Spectral Codes Pin Power Prediction Comparison

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ABSTRACT

Spectral codes are able to produce burnup dependent fuel assembly homogenized neutron cross sections and pin power form factors. Both information are used by diffusion nodal codes to produce fuel assembly powers and intra assembly power distributions. 2D transport codes are usually used for this type of the calculation. Four spectral codes (DRAGON 4, FA2D, NEWT and PSG2/Serpent) were used to calculate pin power distribution for reflected single fuel assemblies during depletion. The NPP Krško 16×16 fuel assemblies without and with IFBAs, for two U-235 enrichments 4.4% and 4.8%, as found in cycle 24 of the plant, were modeled. The heterogeneous depletion calculation was performed up to burnup of 60 GWd/tU. The prediction capabilities of the codes are compared for infinite multiplication factor, and for 2D pin power form factors.

1 INTRODUCTION

Nodal neutron diffusion codes rely, in their pin powers predictions, on data pre-calculated on fuel assembly basis using 2D transport codes. That is true for both, steady state (design and in-core fuel management) and transient, core pin power distribution. Besides the assumptions used during pin power reconstruction, final results depend on the accuracy of performed 2D transport depletion calculation. In the paper different 2D spectral codes were used to calculate pin power distribution for reflected single fuel assemblies during depletion. The assemblies are NPP Krško 16×16 fuel assemblies without and with IFBAs, for two U-235 enrichments 4.4% and 4.8%, as found in cycle 24 of the plant. The heterogeneous depletion calculation was performed up to burnup of 60 GWd/tU. Four spectral codes were used:

DRAGON (Version 4.03 was used) is neutron transport (collision probabilities and method of characteristics) code for calculation of pin cells and fuel assemblies developed at Institut de Genie Nucleaire Ecole Polytechnique de Montreal [1],

FA2D is 2D transport collision probability code developed at Faculty of Electrical Engineering and Computing, University Zagreb,

NEWT (as found in SCALE 6.0) is discrete ordinates transport code developed at Oak Ridge National Laboratory [2] and [3], and

PSG2/Serpent (ver 1.13) is a three-dimensional continuous-energy Monte Carlo reactor physics burnup calculation code, specialized in two-dimensional lattice physics calculations, developed at VTT Technical Research Centre of Finland [4].

The prediction capabilities of the codes are compared for infinite multiplication factor, and for 2D pin power form factors.
In this paper four codes, FA2D, DRAGON 4, NEWT, and PSG2/Serpent were used to perform fuel assembly calculations for selected configurations found in NPP Krško cycle 24. Both, DRAGON and NEWT are well known codes and FA2D was already verified, to some extent, by performing available benchmark calculations [5], internal comparisons in frame of IRIS project [6], and by comparison with NPP Krško design data [7]. Serpent is rather new code, still under development, but is unique being Monte Carlo code dedicated to group cross section calculation. In this paper, as part of continuous verification of different FA2D parts, the comparison is performed for assembly pin-power distributions (indicate intra-assembly flux distribution). As a part of the comparison effective multiplication factors ($k_{\text{eff}}$), and spectral ratios are provided too.

2 FUEL ASSEMBLY TRANSPORT CALCULATION

2.1 Calculational tools

The computer code DRAGON (in this paper version 4.03 was used) contains a collection of models which can simulate the neutronic behavior of a unit cell or a fuel assembly in a nuclear reactor. It performs required interpolation of microscopic cross sections supplied in one of supported formats, resonance self-shielding calculations in multidimensional geometries, multigroup and multidimensional neutron flux calculations which can take into account neutron leakage, transport-transport or transport-diffusion equivalence calculations as well as editing of condensed and homogenized nuclear properties for reactor calculations, and finally it is able to perform isotopic depletion calculations. The code has modular structure with different algorithms being available for both self-shielding calculations and 2D and 3D transport calculation. In this paper EXCELL option which solves the integral transport equation using the collision probability method for general 2D geometries was used. User may select two different types of libraries, 69-group WLUP libraries (the libraries based on ENDF/B-VI.8, ENDF/B-VII, JEF-2.2, JEFF-3.1 and recommended IAEA library are available) or 172-group libraries in DRAGLIB format (the libraries based on ENDF/B-VI.8, ENDF/B-VII, JEF-2.2, JEFF-3.1 are available). In the paper only WLUP based libraries are used due to rather large differences experienced with DRAGLIBs when compared to FA2D and NEWT. DRAGON uses relatively flexible command language to describe calculational set-up and used methods within input file. DRAGON is able to prepare a reactor cross section databases for a full core calculations using code DONJON. In many aspects DRAGON can be mentioned as state-of-the-art, and still freely available code in the category of spectral codes.

