Calculation of PWR Thorium Pin Cell Burnup and Isotope Prediction Using WIMSD-5B Code

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Abstract. The amount of thorium in the world is very abundant and the benefits of using thorium as fuel for nuclear reactors such as PWR are increasingly widespread, so it needs to be analyzed. In the initial phase, the PWR pin cell fuel analysis was carried out using the WIMSD-5B code. The PWR ThO2-UO2 fuel in the cladding with the fuel assembly model 17 x 17 is analyzed by its fuel burnup, neutron flux and isotope composition after maximum operation. The pin cell model consisting of fuel, cladding and coolant with a square pitch of 12.6 cm are calculated using different libraries. Eigenvalues, neutron fluxes and isotope concentrations were compared with the PWR pin cell model to high burnup. The eigenvalues and flux neutron as a function of burnup are good, the maximum difference is within 7.41% and the mean absolute difference is less than 3.12%. The best comparison of fission product isotope concentrations is to use the ENDFB7.1 library with Thorium fuel and is comparable to the uranium fuel reported in the literature. Data sources for actinides and fission products used for fuel depletion calculations for thorium fuel are all documented.

Keywords: Thorium fuel, burn up, isotope composition, WIMSD-5B, PWR pin cell

1. Introduction
Over the past two decades, there have been remarkable improvements in the nuclear data. A number of improved evaluated nuclear data libraries such as ENDF/B-6, JENDL-3, IAEA and JEF2 have become available [1-3]. Meanwhile, computing facilities have been improved to a great extent and more sophisticated neutron transport methods have been developed to deal with large and complex problems. Most of the reactor codes (WIMS is one of them) being employed nowadays for reactor analysis, were developed in 1950s, at the time when most of the nuclear data were based on integral measurements and neutron transport methods and computing facilities were in the early stages of development. As far as improvements in methodology are concerned, these have been made from time to time in the codes, and their revised versions have been released. However, nuclear data libraries, input to most of the reactor codes, have not received a commensurate degree of attention. These are mostly based on old, obsolete data, so most of these codes are being employed in reactor analysis with less confidence. Improved data libraries, if any, are usually restricted. The aforementioned situation forced the reactor physicists around the world to think on various projects regarding updating and improvements in nuclear data libraries of reactor codes. In this connection, the IAEA has initiated various activities to update and improve multigroup nuclear data input to neutronics codes. WIMS/D (Winfirth Improved Multigroup Scheme) [4-6] is a widely used neutronics code for reactor lattice analysis. Its data libraries have been in existence in some form for nearly thirty years. The WIMS
standard library, freely available from NEADB (Nuclear Energy Agency Data Bank) [7], contains old data based on adjustments made to fit integral experiments. It performs well on a wide range of current systems, but is employed with less confidence to more advanced reactor concepts. So IAEA with the collaboration of NEADB initiated a project to produce a new updated WIMS library based on latest improved standard evaluated nuclear data files [8,9]. In this work, WIMSD-5B has been a revival of interest in the use of thorium in light water reactors because it can facilitate the realization of longer intra-refueling intervals and high burnup while reducing spent fuel weapons usability and increasing in-repository durability. These prospects motivated the present work under the strategic nuclear research, focusing on the use of thorium-based fuel in otherwise-conventional, retrofittable, PWR fuel assemblies. Since 1980, fueling of LWRs with thorium was actively explored, including whole-core demonstrations[10,11]. Thorium use was also extensively studied in the world programs, but work was focused on recycled mode fuel cycles, using highly enriched $^{235}$U for startup, and burnup 30 MWd/Kg [12,13]. In this work, the burn-up and isotope prediction of thorium pin cell was calculated using the WIMSD-5B program using various libraries. The purpose of this work is to understand how sensitive and accurate the calculation results are in the cross-sectional libraries used.

