On the utilization of SCALE to generate time dependent cross sections and depletion analysis: the case of Th-Pu cell

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Abstract

This paper shows the utilization of SCALE code package developed by ORNL, to realize fuel depletion analysis by processing time dependent cross section. A short review of the codes used is described. As example of the application of this methodology the IAEA-TECDOC 1349 numerical benchmark for (Th-Pu) O_2 was solved. Numerical results were obtained for the k_{eff}, production of minor actinides, plutonium, ^{233}U bred from thorium, and the one group cross sections versus the heavy metal burn up, showing a reasonable agreement with those reported by the participants in the benchmark exercise.

KEYWORDS: time dependent cross section, depletion analysis, thorium plutonium cell, SCALE code system.

1. Introduction

The analysis of fuel cycles requires in realistic cases several repeated fuel spectrum cell calculation due to spectral changes involved in the burn up process. The spectral cell calculation codes, such as LEOPARD, HAMMER and WIMS, use burn up models which includes few actinides and the fission products are usually treated implicitly. The depletion code ORIGEN can perform depletion calculations using working libraries for certain types of reactors (PWR, HWR). This paper will show that the utilization of the COUPLE module from SCALE is an adequate way for the production of time-dependent (burn up) cross section libraries to be used with ORIGEN-S for any type of reactor cell. This is performed by processing a SCALE or AMPX master library through the SCALE modules [1]: NITAWL, BONAMI and XSDRNPM for any reactor fuel pin lattice to produce a weighted, time–dependent cross sections for input in the ORIGEN-S. In order to qualify this methodology using thorium based fuels, the cell burn up calculation benchmark for a (Pu-Th)O_2 (IAEA-TECDOC 1349[2]) was calculated and results for the k_∞, total neutron flux, fractional amount of Pu, the ^{233}U breed from Th/ initial fissile plutonium and fractional amount of Actinides are compared with those reported by the participants in the Coordinated Research Project(Potential of Thorium based Fuel Cycles to constrain plutonium and reduce the radio toxicity). The calculation of the cell was done using standard master libraries of SCALE, as well as using master libraries up dated with ENDF-B-VI.8 data, processed with NJOY, for ^{233}U, ^{232}Th, and ^{239}Pu.

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2. Calculation Model and the Benchmark on Cell Burn up Calculation

2.1 The Calculation Model

In this work the cell calculation was realized by SAS2H, a module of SCALE 4.4 package. From the definition of the cell geometry, composition and temperature, SAS2H construct a mixing table to be used in the neutronics analyses and fuel depletion.

Besides of nuclides that are in the initial cell composition, it is necessary to add in the SAS2H some traces (10^{-20} g/barn.cm) of nuclides important to the neutronic analyses, like fission products (e.g. Xe), and Minor Actinides. In cases of thorium fuel cells, other important nuclides should be added, like, ^{233}U and ^{233}Pa. The neutronic analysis is performed by BONAMI, NITAWL-II and XSDRNPM, modules of SCALE.

The BONAMI code performs calculations of the Bondarenko´s factor to "correct" neutron cross section due to effects of self-shielding. The code uses cross sections and Bondarenko´s factor from a master library.

Many types of cell geometry and arrangements can be treated using Dancoff approximations. The I/O is in AMPX format, standard of SCALE system.

To access the master library and produce working libraries the SAS2H module use the NITAWL, which perform the Integral Nordheim treatment for self shielding of resonances.

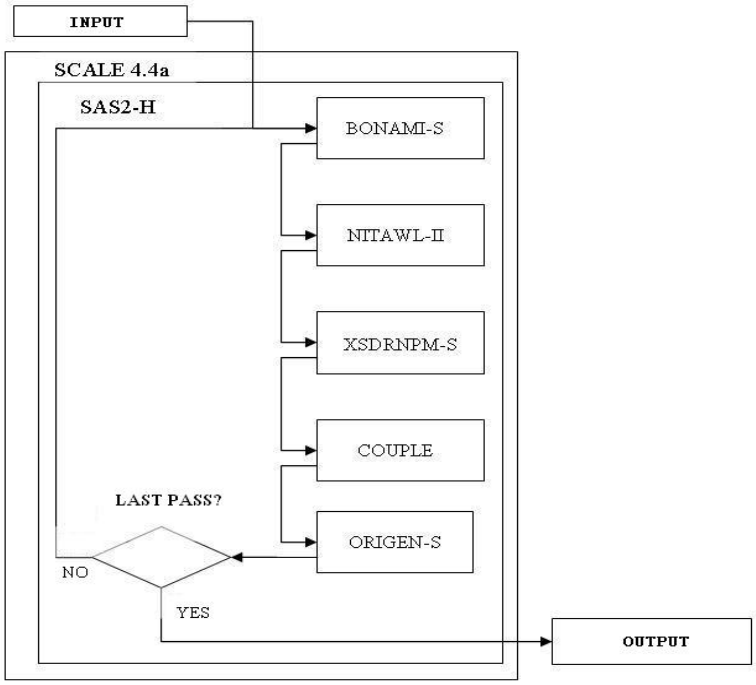
For each composition time dependent of the cell, SAS2H uses the XSDRNPM code to solve by discrete ordinates the one-dimensional multi-group transport equation. The flux calculated by XSDRNPM is utilized to produce cross sections representatives of each burn step. Beside that, the XSDRPM calculates Eigen values (k).

