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An Overview of What's New in SCALE 5

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Introduction

The SCALE (**S**tandardized **C**omputer **A**nalyses for **L**icensing **E**valuations) [1] computer software system developed at Oak Ridge National Laboratory (ORNL) is widely used and accepted around the world for criticality safety analyses. Version 5 of SCALE contains several significant new modules and sequences for criticality safety analysis and marks the most important update to SCALE in more than a decade. This paper highlights the capabilities of these new modules and sequences.

Continuous Energy Flux Spectra For Multigroup Cross Sections

The resolved resonance processor modules CENTRM and PMC [2] provide one of the most significant new capabilities in SCALE 5. CENTRM (**C**ontinuous **En**ergy **Tr**ansport **M**odule) is a one-dimensional (1-D) discrete ordinates code that produces a problem-dependent pointwise continuous energy flux spectra at discrete spatial intervals for each unit cell. Using these fluxes, PMC (**P**ointwise **M**ultigroup **C**onverter) collapses the pointwise continuous energy cross sections into multigroup cross sections for each nuclide in each material in the unit cell. Subsequent modules in SCALE 5 can then use these multigroup cross sections. Discrete-level inelastic cross-section data can also be processed by CENTRM/PMC. Figure 1 shows a flow chart of the CSAS sequence (**C**riticality **S**afety **A**nalysis **S**equence) for cross-section processing using CENTRM and PMC.

CENTRM/PMC avoids many of the inherent assumptions in NITAWL by calculating a problem-dependent flux profile, thus making it a far more rigorous cross-section treatment. Effects from overlapping resonances, fissile material in the fuel and surrounding moderator, and inelastic level scattering are explicitly handled in CENTRM/PMC. Another advantage of CENTRM is that it can explicitly model rings in a fuel pin to more precisely model the spatial effect on the flux and cross sections. CENTRM/PMC enables problem-dependent multigroup cross sections to have the flexibility and accuracy of pointwise continuous energy cross sections for criticality safety analyses.

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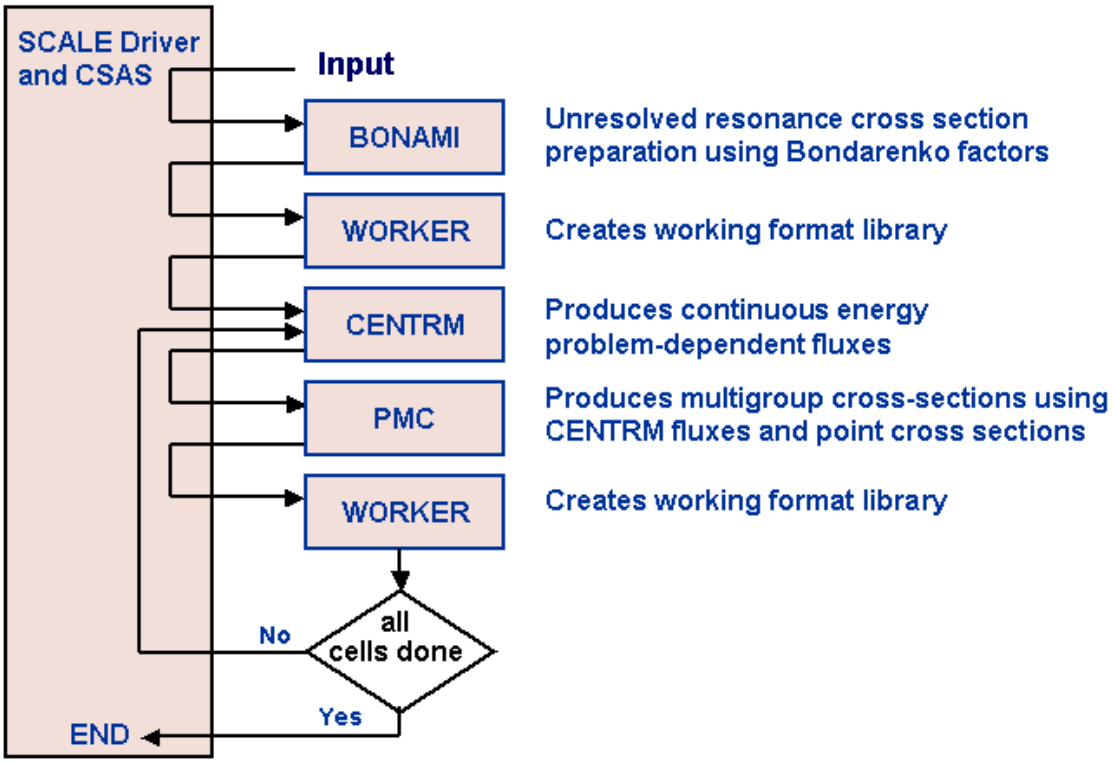

