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February 14, 2007

Dr. Donald E. Carlson
Office of Nuclear Regulatory Research
U.S. Nuclear Regulatory Commission
Mail Stop T-10 F13A
Washington, D.C. 20555-0001

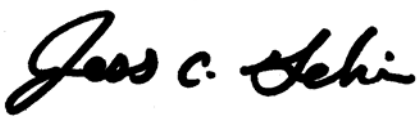
Dear Dr. Carlson:

Final Deliverables for Tasks 6, 7, and 8 of JCG Y6846

Please find attached documentation of the finalization of Task 6 "SCALE S/U Methods and Data for Reactor Physics Validation," Task 7 "Advanced 2-D and 3-D Reactor Lattice Physics methods," and Task 8 "SCALE Tools for Analysis and Plotting of Code Data and Results." The information provided documents the completion of the final deliverables of each task and combined with the previous deliverables marks the finalization of the work under this JCN.

If you have any comments or questions, please do not hesitate to contact me.

Sincerely,



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File NRC/Y6846/Deliverbles

JCN 6846 Task 6 – SCALE S/U Methods and Data for Reactor Physics Validation

TSAR Sensitivity/Uncertainty Tool

As described in Letter Report JCN Y6846/LTR2005/02, a new general purpose sequence has been created to perform the calculation of sensitivities of reactivity changes, which can be used to compute the sensitivity of reactor physics parameters, such as reactivity coefficients to particular cross section data and the uncertainty that results from nuclear data uncertainties.

This tool was originally developed to help assess the uncertainties and biases in the coolant void reactivity (CVR) for the ACR-700, but was developed in a completely general fashion so that it can be applied to other reactor systems as well. As an example of this capability, the overall relative standard deviation in the ACR-700 CVR resulting from nuclear data uncertainties was determined to be approximately 50%. Sensitivity profiles for cross section of interest were plotted using the Javapeno tool I demonstrated in Figure 1 below, which shows the energy dependent sensitivity of the CVR to the hydrogen cross section for a ACR-700 fuel bundle.

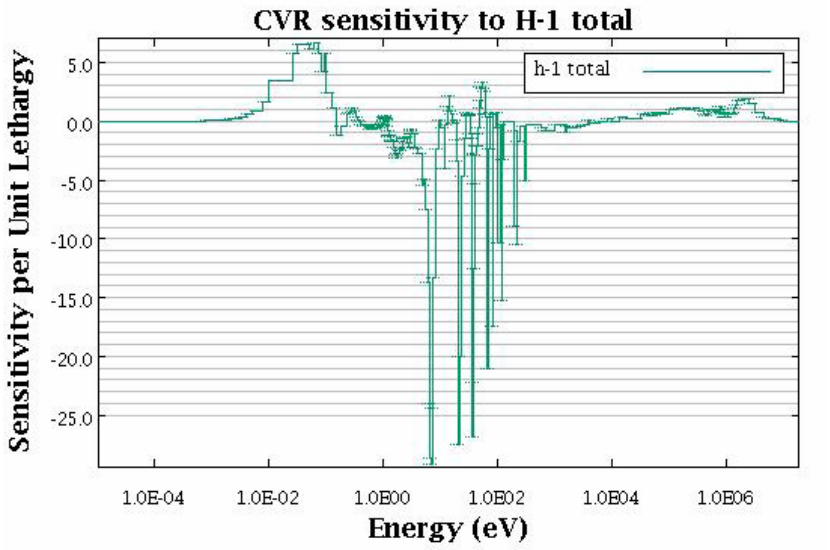

Figure 1. Sensitivity of CVR to hydrogen total cross section.

Minor developments continued in the development of TSAR along with some prototypic applications to problems of interest. Based on the status of the development of the code, it has not yet been released. However, it is available for applications as needed. The theoretical documentation is complete and a limited effort is necessary to provide user documentation. The code has been updated to work with the current release version of SCALE 5.1.

Suggested areas for future use and development include the application of TSUNAMI to the void reactivity coefficients for BWR or ESBWR reactors, development of TRITON to compute the eigenvalue sensitivities so that this two can be used for 2-D lattices, and final testing and release. More generally, development of Generalized Perturbation Theory (GPT) and Depletion

Perturbation Theory (DPT) methods should be pursued to expand the overall capability to perform sensitivity, uncertainty, and bias results for the assessment of margins and limits to support licensing decisions.

