Solution of the Stationary State of the PWR MOX/UO_2 Core Transient Benchmark

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Abstract

The multi-group Discrete Ordinates transport code DORT is applied to solve the stationary state of the OECD/NEA PWR MOX/UO_2 Core Transient Benchmark. Pin cell homogenised cross sections in 16 energy groups and P_1 scattering order have been obtained by fuel assembly burn-up calculations using HELIOS. In this paper, we report on the details of our calculations for this benchmark problem and show our results to be in good agreement with an MCNP Monte Carlo solution with nuclear point data and a multi-group DeCART Method of Characteristics solution.

KEYWORDS: Discrete Ordinates, S_N, DORT, Monte Carlo, MCNP, PWR, MOX, Benchmark

1. Introduction

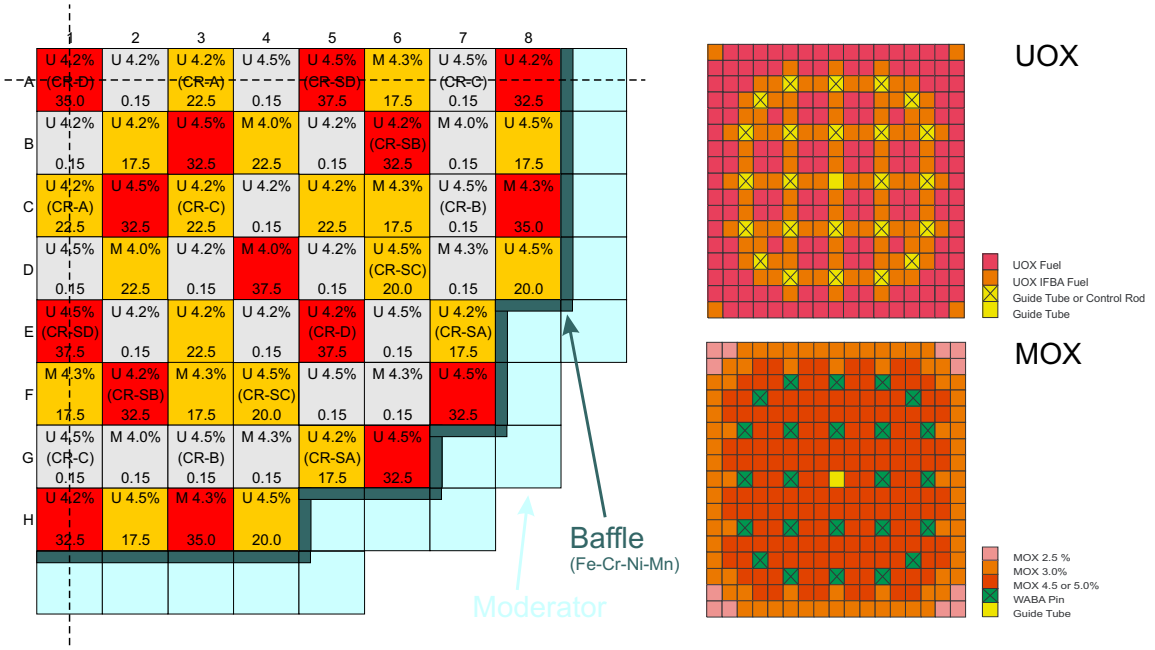
The simulation methods for nuclear design and accident analyses have reached a high level of accuracy and reliability. The code systems, consisting of neutronics models which are also coupled with thermal-hydraulic codes, however, need continuous improvements in order to meet increasingly stringent current and future safety requirements. At the same time, optimisations of the fuel strategy for light water reactors (LWR) are becoming more relevant. The use of improved fuel may also be associated with optimised core loadings to enhance the fuel economics and to reduce the fluence at the pressure vessel. The safety evaluation of such new conditions requires improved and validated analytical methods as well as appropriate computational benchmarks that serve as a means of verifying the numerical solutions obtained with different code systems and nuclear data libraries.

The *PWR MOX/UO_2 Core Transient Benchmark* is an example of the validation of codes and data for the operation of a whole PWR core partially loaded with MOX fuel. In this paper, we report on our solutions of the stationary part of this benchmark obtained with the Discrete Ordinates code DORT using pincell homogenised few-group data and, for comparison, with the Monte Carlo code MCNP using nuclear point data.

