

SCALE Newsletter



William A. Wieselquist
SCALE Director

IN THIS ISSUE

Director's Message.....	1
SCALE Website Update.....	3
Development of ORIGEN Reactor Libraries for HTGRs.....	4
SCALE Modeling of Fluoride-Salt-Cooled High-Temperature Gas-Cooled Reactors.....	6
SCALE Modeling of the Fast-Spectrum Heat Pipe Reactor.....	7
SCALE 6.3 Nuclear Data Updates.....	8
SAMPLER News, SCALE 6.3.....	10
HALEU.....	11
Assessment of Existing Transportation Packages for Use with HALEU (ORNL/TM-2020/1725).....	12
Criticality Safety Validation with VADER.....	13
SCALE 6.2.4 Validation for Criticality Safety Analysis.....	13
SCALE 6.2.4 Validation for Reactor Physics Applications.....	15
SCALE 6.2.4 Shielding Validation.....	15
SCALE User Support and Training.....	17
SCALE Publications, April 2020–April 2021.....	19

Oak Ridge National Laboratory

P.O. Box 2008, Bldg. 5700 MS-6170
Oak Ridge, TN 37831

Email: scalehelp@ornl.gov
<https://www.ornl.gov/scale>

Director's Message

Since our last newsletter, the SCALE Team has become involved in many exciting projects for the US Nuclear Regulatory Commission (NRC), as well as the US Department of Energy (DOE) Nuclear Criticality Safety Program (NCSP).

Non-LWR Severe Accident Analysis

The first NRC project was initiated with the planning document entitled *NRC Non-Light Water Reactor (Non-LWR) Vision and Strategy, Volume 3: Computer Code Development Plans for Severe Accident Progression, Source Term, and Consequence Analysis* (<https://www.nrc.gov/docs/ML1909/ML19093B404.pdf>). This work is a collaboration between the NRC, Oak Ridge National Laboratory (ORNL), and Sandia National Laboratories (SNL). We are using SCALE to provide data to SNL's MELCOR team on nuclide inventory, along with data on decay heat at initiation and during evolution of a severe accident. The MELCOR team is using the data to evaluate the source-term consequences of postulated accidents. So far, we are considering five non-LWR reactor types: (1) the fluoride salt-cooled high-temperature reactor (FHR), (2) the high-temperature gas-cooled reactor (HTGR), (3) the fast-spectrum heat pipe reactor (HPR), (4) the sodium fast reactor (SFR), and (5) the molten salt reactor (MSR).

For the FHR, the prototype chosen was the Berkeley Mark 1. The Pebble Bed Modular Reactor (PBMR)-400 was chosen as the HTGR prototype, Idaho National Laboratory (INL) Design A was chosen as the HPR prototype, the Molten Salt Reactor Experiment (MSRE) was the chosen prototype for MSRs, and the SFR prototype is yet to be determined.



Figure 1. SCALE production coordinator, clearing brush on his property: a fun, COVID-friendly activity.

Planning is underway to develop ORIGEN reactor libraries and ORIGAMI methodologies for each design. For pebble-based systems (HTGRs/FHRs), a strategy has been established for determination of the equilibrium core. The first NRC staff workshop (held May 11–12) covered the HPR and HTGR. The NRC staff workshop for the FHR will be held in August. Public workshops for all three reactor types (HPR, HTGR, FHR) are being held in June, July, and August, after which we will turn our efforts to the MSR and then finally the SFR.

HALEU/HBU/ATF Analysis Activities

At this writing, this phased activity has produced several reports to address High-Assay Low-Enriched Uranium (HALEU) Impact on Storage and Transport Criticality, Isotopic and Fuel Lattice Parameter Trends in Extended Enrichment and Higher Burnup (HBU) LWR Fuel, and Extended Enrichment Accident-Tolerant Fuel (ATF) Isotopic and Lattice Parameter Trends for LWRs. The focus of the NRC HALEU/HBU/ATF code preparedness effort is to assess SCALE for potential confirmatory analysis of this type of new fuel and to familiarize NRC staff members with what they may see in the future. This effort also includes training on how these packages impact storage configurations, the effects of increased enrichment, and whether the benchmark criticality experiments identified are sufficient for computer code validation. Scenarios were evaluated to discern optimum moderation and geometric configurations. Publicly available package designs and their associated data were used for this work. The nuclear industry has achieved high capacity factors and has increased electrical output through measurement uncertainty recapture (MUR: <2% increase in power), stretch power uprates (SPUs: typically up to 7% increase in power), and extended power uprates (EPUs: up to 20% increase in power). It may be possible to increase flexibility and efficiency by allowing for increased enrichment and higher discharge burnups. ATF work is currently focused on assessing near-term concepts for chromium-coated clad, chromium-doped fuel, and FeCrAl cladding. The SCALE validation basis continues to expand as new benchmarks are made available and analysis efforts are prioritized. The reports and links to the supporting input/output files can be found in the references section on our website, and they are also listed here for convenience.

