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APPLICABILITY OF WIMS-ANL TO GENERATE CROSS SECTIONS FOR VERY-HIGH DENSITY UMO FUEL IN PROPOSED MURR LEU ASSEMBLY

B. Dionne, J. Stillman and J. Stevens
RERTR Program, NE Division
Argonne National Laboratory, 9700 S Cass Ave, Argonne, IL, 60439

ABSTRACT

The WIMS-ANL code was used to generate cross sections for the REBUS-DIF3D diffusion theory burnup code used to perform some of the Missouri University Research Reactor (MURR) conversion feasibility studies. This paper presents the analyses performed to verify the capability of WIMS-ANL to generate adequate cross-sections for the MURR proposed LEU assembly. This proposed fuel assembly possesses the following characteristics: i) cylindrical geometry plates, ii) very high density monolithic U-10Mo fuel, iii) varying channel/plate thicknesses within the assembly, and iv) large variation of the thermal flux within the assembly. In order to perform this verification, two types of comparisons are performed. First, condensation spectra obtained from WIMS-ANL are compared to spectra from MCNP to ensure that the 1-D lattice physics methodology is adequate. DIF3D and MCNP comparisons for "cold clean all rods out" cases are then performed. It can be concluded that WIMS-ANL, with the proper selection of computational methodologies, can produced adequate cross-sections for the proposed MURR LEU assembly.

1. Introduction

Historically, reactor physics analyses were performed using a diffusion theory model of the core benchmarked against an accurate but more computationally expensive transport theory model. With the advent of faster computers, it became possible to perform routine reactor physics analyses using transport codes. This trend eventually led to the use of Monte Carlo (MC) methods in depletion calculations due to their more accurate geometry and cross-section treatments. However, compared to the traditional diffusion-based approach, MC-based depletion calculations still require significant simulation time. Therefore, it is still useful to perform diffusion theory calculations for cases requiring a large number of reevaluations of the neutron flux distribution, e.g., when complex fuel shuffling schemes are studied as in the Missouri University Research Reactor (MURR) conversion feasibility studies.

In the RERTR program, diffusion-based depletion calculations are performed using REBUS-DIF3D [1, 2] with cross sections generated by WIMS-ANL [3]. This paper presents the methodology chosen to model a MURR proposed LEU assembly in WMS-ANL as well as the analyses performed to verify the capability of WIMS-ANL to generate adequate cross-sections.

This review of the methodological choices is useful since WIMS-ANL was never tested for a fuel assembly possessing all the following characteristics: i) cylindrical geometry plates, ii) very high density monolithic U-10Mo fuel [4, 5], iii) varying channel/plate thicknesses within the assembly, and iv) rapid variation of the thermal flux within the assembly.

In order to perform this verification, two types of comparisons are performed. First, the condensation spectra in various regions are obtained from WIMS-ANL and compared to MCNP [6] spectra to ensure that a 1-D lattice physics simulation is adequate. Since these cross-sections will be used in the REBUS-DIF3D code, DIF3D/MCNP reactivity comparisons for cold clean all rods out (ARO) cases are then performed. It must be noted that, since MCNP results are also compared to experimental measurement obtained from MURR, benchmarking WIMS-ANL/DIF3D results against MCNP is an adequate approach.

This paper is organized as follows. Section 2 presents a brief description of the WIMS-ANL code. Section 3 discusses the MURR proposed core and the associated computational challenges. Section 4 describes the computational approach chosen to address these challenges. Section 5 shows some key results obtained during this work. Finally, Section 6 presents the conclusions and future work.

2. WIMS-ANL description

Many versions of the Winfrith Improved Multigroup Scheme (WIMS) code have been used throughout the world for power and research reactor lattice physics simulations. WIMS-ANL [3] is the second major revision done in the RERTR program in order to serve the needs of the reactor conversions. Originally, the WIMS-D4 code [7] and library were modified to improve and extend the cross-section data set and implement more accurate methodologies. These modifications led to WIMS-D4M [8] which, following an extensive modernization program, was renamed WIMS-ANL.