FA2D is a lattice burnup code that performs neutron flux and eigenvalue calculations in two dimensions, and solves multi-group neutron transport equation using method of collision probabilities (CP). FA2D was developed mainly at FER, but some elements and ideas from ORNL arbitrary geometric package MARSLIB were used in implementation of geometric capability of FA2D. Linear and curvilinear surfaces can be represented by the combination of primitive geometry elements. Flux calculations are performed using heterogenous geometry and reflective conditions at outside boundary. Input cross section library has 97-group energy structure and it is obtained using NJOY and ENDF/B-VI data. The code performs self-shielding calculations using collision probabilities obtained in ray-tracing algorithm. The self-shielding factors are determined separately for all resonance absorber materials – fuel materials, burnable absorbers materials, and burnable poison materials. FA2D performs a fundamental mode calculation to account for the effects of neutron leakage. The leakage spectrum data are then used to calculate nuclide reaction rates and to perform isotopic depletions. Depletion cases may use any condensed group structure, including the one from microgroup library. The fuel depletion chain consists over 200
nuclides, and isotopic depletion calculations were performed for each material region containing burnable material. The integration is performed using predictor-corrector method.

FA2D calculation flow is similar to any other used in spectral codes and it is shown in Figure 1. The separate calculational procedure was developed at FER to prepare a reactor cross section libraries for a full core calculations (both depletion multi-cycle analyses and transient calculations) using code PARCS [8].

![Diagram of typical calculation flow path of the spectral code (FA2D case)](image)

NEWT (New ESC-based Weighting Transport code) is two-dimensional multi-group transport code. The code solves neutron transport equation on cell level, or fuel assembly level, using discrete-ordinates method. As standalone module NEWT can be used for $k_{\text{eff}}$, critical buckling, B1, source calculations, and for cross sections collapsing. Algorithm for transport equation solving is based on Extended-Step Characteristic (ESC) method over triangular calculational mesh. The two essential assumption of the ESC method are that:

1. within each computation cell all properties (i.e. total macroscopic cross section and neutron source) are uniform,
2. cell boundaries are defined by straight lines.
NEWT with a SCALE control module TRITON and point-depletion code ORIGEN-S provides two-dimensional depletion calculations. TRITON performs iterative calls between NEWT, ORIGEN-S and cross section preparation and processing codes. Burnup-dependent cross sections calculated by NEWT are utilized to update ORIGEN-S library. TRITON uses a predictor-corrector method for fuel assembly and pin cell burnup, and branch-point calculations. Obtained results (homogenized cross sections and their derivations, ADFs, etc) in different burnup points can be used for global reactor calculations (the interface to prepare PARCS TREE libraries exists). The calculational sequence can use ENDFB 6.8 or ENDFB 7.0 based 238-groups libraries.

PSG2/Serpent is a continuous-energy Monte Carlo reactor physics burnup calculation code. The code is designed for two-dimensional lattice physics calculations, but geometry is not restricted to 2D. Burnup calculation capability enables Serpent to perform fuel depletion as stand-alone application. Optimized calculation routines of Serpent code allow detail fuel assembly burnup calculations within a reasonable calculation time. The code can use ENDF/B-VI.8, ENDF/B-VII or JEFF based continuous-energy interaction data from ACE format cross section libraries.