1.1 Pin Cell Model

The work reported here involves analysis of a PWR pin cell excised from a standard 17x17 pin assembly typical of large Westinghouse PWRs [14]. The usual all-UO2 fuel pellets were replaced by aThO2-UO2 mixture at 94% of theoretical density consisting of 75w/o Th, 25 w/o U on a heavy metal basis, with the latter enriched to 19.5 w/o $^{235}$U, to give an overall enrichment of 4.869 w/o $^{235}$U in total heavy metal [15]. Fig. 1 shows the pin cell model representing the unit lattice cell of a Westinghouse PWR fuel bundle. The burnup calculations described in this study are based on this model. Since all actinides in the thorium and uranium chains will be produced during burnup, this calculation is a challenge to all the actinide neutron libraries used by WIMSD-5B, and also a challenge to WIMSD-5B’s treatment of each actinide’s group constants. Table 1 and Table 2 shows detailed parameters of the pin-cell model for a Westinghouse PWR assembly. Parameters at hot full power were used in our calculations.

1.2 WIMSD Code

WIMS is a reactor code for lattice cell calculations applicable to a wide range of reactor types including thermal and fast reactors. It can be applied to rod or plate fuel geometries in regular arrays as well as clusters. Different transport theory options can be applied at various stages of cell analysis. The output of the code provides detailed reaction rates for the reactor lattices, regional and cell averaged constants and multiplication factors. Leakage corrections can also be applied and the lattice can be exposed to burnup. The output parameters are of extensive use in overall reactor calculations. Various reaction rate edits are also given in the output for direct comparison with the experimental measurements. Although the code itself is very versatile and useful, its programming is rather complex. The original version distributed by NEADB used some non-standard Fortran language elements making its portability difficult. The users themselves had to make several changes in the program to make it operational on their systems. Thus, several local versions were made by different laboratories. In some cases different installations would give slightly different results for same problems and the implementation dependent uncertainties need also to be checked and removed. The very first version of WIMS was developed in late 1963. Its library was restricted to 58 groups due to the limitations of computing facilities. In 1965 the code was transferred to extend to the present 69 groups (14 fast, 13 resonance, and 42 thermal groups). In the fast neutron energy range, above 9.118 KeV, there are 14 groups with an equal lethargy width of 0.5. This group division is adequate to describe the leakage events in light-water lattices and to cover fast fission in $^{238}$U above its fission threshold at about 1 MeV. In the resonance range, from 9.118 KeV to 4 eV, there are 13 groups. In the lower part of that range, the boundaries were chosen so as to locate the most important $^{238}$U resonances in the middle of the groups. Finally, in the range below 4 eV there are 42 groups, including 12 groups
clustered around the 1.05 eV 24~ resonance [16]. 1.05 eV $^{240}$Pu resonance and 5 groups around the 0.30 eV $^{239}$Pu The 69-group division of the WIMS library is good enough to apply it to a wide variety of lattice types, ranging from light and heavy water moderated fuel assemblies to steam-cooled fast reactor assemblies. The computational efficiency of a particular type of reactor can be improved by condensing the library to a smaller number of groups, with condensation spectra generated in that reactor.

2. Methodology
For the analysis, the lattices of the PWR pin cell were converted to equivalent cylindrical cells with radii given in Table 1. The other physical parameters employed in the calculations are also given in this table. For these calculations, 69-group WIMS library has been used. The solution of the transport equation has been carried out using discrete ordinate (WDSN option) method [17]. To account for leakage, the values of buckling have been supplied as input and the calculations have been performed using a transport corrected flux solution with a transport diffusion coefficient option. Reaction rates have been calculated for materials $^{235}$U and $^{238}$U in two groups with thermal cutoff at 0.625 eV. All the calculations have been carried out at Hot Full Power (HFP). These inputs are termed as pin cell inputs. To check differences due to installation changes or numerical accuracy of different library computer codes, IAEA has prescribed inputs for the above mentioned benchmark lattice. Moreover, for PWR Pin cell discrete ordinate method has been employed for the solution of the transport equation. The order of scattering for this solution is taken as 4. For other benchmark collision probability method (PERSEUS option) has been adopted. Flux solution with the Benoist diffusion coefficient option in WIMS. Reaction rates for $^{235}$U and $^{238}$U have been calculated in 69 groups with thermal cutoff at 0.625 eV. The calculated results of pin cell inputs and the prescribed inputs have been utilized to calculate lattice parameters defined in an earlier section. Stage-1 of the research has been completed and the results have been sent to the BATAN for evaluation. A summary of these results is presented in the next section.