Robert Hall, B.J. Marshall, William A. Wieselquist, [*Assessment of Existing Transportation Packages for Use with HALEU*](#), ORNL/TM-2020/1725, UT-Battelle, LLC, Oak Ridge National Laboratory (September 2020). [[supporting files](#)]

Robert Hall, Ryan Sweet, Randy Belles, and William A. Wieselquist, [*Extended-Enrichment Accident-Tolerant LWR Fuel Isotopic and Lattice Parameter Trends*](#), ORNL/TM-2021/1961, UT-Battelle, LLC, Oak Ridge National Laboratory (March 2021). [[supporting files](#)]

Riley Cumberland, Ryan Sweet, Ugur Merturek, Robert Hall, and William A. Wieselquist, [*Isotopic and Fuel Lattice Parameter Trends in Extended Enrichment and Higher Burnup LWR Fuel Vol. II: BWR Fuel*](#), ORNL/TM-2020/1835, UT-Battelle, LLC, Oak Ridge National Laboratory (March 2021). [[supporting files](#)]

Robert Hall, Riley Cumberland, Ryan Sweet, and William A. Wieselquist, [*Isotopic and Fuel Lattice Parameter Trends in Extended Enrichment and Higher Burnup LWR Fuel Vol. I: PWR Fuel*](#), ORNL/TM-2020/1833, UT-Battelle, LLC, Oak Ridge National Laboratory (February 2021). [[supporting files](#)]

Our work with NCSP has focused on extending our criticality safety validation database and making this high-quality database openly available to all users. SCALE team members are also contributing to new International Criticality Safety Benchmark Evaluation Project (ICSBEP) benchmarks, reviewing critical experiments, and even designing new ones. We are especially excited about elevated temperature benchmarks, which should provide valuable validation data for thermal scattering law data and Doppler broadening methods used in Monte Carlo codes.

SCALE Development

In February of 2021, the addition of new features to SCALE 6.3.0 was halted. An integrated SCALE manual is now in the repository to serve as an online and PDF version. The team is working on surveying and improving SCALE performance, as discussed in more detail in this newsletter. In addition to the new features in SCALE 6.3.0, more than 100 minor fixes/improvements have been made to the codebase since SCALE 6.2.4—the final release in the 6.2 series.

Outlook

Like many of our users and colleagues, the majority of the SCALE team has been working from home for more than a year now. We are beginning to return to the office at least part time in June and July. Our upcoming SCALE Users' Group Meeting is on the calendar for August 4–6, 2021, and a non-LWR workshop will be held as part of the International Conference on Mathematics and

Computational Methods Applied to Nuclear Science and Engineering (M&C) 2021 conference. We hope to see you there!

SCALE Website Update

The SCALE website has been refreshed with a new layout, as shown in Figure 2 below.