The routine COUPLE automatically couples the flux and the cross sections with the code ORIGEN-S, to solve the decay and transmutation equations to produce concentrations for a new burn step. The input of the COUPLE is a working library produced by the analyses performed by XSDRNPM, BONAMI and NITAWL.

This methodology permit that the ORIGEN-S utilizes cross sections representatives of the operation history of the simulated reactor in each burn up step. The ORIGEN solve the transmutation and decay equations using a one group cross section, weighted by three variables calculated in the neutronics analyses: TERM, RES and FAST.

The standard MASTER libraries available in SCALE 4.4 are a 238 groups ENDFB-V based library and a 33 groups collapsed from the 238 group library. The SCALE have some tools to process these libraries based on the AMPX format. In this work we update some main nuclides with the ENDFB-VI.8 data, using NJOY system. Fig. 2.1.1 shows schematically the calculation methodology.

Figure 2.1.1-Methodology used in SCALE



2.2 The IAEA Benchmark on Th-Pu Cell Burn up Calculation.

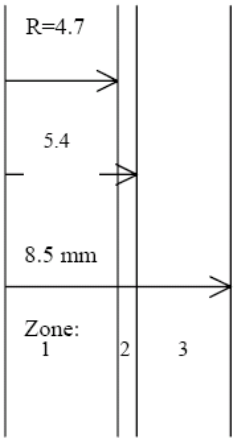
As part of the International Atomic Energy Agency (IAEA) Coordinated Research Project (CRP) on " Potential of Thorium based Fuel Cycle to constrain Plutonium and to reduce Long Term Waste Toxicity", in which participated: China, Germany, India, Israel, Japan, Republic of Korea, Netherland, Russia Federation, and the United States of America, a benchmark was established to compare the effect of different methods and databases for cell burn up calculation: "Calculation of the isotopic composition, cross sections, and fluxes for a typical PWR cell loaded with (Pu-Th)O_2 fuel as function of the fuel burn up".

The Benchmark geometry of the reference cell is show in Figure 2.2.1, and Table 2.2.1 gives the description of material composition in terms of nuclide concentration for the different zones.

The task to be performed for this benchmark was defined as follows: Calculate the fuel burn up at a constant power (211 W/cm) as a function of time, not using any neutron poison for reactivity control, for a burn up of 0, 30, 40, and 60 MWd per kg of Heavy Metal, and comparing the following items: 1) Neutron multiplication(k_{eff}); 2)Total neutron fluxes; 3)Average energy per fission; 4) Residual amount of Plutonium; 5) Fraction of fissile plutonium; 6)Amount of generated minor actinides; 7) Average one-group microscopic cross section, and fission for the heavy metal isotopes from ^{232}Th through ^{244}Cm.

The calculation methods used by the CRP participants varied from country to country. Thus, China and Germany used the VSOP system, a German system developed by FZJ (Julich), with database from ENDF-B-V and JEF 1, India used the WIMSD/4 code with 69 WINS Library, Israel and the USA the ELCOS system, Japan the SWAT code system, Korea the HELIOS/ MASTER code system, Russia WIMS-ABBN, a modernized version of WIMSD/4, and Netherland the OCTOPUS system[8].