2.2 Calculational model

Four selected configurations from NPP Krško cycle 24 were selected for comparison [9]. The configuration is unique combination of fuel type, enrichment and number and distribution of IFBA (Integral Fuel Burnable Absorber) absorbers. NPP Krško uses standard Westinghouse 16×16 fuel assemblies. Selected configurations are: 4.4% enriched fuel with 64 and 80 IFBAs, and 4.8% enriched fuel with 0 and 116 IFBAs. The heterogeneous depletion calculation was performed at constant power density of 40.5 W/gU up to burnup of 60 GWd/tU (using prescribed 33 burnup steps). Assumed state point thermal-hydraulic variables were: fuel temperature 810.9 K, cladding temperature 616.5 K, coolant pressure and temperature 15.5 MPa and 580.6 K, boron concentration 500 ppm. Cold nominal dimensions were assumed. Inter assembly gap and fuel rod gap were explicitly treated. In Figure 2 geometry of 16×16 fuel assembly with 116 IFBAs as interpreted by NEWT code is shown.

DRAGON 4 used 69-groups WLUP ENDFB 6.8 library, FA2D used 97-groups ENDFB 6.5 based library, NEWT used 238-groups ENDF/B-VI.8 SCALE library and Serpent used continuous-energy ENDF/B-VI.8 ACE format library (format shared with MCNP code).

In order to produce FA2D collision probability matrix fuel assembly was covered by mesh of parallel lines (distance between lines 0.05 cm) and 16 equally spaced angles. Tracking distance was 6 MFPs (Mean Free Paths). Convergence criterion for inner iterations was $10^{-4}$ and for fundamental mode calculations was $10^{-5}$. Total number of constant flux regions in FA2D was 1238. DRAGON used 1003 regions and ray-tracing mesh with 12 tracking angles. In the same time NEWT used 11304 calculation cells. In order to perform depletion calculation FA2D needed around 5 CPU hours, DRAGON around 10 CPU hours and NEWT (SCALE 6.0) needed almost 24 hours of CPU time. Serpent spent around 4 hours of CPU (Intel Core i7 3.05 GHz) and allocated almost 8 GB or RAM for execution of 36 predictor-corrector burnup steps (500 active cycles per step with 2000 neutrons per cycle).

The prediction capabilities of the codes are compared for infinite multiplication factor, spectral ratio, and for 2D pin power form factors.
3 CODE COMPARISON

Initial comparison was performed for infinite multiplication factor. Small difference in infinite multiplication factor means that overall transport calculation was performed in proper way, but there is no guarantee that calculated homogenized cross sections or relative pin powers are suitable for nodal calculation. In Figure 3 calculated infinite multiplication factor for fuel assembly with enrichment of 4.4% and configurations with 64 and 80 IFBA rods (left figure), and for fuel assembly with enrichment of 4.8% without IFBAs and with 116 IFBAs are shown. The characters d4, std/fa2d and newt are used to label DRAGON 4, FA2D and NEWT results. Rest of the label is related to enrichment and number of IFBAs in fuel assembly. All three codes predict infinite multiplication reasonably well. $k_{inf}$ calculated by DRAGON 4 is higher than $k_{inf}$ calculated by FA2D and NEWT. The difference between the values calculated by FA2D and NEWT is generally small, with FA2D results always being above NEWT results. At the end of calculated interval all three values are the same, but slope of NEWT results is little bit different than for DRAGON and FA2D. Just one run was performed using Serpent code (4.80% no IFBAs) and results are very close to corresponding FA2D results.

Figure 3: $k_{inf}$ for 4.4%, 64/80 IFBA (left) and 4.8% 0/116 IFBA (right), DRAGON4, FA2D and NEWT
It is expected that larger relative differences in predicted spectral ratios (ratio of fast and thermal collapsed macro group fluxes) exist. Usually, differences in spectral ratio can be later correlated to differences in isotopic compositions of the fuel during depletion and are responsible for history effects in cross section data. The spectral ratios for fuel assembly with enrichment of 4.4% and configurations with 64 and 80 IFBA rods (left), and for fuel assembly with enrichment of 4.8% without IFBAs and with 116 IFBAs (right) are shown in Figure 4. For first enrichment FA2D and NEWT predict almost the same values up to burnup range 15-25 GWd/tU, and after that have different slopes. In the first part of burnup range DRAGON calculates the smallest spectral ratio, and at the end of the interval FA2D predicts the smallest spectral ratio. The largest difference between the codes is about 6%. For enrichment of 4.8%, in first part of burnup range DRAGON predicts the smallest ratio and FA2D the largest (NEWT is approximately in the middle of them). After 30 GWd/tU FA2D calculates faster decrease of spectral ratio and gives smallest absolute values at the end of the interval. The largest difference between deterministic codes is within 3%. Spectral ratio calculated using Serpent for fuel assembly without IFBAs enriched at 4.80% was in first part of burnup range below all others and at the end of calculation slightly above other results.