2. The OECD/NEA and U.S. NRC PWR MOX/UO_2 Core Benchmark

The PWR MOX/UO_2 Core Transient Benchmark [1] has been designed at the Purdue University under the auspices of the OECD/NEA Working Party on the Physics of Plutonium Fuels and Innovative Fuel Cycles (WPPR) and the U.S. NRC. Its purpose is to assess the ability of modern reactor kinetics codes to simulate a control rod ejection transient of a core partially

Figure 1: Core configuration (left) and fuel assembly layout for the UO_2 (upper right) and MOX (lower right) assembly. In the core configuration, CR-A to CR-D denote four different control rod banks, and CR-SA to CR-SD refer to the four shutdown rod banks. The control rod ejection occurs in assembly E5. Reflective boundary conditions apply along the dashed lines.



loaded with MOX fuel. In order to allow for a realistic simulation, the problem chosen for this benchmark represents a four-loop Westinghouse PWR core with a 30% MOX fuel loading.

The fuel assembly arrangement of one quarter of the core is shown on the left hand side of Figure 1. The core has 90° rotational symmetry and contains UO_2 and MOX fuel assemblies (in total 193) with different enrichments and at several burn-up levels. The enrichments are 4.2% and 4.5% for UO_2, and for the MOX fuel, the Pu_{fiss} content is 4.0% and 4.3%. Up to seven burn-up states are taken into account, ranging from 0.15 GWd/tHM to 35.0 GWd/tHM.

The core is surrounded by a single row of reflector assemblies of the same width as the fuel assembly containing a 2.52 cm thick baffle. The outer radial boundary condition is vacuum. Each assembly consists of a 17×17 square pin cell lattice as shown on the right hand side of Figure 1. The pin cell pitch equals 1.26 cm corresponding to an assembly width of 21.42 cm. In addition to the conventional fuel and control rod/guide tube pin cells, the UO_2 assemblies also contain 104 *Integrated Fuel Burnable Absorber (IFBA)* pins. Located at the highest worth regions in the vicinity of the guide tubes, their purpose is to compensate for excess reactivity of the fresh fuel. This is achieved by a thin coating of ZrB_2 on the fuel pellet. For the MOX assemblies, 24 *Wet Annular Burnable Absorber (WABA)* pins have a similar purpose. They are located at the guide tube positions and consist of annular pellets of Al_2O_3-B_4C with water-filled central Zircaloy claddings.

The benchmark consists of a stationary and a transient part simulating the control rod ejection. In this paper, we consider the "All Rods Out" (ARO) stationary state for which the effective multiplication constant (k_{eff}) is to be determined for a two-dimensional representation of the core. In addition, the assembly-wise power distribution of the whole core and the pin-wise power distribution of the fuel assemblies along the diagonal of the core (A1, B2, ..., F6 in Fig-

ure 1) are also requested. The thermal-hydraulic conditions of the stationary state correspond to the Hot Zero Power (HZP) state, specified by a core temperature $T_{core} = 560\ K$, a moderator density $\rho_{mod} = 752.06\ kg/m^3$ and a soluble Boron concentration of $SB = 1000\ ppm$.

3. Calculational Details

The eigenvalue and flux calculations of the specified ARO core state were performed using the S_N code DORT 3.2 [2] as distributed by the OECD/NEA Data Bank. DORT is a module of the DOORS code system and solves the 2-D stationary Boltzmann transport equation in Discrete Ordinates representation for an arbitrary number of energy groups in both Cartesian and curvilinear regular geometries. Anisotropic scattering is treated using a Legendre scattering cross section expansion.