Figure 1. CSAS cross-section processing using CENTRM/PMC

ENDF/B-V continuous energy cross-section data files for CENTRM have been developed as part of SCALE 5. These data files correspond to the ENDF/B-V 238- and 44-group cross-section libraries in SCALE. ENDF/B-VI continuous energy data for CENTRM are under development for a future release of SCALE.

ENDF/B-VI Multigroup Resonance Cross-Section Processing

SCALE 5 is the first version to have the capability to handle ENDF/B-VI resonance data. NITAWL-III [2] is a new version of the Nordheim Integral Treatment resonance data processor that has the capability to process multi-pole data, thus enabling it to process an ENDF/B-VI cross-section library with the Reich-Moore resonance parameters converted to multi-pole parameters. Although an ENDF/B-VI multigroup cross-section library is not available in SCALE 5, work is currently underway to generate and validate such a library for a future release of SCALE.

Sensitivity and Uncertainty for Criticality Safety Analyses

ORNL has invested a significant effort in the development of sensitivity and uncertainty (S/U) analysis capabilities for criticality safety [3]. Both 1-D and three-dimensional (3-D) sequences have been developed, plus several auxiliary codes.

SEN1, a 1-D sensitivity sequence, generates sensitivity coefficients that represent the percent change in the system k_{eff} for a one percent cross-section value change in a given energy group for each reaction type and isotope of interest (nuclide-reaction pair). This sequence performs standard resonance-processing tasks using BONAMI and NITAWL, then determines the forward and adjoint angular fluxes and flux moments needed for sensitivity coefficient generation using the 1-D transport XSDRNPM code.

The SEN3 sequence has been developed for cross-section sensitivity analysis of 3-D criticality safety models. SEN3 performs automated problem-dependent cross-section processing exactly as is done in the CSAS/KENO V.a sequence in SCALE. It then uses the updated KENO V.a Monte Carlo code to produce forward and adjoint angular flux solutions necessary for sensitivity calculations. Sensitivity calculations are subsequently performed using first-order-linear perturbation theory in the SAMS module. The input specification for SEN3 is very similar to CSAS, but there are some additional optional parameters that may be entered. If only CSAS input is entered, SEN3 will execute with a set of default values for the optional parameters. This will yield reasonable results for most cases.

Plotting routines have been developed to read the energy-dependent sensitivity data files and produce two-dimensional (2-D) plots for visualizing the data. Javapeno (**Java** **P**lots **E**specially **N**ice **O**utput) is a Java program designed to plot data from the sensitivity sequences SEN1 and SEN3 as well as the material optimization sequence SMORES discussed later in this paper. A sample plot of SEN3 results displaying a comparison of the sensitivity of k_{eff} to the ^{239}Pu fission cross section for two critical experiments is presented in Figure 2. Because of the cross-platform capabilities of Java, Javapeno can execute on any computer for which the Java Runtime Environment is available. Further capabilities of Javapeno are discussed more fully in another paper [4] at this meeting.