A typical WIMS-ANL simulation is performed in two steps. First, fine-group neutron fluxes (WIMS library 69 fine groups structure) are calculated for a simple average fuel cell in order to generate intermediate group constants for a transport calculation over a more detailed one-dimensional geometry. These fluxes are then used to condensed cross-sections over the few-group (broad group) structure used in a diffusion theory simulation. Note that WIMS-ANL contains a Supercell option [9] that allows the user to break down a complex problem into simpler auxiliary cells to obtain improved spectra, resonance corrections and homogenization.

Typically, the first step of a WIMS-ANL simulation uses the SPECTROX (simplified collision probability) solver to obtain the intermediate group structure neutron fluxes and resonance corrected cross-sections. For the Supercell option, it is possible to use a discrete ordinates (DSN) solver for this first step, i.e., during the simulation of the auxiliary cells. For the second step, it is possible to select either a collision probability (referred to as the PERSEUS solver in WIMS-ANL) or discrete ordinates (DSN) solver.

3. Computational challenges for MURR proposed LEU core

3.1. MURR description

MURR is a tank-type light-water cooled 10 MWth reactor with curved plates fuel assemblies as well as beryllium and graphite reflectors. Each of its eight (8) proposed LEU fuel assembly consist of twenty-four (24) curved plates composed of U-10Mo monolithic foils clad in aluminum. These 24 fuel plates are held together by two grooved side plates forming a wedge-like structure. The coolant channels are formed by the space between two adjacent fuel plates. These fuel assemblies, located between an inner and outer pressure vessel (PV), are arranged such that a water-filled central flux trap is formed. This flux trap is typically used to irradiate samples placed in three holder tubes. Since the MURR core relies on neutron reflection to achieve criticality, boral control blades located outside the outer pressure vessel control reactivity by adjusting the amount of reflection. Figure 1 shows a schematic of one quadrant of the MURR core.

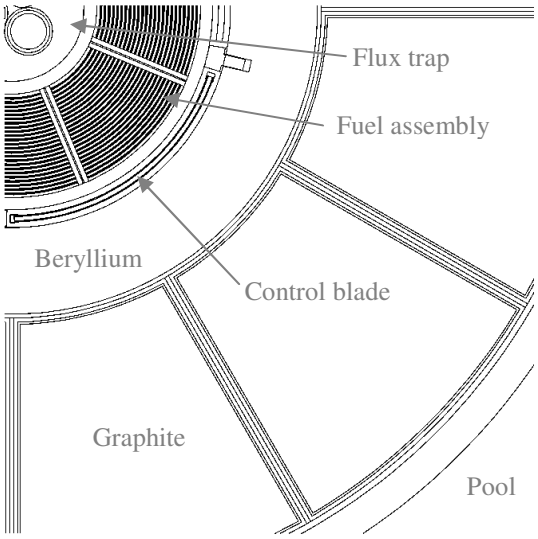

Figure 1 MURR core schematic

3.2. Challenges

Due to the presence of the flux trap and beryllium reflector at the edges of each fuel assembly, strong thermal flux gradients are observed within the assemblies. These changes in thermal flux stretch the typical WIMS methodology and require a more detailed modeling of the fuel assembly environment to capture these variations and obtain accurate cross-sections. Note that the combination of large thermal fluxes at the edges of the assembly and high density U-10Mo fuel forced the redesign of the assembly to introduce inner and outer plates (plates 1, 2 and 24[1]) with thinner meat and different clad thicknesses [10]. The changes in meat thickness affect the evaluation of the self-shielding for these plates and require special attention. Note that since the

[1] As a convention, the plates are numbered sequentially from 1 to 24 starting from the one closest to the inner PV.

flux trap has a large impact on the assembly spectrum, it is important to consider the flux trap content when generating fuel cross-sections.