JCN 6846 Task 7 – Advanced 2-D and 3-D Reactor Lattice Physics Methods

Updated TRITON with improvements in collapsed library generation, resonance processing, and particle fuel depletion capability

Introduction

SCALE 5.1 released in 2006 contains several enhancements to improve the lattice physics and resonance processing capabilities. Enhancements were made to the resonance processing methods to allow a simplified two-region treatment to allow more efficient resonance processing that is accurate for many types of problems, the ability to treat double-heterogenity in the fuel for criticality problems, and the ability to perform 3-D Monte Carlo Depletion calculations with KENO Va and KENO-VI within the TRITON sequence. These capablities are described in detail in the SCALE 5.1 manual.

The fuel used in pebble bed and prismatic reactor concepts, such as the Pebble Bed Modular Reactor (PBMR) and the Gas-Turbine Helium Modular Reactor (GT-MHR) consists of small fuel grains (~400 microns in diamater) surrounded by layers of graphite and silicon carbide embedded in either a graphite pebble or cylindrical fuel compact. These fuels are said to have a "double heterogeneous" structure because of the local fuel grain heterogenity as well as the pebble-to-pebble or compact-to-compact heterogenity. This double-heterogenity structure must be taken into account during cross section processing to obtain accurate results. The cabilitity included in SCALE 5.1 allows the analysis of systems containing double heterogeneous materials but did not include the capability to perform depletion. Under this task, the TRITON sequence was modified to work with the double-heterogeneous processing capability to allow depletion to be performed, and is described in more detail below.

Overview of the Double Heterogenity Capability in SCALE

The standard approach for the treatment of double heterogenity in resonance processing is based on the calculation of Dancoff factors for the specific material of interest. Analytic formulations and Monte Carlo approaches are available for providing the Dancoff factors. Indeed, this method can be used in SCALE with the NITAWL module or the two-region option of CENTRM. The approach implemented in SCALE, however, does not use Dancoff factors and is based on the solution of the continuous energy equations for the particle and then pebble or compact. In this manner, spatial resonance shielding effects are handled directly.

Cross sections are resonance-shielded using the CENTRM/PMC/CHOPS modules of the SCALE code system. CENTRM solves the 1-D transport equation using point-wise cross sections to calculate the corresponding point-wise spectrum, over an energy range specified by the user (usually the resonance range). PMC uses the point-wise cross sections, the CENTRM-calculated point-wise spectrum, and the multigroup data (where point-wise spectrum is not calculated) and generates multigroup cross sections. Double heterogeneity is accounted for by first calculating the point-wise flux disadvantage factors for the particle-matrix unit cell and then using these factors to create the homogenized point-wise particle/matrix mixture cross sections. The homogenized point-wise cross sections are used on the second pass to create the final resonance-shielded multigroup cross sections that represent the fuel pebbles. This scheme is very rigorous and does

not rely on calculating Dancoff factors as is the case for most other multigroup resonance processing codes. Lattice effects are approximated by using the white boundary condition. The flowchart of the CSAS code sequence execution is shown in Fig. 1. Further information is available in the Material Information Processor for SCALE manual, Vol. III, Sect. M7 of the SCALE 5.1 manual.

