Comparison of PWR – Pin Cell burnup calculations with SCALE 5.0/TRITON – KAPROS/KARBUS - MONTEBURNS

Ph.Oberle, C.H.M.Broeders, R.Dagan
Forschungszentrum Karlsruhe, Institut für Reaktorsicherheit
Hermann-von-Helmholtz-Platz-1, 76344 Eggenstein-Leopoldshafen
oberle@irs.fzk.de

1. Introduction

The fuel unit cell is the basic portion of a nuclear reactor studied in reactor analysis. It consists of a single fuel rod, its cladding and its representative surrounding coolant. Fuel assemblies which are clusters of single fuel cells are regarded as the basic components of reactor calculations.

One of the common ways to generate relevant data for a subassembly is based on one dimensional cylindrized Wigner-Seitz unit cells while preserving the unit cell volume of the original square or hexagonal array. The KAPROS system [1] uses this approach utilising the collision probability methods. Such methods allow neutron probability transfer from each mesh to all other meshes defined within the unit cell.

Another more complex but also more accurate way is to represent the geometry of the unit cell with a flexible cell structure to give a better approximation of both rectangular and curved geometries inside the unit cell. Such a geometric solution was established in the new transport program NEWT which is part of SCALE 5.0/TRITON [2]. NEWT uses the *Extended Step Characteristic Method* in which the neutron probability transfer is constrained to the governing characteristic line.

This study evaluates the two methods by means of a single pin cell burnup calculation. Both deterministic codes are also compared to the MONTEBURNS [6] system which couples Monte Carlo code (MCNP) with the burnup code ORIGEN. Furthermore the sensitivity to the cross section libraries including its fission energy release is discussed.

2. Short description of the transport calculation methods in SCALE5.0/TRITON/NEWT, KAPROS/KARBUS and MONTEBURNS

The Extended Step Characteristic (ESC) method is based on the Step Characteristic method (SC). In both methods the average fluxes on the sides of the cells have to be determined to calculate cell-averaged fluxes. That's made possible by deriving analytical solutions for the angular flux on unknown sides based on known fluxes on the remaining sides. In contrary to the ESC method the SC method only deals with orthogonal four sided grid meshes. The mathematical solution of the step characteristic method of the Boltzmann transport equation does not restrict to a particular geometry [3] and therefore it is possible to use arbitrary geometry cells. The only need is that the geometrical relationships between the sides of these arbitrary cells must be known.

While conventional discrete ordinate codes only can handle regular geometries like (R,Z), (X,Y), (X,Y,Z), (R,θ,Z), SCALE 5.0/TRITON/NEWT which applies the ESC method, can perform a completely arbitrary problem grid by using a polygon grid structure instead of an orthogonal grid structure. The number of polygons in a geometric problem is not limited.

A simple discrete ordinate method is used in KARBUS. KARBUS applies the First Collision Probability (FCP) Method (Bonalumi Method [4]). The problem geometry in the FCP method is represented by a structured grid which only provides a single geometrical shape of grid meshes. In the Wigner-Seitz cell calculation in KARBUS the appropriated geometrical form of the meshes to represent the geometrical problem are rings. The advantage of the FCP

method applied in KAPROS/KARBUS in contrary to the ESC method applied in SCALE5.0/TRITON/NEWT is that in the FCP method a neutron can move from each mesh into every mesh while in the ESC method a neutron can only move from one mesh to a second mesh if these meshes are lying along a certain characteristic line.
In the depletion code MONTEBURNS the transport calculations are performed by the Monte Carlo code MCNP4C.

3. Specifications of the test problem

The pin cell configurations have been taken from the specification of a modern 18x18-24 UO_2 PWR-assembly [5]. The material composition in the fuel is UO_2 with 4 w/o enrichment of U-235. The clad consist of Zircaloy-4. The boron concentration in the moderator (water) stays constant along the burnup calculation at 500 ppm. In figure 1 both pin cells of the deterministic codes are shown. In the KAPROS/KARBUS model the pin cell is divided into 16 fuel meshes, 3 clad meshes and 4 moderator meshes to a total of 23 cylindrical meshes (not all meshes are indicated in the KAPROS/KARBUS pin cell in figure 1).
In SCALE5.0/TRITON/NEWT the pin cell is divided into 9 zones, 8 consisting of 3 polygonal meshes each (one mesh for each material) and one zone consisting of one mesh (the middle fuel zone) to a total of 25 meshes.
In MONTEBURNS the pin cell was approximated by 3 cylindrical zones (fuel, clad, moderator).