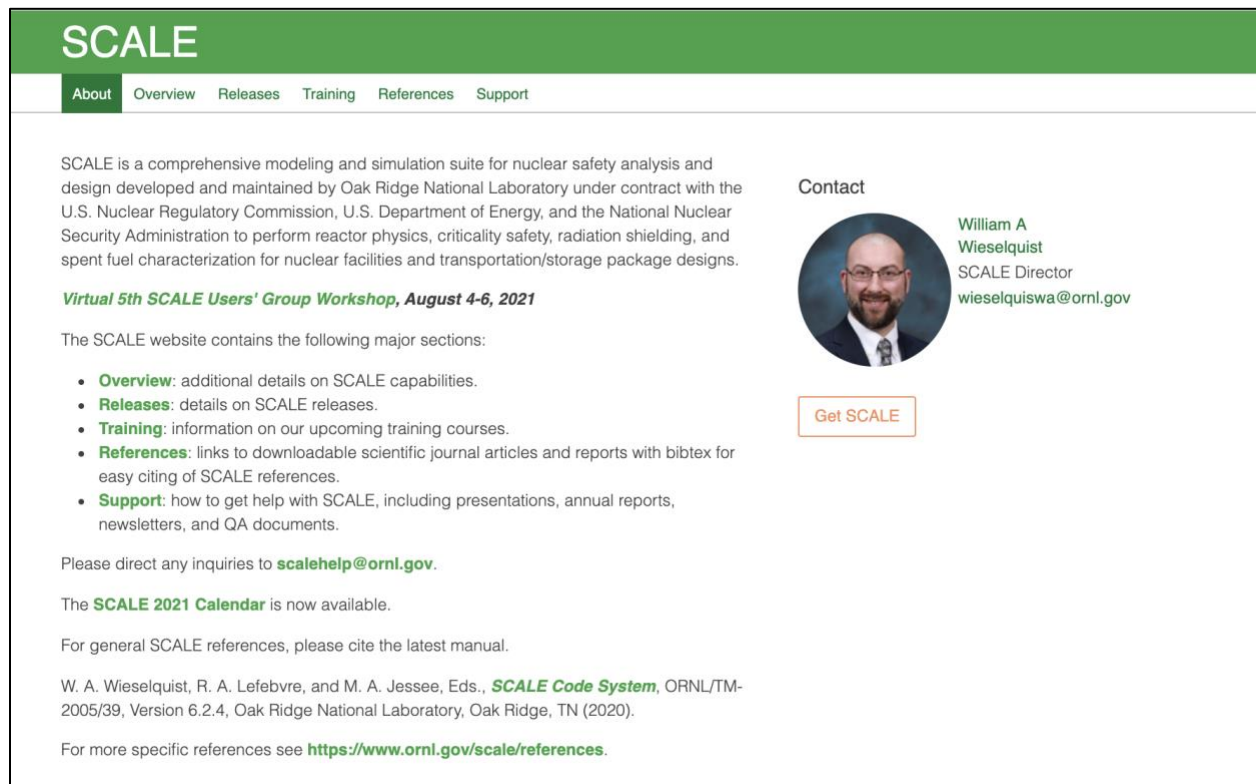


Figure 2. New website layout.

The main goal for this rework was to enable new landing pages for SCALE releases and useful reference material. The releases page (<https://www.ornl.gov/scale/releases>) provides links to the SCALE version's landing page. To optimize maintenance efforts, the first thing we will do with a potential discrepancy is to verify that the issue still exists in the *latest production release*. If the issue *does not exist* in the latest production release, then we may ask you to upgrade to this version, and we will only minimally look into the issue further. This process will also affect how we document issues. We will only formally document minor issues for the latest production release. Significant issues will continue to have the extent of their condition investigated for many SCALE versions.

When v6.3.0 is released, the v6.2.4 landing page will include a banner at the top of the page stating, "This version is no longer supported" (Figure 3). This means that we will no longer update the webpage with any newly discovered discrepancies in the v6.2 series, and we encourage all users to upgrade to SCALE v6.3.0. We will continue to support users with questions about the v6.2 series, but support for verifying and fixing discrepancies will only apply to the *latest production release*. Starting with SCALE v6.3.0, we will maintain a list of known discrepancies on the v6.3.0 version landing page as they are found. When we release the v6.3.1 maintenance update, we will explicitly note which discrepancies were fixed and which ones remain. For example, we may

choose not to fix minor issues with a clear workaround until the next major release (v7.0.0). Hopefully this approach will give current and potential users an easy way to check the contents of a release to see if it meets their needs.

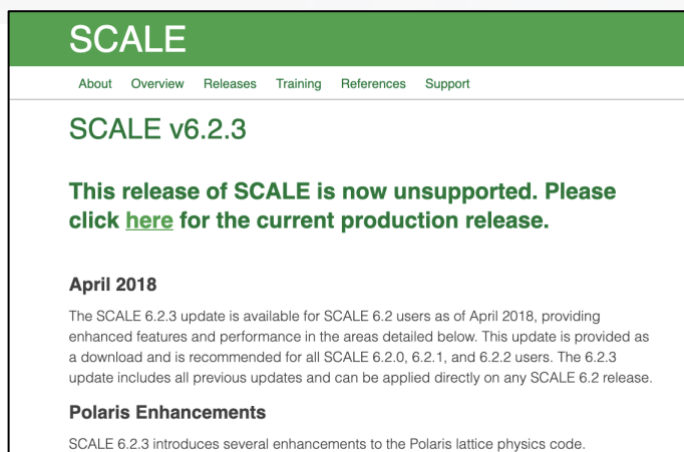


Figure 3. Release unsupported message.

