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OVERVIEW OF THE SCALE CODE SYSTEM

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INTRODUCTION

The Standardized Computer Analyses for Licensing Evaluation (SCALE)[1] computer software system developed at Oak Ridge National Laboratory (ORNL) is widely used and accepted around the world for nuclear applications such as problem-dependent resonance self-shielding of cross-section data, criticality safety, radiation source terms and shielding, sensitivity and uncertainty, and reactor physics analyses. Version 5.1 of SCALE was released in November 2006, and Version 6.0 is scheduled for release in October 2008. SCALE 5.1 has been implemented and tested on Linux, Unix, and Windows computing platforms. Executables for Linux and Windows are included in Version 5.1. This paper presents an overview of the capabilities in Versions 5.1 and 6.0.

RESONANCE SELF-SHIELDING OF CROSS-SECTION DATA

SCALE 5.1 includes both continuous energy and multigroup ENDF/B-VI cross-section libraries. The multigroup library is a 238-group general purpose criticality safety library with the same energy group structure as the 238-group ENDF/B-V library in SCALE. All cross-section libraries in SCALE have been generated with the AMPX code system.[2]

The resolved resonance processor modules CENTRM (Continuous Energy Transport Module) and PMC (Pointwise Multigroup Converter) provide a rigorous method for generating problem-dependent multigroup cross sections. CENTRM performs a 1-D discrete ordinates calculation to generate a continuous energy spectrum for a unit cell using pointwise cross-section data. PMC uses the continuous energy flux and cross sections from CENTRM to generate problem-dependent multigroup cross sections. Because CENTRM/PMC calculates a problem-dependent flux profile, it provides a rigorous cross-section treatment that explicitly handles effects from overlapping resonances, fissile material in the fuel and surrounding moderator, anisotropic scattering, and inelastic level scattering. An efficient two-region solution method is also available with CENTRM. The two-region approximation usually runs much faster than the discrete-ordinates solution and is adequate for a wide range of standard applications, such as reactor fuel assembly lattices.

A new resonance self-shielding option in the SCALE criticality safety calculational sequences can address doubly heterogeneous cells (e.g., pebble bed or prismatic fuel where small micrograins of fuel and moderator matrix are contained in larger spheres or rods) by applying sequential CENTRM/PMC resonance calculations for the low-and high-level heterogeneities. This method computes PW disadvantage factors to obtain cell-homogenized PW cross sections from the low-level unit cell to use in the high-level unit cell resonance-shielding computation.

KENO V.A AND KENO-VI: CRITICALITY SAFETY

The KENO V.a and KENO-VI Monte Carlo codes are designed for criticality safety calculations. In SCALE 5.1, these codes perform multigroup calculations. In SCALE 6, both versions will also be capable of performing continuous energy calculations.

KENO V.a uses basic geometrical bodies for defining a geometry model: cuboids, spheres, cylinders, hemispheres, hemicylinders, and arrays. KENO V.a does not allow intersecting regions or non-orthogonal orientations. Because of the simplified geometry design of KENO V.a, it runs much faster than other widely used Monte Carlo codes for criticality safety. KENO-VI uses a generalized geometry scheme known as the SCALE Generalized Geometry Package (SGGP). It constructs and processes geometry data as sets of quadratic equations. KENO-VI has a much more extensive set of geometric shapes, including cones, wedges, parallel planes, and hexprisms. The code's flexibility includes the following features: intersecting geometry regions; hexagonal as well as rectangular arrays; rotations of bodies to any angle and truncated to any position; and the use of an array boundary that intersects the array. Users should be aware that the added geometry features in KENO-VI can result in longer run times than KENO V.a, but these are comparable to other Monte Carlo criticality safety codes. A KENO-VI problem that can also be modeled with KENO V.a will typically run four times as long as the same problem using KENO V.a. Thus, version VI is not a replacement for the existing version V.a, but an additional version for complex geometries that could not be modeled previously.

Plotting capabilities for both KENO V.a and KENO-VI include 2-D color plots and 3-D interactive visualization using KENO3D. The Windows graphical user interface (GUI) named GeeWiz (Graphically

Enhanced Editing Wizard) in SCALE can be used to set up and run both KENO V.a and KENO-VI.

An advanced HTML-formatted output interface for KENO V.a has been developed as part of SCALE 5.1 and will be available in KENO-VI in SCALE 6. The use of HTML as an alternative output interface for SCALE codes provides the user with a convenient and familiar means of navigating and visualizing data. HTML presents a wide variety of formatting options for differing fonts, colors, and data tables. More advanced technologies such as Java applets and JavaScript are incorporated into the output for advanced navigation and data visualization.

ORIGEN-ARP: SPENT FUEL CHARACTERIZATION, DECAY HEAT AND RADIATION SOURCE TERMS

The preeminent computer code used internationally to predict spent fuel isotopic concentrations and associated radiation sources is ORIGEN (Oak Ridge Isotope GENeration). The modern version is ORIGEN-S, which is one of the key functional modules in SCALE.

