradiation time. One of the coarse control arms is shown in Fig. 3. The outer ring of the circular fuel assemblies contain boron which will be depleted during irradiation and therefore this zone was also subdivided to account for the spatial burn-up. The six coarse control arms were modeled using individual transformation cards for every arm to define easily the control rod position. The moderator and fuel temperatures were taken as constant for all zones since there was no significant local variation of these temperatures.

### burn-up model

The number densities for the nuclides of the material compositions for the MCNP model were calculated via the burn-up program BURN of the applied coupled MCNP-burn-up program system which solves the depletion equations for a reduced nuclide chain model. This model regards 20 actinides and 85 fission products. Additionally also boron as a burnable poison can be depleted. An interface between BURN and MCNP organizes the material specification for the MCNP run and prepares effective cross sections for the burn-up step from MCNP results. For fresh fuel elements the corresponding U-235, U-236 and U-238 composition are used for material composition. The fuel elements can be replaced or shuffled via a special interface program re-ordering the zone wise nuclide vectors. The cross sections for the depletion calculation are calculated from the MCNP step before the burn-up step. For the main actinides and a few important fission products the zone wise cross section were directly calculated from MCNP tallies for reaction rates and total fluxes. For the rest of actinides and fission products the cross sections for the depletion calculation were calculated from pre-determined few group cross sections (8 groups) from a MCNP calculation with an average burn-up distribution for a coarser subdivision of the fuel zones. The individual zone cross sections for the depletion step for these nuclides are calculated from few group cross fluxes for the fine subdivision of the fuel assemblies calculated from the most actual MCNP step. By this procedure the number of tallies per zone could be reduced remarkably. The flow chart of the calculation scheme is shown in Fig. 4. The flow chart for the pre-calculation of few group cross sections is shown in Fig. 5.

### 3.2 The coupled MCNP –

Since the number of burn-up cells was more than 10.000 the request on memory could be reduced by the described method so that MCNP could run on a CRAY-T3E with 512 MB memory/processor. Furthermore, the reduced number of tallies required much less communication time and dynamic memory for parallel processing and improved therefore the efficiency of the calculations. On the new parallel computer available now, the IBM p690, the memory/processor is 2GB but the communication time and the performance is still the limiting factor for effective parallel computing.



**Fig. 4: Coupled MCNP burn-up calculation**

For the calculation of a complete operating cycle of about 25 days at 20 MW power the cycle is divided in certain burn-up steps and MCNP steps respectively. After refueling a first MCNP calculation is performed for cold conditions to proof the critical control arm position after reloading. Then MCNP is run for hot conditions. For an assumed dependency of the critical control arm position as a function of cycle burn-up the control arm positions for all time steps were defined and all time steps BURN-MCNP until EOC were run. All intermediate results (number densities as a function of time step, k-eff, reaction rates etc.) are stored on an archive so that every time MCNP calculations can be performed with corresponding material compositions e. g. for other temperatures, control arm positions, other tallies for special investigations etc.