4. Description of WIMS-ANL computational approach for MURR

It is well known that large changes in flux spectrum and magnitude are difficult to model accurately using diffusion theory. Therefore, to obtain accurate results, the approach in WIMS-ANL must be tightly tied to the approach use in REBUS-DIF3D. It is therefore important that the MURR WIMS-ANL model take all these aspects into consideration. Other considerations such as self-shielding, transport solver and phase-space discretization must also be addressed

4.1. REBUS-DIF3D

Finite-difference diffusion theory models are more accurate and have better convergence rate when mesh sizes are as close as possible to one diffusion length. MURR core components larger than one diffusion length (control blades, reflectors and flux trap content) are subdivided in a few regions. Each of those regions can be assigned a different set of cross sections that is condensed over the appropriate volume in WIMS-ANL. Consequently, large changes in spectra will be captured in WIMS-ANL and reflected in the cross sections.

Since a MURR fuel assembly is also subjected to large changes in spectrum, it is also important to generate different cross-section *color sets* for the various regions. These *color sets* were chosen by looking at the thermal flux in each plate obtained from MCNP for both HEU and LEU assemblies with and without the control blades. Both the HEU and LEU assemblies were studied so the *color sets* would be appropriate for both assemblies. To illustrate this, Figure 2 shows the MCNP thermal flux (less than 4 eV) for each plate and the seven *color sets* for a cold clean LEU assembly with ARO and an empty flux trap.

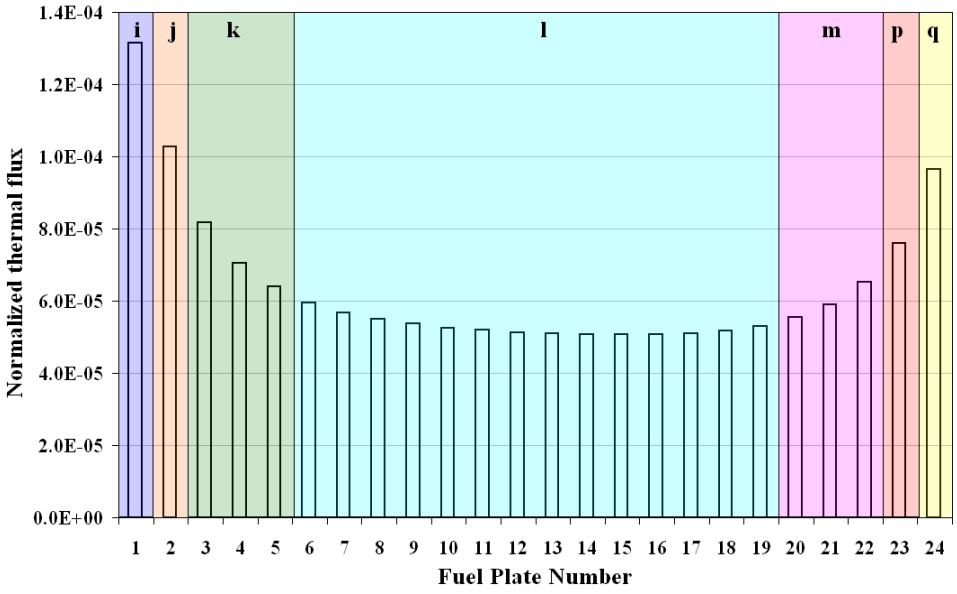

Figure 2 Fuel assembly cross-section color sets and maximum thermal flux

Note that when a when a *color set* is comprise of many plates, the average cross-sections are obtained by smearing these plates in WIMS-ANL. To take into account the impact of the flux trap content in the DIF3D model, it was determined that it sufficient accuracy is obtained by recalculating the *color sets* labeled *i* and *j* for the various flux trap content.

Generating the different cross-section sets for the various regions will not be sufficient to produce accurate DIF3D results if the energy group structure used in the diffusion model is not detailed enough to capture the bulk of the spectrum changes. Therefore, it is important that the few-group structure over which WIMS-ANL will condense the cross-sections is appropriate.

Previous experience [11] in modeling light water cooled and moderated research reactors using DIF3D and WIMS suggested that the standard ANL-RERTR seven groups structure might not be sufficient to model a reactor with strong thermal flux gradient. It also showed that using fewer than five (5) library groups for the highest broad group will lead to a positive bias as compared to MC simulations.