| Table 1. Pin-cell Model Parameters [18] |
|----------------------------------------|
| Parameter                              | Cold zero power | Hot Full power |
| Fuel Temperature (K)                   | 300             | 900            |
| Power Density (KW/KgHM)                | 0.0             | 38.1347        |
| Power Density (KW/liter cell)          | 0.0             | 107.284        |
| Fuel Density (g/cm$^3$)                | 9.614           | 9.424          |
| Cladding Temperature (K)               | 300.0           | 621.1          |
| Cladding Density (g/cm$^3$)            | 6.550           | 6.505          |
| Coolant Pressure (bars)                | 155.13          | 155.13         |
| Coolant Temperature (K)               | 300.0           | 583.1          |
| Coolant Density (g/cm$^3$)             | 1.003           | 0.705          |
| Fuel Pellet Radius (mm)                | 4.096           | 4.1274         |
| Cladding Inner Radius (mm)             | 4.178           | 4.1896         |
| Cladding Outer Radius (mm)             | 4.750           | 4.7609         |
| Pin Pitch (mm)                         | 12.6            | 12.626         |
Table 2. Initial Compositions (Hot Full Power Conditions) [19]

| Material | Nuclide | ID | WIMSD | Atomic Density (/barn cm) |
|----------|---------|----|-------|--------------------------|
| Fuel     | \( {^{90}}\text{Th}^{232} \) | 2232 | \( 1.612150\times10^{-02} \) |
|          | \( {^{232}}\text{U} \)    | 234  | \( 8.245180\times10^{-06} \) |
|          | \( {^{234}}\text{U} \)    | 2235 | \( 1.036150\times10^{-03} \) |
|          | \( {^{235}}\text{U} \)    | 8238 | \( 4.229570\times10^{-03} \) |
|          | \( {^{8}}\text{O}^{16} \) | 6016 | \( 4.268350\times10^{-02} \) |
| Cladding | Zr      | 91  | \( 4.2.46100\times10^{-02} \) |
|          | Fe      | 2056| \( 1.412700\times10^{-04} \) |
|          | Sn      | 118 | \( 4.984500\times10^{-04} \) |
|          | Ni      | 58  | \( 4.705100\times10^{-06} \) |
|          | Cr      | 52  | \( 7.586600\times10^{-05} \) |
| Coolant  | \( {^{1}}\text{H} \)     | 3001 | \( 4.710530\times10^{-02} \) |
|          | \( {^{16}}\text{O} \)    | 6016 | \( 2.356620\times10^{-02} \) |

3. Result and calculation

Figure 2 shows the eigenvalue history using WIMSD-5B code. The eigenvalue (K-inf) decreases as a function of time operation. The decrease in k-inf value indicates that the reduction of Th and U material as fuel in the PWR pin cell formation in the model.