Table 1: Range of relative pin powers

<table>
<thead>
<tr>
<th>Code</th>
<th>IFBA</th>
<th>Enrich (%)</th>
<th>Burnup [GWd/tU]</th>
<th>Min pin power</th>
<th>Max pin power</th>
</tr>
</thead>
<tbody>
<tr>
<td>D4</td>
<td>64</td>
<td>4.40</td>
<td>0/60</td>
<td>0.9147/0.9382</td>
<td>1.051/1.071</td>
</tr>
<tr>
<td>D4</td>
<td>80</td>
<td>4.40</td>
<td>0/60</td>
<td>0.9361/0.9381</td>
<td>1.045/1.071</td>
</tr>
<tr>
<td>D4</td>
<td>0</td>
<td>4.80</td>
<td>0/60</td>
<td>0.9431/0.9368</td>
<td>1.066/1.071</td>
</tr>
<tr>
<td>D4</td>
<td>116</td>
<td>4.80</td>
<td>0/60</td>
<td>0.9511/0.9370</td>
<td>1.032/1.072</td>
</tr>
<tr>
<td>FA2D</td>
<td>64</td>
<td>4.40</td>
<td>0/60</td>
<td>0.863/0.927</td>
<td>1.056/1.032</td>
</tr>
<tr>
<td>FA2D</td>
<td>80</td>
<td>4.40</td>
<td>0/60</td>
<td>0.880/0.926</td>
<td>1.050/1.032</td>
</tr>
<tr>
<td>FA2D</td>
<td>0</td>
<td>4.80</td>
<td>0/60</td>
<td>0.803/0.925</td>
<td>1.072/1.030</td>
</tr>
<tr>
<td>FA2D</td>
<td>116</td>
<td>4.80</td>
<td>0/60</td>
<td>0.900/0.924</td>
<td>1.040/1.033</td>
</tr>
<tr>
<td>NEWT</td>
<td>64</td>
<td>4.40</td>
<td>0/60</td>
<td>0.8770/0.8859</td>
<td>1.058/1.068</td>
</tr>
<tr>
<td>NEWT</td>
<td>80</td>
<td>4.40</td>
<td>0/60</td>
<td>0.8976/0.8897</td>
<td>1.051/1.069</td>
</tr>
<tr>
<td>NEWT</td>
<td>0</td>
<td>4.80</td>
<td>0/60</td>
<td>0.9198/0.9132</td>
<td>1.075/1.082</td>
</tr>
<tr>
<td>NEWT</td>
<td>116</td>
<td>4.80</td>
<td>0/60</td>
<td>0.9231/0.8913</td>
<td>1.033/1.065</td>
</tr>
<tr>
<td>Serpent</td>
<td>0</td>
<td>4.80</td>
<td>0/60</td>
<td>0.910/0.937</td>
<td>1.103/1.056</td>
</tr>
</tbody>
</table>
Figure 5: Relative pin power vs. burnup for 4.40% 64 and 80 IFBAs

Figure 6: Relative pin power vs. burnup for 4.80% 0 and 116 IFBAs
The differences between spectral codes are again expected in calculated pin power distribution, both in predicted maximum peak power and in predicted 2D shape of pin power. The differences can be related to calculation method used in each code, available discretization and used library (fission energy). The relative pin powers (pin power form factors) are important due to their usage in nodal codes in pin power reconstruction procedure. Obtained local pin powers are responsible for local fuel temperatures and pin burnup calculation (both safety and licensing aspects).
Figure 10: Pin power distribution for 4.8%, 116 IFBA, 0 (left) and 60 GWd/tU (right), D4

Figure 11: Pin power distribution for 4.8%, 116 IFBA, 0 (left) and 60 GWd/tU (right), FA2D