To develop the MURR ten (10) broad groups structure, starting from the typical ANL-RERTR seven groups structure, the few-group group boundaries were compared to a detailed WIMS-ANL library sixty-nine (69) groups spectrum for the flux trap, for an average of all fuel plates and for the control blades. The boundaries were then adjusted to best represent the various components of the detailed spectrum. For each spectrum region, the main considerations were;

- Fast (groups 1 and 2): minimum of 5 library groups in the highest broad group
- Epithermal (group 3): all library resonance groups are condensed together
- Thermal (groups 4 to 10): set boundaries and additional groups to properly represent large changes in various core components, e.g., increase in flux between 0.14 and 0.32 eV due to the flux trap.

Figure 3 shows the boundaries chosen for the few-group structure used in REBUS-DIF3D overlaid over the 69 groups spectrum obtained from the WIMS-ANL model (see later sections for more detailed discussion about the WIMS-ANL model).

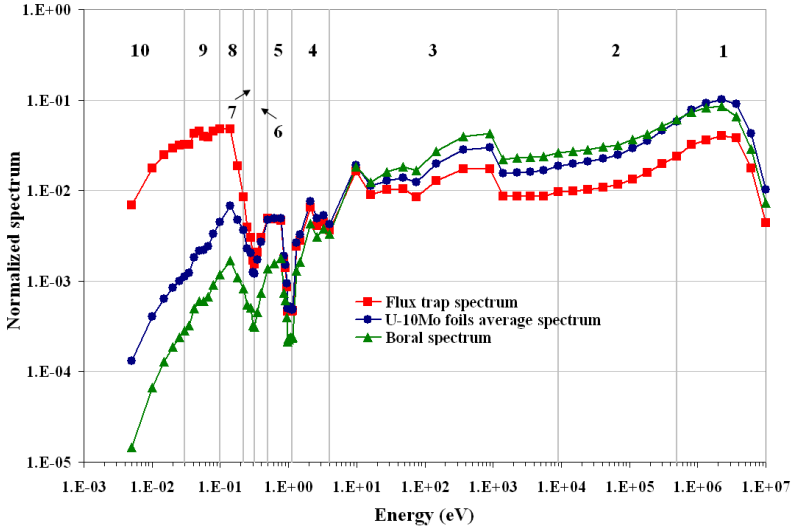

Figure 3 MURR custom 10 energy groups structure

Note that the energy group structure was also used to generate cross sections for the HEU MURR core model to ensure adequate k-effective consistency with MCNP.

4.2. Resonance self-shielding

One important aspect of collapsing cross-sections is the evaluation of the resonance self-shielding. Typically, self-shielding models assume a single lump of fuel surrounded by an infinite moderator. Then, "rod shadowing" effects (the impact on the spectrum in a fuel lump region from being surrounded by a lattice of identical lumps) are introduced for the unit cell through correction factors such as the Bell and Dancoff factors. If these factors are inaccurate for a given lattice geometry, the resonance capture cross-sections can be under- or over-predicted. In the case of the MURR proposed LEU geometry, this is complicated by the fact that different fuel thicknesses are present within one assembly therefore requiring many such correction factors.

In order to minimize the error on the resonance capture introduced by using inaccurate self-shielding correction factors, the main transport simulation is performed over full assembly for the 69 energy groups of the WIMS-ANL library. Performing a fine group calculation over the detailed assembly ensures that changes in spectrum from surrounding fuel plates are explicitly modeled during the transport simulation. Therefore, for a given region, explicit variations in spectrum and magnitude of the flux are taken into account when collapsing cross-sections. In WIMS-ANL, this can be done by defining a Supercell of the whole assembly and various auxiliary cells.

The errors from inaccurate self-shielding factors will therefore mainly affect the cross-sections used in the main transport calculation. Moreover, the Supercell option allows the definition of two resonant materials in a given auxiliary cell. This can be used to reduce the errors on self-shielding corrections for the transport cross-sections by defining auxiliary cells that contain plates 1 and 2 as shown in Figure 4.