For all materials and burnup levels, pin cell homogenised group constants in 8 energy groups and P_0 scattering order have been provided on the benchmark web site. However, we found that considering only isotropic scattering does not yield the correct solution. Therefore, we performed own burnup calculations for all four UO_2 and MOX fuel assemblies using the 2-D cell and depletion code HELIOS 1.8 [3] for generating pin cell homogenised cross sections in 16 energy groups and P_1 scattering expansion. The burn-up calculation is based on the nuclide inventory of the fresh state of the different Uranium and MOX fuels as given in the benchmark specification. The specific power (W/g initial heavy isotopes) was estimated from the specified thermal reactor power level, the number of fuel rods and an average fuel density of 10.3 g/cm^3 to be 37.87 W/g. The condensation of the cross sections to 16 energy groups is based on the HELIOS 190 energy group data library. The lower energy limits of this 16 energy group structure are listet in Table 1.

Table 1: Lower energy limits of the 16 energy group structure used in the HELIOS calculation.

Group index	Lower energy limit	Group index	Lower energy limit	Group index	Lower energy limit	Group index	Lower energy limit
1	3.6788 MeV	5	9.1188 keV	9	29.023 eV	13	625.06 meV
2	2.2313 MeV	6	2.0347 keV	10	12.099 eV	14	270.52 meV
3	820.85 keV	7	130.07 eV	11	3.9279 eV	15	56.922 meV
4	67.379 keV	8	78.893 eV	12	1.0137 eV	16	$1.0 \cdot 10^{-4}$ eV

For the baffle alloy, this library contains data for isotropic scattering only. Since the use of P_0 scattering cross sections turned out to be inadequate for a sufficiently accurate treatment of the baffle, a set of cross sections containing P_1 matrices was generated for the baffle material composition. This was done with the collision probability code RESMOD [4] by performing a spectral calculation for a single pin cell with a JEF-2 based nuclear data library with 292 energy groups and a hyperfine representation of the resolved resonance region.

Using these pin cell homogenised cross sections, the DORT calculation was performed for one quarter of the core in Cartesian geometry. Each pin cell is divided into 2×2 meshes which results in 289×289 meshes in $x - y$ plane with the mesh size equal to half a pitch, i.e. 0.63 cm. Concerning the angular discretisation, we used the level-symmetric quadrature

sets S_4, S_8 and S_{16} as supplied with DORT. Not counting the zero-weight angles that are necessary in cylindrical geometry, they comprise 12, 40 and 144 discrete angular directions in two spatial dimensions, respectively.

In addition to our DORT solution for the ARO reactor state, we also performed an MCNP-4C [5] calculation with nuclear point data based on JEF-2.2. About 200 million histories have been sampled in the MCNP calculation. The corresponding nuclide inventories for the various burnup states were also provided by HELIOS.

4. Results and discussion

According to the benchmark specification, the objectives are to calculate the eigenvalue k_{eff}, the assembly-wise power distribution of the whole core and the pin-power distrubution of selected fuel assemblies along the diagonal of the core. The effective multiplication factors of our DORT and MCNP solution are listed in Table 2 and compared with the eigenvalue of a multi-group Method of Characteristics solution obtained by the DeCART code. The latter has been made available on the benchmark website [1] and was prepared using transport-corrected P_0 scattering order cross sections in 47 energy groups with no homogenisation at the level of pin cells. The group parameters have been generated in HELIOS fuel assembly burnup calculations.

Table 2: Effective multiplication constants (k_{eff}) of pin-by-pin calculations for the ARO reactor state of the PWR MOX/UO_2 benchmark: DORT with 16-group cross sections (P_1 scattering order) and S_4 quadrature order, MCNP-4C with JEF-2.2 nuclear point data and DeCART with 47-group cross sections (transport-corrected P_0 scattering order).

Code	DORT	MCNP	DeCART
k_{eff}	1.06036	1.06065 ± 0.00005	1.05852

The eigenvalues compare very well with each other. Test calculations with S_4, S_8 and S_{16} quadratures reveal that there is almost no dependence on the quadrature order used in DORT, i.e. even S_4 quadrature order turns out to be sufficient, thereby significantly saving CPU time which amounts to about 1 hour on a conventional workstation.