Figure 3 shows burn up as a function of time operation. In the results of this calculation, the fuel burn up increases according to the operating time. The greater the fuel burn-up value, indicating that the greater the amount of fuel burned, meaning that the amount of fuel with Th and U materials is reduced. At one point, the reactor could no longer be operated in a critical condition, so refueling was needed. In the PWR type reactor after operating at full power for 3 years, refueling is required.
Figure 3. Burn up as a function of operating time

Figure 4 shows the atom density of $^{232}$Th after 1599 days of operation at selected time steps. Considering that the point of major concern is the burnup value where maximum reaches 60.977 MWd/kg. This eigenvalue comparison shows almost no difference at that point. This is encouraging because one must achieve better accuracy for thorium fueled cores than for all-uranium fuel (since the slope of k-inf vs burnup is less steep) to achieve equal accuracy in cycle length estimates. At 60 MWd/Kg (corresponding to projected end-of-life core average burnup), the eigenvalue difference increased to approximately 0.015. The result had about 0.02 lower K-inf at the first point, but agrees well with reference results later because the different cladding compositions used in the reference model acted as a small amount of “burnable poison”. Reference discusses how to decrease this oscillation and how to improve the burn-up and benchmark comparison.

Figure 4. Thorium atom density as a function of operating time

Figure 5 shows the isotope concentration comparison of $^{235}$U and $^{238}$U at 60.977 MWd/Kg (1599 days) which is at the upper limit of discharge burnup core refueling scheme is considered. All-in-all, it appears that our results agree as well or better than these other contemporary comparisons. One observation is that the concentrations of thorium chain actinides calculated by WIMSD-5B are almost all larger than those of the IAEA library by about 4%, whereas the concentrations of uranium chain actinides are on average smaller by 4%. Further calculations show that increasing the initial $^{232}$Th concentration by 2% and at the same time decreasing $^{238}$U concentration by the same amount in
WIMSD-5B eliminated roughly half of the differences. This suggests that refinement in the thorium and uranium cross section sets should be looked into. Total end-of-life heavy metal destruction was about 1% higher in WIMSD-5B, which supports the conclusion that overall average energy per fission plus capture differs slightly. This is a well-known dilemma, since few codes disaggregate the capture contribution: use of a constant overall approximation of 8 MeV is common. This means that WIMSD-5B will grind through more of the nuclide chains for the same EFPD (energy full power day). Another point of interest is the large difference in $^{234}$U concentrations, which merits further attention, even though this nuclide has a small effect on k-inf.

The results of the isotope concentration of heavy metal elements can be seen in Figure 6a. This result comes from WIMSD-5B calculation and can be seen clearly that the isotope concentration of $^{233}$U is very dominant. This isotope is obtained from the $^{232}$Th isotope by trapping neutron particle in the fuel material.

The results of the isotope concentration of heavy metal elements can also be seen in Figure 6b. This result also comes from WIMSD-5B calculation and can be seen clearly that the isotope concentration of $^{241}$Pu is very dominant and then $^{240}$Pu. This isotope is obtained from the $^{238}$U isotope by trapping neutron particle in the fuel material.
The burnup calculation was performed over a period of 1500 days, which corresponds to a 55% reduction in the initial $^{235}$U concentration. The variations during the burning of the concentrations of some nuclides for the seven nuclear data libraries evaluated were plotted in graphs and can be consulted in Figures 6a and 6b. It can be seen that at the end of the simulation of the burning, in 1599 days, the concentrations obtained using the seven nuclear data libraries evaluated do not differ in most cases. However, not all libraries produced similar results in the following related cases: $^{241}$Pu, $^{242}$Pu, $^{242}$Cm, $^{243}$Cm, $^{244}$Cm, $^{241}$Am, $^{242}$Am and $^{243}$Am.