The other important page added to the website is the “References” tab (Figure 4). From this point forward, this part of the website will list publications authored by SCALE team members that document the development or application of SCALE capabilities.

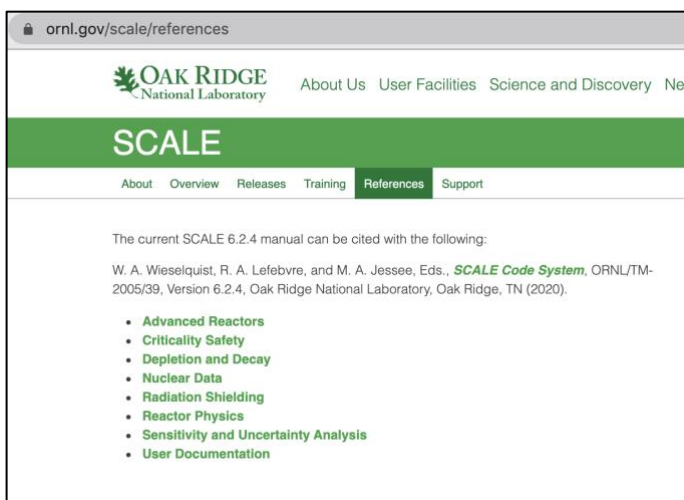


Figure 4. References tab.

Publications will be listed by topic area (Figure 5). As shown in the screenshot of the Criticality Safety page below, relevant documents will be organized by year of publication and will be linked on <https://www.osti.gov/>.

For key ORNL reports, links to supporting files—typically all the model inputs and outputs that facilitated an analysis—will be included. This will provide the SCALE user community with easier access to high-quality models to use as starting points for their own analyses.

We are aware that this is a significant change to the website, and if we have not preserved some important content for you as a SCALE user, please let us know by sending an email to scalehelp@ornl.gov.

Development of ORIGIN Reactor Libraries for HTGRs

As part of a larger NRC-funded effort focused on quantifying severe accident source terms for non-LWRs, ORNL staff members have been using SCALE to model and evaluate several advanced reactor systems based on open literature concepts.

One such reactor system is the PBMR, a Generation IV concept based on continuous circulation of graphite-based pebbles composed of microscopic tristructural isotropic (TRISO) fuel particles. These TRISO fuel particles consist of a uranium oxide fuel kernel surrounded by layers of silicon carbide and graphite which serve as a fission product barrier and buffer. A key advantage of the TRISO fuel concept is its inherent safety features, including strongly negative temperature feedbacks and excellent fission product retention capabilities. The PBMR concept has a long pedigree that stretches back to the German AVR reactor, and it also draws from features of the prismatic block HTGR concepts developed in the United States. Although no commercial-scale PBMR units currently exist, some of the more well-known HTGR examples include the HTR-10 research reactor in China, as well as the proposed (and later abandoned) PBMR-400 project in South Africa, a 400 MW pebble bed design using low-enriched uranium fuel and designed to achieve very high fuel burnups (~90,000 megawatt days [MWd]/metric tons of initial heavy metal [MTIHM])—nearly double the average burnup of conventional LWRs.

Though it was never constructed, the PBMR-400 lives on as an international reactor physics benchmark (Figure 6).