Similarly good agreement has been found concerning local quantities. This is shown for the normalised assembly-wise power distribution of the whole core that has been obtained from the DORT S_4-P_1 calculation and is depicted on the left of Figure 2. It is characterised by its maximum close to the core center and a very steep gradient towards the core boundary which can be attributed to the presence of the peripheral ring of almost fresh (0.15 GWd/tHM) fuel assemblies (see Figure 1). As shown in the two graphs on the right hand side of Figure 2, the DORT distribution compares well with the DeCART and our MCNP solution: Regarding the comparison with DeCART, the relative deviations are of the order of at most 1...2%, with a minimum of -2.2% and a maximum of $+1.9$% occuring only for very few assemblies. This also applies to the pin-wise power distribution within individual fuel assemblies. For the six assemblies along the core diagonal (A1, B2, ..., F6 in Figure 1) that were evaluated according to the benchmark specification, the typical differences of the pin-wise power distribution with respect to DeCART are of the same order as for the assembly-wise distribution: The differences range from -1.4% to $+0.9$%, and again the minimum and maximum values are observed only

Figure 2: Left: Normalised whole core assembly power distribution of the ARO reactor state obtained from the DORT S_4-P_1 calculation using pin cell homogenised 16-group cross sections in P_1 scattering order. Right: Relative deviations of this distribution with respect to the DeCART 47-group and our MCNP nuclear point data solution.

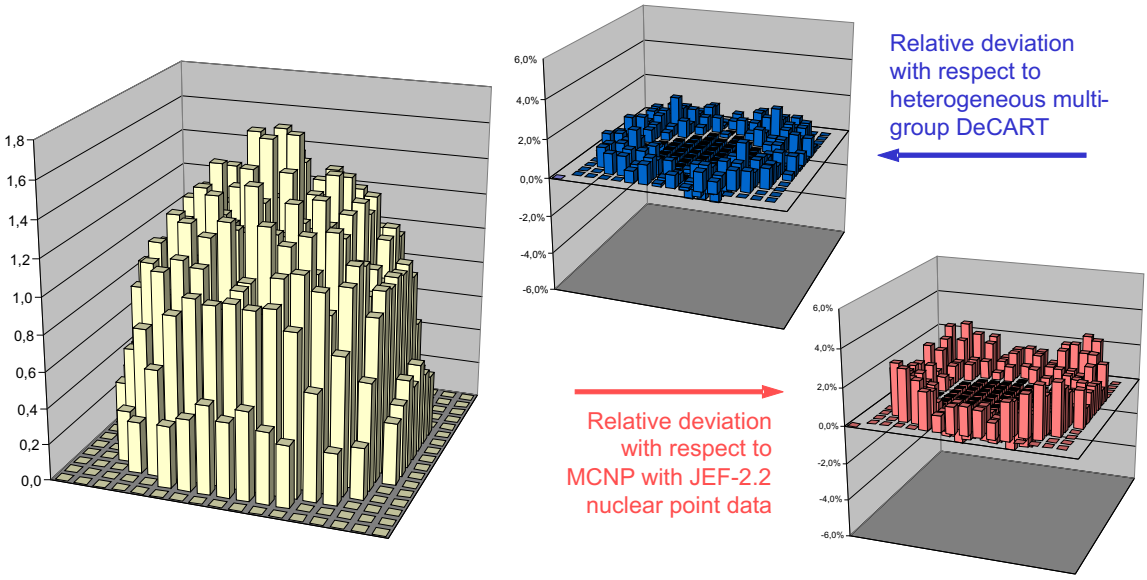
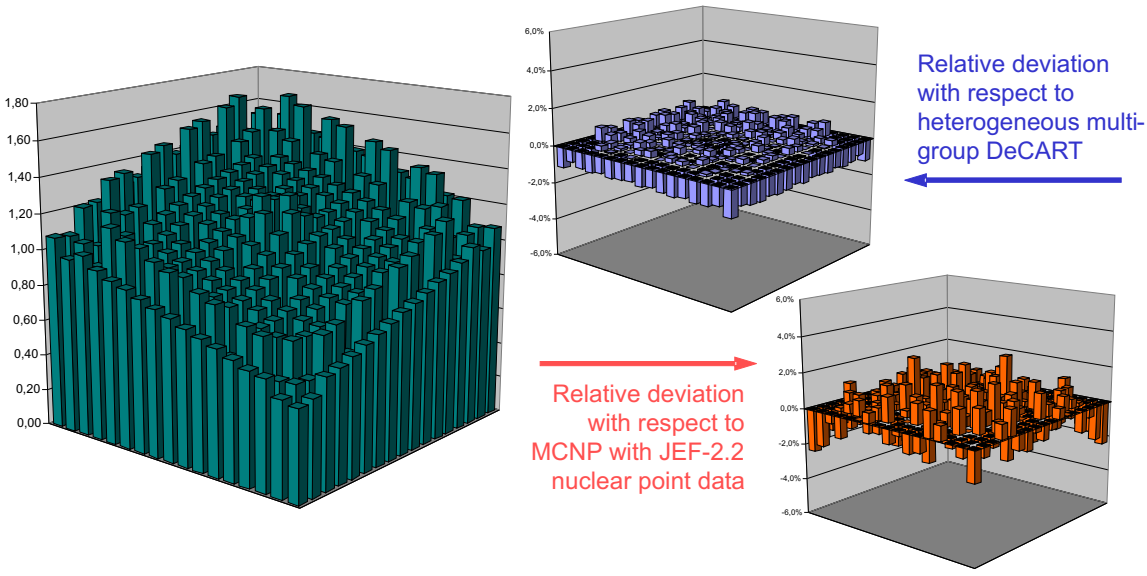