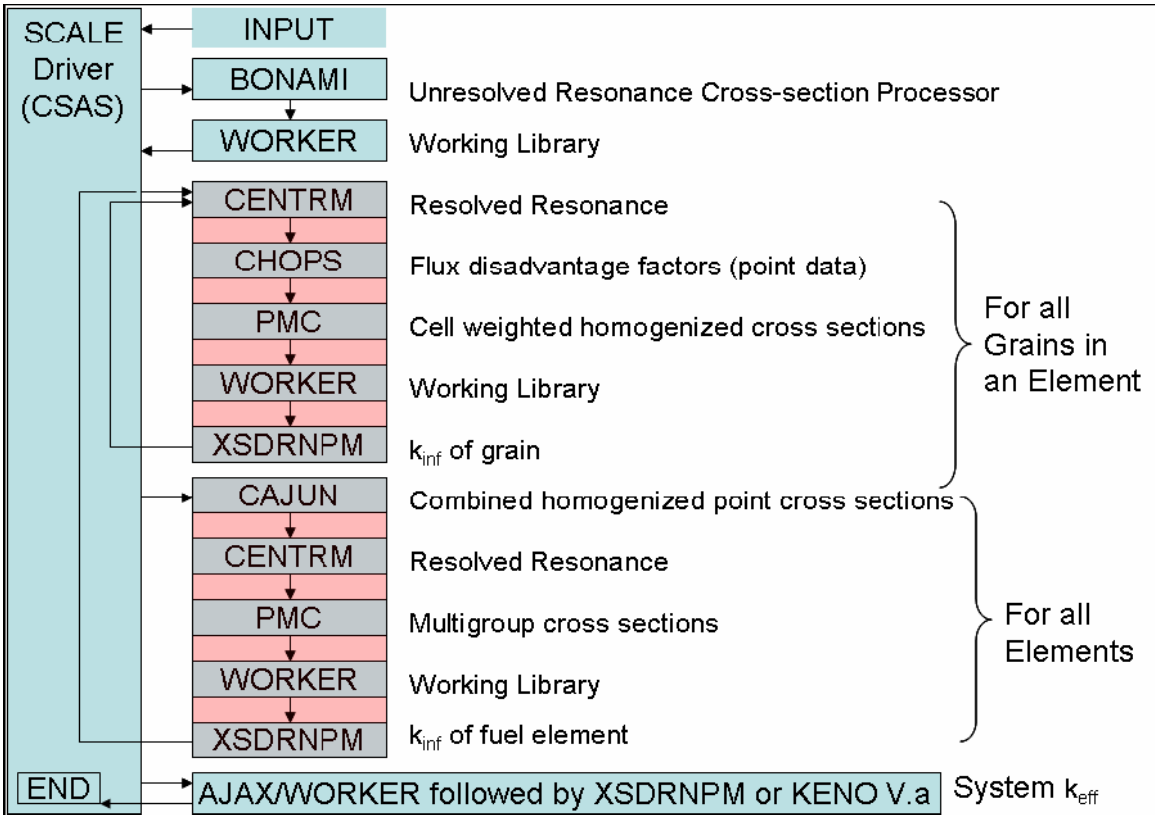

Fig. 1. Flow diagram for the double heterogenity processing in SCALE 5.1

Description of Work Performed Under this Task

The process described above and presented in Fig. 1, while general, was intended for a single state-point calculation and not for the depletion process. It's incorporation into the TRITON depletion sequence required modifications to exchange volume and atom density information to be able to execute this two-pass option within the depletion loop of TRITON. Note that since the fuel homogeniziation is performed outside of the TRITON NEWT calcluation (unlike the case for light water reactor lattices), the resulting homogeized atom densities had to be "un-homogenized" using their volume information. While, not difficult in theory, several changes to TRITON were required to pass the necessary volume information. These changes have been made and two-step process can now be called from within TRITON to deplete double-heterogeneous materials.

An annotated input file is included in Fig. 2, that shows the key features of a TRITON input file for the modeling of an infinite lattice of fuel compacts containing particle fuel. The key input is provided in the celldata block, as repeated below:

```
read celldata
doublehet  right_bdy=white fuelmix=10 end
gfr=0.025  101 coatt=0.009 102 coatt=0.004 103 coatt=0.0035 104 coatt=0.004 105
matrix=106 numpar=15000 end grain
rod squarepitch right_bdy=white hpitch=3.0 108 fuelr=2.5 cladr=3.0 107 fuelh=365 end
centrm data ixprt=1 isn=6 nprt=2 end centrm
```

This input provides the fuel mixture (10), the outer radius of the fuel kernel (0.025 cm), several coatings (0.009, 0.004, 0.0035, and 0.004 cm in thickness), the matrix material (106), the number of fuel particles (15000), and the dimension of the fuel compact.

This compact was depleted within TRITON and provided the kinf vs depletion curve as presented in Fig. 3. This sample case provides the indication that the capability is now functional within the TRITON depletion sequence. Previous benchmarking has been performed for the double-heterogeneity treatment for fresh fuel, but the depletion capability has not been validated. It is currently available for use at ORNL for testing and validation before release in the next version of SCALE.

Recommendations for Future Work

Under this task, the ability to perform fuel depletion with the SCALE 5.1 double heterogeneity treatment has been implemented. Sample cases have been used to test the functionality, but there has been no verification and validation of the capability. The following areas are recommended as future activities to validate this capablity and to improve the approach for pebble bed reactors:

1. Verification and Validation: Limited data is available for the verification and validation of the depletion of double-heterogeneous fuel material. Results can be obtained from benchmarks performed under the OECD/NEA Working Party on the Scientific Issues of Reactor Systems. Isotopic assay data for these fuels are very limited and additional data is needed to validation.

2. Analysis of the PROTEUS and HTR-10 Experiments: Data is available for the PROTEUS and HTR-10 facilties to provide benchmarking for pebble bed reactors. The available data is for criticality with fresh fuel and therefore, will not provide a verification of the depletion capablition. These benchmarks, however, will provide valuable validation of the application of SCALE to such systems.

