SCALE AND AMPX ADVANCEMENTS TO SUPPORT NCS APPLICATIONS

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INTRODUCTION

The objective of the US Nuclear Criticality Safety Program (NCSP) Analytical Methods program element is to sustain state-of-the-art radiation transport modeling capabilities and the expertise necessary to develop, maintain, and disseminate the analytical tools and data libraries in a manner that is responsive to the needs of those responsible for developing, implementing, and maintaining criticality safety. To this end, ORNL develops and maintains the AMPX cross-section processing system [1] and the SCALE code system[2] to provide nuclear data libraries and radiation transport analysis tools needed to support nuclear criticality safety (NCS) analyses of systems with fissionable material. The objective of this summary is to document new capability enhancements that have been completed for both the SCALE and AMPX code packages at ORNL through the support of the NCSP program as a general sponsor of both packages while many of the targeted capability enhancements have been supported by multiple sponsors.

SCALE

SCALE is an industry-leading suite of tools for nuclear systems modeling and simulation that provides comprehensive, verified and validated, user-friendly capabilities for criticality safety, reactor physics, radioactive source term characterization, radiation shielding, and sensitivity and uncertainty analysis, and includes recent nuclear data. SCALE is developed and maintained within the Reactor and Nuclear Systems Division of the Oak Ridge National Laboratory (ORNL). For more than 30 years, regulators, licensees, and research institutions around the world have used SCALE for nuclear safety analysis and design. SCALE provides a "plug-and-play" framework that includes three deterministic and three Monte Carlo radiation transport solvers that are selected based on the desired solution. SCALE includes the latest nuclear data libraries for continuous-energy (CE) and multigroup (MG) radiation transport as well as activation, depletion, and decay calculations. SCALE's graphical user interfaces assist with accurate system modeling, visualization, and convenient access to desired results. SCALE 6.2 provides several new capabilities and significant improvements in many existing features, especially with expanded CE Monte Carlo capabilities for criticality safety, shielding, depletion, and sensitivity and uncertainty analysis. A brief overview of SCALE capabilities is provided with emphasis on new features for SCALE 6.2.

Quality Assurance

The SCALE quality assurance (QA) program has been updated in 2013 to provide an improved means of providing high quality software and data for the user community. A new QA program has been implemented, which is compliant with ISO 9001,[3] DOE 414.1D,[4] and the ORNL Standards Based Management System, and is consistent with ASME NQA-1.[5]. With the new SCALE QA program, a streamlined Kanban process is implemented with continual integration of new features and an automated test system that performs approximately 50,000 tests per day on Linux, Macintosh, and Windows operating systems. The QA program provides for rapid introduction of new features for deployment to end-users.

Criticality Safety

The KENO Monte Carlo neutron transport codes for eigenvalue problems have realized a number of enhancements for SCALE 6.2. A comprehensive review of the CE treatment in KENO has led to a number of improvements providing reduced biases and substantially reduced memory footprint. Additional improvements in the initialization of the problem-dependent fission spectrum data and implementation of Doppler broadening rejection correction techniques provide further enhancements in some cases.

Parallel computation capabilities have been added to KENO to provide faster results on multicore PCs and Linux clusters, and fission source convergence diagnostic techniques have been implemented to provide improved confidence in the computed results.

CE Depletion

SCALE 6.1 provided MG Monte Carlo depletion that coupled SCALE MG cross-section processing capabilities with KENO and ORIGEN. A new CE-based

KENO/ORIGEN Monte Carlo depletion capability has been developed and can be utilized by simply changing the input library specification. CE depletion is especially useful for models with complex geometry that present difficulties in obtaining accurate resonance self-shielded MG data and for models with many depletion regions where run-time to generate and store the resonance self-shielded cross-section data for each material is prohibitive.

Radioactive Source Term Characterization

SCALE includes the ORIGEN (Oak Ridge Isotope GENeration) code and its comprehensive depletion, activation, decay, gamma-ray, and x-ray library with over 2,200 nuclides. ORIGEN and its nuclear data libraries have been updated to provide convenient modular interfaces within SCALE, and these interfaces also provide easy access to ORIGEN's robust capabilities by other software packages.