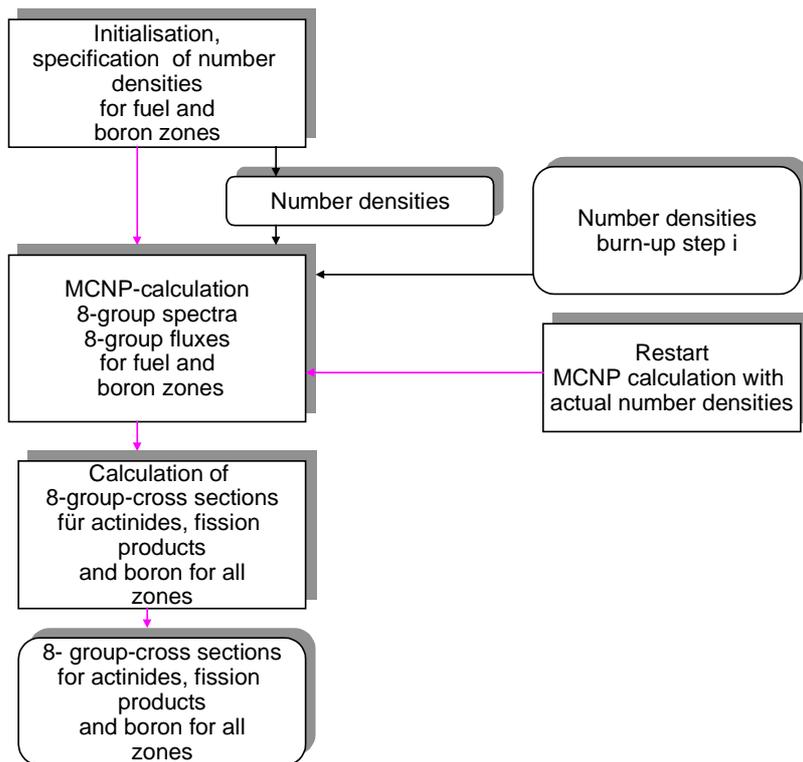


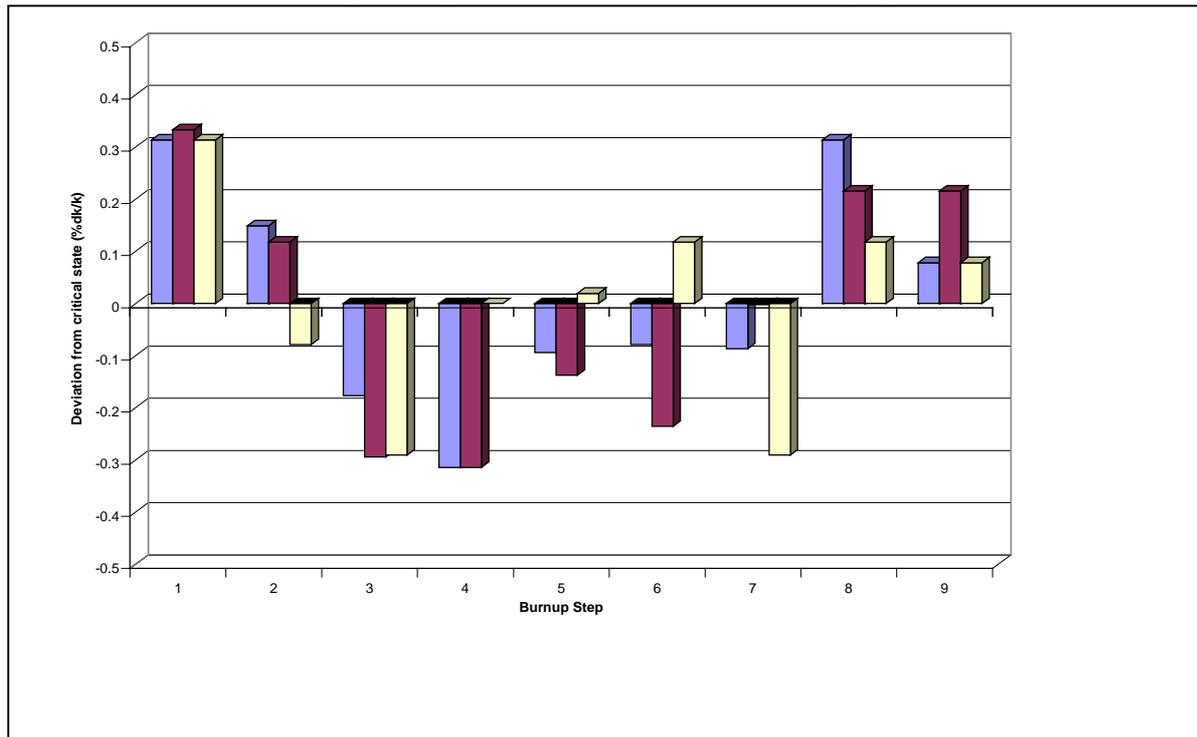
Fig. 5: Calculation flow chart for the determination of microscopic few group cross sections in depletion zones