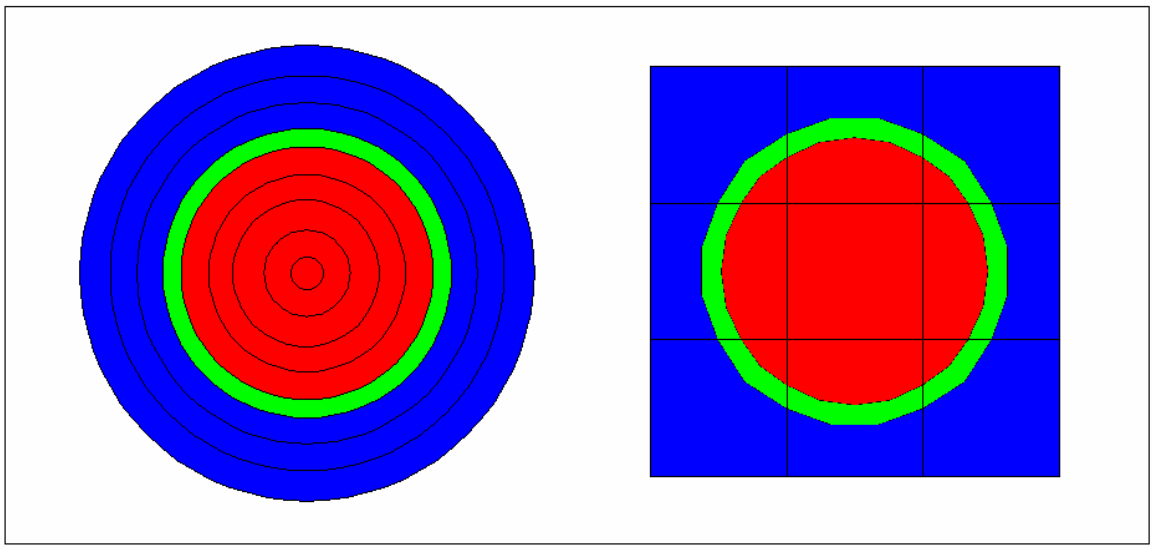

Figure 1: Basic pin cell meshes used in KARBUS (left) and NEWT (right)

In both deterministic codes the radial boundary conditions were specified as reflective, so the problem can be seen as infinite in radial direction. The length of the pin is about 390 cm. In SCALE 5.0/TRITON/NEWT an axial buckling correction is performed to calculate leakage normal to the plane of the 2-D model. In KAPROS/KARBUS no treatment of axial leakage is taken into account. Both deterministic calculations have been performed with S_n order 8 and a convergence criterion of 10^{-5} for k_{inf}. The cross section libraries used are basically ENDF/B 5 in the SCALE 5.0/TRITON and the MONTEBURNS calculation and ENDF/B 6.5 in the KAPROS/KARBUS calculation. For three calculations average fission energy of 200 MeV was applied. An extra KAPROS/KARBUS calculation with an average fission energy of 208 MeV was performed to investigate the influence of fission energy to burnup.

4. Results

The two deterministic calculations were performed up to a burnup of 80 MWD/kg HM. The Monte Carlo calculation with MONTEBURNS was progressed up to 60 MWD/kg HM. Figure 2 shows the comparison of k_{inf} as function of burnup for the four cases. The two KAPROS/KARBUS curves are nearly identical in this representation.