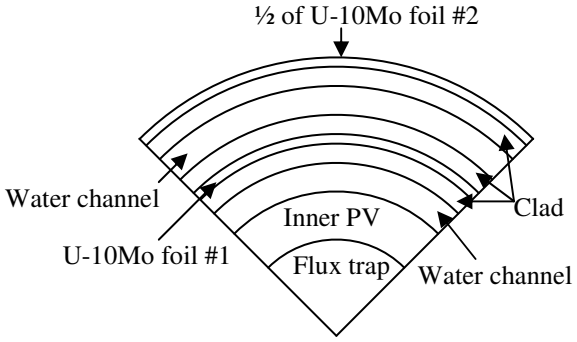

Figure 4 Auxiliary cells for fuel plates 1 and 2

Such an auxiliary cell should provide a better approximation of the "rod shadowing" effects in plate 2 from plate 1 and vice versa than a simple cell. Moreover, it is also possible to take into account the content of the flux trap when generating the transport cross-section.

4.3. WIMS-ANL Supercell model

Considering that, for a MURR fuel assembly, the representation of environment is especially important to obtain accurate cross-sections, it was decided that the1-D radial model should include all possible structures with the limits of WIMS-ANL. In the WIMS model shown in Figure 5, each core component is represented using one or more materials (see discussion in section 4.1).

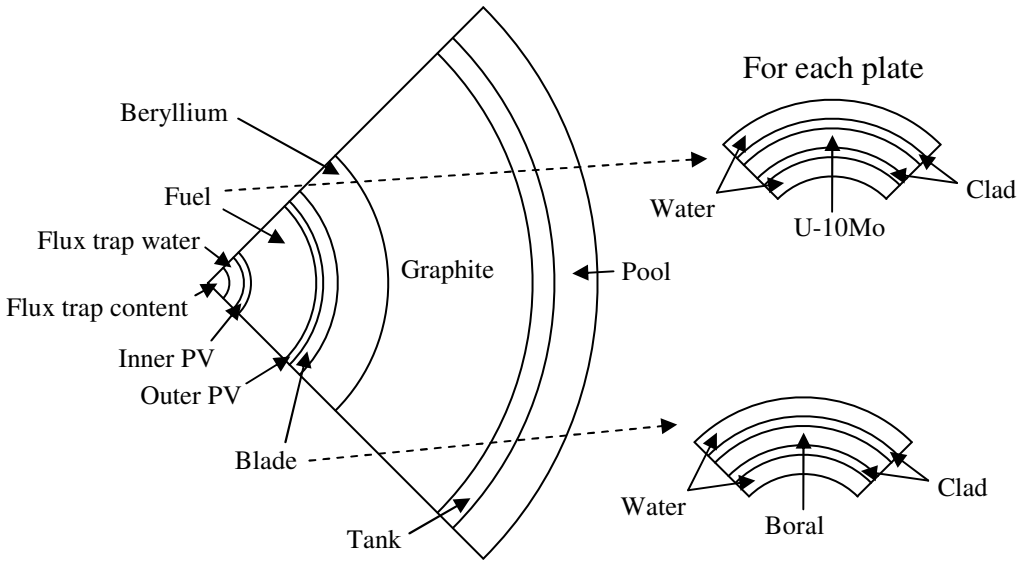

Figure 5 WIMS-ANL Supercell model for MURR proposed LEU core

Representing each fuel plate independently allows "edge-plates" to be treated differently than other plates in order to improve the self-shielding of these plates as discussed in the previous section. Many auxiliary cells were also defined for the MURR WIMS-ANL model. Moreover, this approach ensures that depletion will be performed using the proper flux spectrum and magnitude for each plate. In addition to the auxiliary cells described in section 4.2, other cells were created for the flux trap, each fuel plate, the control blade, as well as the reflectors and tank. Figure 6 shows these various types of auxiliary cells.