Figure 2.2.1- Reference Cell for the Benchmark



Infinite lattice

Average power: P = 211 W/cm

Average temperature of the fuel: T_{fuel} = 1023 K

Average temperature of the water: T_{mod} = 583 K

Table 2.2.1 - Initial nuclide densities in the cell (atoms/cm^3).

	average in cell	zone 1	zone 2	zone 3
Th-232	6.45E+21	2.11E+22		
Pu-238	2.97E+18	9.72E+18		
Pu-239	1.83E+20	5.99E+20		
Pu-240	7.10E+19	2.32E+20		
Pu-241	2.35E+19	7.69E+19		
Pu-242	1.46E+19	4.78E+19		
Cr	1.99E+20		8.14E+19	3.20E+20
Mn	1.26E+19			2.11E+19
Fe	5.20E+20		1.60E+20	8.46E+20
Ni	2.24E+20			3.76E+20
Zr	4.27E+21		4.37E+22	
C	1.60E+18			2.68E+18
H	2.86E+22			4.80E+22
O	2.78E+22	4.41E+22		2.40E+22

3. Results

The comparisons of the results published by the participants in the CRP and the results obtained by this work are show in Figs 3.1-3.7. This work 1 means the results obtained by the SCALE standard library, and 2, using the library generated using ENDF-B VI.

Figure 3.1 - Neutron multiplication vs. heavy metal burn up

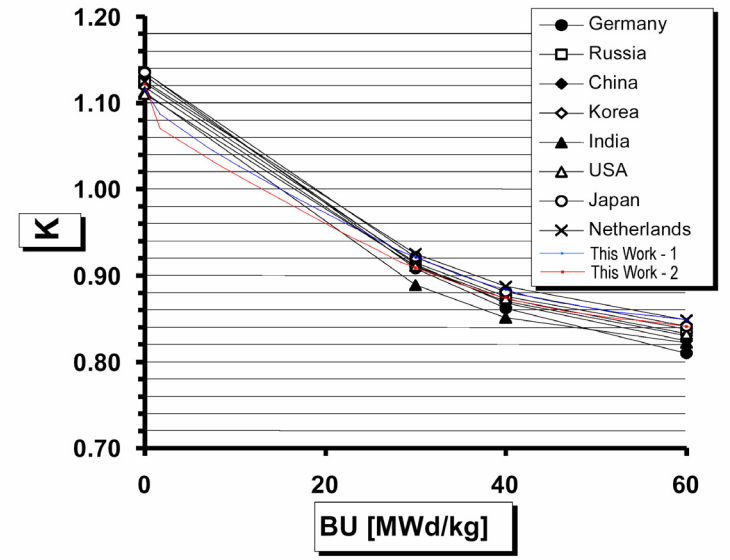


Figure 3.2 - Minor Actinides/ initial plutonium

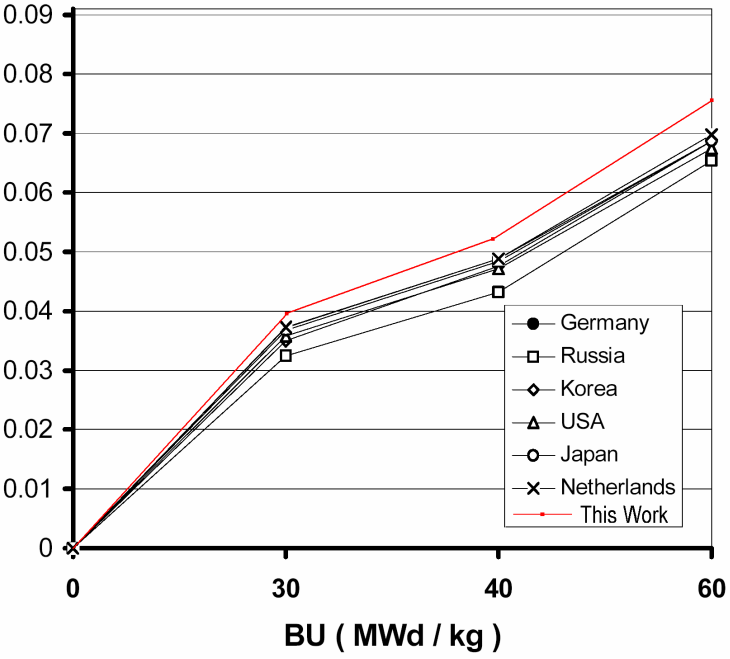


Figure 3.3 -(Pu/Pu initial) vs. heavy metal burn up (MWd/t)