3. Incorporation of XSDRN into TRITON: The NEWT transport module of the TRITON system cannot be used for the analysis and cross section generation for fuel pebbles because it is limited to 2-D (X-Y) geometry. It can be applied to the prismatic concepts. Currently the analysis requires the use of the KENO-Va and KENO-VI Monte Carlo codes. Incorporation of the 1-D transport code, XSDRN in to TRITON would allow the analysis of fuel pebbles with a deterministic code and in a more efficient manner.

4. Double-Het Depletion with KENO V.a and KENO-VI: The Monte Carlo codes use a different mixing table than is used by NEWT within TRITON. A minor extension of the work performed under this task is needed to use KENO V.a and KENO-VI for depletion using the double-heterogeneous option.

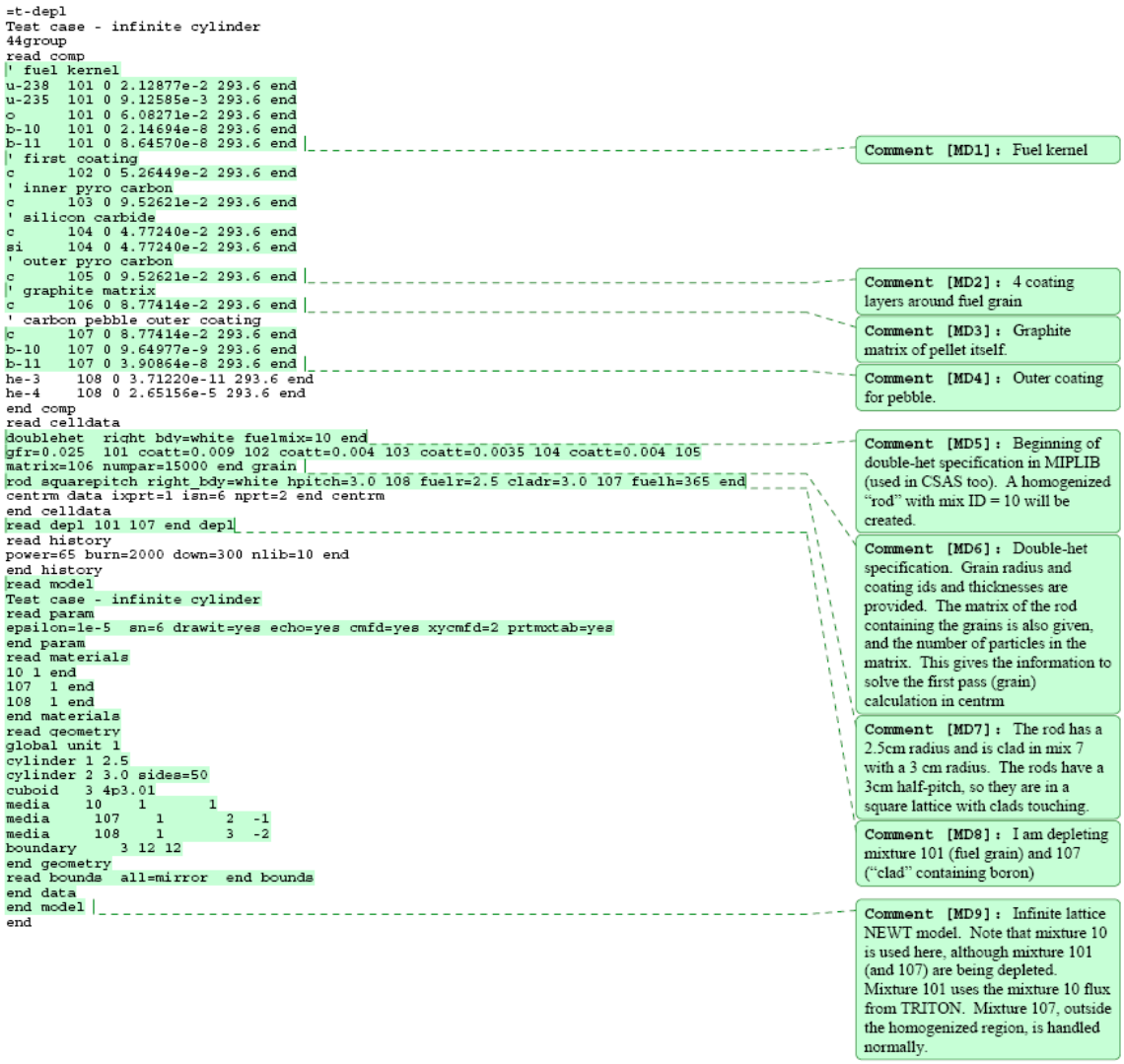

Fig. 2. Annotated TRITON input file for the depletion of an infinite lattice of fuel compacts.