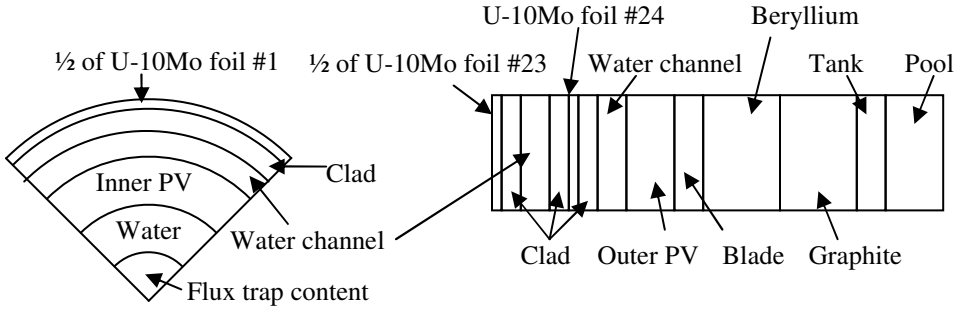

Figure 6 Other WIMS-ANL auxiliary cell models

4.4. Transport solver selection

Based on the previous discussion, it is clear that the Supercell option will be needed to obtain more accurate results for the MURR LEU assembly. Using that option, it is possible to select different transport solvers for the detailed Supercell model and each auxiliary cell.

For the auxiliary cells, the SPECTROX solver assumes that every material must be fuel, can, coolant and/or moderator averaged accordingly into a 3 or 4 region model. Considering the relative complexity of certain auxiliary cell (see sections 4.2 and 4.3) in the MURR model, a single average fuel cell approach is inappropriate. Therefore, the DSN solver was selected for the auxiliary cells. Note that for the set of auxiliary cells with only 3 regions (fuel plates 3 to 22), the selection of SPECTROX or DSN does not change significantly the solution.

For the second step, where the more detailed geometric model includes large regions where the flux can change significantly, it is more appropriate to use the DSN solver since it provides more control over angular quadrature and mesh sizes. Moreover, the flat flux assumption inherent to collision probability methods would require dividing each MURR component in many more regions to obtain accurate results.

4.5. WIMS-ANL phase-space discretization

Once the problem is broken into various regions and auxiliary cells, it is important to select the appropriate discretisation for the problem in order to obtain the most accurate multigroup fluxes. Because WIMS-ANL performs transport calculations for 1-D geometries, fine discretisation parameters can be chosen while maintaining reasonable simulations times.

For LEU assemblies, selecting an appropriate intermediate energy group structure is important to properly model the resonance capture in the epithermal region. To circumvent this possible difficulty, the transport simulations were performed for the 69 energy groups of the WIMS-ANL library.

Considering that the environment of the fuel assembly was modeled as completely as possible, solving for the neutron flux in regions such as the graphite, tank and pool can be considered “deep penetration” problems. Since this type of problem requires a high order angular representation, an S_{16} quadrature set was selected. This is also useful to accurately model the change in thermal flux in the control blades.

The implementation of the S_N method in WIMS-ANL uses a simple linear diamond differencing scheme making it possible to obtain negative scalar fluxes. Therefore, special care was taken to ensure that mesh sizes were of the order of the thermal mean-free-path of each region. This does not guarantee positivity as a stricter criterion [12] based on the quadrature set would but it does minimize the likelihood of obtaining negative fluxes. Note that when selecting mesh sizes, it was also taken into account that when high burnup depletion calculation will be performed, the fuel properties will change and certain region may require slightly smaller mesh sizes to prevent negative fluxes.

5. Results

5.1. WIMS-ANL versus MCNP spectra

In order to obtain adequate broad-group cross-sections, it is essential to perform the energy condensation using an accurate spectrum. Therefore, as the methodology described in the previous section was being developed, frequent comparisons of WIMS-ANL and MCNP spectra were performed. Among other things, these comparisons identified the need to use leakage corrected critical spectra in WIMS-ANL. Note that for REBUS-DIF3D calculations, the axial and radial buckling values used in WIMS-ANL to determine the critical spectrum are not important since no directional information is used. Figure 7 compares the WIMS-ANL 10-group condensation spectra averaged over the flux trap, all fuel plates and the control blade with the equivalent spectra tallied in an MCNP simulation.