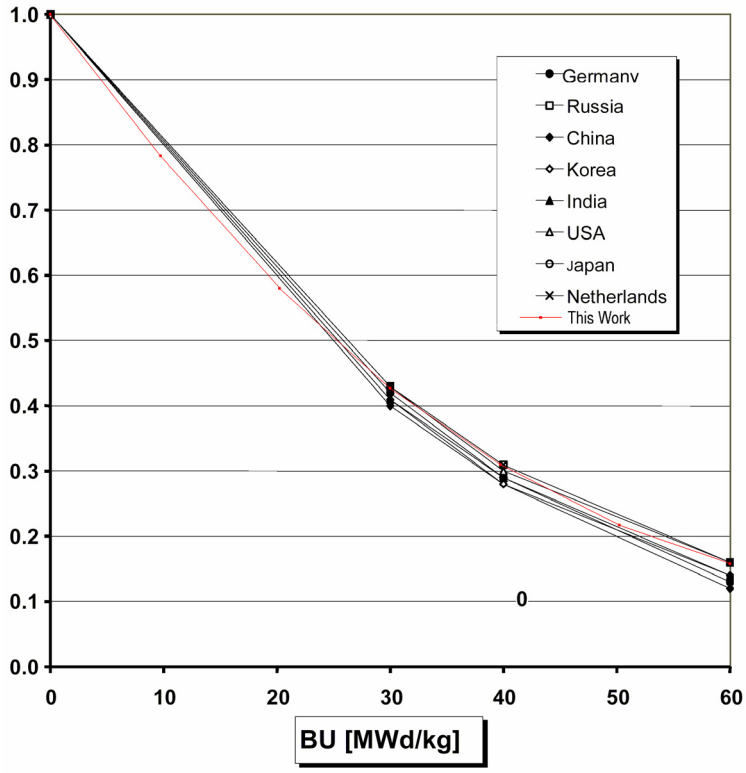


Figure 3.4 - (Pu-fiss/Pu-total) vs. Heavy metal burn up.