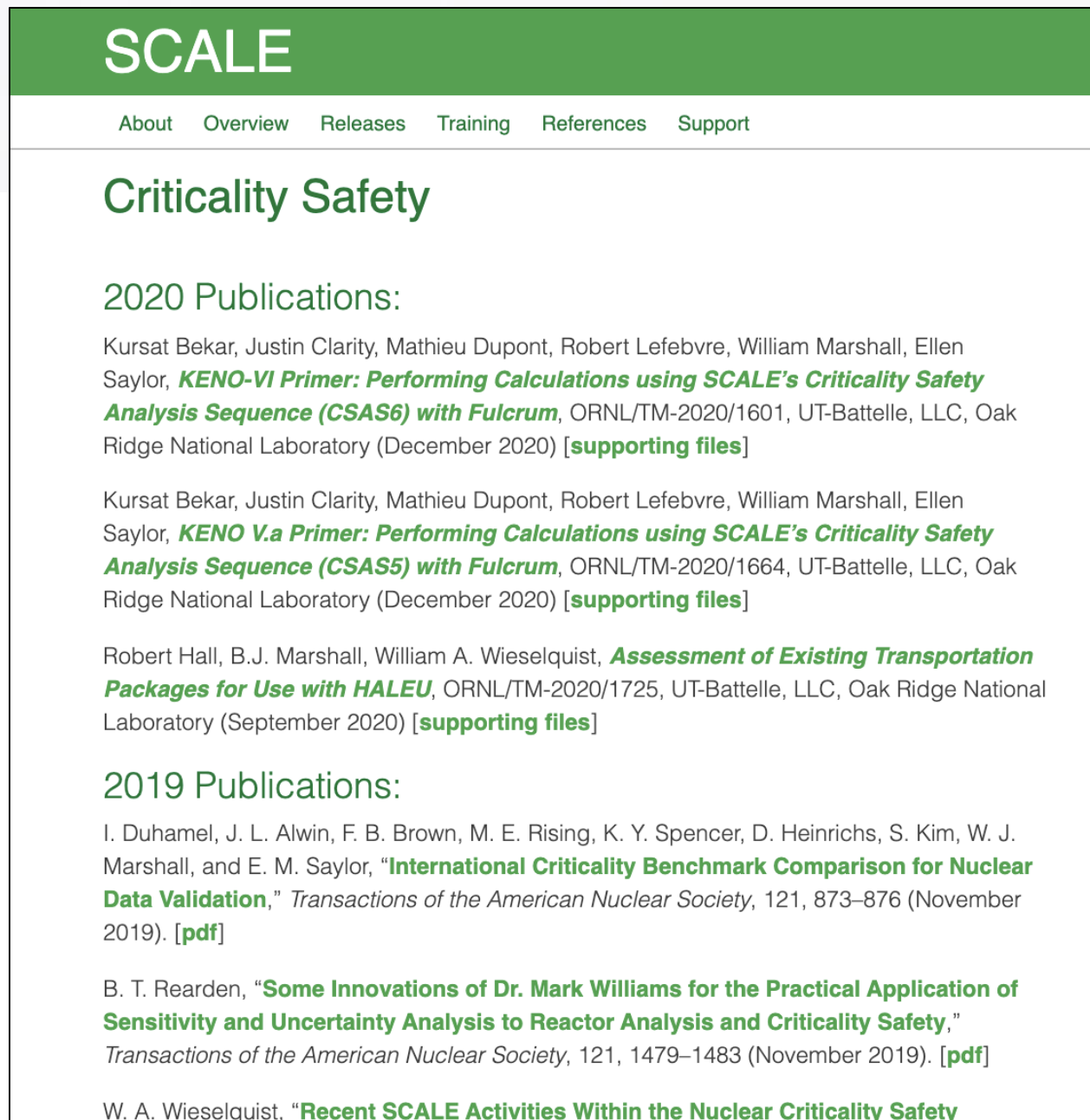


Figure 5. Publications by topic area.

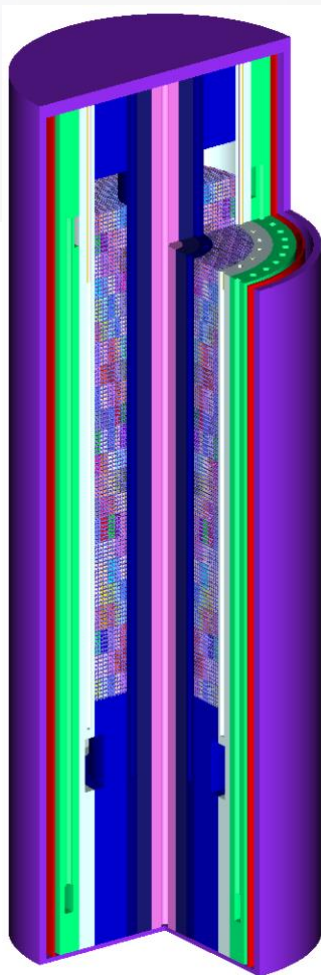


Figure 6. PBMR400 model.