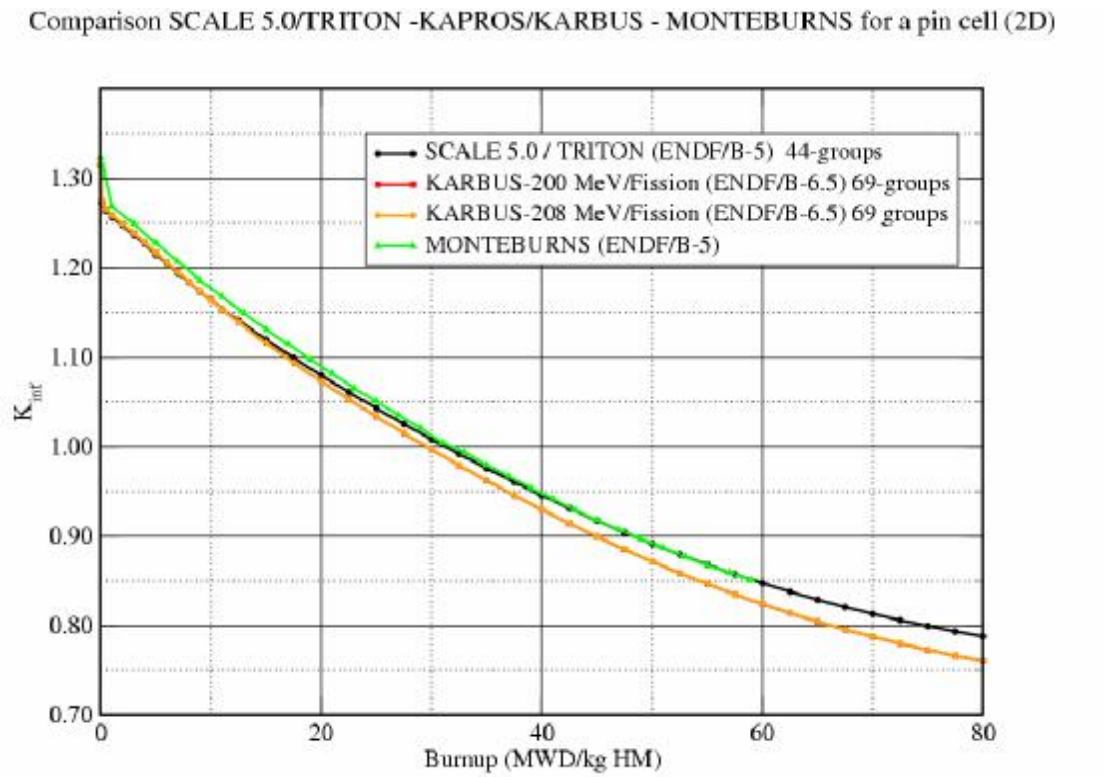

Figure 2: K_{inf} as function of burnup in MWD/kg HM, for four pin cell calculations

Both deterministic codes show a very good agreement up to 20 MWD/kg HM burnup. Over the total burnup range figure 2 shows that the SCALE 5.0/TRITON curve is flatter than the KAPROS/KARBUS curve while the MONTEBURNS curve converges towards the SCALE5.0/TRITON curve. In figure 3 the differences of k_{inf} for the four burnup calculations are shown. The standard deviation of the MONTEBURNS/MCNP calculations was $3*10^{-4}$.
At zero burnup k_{inf} determined by KAPROS/KARBUS differs compared to MONTEBURNS/MCNP by 0,6% while SCALE5.0/TRITON/NEWT differs from MONTEBURNS/MCNP by 0,7%. At ≈ 60 MWD/kg HM burnup k_{inf} of SCALE5.0/TRITON and MONTEBURNS differs only 0,1%. The two KAPROS/KARBUS calculations, with different energy per fission release, do not show any difference in figure 2. The maximum deviation in the plot of differences in figure 3 is about 0,42%.

5. Summary and outlook

Systematic comparisons of burnup calculation methods have been started for a PWR burnup benchmark proposed by GRS. Two deterministic codes, KAPROS/KARBUS developed at Forschungszentrum Karlsruhe and TRITON/NEWT a new option in the SCALE 5.0 standard code for LWR licensing, have been compared with the MONTEBURNS Monte Carlo based code system. Despite the applied different data library bases ENDF/B-5 and ENDF/B-6.5 reasonable agreement for the reactivity loss due to burnup may be observed. The systematic deviations need further analyses. For this purpose additional burnup calculations with the Monte Carlo codes MCB and MCNPX will be applied and nuclear data sensitivities will be

analysed. Further comparisons of the different codes and data with a PWR burnup experiment at the Obrigheim reactor (ICE experiment [7]) will be performed.