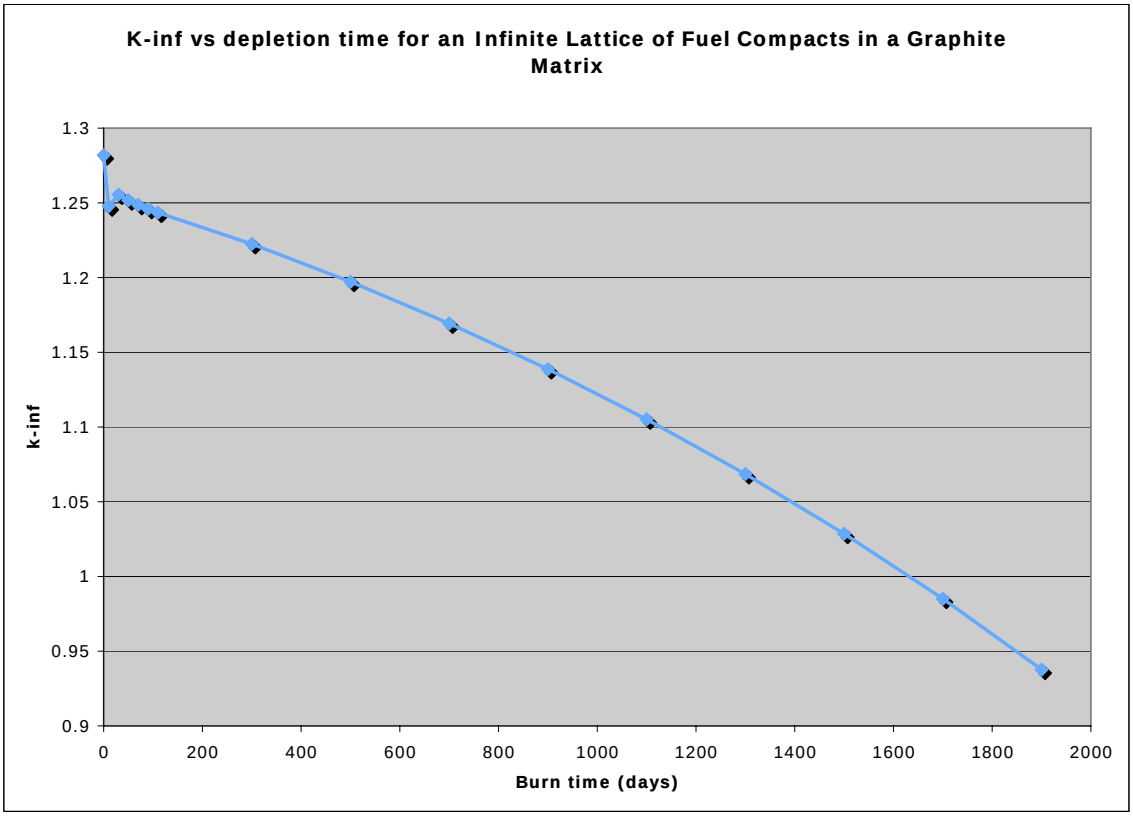

Fig. 3. K-inf vs depletion time for the sample case of an infinite lattice of fuel compacts.

JCN 6846 Task 8 – SCALE Tools for Analysis and Plotting of Code Data and Results

Updated Javapeno with Plotting Enhancements

Javapeño (**Java P**lots, **E**specially **N**ice **O**utput) is an interactive two-dimensional (2D) and three-dimensional (3D) plotting package that is written in Java and operates on numerous computing platforms. Javapeño enables the plotting of data from TSUNAMI-A and TSUNAMI-B sensitivity data files, KENO V.a and KENO-VI data files generated with KMART and KMART6, XSDRNPM data files, and SMORES data files. A new version of Javapeno with plotting enhancements was released with SCALE 5.1. Many new features have been added to Javapeno since its version 1.0 release. Below is a list highlighting the major (and some minor) new features:

1. 3D plotting capability
2. Support for multigroup cross-section data (AMPX)
3. Support for multigroup cross-section covariance data (COVERX)
4. Modern, floating window layout for Javapeno's application mode
5. Advanced 3D plotting customization such as zooming, panning, rotating
6. Auto-rotate ability on 3D plots
7. Simple mathematical operation capability for 2D plots
8. Addition of a general 3D plot data type.
9. Printer Page Layout customization
10. Improved applet mode capabilities and layout