Table 3. K-inf values as a function of operating time

| Time (days) | k-inf IAEA | k-inf JEF2.2 | k-inf JEF3.1 | k-inf JENDL3.1 | k-inf ENDFB6.8 | k-inf ENDFB7.0 | k-inf ENDFB7.1 |
|-------------|------------|---------------|-------------|----------------|----------------|----------------|----------------|
| 0.000       | 1.25947    | 1.24966       | 1.23398     | 1.25755        | 1.23381        | 1.24607        | 1.24578        |
| 1.500       | 1.22480    | 1.21525       | 1.19972     | 1.22286        | 1.19994        | 1.21161        | 1.21134        |
| 6.000       | 1.22134    | 1.21194       | 1.19641     | 1.21945        | 1.19664        | 1.20823        | 1.20786        |
| 156.000     | 1.16595    | 1.15743       | 1.14410     | 1.16509        | 1.14430        | 1.15501        | 1.15579        |
| 277.800     | 1.13735    | 1.12988       | 1.11812     | 1.13705        | 1.11815        | 1.12800        | 1.12963        |
| 515.999     | 1.08649    | 1.08127       | 1.07164     | 1.08678        | 1.07164        | 1.07970        | 1.08253        |
| 817.799     | 1.03035    | 1.02788       | 1.01996     | 1.03097        | 1.02025        | 1.02593        | 1.02972        |
| 1057.799    | 0.98931    | 0.98885       | 0.98211     | 0.99006        | 0.98269        | 0.98645        | 0.99077        |
| 1299.002    | 0.95182    | 0.95309       | 0.94748     | 0.95257        | 0.94844        | 0.95037        | 0.95511        |
| 1357.802    | 0.94299    | 0.94465       | 0.93930     | 0.94372        | 0.94035        | 0.94184        | 0.94667        |
| 1599.004    | 0.91032    | 0.91330       | 0.90894     | 0.91092        | 0.91035        | 0.91022        | 0.91542        |

Table 3 shows the results of calculating k-inf values from different libraries, namely IAEA, JEF2.2, JEF3.1, JENDL3.1, ENDFB6.8, ENDFB7.0 and ENDFB-7.1. The results of the initial calculations without burning up show that the smallest k-inf value is the result of the calculation of WIMS-5B with the ENDFB6.8 library, namely 1.23381, while the largest is the IAEA library which is 1.25947 and the difference between the two is 2.02%. After operating 1599 days with a maximum burn up, the smallest k-inf value is the calculation result with the JEF3.1 library, which is 0.90894, while the largest is the calculation result with the ENDFB7.1 library, which is 0.91542. The difference between these two results is 0.71%. From the results of these calculations, it is found that the best library is...
ENDFB7.1 because the initial k-infinity value is not the maximum, but when it has been operating for 1599 days it produces the largest k-infinity value. The ENDFB7.1 library is the newest and most comprehensive library of macroscopic constants and its spectrum according to the type of thorium PWR fuel.

### Table 4. Average total fluxes as a function of operating time (x 10^14)

| Time (days) | IAEA | JEF2.2 | JEF3.1 | JENDL3.2 | ENDFB6.8 | ENDFB7.0 | ENDFB7.1 |
|------------|------|--------|--------|----------|----------|----------|----------|
| 0.000      | 2.843| 2.864  | 2.852  | 2.839    | 2.886    | 2.858    | 2.863    |
| 1.500      | 2.915| 2.937  | 2.925  | 2.912    | 2.959    | 2.931    | 2.936    |
| 6.000      | 2.923| 2.945  | 2.933  | 2.920    | 2.967    | 2.939    | 2.945    |
| 156.000    | 3.074| 3.095  | 3.079  | 3.072    | 3.116    | 3.088    | 3.091    |
| 277.800    | 3.161| 3.180  | 3.160  | 3.159    | 3.199    | 3.172    | 3.174    |
| 515.999    | 3.332| 3.344  | 3.318  | 3.333    | 3.360    | 3.337    | 3.335    |
| 817.799    | 3.545| 3.548  | 3.515  | 3.546    | 3.560    | 3.547    | 3.538    |
| 1057.799   | 3.718| 3.712  | 3.674  | 3.721    | 3.720    | 3.710    | 3.703    |
| 1299.002   | 3.890| 3.874  | 3.830  | 3.895    | 3.877    | 3.876    | 3.867    |
| 1599.004   | 4.095| 4.069  | 4.018  | 4.103    | 4.065    | 4.074    | 4.063    |