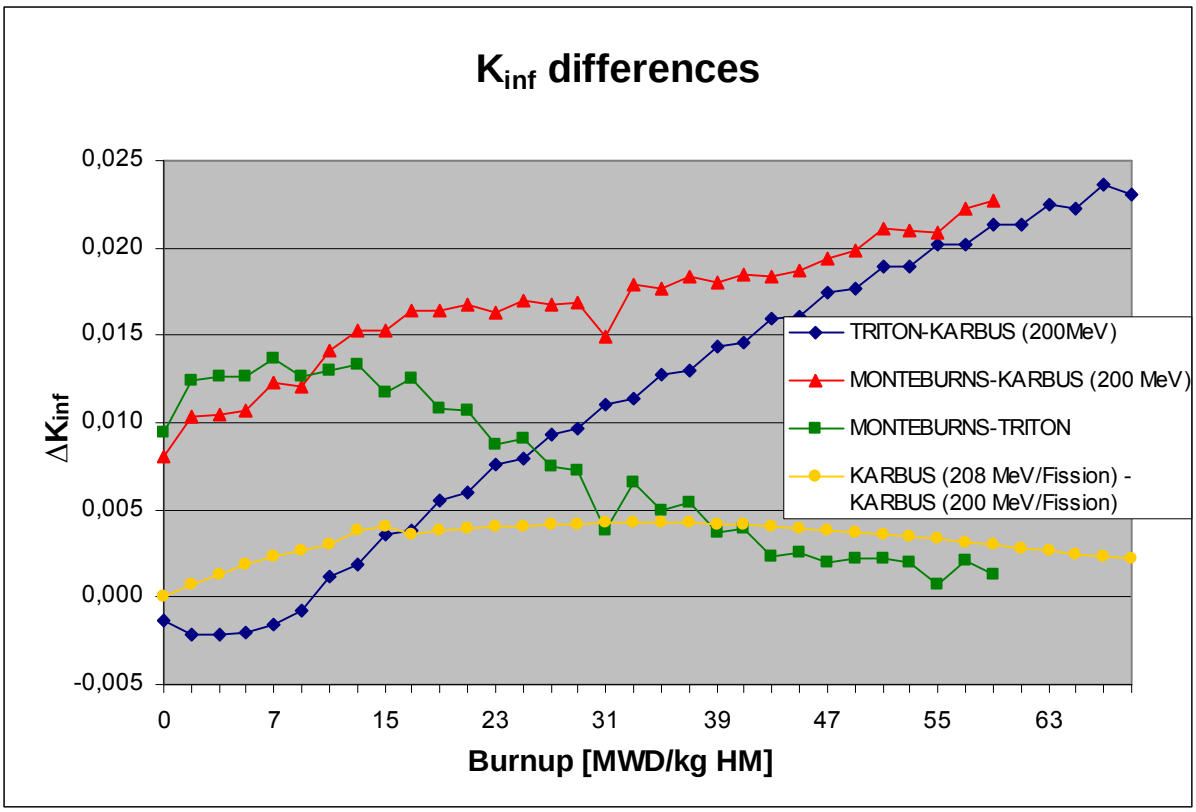

Figure 3: ΔK_{inf} of the four results from SCALE5.0/TRITON, KAPROS/KARBUS and MONTEBURNS

6. References

[1] C.H.M. Broeders, „Entwicklungsarbeiten für die neutronenphysikalische Auslegung von fortschrittlichen Druckwassereaktoren (FDWR) mit kompakten Dreiecksgittern in hexagonalen Brennelementen“, KFK 5072, 1992

[2] “SCALE: A Modular Code System for Performing Standardized Computer Analyses for Licensing Evaluation”, ORNL/TM-2005/39, Version 5, Vols. I-III, April 2005

[3] M.D. DeHart, R.E. Pevey, T.A. Parish, “An Extended Step Characteristic Method for Solving the Transport Equation in General Geometries”, Nuclear Science and Engineering, 118, 79-90, 1994

[4] Bonalumi, R., “Neutron first collision probabilities in reactor physics”, Energia Nucleare, 8, 326, 1961

[5] D. Porsch, at al; „Spezifikationen eines DWR-Brennelementes, UO_2 (4 w/o U-235) 18x18 – 24, für Vergleichsrechnungen“, Framatome ANP GmbH Erlangen Juli, 2004

[6] D.I. Poston, H.R. Trellue,“User´s Manuel, Version 2.0 for MONTEBURNS, Version 1.0“, LA-UR-99-4999, September 1999

[7] L. Koch, S. Schoof,”The Isotope Correlation Experiment ICE”, ESARDA 2/81, EUR 7766 EN, KfK 3337 (1981)