#### 4 VALIDATION AND APPLICATION OF THE MODEL

The described model is implemented and applied for FRJ-2 since 1997. A large number of cycles were simulated since this time and many comparisons of calculations and experimental data were performed. The criticality state corresponding to the multiplication factor of the reactor core of each operating cycle will be compared with those predicted by the calculation for each irradiation step. An example of such comparisons is shown in Fig. 6 for three operating cycles. The figure shows that for the selected cycles at each burn-up step corresponding to an irradiation time the criticality state is reproduced with a precision of better than 0.3 % dk/k. The statistical error of the individual  $k_{\text{eff}}$  values of the MCNP runs is always less than 0.2 % dk/k (  $2\sigma$  confidence interval). This accuracy was achieved by simulating about  $10^6$  neutrons per MCNP run. Additionally, the calculated total burn-up values for the individual fuel elements at the end of each cycle are compared with corresponding experimental values obtained from flux measurements. For example, from foil activation (Co-60) measurements performed during the operating cycle 3 in 1999, the average neutron flux at the inner channel of the fuel elements were derived and compared with corresponding calculated values derived from MCNP results for the measuring positions of corresponding flux and reaction rate tallies. The normalized results of measurements and calculations are shown in Fig. 7. Taking into account the uncertainties of the measuring method resulting from irradiation time and positioning of the foils in the inner fuel element channels as well as the statistical error of the calculated values the agreement between measurement and calculation is really good for all positions of the fuel elements. Also

comparisons of the calculated and measured axial activation rates (Co-90 foils) for a highly rated fuel element showed very good agreement as it was shown in [3].

The experience with the coupled program system and the results achieved up to now showed that the chosen models of this system are suitable for the precise predicting of reactivity, assembly burn-up and flux values. Therefore, the program system can be used for the predicting of all necessary safety related parameters for the next cycles and for optimization calculations. It could also be used for the planning of the HEU-LEU conversion project for the FRJ-2 [4].



**Fig. 6** Difference of calculated multiplication factors from the reference value for the critical state as a function of burn-up step. Control arm positions for burn-up steps according to measurement

## 5 CONCLUSIONS

The method described allows the detailed and precise analysis of integral and differential neutronics parameter for all time steps of operating cycles of a research reactor. For the FRJ-2 this was very important since the core and the reactivity control system is very complex and not realistic describable by deterministic methods based on orthogonal grids. The detailed burn-up distributions calculated by this method requires a very large number of data which can overflow the capacity also of modern high performance computers. Therefore, a model was developed to reduce the requirement of data to a reasonable amount without significant loss of accuracy. Due to the relatively short operating time of one cycle there is a need for the fast processing of all necessary investigations and predictions for the next cycle. Since the detailed Monte Carlo model needs substantial computing time for one step a complete cycle with up to 10 steps and all subsequent MCNP calculations would require a very long turnaround time with single processor workstations. Therefore, multiprocessor computers were used for these calculations. The PVM version of MCNP-4C3 on CRAY-T3E and later on IBM-p690 has been used successfully for a

great many of MCNP-runs. The large number of tally data, however, limit the number of processors which can be efficiently used on these computers. At the CRAY-T3E therefore 32, at the IBM-p690 8-10 processors were respectively will be used to get typical running times for one MCNP calculation with  $10^6$  neutrons of about 40 to 60 minutes which is sufficiently fast for the fuel management calculations for the next cycles.