Figure 3: Left: Normalised pin-wise power distribution of assembly F6 of the ARO reactor state obtained from the DORT S_4-P_1 calculation using pin cell homogenised 16-group cross sections in P_1 scattering order. Right: Relative deviations of this distribution with respect to the DeCART 47-group and our MCNP nuclear point data solution.



for few pin cells. A similarly good agreement has been found when the DORT solution is compared with the MCNP result: The relative deviations in the assembly-wise power distribution range from -1.6% to $+2.7\%$. For the pin power distribution of the peripheral fuel assembly, the differences are slightly higher (the minimum of -3.9% and the maximum of $+3.4\%$ is encountered only for few pin cells) than between DORT and DeCART; this may be attributed to the statistical nature of the Monte Carlo method. This is shown in Figure 2 which displays pin power distribution and relative differences for the peripheral fuel assembly (F6) in a representation analogous to Figure 1. We found an appropriate treatment of the baffle alloy to be crucial for obtaining the correct power distribution: Test calculations have shown that describing the baffle material by only isotropic scattering cross sections in an otherwise unchanged DORT S_4 P_1 calculation causes the deviations in the power distribution to rise to up to 4%, in particular at the core boundary.

5. Summary and Conclusion

In this paper, we present our solutions of the stationary *All Rods Out* state of the PWR MOX/UO_2 Core Transient Benchmark that have been obtained by the multi-group Discrete Ordinates (S_N) transport code DORT and the Monte Carlo code MCNP. Fuel assembly burnup calculations have been performed using the 2-D cell and depletion code HELIOS in oder to generate few-group constants including P_1 scattering order. Separate treatment of the baffle alloy was necessary because for the baffle materials, the HELIOS library only accounts for isotropic scattering. This has been done by a spectral calculation for an individual pin cell using the collision probability code RESMOD. The burnup-dependent macroscopic cross sections have been homogenised over individual pin cells and condensated to 16 energy groups. The MCNP Monte Carlo solution is based on an exact geometric representation of the core and JEF-2.2 nuclear point data. Both the DORT and MCNP solution are compared to the results of a Method of Characteristics DeCART calculation based on a 47 energy groups set of transport-corrected P_0 scattering cross sections with no homogenisation at the level of pin cells. Very good agreement is obtained between the solutions, both with respect to integral and local quantities, i.e. the multiplication constants, the fuel assembly wise power distributions and the pin wise power distributions of selected fuel assemblies.

The good experiences with the application of DORT to this benchmark demonstrate that few-group deterministic transport methods using cell-homogenised nuclear group data are capable of accurately modelling static MOX cores. This has been demonstrated by comparing the DORT result with high-resolution calculations. It is found that the accuracy of the DORT solution is comparable to the results obtained with the multi-group Method of Characteristics or the Monte Carlo method. In addition, the few-group S_N method significantly saves CPU time, in particular with respect to MCNP.

Acknowledgements

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