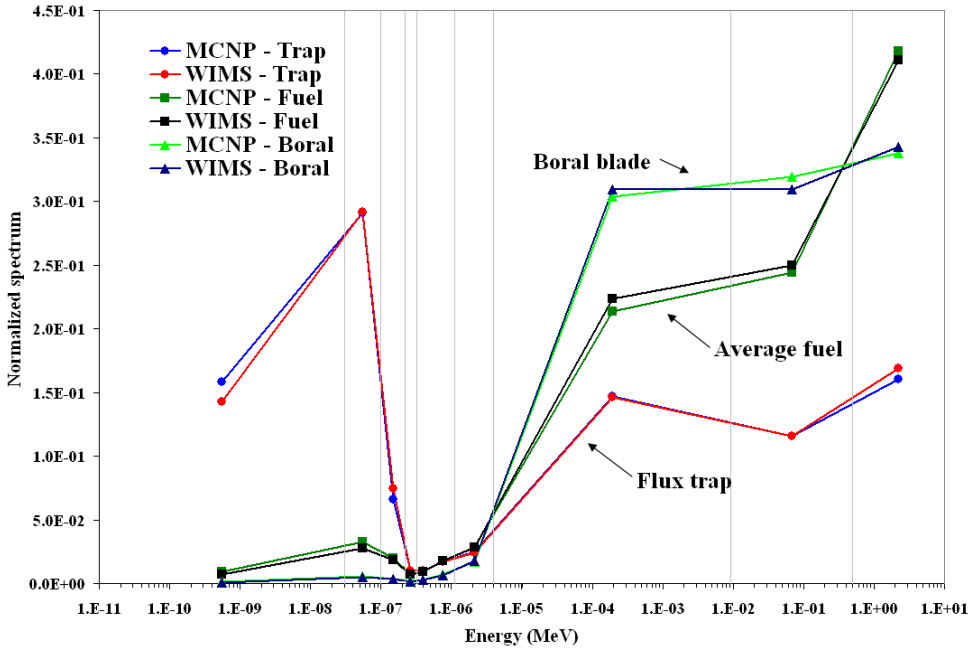

Figure 7 WIMS-ANL and MCNP 10-group spectra for the control blade, flux trap and fuel

Looking at Figure 7, it obvious that, using the methodology described previously, relatively accurate condensation spectra can be obtained.

5.2. k-effective comparison

Again, throughout the development of the approach, predicted k-effectives (k_{eff}) from MCNP and DIF3D were used to verify the WIMS-ANL cross sections and DIF3D model. For the MURR proposed LEU core, the following three cases were used; i) ARO with an empty flux trap, ii) ARO with holder tubes inserted in the flux trap, and iii) control blades inserted at a BOL critical position with holder tubes present ("Step 3" in ref. [13]). Table 1 presents the latest DIF3D and MCNP k_{eff} comparison for MURR proposed LEU core.

Table 1 DIF3D and MCNP k_{eff} comparison for MURR proposed LEU core

Case	Description	MCNP k_{eff}	DIF3D k_{eff}	$\Delta k/k$ (%)
1	ARO empty trap	1.10003	1.09646	-0.296
2	ARO with holder	1.10370	1.00700	-0.247
3	Blades inserted with holder[2]	1.00891	1.00598	-0.289

By looking at Table 1, it can be concluded that, using WIMS-ANL cross-sections generated as previously described, DIF3D and MCNP k_{eff} are in good agreement. From Table 1, the predicted reactivity worth of the holder tubes from the two methodologies are 0.302% (MCNP) and 0.351% (DIF3D). Note that similar comparisons were also performed for the HEU MURR core with similar agreement [15].

6. Conclusions and Future Work

From the review performed in this work, it can be concluded that WIMS-ANL, with the proper selection of computational methodologies, can produced adequate cross-sections for the proposed MURR LEU assembly. More detailed comparisons of power and burnup distributions will be performed to ensure that the current methodology remains valid during depletion.

7. References

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[2] In order to get good agreement for control blade worths in diffusion theory; it was necessary to use internal blackness coefficients [14]. Note that for MURR, the theoretical blackness coefficients were calculated for cylindrical geometries for energy groups 7 to 10.

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