CE Fixed-Source Radiation Transport

The SCALE fixed-source Monte Carlo capability with automated variance reduction has been enhanced to enable CE calculations. The new CE capabilities provide enhanced solution fidelity while still implementing the unique acceleration techniques of the FW-CADIS (Forward-Weighted Consistent Adjoint Driven Importance Sampling) methodology for deep penetration shielding and criticality accident alarm system modeling.

Sensitivity and Uncertainty Analysis

The MG TSUNAMI eigenvalue sensitivity and uncertainty analysis methods that use KENO for transport analysis are extended to provide CE capabilities through the implementation of the CLUTCH (Contributon-Linked eigenvalue sensitivity/Uncertainty estimation via Tracklength importance CHaracterization) methodology and Iterated Fission Probability method. [6] CLUTCH is an efficient methodology that has been demonstrated to provide high-fidelity results with manageable runtimes and memory requirements.

A new stochastic uncertainty quantification capability has been added with the SCALE 6.2 Sampler module that implements stochastic techniques to quantify the uncertainty in any computed result from any SCALE sequence due to uncertainties in

- neutron cross sections,
- fission yield and decay data, and
- any user input parameter, such as geometry, material density, isotopic composition, temperature, etc.

Sampler propagates these uncertainties through complex analysis sequences such as depletion calculations, and provides the variation in the output quantities due to variations in any combination of input data. Correlations between systems with shared uncertainties are also computed, which is especially useful for quantifying correlated uncertainties in benchmark experiments, as required for generalized linear least-squares techniques as implemented by the SCALE module TSURFER.

Additional SCALE Updates

SCALE 6.2 includes a number of other improvements, such as the extension of the maximum allowed number of materials from around 2,000 to around 2 billion. Additionally, some older features are removed such as Evaluated Nuclear Data File Version V and VI data libraries (i.e., ENDF/B-V and –VI, respectively), the point kernel shielding capability, and a material optimization search sequence.

AMPX

AMPX is a cross-section processing software package that has been developed at ORNL for more than 30 years and is completely independent from any other cross-section processing software package. AMPX is used to process ENDF-formatted nuclear data evaluations and provide nuclear data libraries for the SCALE radiation transport package. AMPX provides CE, MG, and covariance data libraries for SCALE. The following summary identifies the recent AMPX updates that have led to improved nuclear data libraries for the SCALE code system.

Nuclear Data Updates for SCALE

Investigations into the CE data generated by the AMPX code system for deployment with SCALE revealed a need for improvement in the $S(\alpha,\beta)$ treatment, especially for forward-peaked kinematics. For thermal moderators like hydrogen in H_2O, ENDF evaluations give detailed angular and exit energy information for incoherent elastic scattering. Information is given in the form of a $S(\alpha,\beta)$ function, where α is the momentum transfer and β the energy transfer. AMPX uses the information from the ENDF/B evaluation to reconstruct the double differential scattering distribution. Prior to the development of the CE capabilities in SCALE, AMPX was primarily used to produce MG libraries, and AMPX collision kinematics distributions were provided as a function of cosine moment distributions instead of CE distributions. To support the CE capability development in SCALE, AMPX modules were developed to post-process the cosine moment distributions and recreate the original CE collision kinematics distributions. Once the CE distributions were reconstructed, the marginal and conditional probability distributions for exit angles and energies were generated (i.e., “legacy” CE kinematics distribution approach). For the CE libraries distributed with SCALE 6.0 and SCALE 6.1, AMPX used this legacy procedure to generate CE double-differential data from the cosine moment distributions. Following the release of SCALE 6.1, investigations revealed that the legacy procedure of generating CE probability distributions from the cosine moments introduced non-physical structure in the thermal scattering law data for water that resulted in a bias from some benchmark calculations. Based on the investigation, the AMPX collision kinematics processing procedures have been updated and modernized to produce CE probability distributions directly from the CE collision kinematics distributions thereby eliminating the cosine moment distribution processing step. The SCALE ENDF/B-VII.0 data libraries have been re-generated using the new AMPX processing procedures, and the benchmark testing results with SCALE 6.2 show substantially improved results with the new CE data libraries. Select critical benchmark results for thermal plutonium systems are provided in Figure 1, and the bias in the SCALE 6.2 CE results is reduced relative to SCALE 6.1.