It is the basis of a current effort to determine how to develop future ORIGIN reactor data libraries to accommodate the unique features of this design. Some of the more prominent modeling challenges center around accounting for the continuous flow of pebbles through the core, which is further complicated by the fact that pebbles are irradiated in multiple passes through the core. The goal is not to reinvent decades of methods development to describe the physics of the core evolution toward an equilibrium, but rather to develop a rigorous means of developing reactor libraries that can be used to rapidly estimate pebble isotopic inventories with the same ease and relative accuracy that the present suite of ORIGIN reactor data libraries provides.

Given the substantial differences between the PBMR and LWR cores, much of this effort involves characterizing appropriate dimensions for which library interpolation

parameters will be defined. Users of ORIGIN are no doubt familiar with the traditional parameters used for library interpolation, such as initial enrichment, average moderator density, burnup for uranium oxide fuel, fissile plutonium content, and total plutonium fraction for mixed-oxide fuels. As we continue to apply SCALE tools to a broader class of reactors, its capabilities will continue to expand. In the case of non-LWR systems, this means generalizing the approach to handle reactor data library interpolation—a feature planned for the SCALE 7.0 series. The findings of this study will be released in a forthcoming ORNL technical report, “Assessment of ORIGIN Reactor Library Development for Pebble-Bed Reactors Based on the PBMR-400 Benchmark.”

SCALE Modeling of Fluoride-Salt-Cooled High-Temperature Gas-Cooled Reactors

An FHR combines the HTGR fuel form with liquid fluoride salt coolant in a graphite-moderated environment. A pebble-bed FHR has a core filled with a large amount of graphite moderator and fuel pebbles surrounded by graphite reflector structures (Figure 7). Like an HTGR, the fuel pebbles contain thousands of TRISO particles distributed in a graphite matrix. However, the pebbles in an FHR are significantly smaller at ~3 cm diameter, and the fuel particles within the pebble are tightly packed in a spherical shell that is 1.5 mm thick (Figure 8).

Current FHR modeling efforts with SCALE are supporting NRC-sponsored projects for nuclear data performance assessment and for the generation of nuclide inventory for severe accident analysis. In preparation for full core multigroup (MG) calculations, the performance of SCALE’s *doublehet* approach for MG calculations for particles placed in shells was verified through comparisons with continuous-energy (CE) calculations. (Note that significant verification has already been performed for spheres.) TRITON/KENO-VI depletion calculations for an infinite lattice of fuel pebbles with reflective boundary conditions were compared for the following models: (1) an MG model using the *doublehet* treatment for the self-shielding calculation, (2) a CE model with TRISO particles placed in a square lattice, allowing particle clipping, (3) a CE model with TRISO

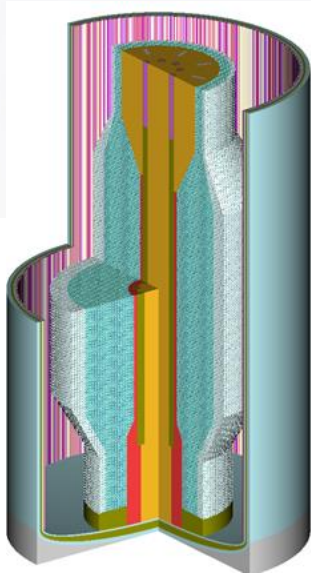


Figure 7. SCALE model of the UC Berkeley pebble-bed FHR.

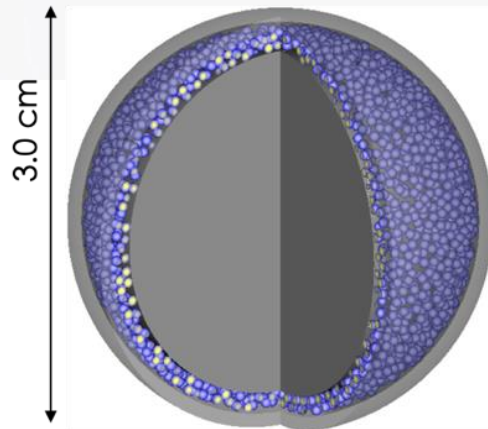


Figure 8. SCALE model of an FHR fuel pebble with TRISO particles randomly distributed.

particles in a square lattice, avoiding particle clipping, and (4) a CE model with TRISO particles randomly distributed in the fuel region, avoiding particle clipping. The fuel mass in these models was identical, and a CE model (4) was taken as reference, as it seemed to be the closest to reality. Very good agreement was obtained for k_{eff} between the MG calculation and the CE reference, with differences smaller than 300 pcm throughout depletion. Models (3) and (4) showed excellent agreement, with differences smaller than 60 pcm. It was noted that particle clipping caused a bias of up to 500 pcm. With respect to the variation of nuclide mass content during depletion, very good agreement was observed among all CE calculations. The MG calculation resulted in differences smaller than 3.5% for all relevant observed nuclides.