A data processing code called CANDE (**C and E**) was created to perform the integral parameter analyses using the sensitivity data created from the SEN1 and/or SEN3 sequences. The user of CANDE provides a list of applications, which will be compared to a list of critical experiments. CANDE assigns numerical correlations between each application and critical experiment for parameters of interest.

Flexible Mesh 2-D Discrete Ordinates

Since its initial release, SCALE has offered capabilities for 1-D and 3-D criticality safety analyses using the XSDRNPM 1-D discrete ordinates code and the KENO 3-D Monte Carlo code. SCALE 5 introduces 2-D analytical capability via the NEWT [5] (**NEW** **T**ransport algorithm) flexible mesh discrete ordinates code. Unlike traditional S_n codes, NEWT is not limited to Cartesian or cylindrical coordinate systems. NEWT's arbitrary geometry, or flexible

mesh, allows users to combine orthogonal, radial, and other more unusual geometry shapes in the same model. The modeling capabilities of NEWT are discussed more fully in another paper at this meeting [5]. Figure 3 depicts the NEWT 2-D flexible mesh model for a BWR fuel assembly and the visualization of the flux distribution over the assembly.

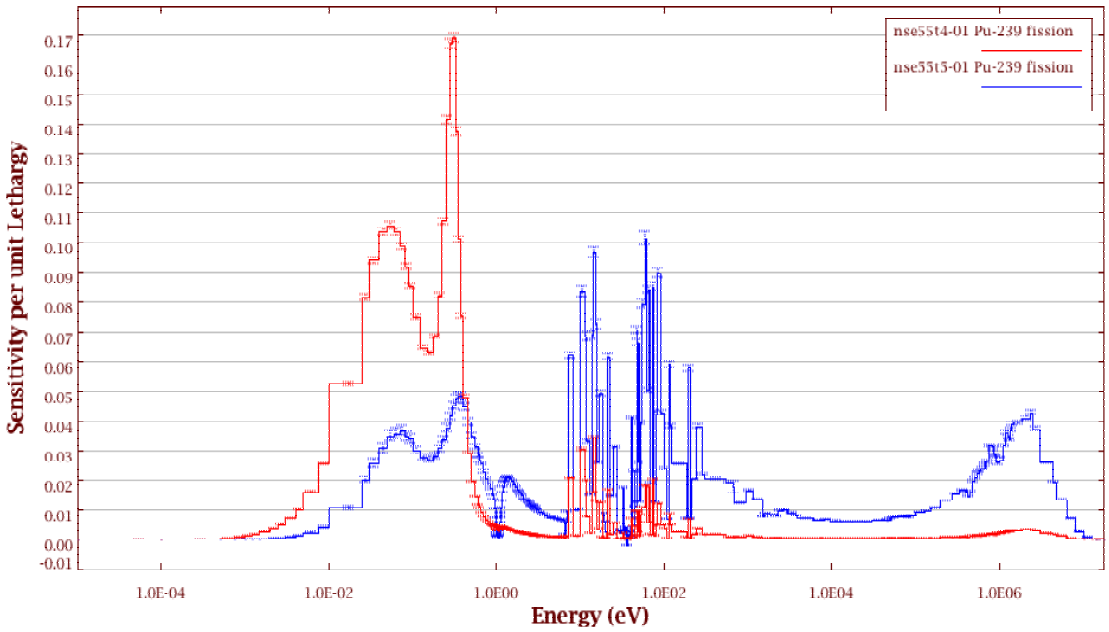

Figure 2. Comparison of sensitivity of k_{eff} to ^{239}Pu fission cross section.

Problem-dependent cross sections can be generated by BONAMI/NITAWL or CENTRM/PMC via the new SAS2D control module [6]. SAS2D provides automated sequences for 2-D criticality safety analyses and 2-D lattice cell depletion.