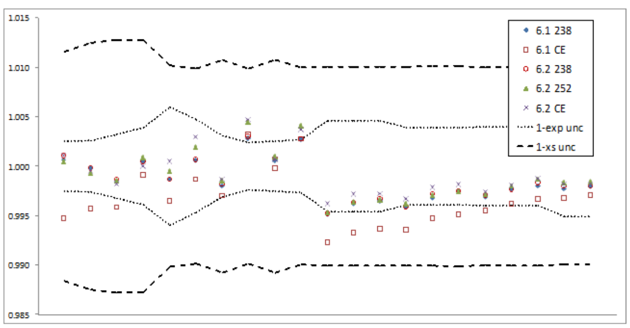

Fig. 1. SCALE calculated results for International Criticality Safety Benchmark Evaluation Project (ICSBEP)[7] thermal plutonium critical systems.

Additionally, the probability tables that provide CE treatment in the unresolved resonance range have been improved, primarily through the inclusion of additional resolution and error correction. Testing with the new probability tables has shown reduced biases for systems that are sensitive to the intermediate energy range.

With regard to MG analyses, ORNL has performed detailed comparisons between SCALE CE and MG results, and a consistent bias has been observed between the 238-group and CE calculations. Subsequently, a detailed investigation was performed to develop a new group structure that would eliminate the consistent bias observed with the 238-group library, especially for light-water moderated systems. A new 252-group structure has been developed that provides a more detailed representation of the ^{238}U resonance structure, and AMPX has been used to develop a new 252-energy-group ENDF/B-VII.0 neutron cross-section library for SCALE 6.2. In addition to the new group structure, the 252-group library has been generated using a new weighting spectrum with improved resonance self-shielding parameters. Specifically, for actinides and hydrogen in H_2O, a temperature-dependent CE flux spectrum has been generated with the CENTRM module for a PWR pin cell, and the CE flux spectrum has been used to generate the 252-group library. Intermediate resonance parameters (lambdas) for all isotopes have been included in the library, which provides a capability for improved self-shielding with the Bondarenko method [8]. Bondarenko shielding factors, as a function of background cross section and temperature, were computed for all actinides (except ^{235}U, ^{238}U, ^{239}Pu, ^{240}Pu, and ^{241}Pu) using CE spectra calculated by CENTRM for homogeneous mixtures of the resonance material and hydrogen, corresponding to the respective background cross section. For the nuclides ^{235}U, ^{238}U, ^{239}Pu, ^{240}Pu, and ^{241}Pu, the Bondarenko factors are based on CENTRM CE calculations for heterogeneous pincell models that span the range of anticipated self-shielding conditions. The thermal cutoff in the 252-group library for thermal moderators and the free-gas approximation has been raised from 3 eV to 5 eV. The new library has been tested by analyzing a wide variety of critical benchmark experiments and by comparing results with CE Monte Carlo results. The 252-group results that are presented in Figure 1 demonstrate consistent performance with the SCALE 6.2 CE results for the thermal plutonium critical benchmark experiments. Based on additional studies with the 252-group library, computational benchmark comparisons with CE results at room temperature and elevated temperatures show agreement within 100 pcm in most cases. In addition to the 252-group library, a new ENDF/B-VII.0 broad group library, with 50–70 energy groups, will also be available with SCALE 6.2.

Additional AMPX updates

AMPX has also been used to generate prototypic ENDF/B-VII.1 CE, MG, and covariance data libraries. ORNL is in the process of testing the new ENDF/B-VII.1 libraries in order to QA the libraries prior to release with SCALE. The ENDF/B-VII.1 library release is planned to occur after the release of SCALE 6.2.

CONCLUSION

ORNL has completed significant accomplishments for the AMPX and SCALE analytical methods capabilities, and the new nuclear data and radiation transport capabilities provide improved results for NCS analyses. These new nuclear data and analysis capabilities will be available in SCALE 6.2. With these developments, SCALE 6.2 continues a 30-year legacy of nuclear systems modeling and simulation by providing comprehensive, verified and validated, user-friendly capabilities for criticality safety, reactor physics, radioactive source term characterization, radiation shielding, and sensitivity/uncertainty analysis. In addition, SCALE 6.2 includes recent ENDF/B nuclear data libraries. The new capabilities within SCALE 6.2 provide significant advances over the previous versions, thanks especially to the expanded CE Monte Carlo capabilities for criticality safety, shielding, depletion, and sensitivity/uncertainty analysis.

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