In Table 4 present the results of total neutron fluxes from different libraries (IAEA, JEF2.2, JEF3.1, JENDL3.1, ENDFB6.8, ENDFB7.0 and ENDFB-7.1). The total neutron flux value increases with the decrease in the amount of uranium and thorium in the reactor core. All calculation results show the same results. The highest total neutron flux value at zero burn up is the result of calculations using the ENDFB6.8 library, but the big difference with other calculation results is 1.63%. After the reactor has operated for 1599 days or a maximum burn-up of 60,977 MWd/Kg, the largest total neutron flux value is calculated by JENDL3.2. The biggest difference from other calculations was 2.07%.

### Table 5. Average fast flux as a function of operating time (x 10^12)

| Time (days) | IAEA | JEF2.2 | JEF3.1 | JENDL3.2 | ENDFB6.8 | ENDFB7.0 | ENDFB7.1 |
|------------|------|--------|--------|----------|----------|----------|----------|
| 0.000      | 2.419| 2.270  | 2.386  | 2.290    | 2.400    | 2.414    | 2.437    |
| 1.500      | 2.488| 2.334  | 2.455  | 2.355    | 2.468    | 2.483    | 2.506    |
| 6.000      | 2.495| 2.340  | 2.462  | 2.362    | 2.475    | 2.490    | 2.514    |
| 156.000    | 2.635| 2.471  | 2.597  | 2.496    | 2.611    | 2.628    | 2.650    |
| 277.800    | 2.717| 2.546  | 2.673  | 2.574    | 2.688    | 2.707    | 2.727    |
| 515.999    | 2.870| 2.683  | 2.813  | 2.723    | 2.831    | 2.854    | 2.872    |
| 817.799    | 3.053| 2.846  | 2.981  | 2.895    | 3.000    | 3.032    | 3.045    |
| 1057.799   | 3.198| 2.974  | 3.112  | 3.033    | 3.133    | 3.167    | 3.181    |
| 1299.002   | 3.339| 3.099  | 3.239  | 3.168    | 3.260    | 3.302    | 3.315    |
| 1357.802   | 3.374| 3.129  | 3.271  | 3.201    | 3.292    | 3.335    | 3.347    |
| 1599.004   | 3.507| 3.247  | 3.391  | 3.329    | 3.412    | 3.462    | 3.473    |

In Table 5 present the results of total neutron fluxes from different libraries (IAEA, JEF2.2, JEF3.1, JENDL3.1, ENDFB6.8, ENDFB7.0 and ENDFB-7.1). The fast neutron flux value increases with the decrease in the amount of uranium and thorium in the reactor core. All calculation results show the same results. The highest fast neutron flux value at zero burn up is the result of calculations using the ENDFB7.1 library, but the big difference with other calculation results is 6.85%. After the reactor has operated for 1599 days or a maximum burn-up of 60,977 MWd/Kg, the largest total neutron flux value is calculated by IAEA library. The biggest difference from other calculations was 7.41%.
4. Conclusion
Calculations of the WIMSD-5B with different libraries for the prediction of burn up and other isotope and neutronic parameters, based on comparisons between nuclear data it appears that they can perform thorium calculations with acceptable compatibility. The thorium utilization study uses the simpler and more user-friendly WIMSD-5B code to evaluate which fuel assembly are very popular with users. The pin cell model used to calculate the power distribution in the different effects library is very decisive. Preliminary results show that the results of WIMSD-5B match the reference quite well [IAEA], but using the ENDFB7.1 library is better than all because it is the newest and contains the highest number of isotopes and materials. Tracing the source of this difference should prove to be of benefit to the overall challenge of modeling thorium enriched terraces. It is also hoped that other groups interested in thorium fuel will be able to use the ENDFB7.1 library. The biggest difference with other libraries is 7.41 % and the average difference is around 3.12%.

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