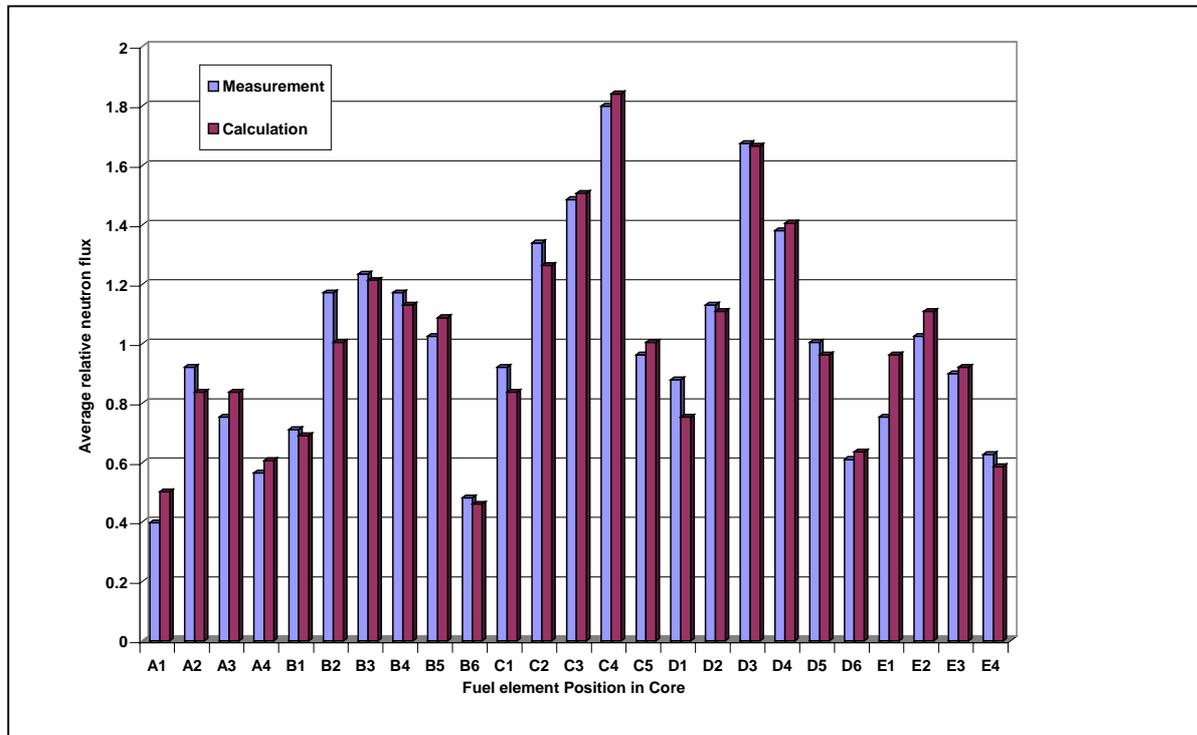


Fig. 7 Calculated and measured average neutron flux densities at the inner channel of FRJ-2 fuel elements for the core configuration 3/1999

## 6 REFERENCES

- [ 1] Nabbi, R.; Wolters, J., "Coupling MCNP and a Depletion Code for Detailed Neutronic Analysis and Optimum Core Management at the German FRJ-2 Research Reactor" *Intern. Meeting on: Math. Methods for Nuclear Applications* (Sept. 2001), Salt Lake, USA
- [ 2] J. F. Briesmeister, Editor, "MCNP -- A General Monte Carlo N-Particle Transport Code", *Los Alamos National Laboratory report LA-12625-M* (March, 1997)
- [ 3] Nabbi, R.; Wolters, J., "Investigation of Radiation Damage in the Aluminum Structures of the German FRJ-2 Research Reactor". 2000 Int. Meeting on Reduced Enrichment for Research and Test Reactors, Las Vegas, Nevada, October 1-6, 2000
- [ 4] Nabbi, R.; Thamm, G. Wolters, J., "A Sophisticated Computational Method for HEU-LEU Conversion of the German FRJ-2 Research Reactor Using MCNP". 2000 RERTR meeting, Las Vegas, Nevada, USA, 1-6 October, 2000