Burnup-Credit Analysis Sequence

STARBUCS [7] (**St**andardized **A**nalysis of **R**eactivity for **Bu**rnup **C**redit using **S**CALE) is a new sequence to perform criticality calculations for spent fuel systems employing burnup credit. STARBUCS automates the coupling of the depletion and criticality aspects of the calculation, thereby eliminating the need to manually process spent fuel isotopic compositions from a burnup calculation into the units and formats required by criticality codes. STARBUCS automatically prepares the input for all codes in the analysis sequence, executes the codes through the SCALE driver, and performs all module interface and data management functions for the user.

STARBUCS uses the ORIGEN-ARP methodology to perform the burnup analysis for each spatially varying burnup region of a fuel assembly. The final spent fuel compositions are used to generate macroscopic fuel cross sections using CSAS. Finally, KENO V.a or KENO-VI is used to perform a 3-D criticality calculation. The flowchart in Fig. 4 illustrates the calculational process.

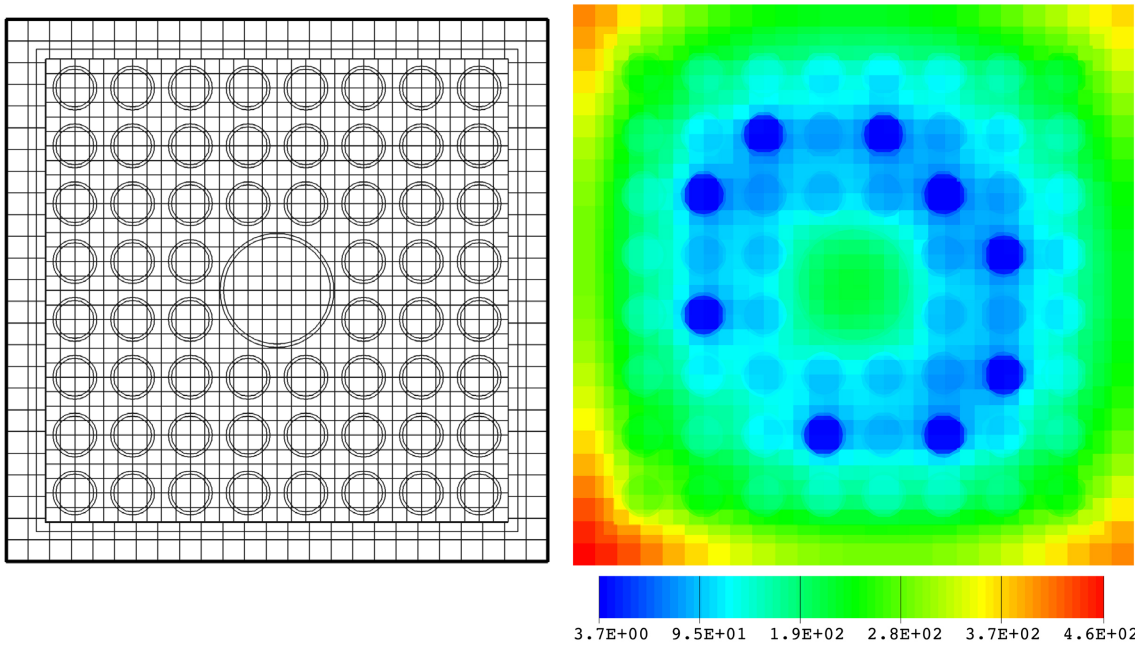

Figure 3. NEWT 2-D BWR fuel assembly lattice.