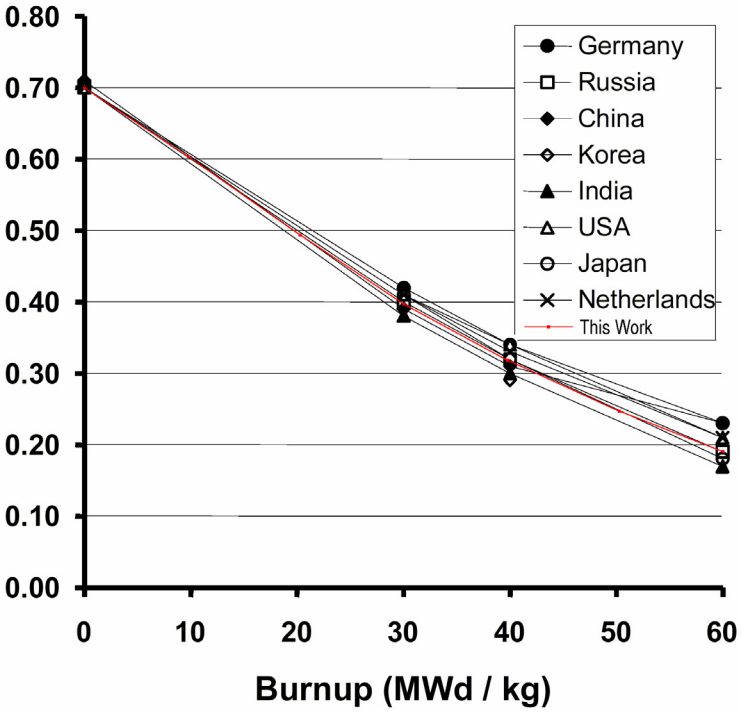


Figure 3.5 - ^{233}U bred from Th/ initial fissile plutonium

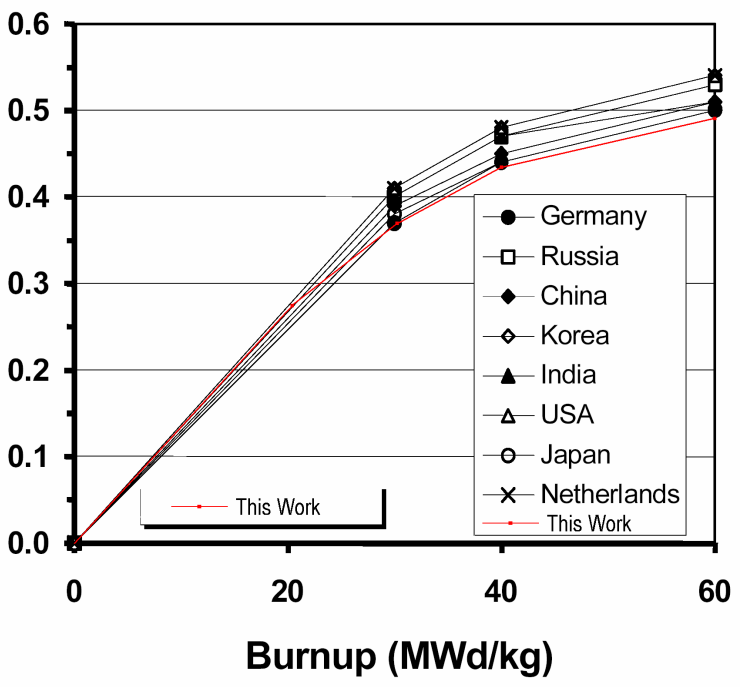


Figure 3.6 -(.Fission/ absorption) cross sections (BOL)

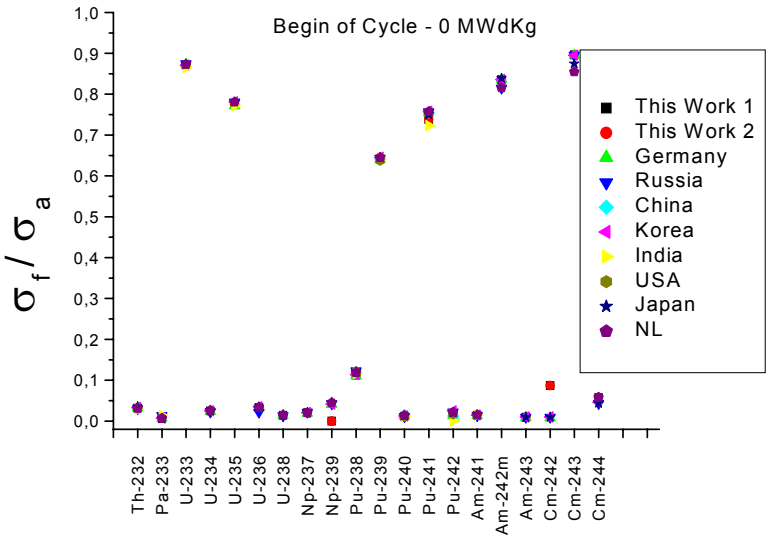
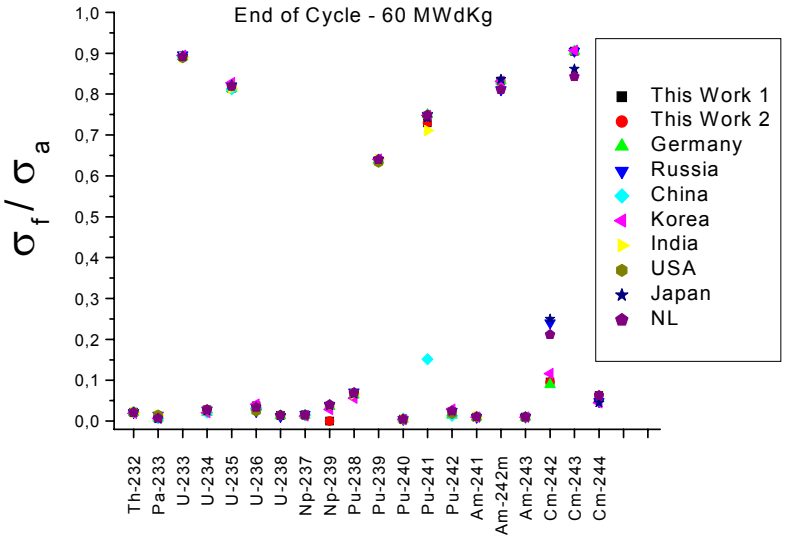


Figure 3.7 - (Fission/ absorption) cross sections (EOL).



4. Conclusions

The comparison of the results obtained by the participants and our results are in agreement within ~2 %(BOL) - and 5% (EOL) for the calculated cell reactivity ($\Delta\rho$), as show in Fig. 3.1. The results for the production of Minor Actinides per initial plutonium, overestimate the results obtained by the CRP participants, however the Plutonium consumed are in agreement with them. The results of the one group cross sections (fission and absorption), are in general in agreement with those reported by the CRP participants. Therefore in general, the calculation method using SCALE reproduces satisfactorily the results of the benchmark, indicating that it can be used in thorium-plutonium cells to depletion calculation and to generate one group time dependent cross sections to be used by ORIGEN. The case of U-Pu cells has been demonstrated in a previously work [9].

Acknowledgements

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