Figure 12: Pin power distribution for 4.8%, 116 IFBA, 0 (left) and 60 GWd/tU (right), NEWT

Figure 13: Pin power deviation from 1 for 4.8%, 116 IFBA, 60 GWd/tU, FA2D and NEWT
The pin power was not directly available in DRAGON calculation and program was changed in order to get pin power map as a part of standard cross section edit (based on available region reaction rates and isotopic fission energy gains). Minimum and maximum relative pin power values for four fuel assembly configurations calculated using DRAGON, FA2D and NEWT at 0 and 60 GWd/tU are shown in Table 1. Maximum pin powers calculated by mentioned codes for two IFBA configurations at enrichment of 4.4% and 4.8% are shown in Figure 5 and Figure 6. Normalization is performed based on actual number of fuel pins and not on the available fuel assembly matrix locations. For zero burnup all codes predict maximum pin power reasonably well (within 1%). That is especially true for FA2D and NEWT. After about 15 to 20 GWd/tU the behavior of the calculated values is different. DRAGON and NEWT have rather similar behavior and they finally predict larger maximum relative pin powers for increased burnup. Opposite is true for FA2D results. In Figure 7 to Figure 9, 2D distributions of relative pin powers are shown for enrichment of 4.4% and 64 IFBAs, as calculated by DRAGON, FA2D and NEWT. For zero burnup FA2D predicts relatively lower pin power at the periphery of fuel assembly and for end of the depletion its pin powers are more uniformly distributed (more flatten power shape). Similar information is shown for fuel assembly enriched at 4.8% with 116 IFBAs in Figure 10 to Figure 12. Maximum relative pin power versus burnup for fuel assembly enriched at 4.8%, without IFBAs and with 116 IFBAs is shown in Figure 6. The trend of the change predicted for configuration without IFBAs with FA2D is completely different than trends predicted by DRAGON and NEWT. It should be mentioned that initial calculated values are rather close for all three codes. In addition maximum relative pin powers calculated by DRAGON and FA2D for the cases without and with IFBAs converge to the same value for high burnups and diverge for NEWT. In the same figure Serpent results for fuel assembly enriched at 4.80% without IFBAs are shown. They are more oscillatory and higher than the results predicted by deterministic codes. The label 1c means that all fuel pins are depleted as one material and label 2c means that each pin is individually depleted. The individual depletion, similar as with deterministic codes, gives decrease of peaking factors with burnup and more uniform relative pin power distribution across fuel assembly. In the same time it should be mentioned that predicted multiplication factor does not depend on assumption used in depletion of the pins (individual or material based depletion).

This kind of behavior obviously affects pin power reconstruction capability implemented in nodal code based on pin power factors predicted with spectral code, but it should be mentioned that the largest experienced difference between deterministic codes is below 5%. The reason for the differences in the prediction between DRAGON and NEWT on one side and FA2D on other side is related to the fact that first two codes deplete defined fuel mixtures and FA2D depletes each fuel pin region independently. That results in decreased min-max relative power range for higher burnup in case of FA2D as compared to NEWT calculation, as shown in Figure 13 for fuel assembly enriched at 4.8% with 116 IFBAs (power deviation from 1 means difference between local and average relative pin power).

4 CONCLUSION

The shown comparison of different code predictions at assembly level can help initially in verification of the codes and later in estimating uncertainties in reactor core calculations. It was possible to identify data where differences can be expected even if predicted multiplication factors are similar (e.g. spectral ratios and pin powers). Even with well known and established codes rather different predictions are possible as well as hidden errors. The demonstrated differences stay within usual required error margins, but it is still necessary to
check and understand reasons for the differences, especially when that affects even trend of changes, and when the change is in non-conservative direction. The example for that kind of behavior is the calculated decreased maximum relative pin power in FA2D case, even though, in that particular case, the reason for the difference is probably in individual depletion of each pin, what is a more realistic assumption. This type of code comparison is rather challenging, but it is far less time consuming than complete calculation procedure that includes both generation of full set of cross section data and nodal diffusion calculation. It can help to identify errors or weak points in calculated data before performing nodal diffusion calculation using that data. Initial effort is performed to introduce Monte Carlo code in comparison, to be used as both, reference and cross section generation tool.

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