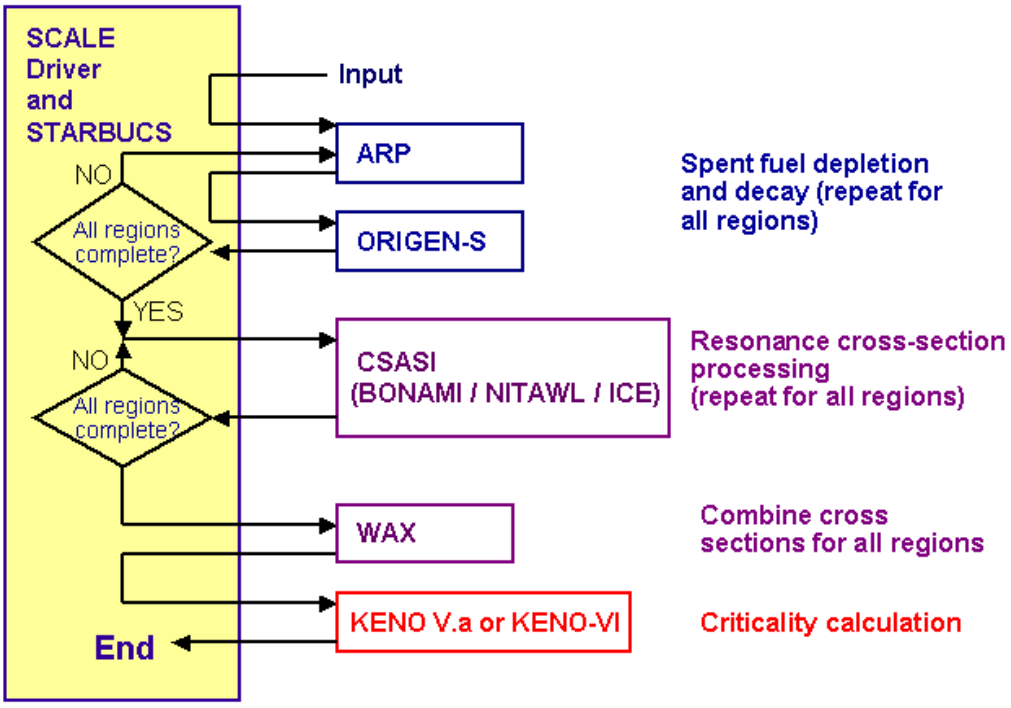

Figure 4. STARBUCS calculational sequence.

Options are provided to allow simulation of many of the dominant burnup-credit phenomena. An arbitrary axial and/or horizontal burnup profile may be specified. Default "built-in" profiles are also available. The user may select the specific actinides and fission products to be used in the criticality calculation and optionally specify isotopic correction factors to account for bias and uncertainty in the calculated inventories. The user may also specify any irradiation and cooling time history. The input format is fashioned around the existing depletion (SAS2H) and criticality (CSAS) sequences of SCALE. Only a minimal amount of input beyond that typically required for a fresh-fuel calculation is needed to perform a burnup-credit calculation using STARBUCS.

Material Optimization for Criticality Safety Analysis

A new SCALE control module named SMORES [8] (**S**CALE **M**aterial **O**ptimization and **RE**placement **S**equence) has been developed as part of the Applicable Ranges of Bounding Curves and Data (AROBCAD) Task undertaken by the DOE Nuclear Criticality Safety Program. The purpose of SMORES is to perform automated 1-D optimization for criticality safety analysis.

The SMORES sequence consists of three major steps: (1) preparation of the problem-dependent cross sections, (2) execution of the 1-D XSDRNPM discrete ordinates code to calculate the angular forward and adjoint fluxes, and (3) calculation of effectiveness functions and optimization of the system using the SWIF module developed by the University of California, Berkeley [9]. SMORES/SWIF optimizes a specified parameter (k_{eff} or minimum mass) by calculating effectiveness functions determined from first-order linear perturbation theory by using the fluxes calculated by XSDRNPM and the problem-dependent cross sections. Since the optimization process is iterative, the above steps are repeated until convergence is achieved.

Conclusions

SCALE 5 contains many new capabilities, including: continuous energy flux spectra for processing multigroup problem-dependent cross sections; END/B-VI resonance processing for multigroup cross sections; 1-D and 3-D S/U analyses for criticality safety evaluations; 2-D flexible mesh discrete ordinates code; automated burnup-credit analysis sequence; and 1-D material distribution optimization for criticality safety.

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