ORIGEN-S currently tracks 1119 individual fission products generated in the fuel during irradiation, 129 actinides, and 698 isotopes associated with structural and/or activation components. The nuclear data have been recently updated with most of the decay data, cross sections, and fission product yields based on ENDF/B-VI evaluated nuclear data. Data not available from ENDF/B-VI are obtained from the Evaluated Nuclear Structure Data File (ENSDF), the Fusion Evaluated Nuclear Data Library (FENDL), and the European Activation File (EAF). Explicit fission yields for 30 fissile and fissionable actinides, including 240 new fission product nuclides, are contained in the new data. New activation and decay data from ENDF-VII will be added for SCALE 6.

The methods in the SCALE code system use the ORIGEN-ARP sequence to perform the rapid and accurate fuel analysis using ORIGEN-S that relies on the ARP (Automated Rapid Processing) module to interpolate pregenerated cross-section libraries that cover a wide range of potential fuel types and irradiation conditions. Thus, the computing effort to generate the problem-dependent cross sections is performed in advance, allowing ORIGEN-ARP to calculate the spent fuel properties typically in a few seconds, with accuracy equal to that of detailed reactor physics calculations.

To support spent fuel analysis, ORNL has developed ORIGEN-ARP libraries for many commercial light water reactor (LWR) fuel designs used worldwide as well as European MOX, CANDU, AGR, VVER, and MAGNOX fuel types. ORIGEN-ARP also has a fast and easy-to-use Windows graphical interface that assists users in performing fuel irradiation and decay calculations, including the interactive plotting of results.

TSUNAMI: SENSITIVITY AND UNCERTAINTY FOR CRITICALITY SAFETY ANALYSES

SCALE contains advanced sensitivity and uncertainty (S/U) analysis capabilities for criticality safety. Both 1-D and 3-D sequences plus several auxiliary codes have been developed into a new suite of S/U analysis codes called TSUNAMI (Tools for Sensitivity and UNcertainty Analysis Methodology Implementation).

TSUNAMI contains a number of codes that were developed primarily to assess the area of applicability of benchmark experiments for use in criticality code validations. However, the S/U data produced by these codes can be used in a wide range of studies. Sensitivity coefficients produced by the TSUNAMI sensitivity analysis sequences predict the relative changes in a system's calculated k_{eff} value due to changes in the neutron cross-section data, using first-order eigenvalue perturbation theory. TSUNAMI produces sensitivity data on a groupwise basis for each region defined in the system model. The TSUNAMI-1D control module generates sensitivity coefficients using XSDRNPM. The TSUNAMI-3D control module is based on KENO V.a.

Both TSUNAMI-1D and TSUNAMI-3D fold the sensitivity data with cross-section covariance data to calculate the uncertainty in the calculated k_{eff} value due to tabulated uncertainties in the cross-section data. ENDF/B-V and ENDF/B-VI covariance libraries for sensitivity/uncertainty analyses with the TSUNAMI sequences are also included in SCALE 5.1. Covariance data from JENDL based on an integral approximation are used for nuclides that have no covariance data in ENDF.

The applicability of benchmark experiments to the criticality code validation of a given application can be assessed using S/U-based integral parameters. The TSUNAMI-IP (Integral Parameters) code uses sensitivity data and cross-section covariance data to produce a number of relational integral parameters that can be used to assess system similarity, including integral indices. These indices are correlation coefficients that quantify the amount of shared sensitivity or uncertainty in the k_{eff} values of an application and a benchmark due to particular nuclide cross sections. The TSURFER code uses a generalized least-squares adjustment to consolidate benchmark experiments with calculated results, reducing the uncertainty in predicted k_{eff}.

TRITON: Reactor Physics

The TRITON control module in SCALE performs 2-D depletion calculations using the New ESC-based Weighting Transport code (NEWT) flexible mesh discrete ordinates code coupled with CENTRM/PMC resonance self-shielding and with ORIGEN-S depletion. The NEWT geometry input is based on the SGGP combinatorial input format employed by KENO-VI. The use of a common input format reduces the learning curve in model development for SCALE users. Although limited to two dimensions, the use of the SGGP input format provides the geometric flexibility of Monte Carlo for a deterministic solution. It also allows a means for direct comparison of Monte Carlo vs. deterministic methods. Using the same cross-section data and virtually identical geometric configurations, differences in results can be attributed to differences in the two transport techniques.

The TRITON control module also can perform 3-D depletion calculations using the KENO V.a or KENO-VI Monte Carlo transport codes. TRITON couples these neutron transport codes with ORIGEN-S in a method similar to that used in 2-D depletion calculations with NEWT. This capability allows the user to perform detailed calculations such as tracking the isotopic depletion by individual fuel rods, axial portions of a fuel rod (in 3-D), or concentric rings in a rod loaded with burnable poison.

CONFIGURATION CONTROL, DOCUMENTATION, AND TRAINING

The SCALE package is developed in a configuration-controlled environment and distributed through the Radiation Safety Information Computational Center. SCALE has been used in domestic and international licensing environments since the 1980s. The input, output, and theory of the SCALE codes are described with over 5000 pages of documentation, and hands-on training with instruction by the code developers. Training is offered in a multiday format twice each year. Up-to-date information for users is available on the SCALE website (http://www.ornl.gov/sci/scale), including semiannual newsletters, updates to download, user notebooks, and training course information.

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