Based on the good performance of the MG treatment for this type of fuel pebble, modeling efforts began for the University of California Berkeley pebble-bed FHR. The goal is to estimate a realistic nuclide inventory for an equilibrium state of the reactor, considering that the pebbles travel multiple times through the reactor before they reach their final discharge burnup. Initially, a simplified approach was used to obtain representative nuclide inventories for a model that will be used in nuclear data sensitivity and uncertainty calculations. This

study is ongoing, and results will be published later this year in a technical report.

SCALE Modeling of the Fast-Spectrum Heat Pipe Reactor

As part of the severe accident analysis collaboration with SNL and the NRC, SCALE models were developed for a fast-spectrum heat pipe reactor (Figure 9). These models were based on the INL Design A concept, which is an alternative design to the Los Alamos National Laboratory (LANL) Special Purpose Reactor, also known as the *Mega-Power Reactor*. The original model contains 1,134 heat pipes with a potassium working fluid. The heat pipes are surrounded by hexagonal fuel elements, and the fuel is UO_2 with 19.75 wt% ^{235}U enrichment. The model contains axial BeO reflectors above and below the active fuel region, along with a radial alumina reflector containing twelve B_4C control drums. The center of the core is left unfueled to make room for two shutdown control rods—one annular and one solid. The active region of the core was discretized into twenty axial and five radial zones to analyze spatial variations in power and burnup.

Infinite lattice unit cell sensitivity studies were used to perform verification between the SCALE and INL models. The results agreed well: the reported eigenvalues were

within roughly 50 pcm for these unit cell models. Full-core model verification was also performed to analyze system eigenvalues with differing configurations of control drum and shutdown rod positions. All of these full-core results had eigenvalue differences of less than 190 pcm. Control drum and shutdown rod worths were also compared, and the results showed differences of 3.5% or less. Now that the model has been verified, it is being used to provide isotopic inventories and decay heat to SNL as input to the MELCOR severe accident code to analyze potential releases from this reactor design.

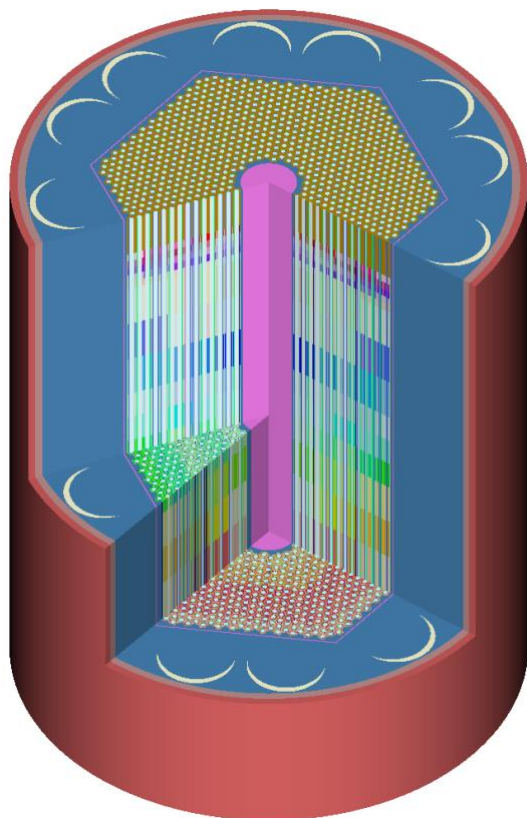


Figure 9. SCALE model for heat pipe reactor.

SCALE 6.3 Nuclear Data Updates

The SCALE 6.3 release includes a new release of the SCALE data. This release includes new Evaluated Nuclear Data File (ENDF)/B-VIII.0 data and updated ENDF/B-VII.1 data, and the ENDF/B-VII.0 data have been removed. The National Nuclear Data Center released the ENDFB-VIII.0 evaluated data in February 2018. ORNL performed processing and extensive testing before and after the

ENDF/B-VIII.0 data library release [1] [2]. The latest ENDF release contains neutron cross section data for 556 isotopes, including metastable targets, as well as 34 thermal scattering law evaluations, including multiple versions of graphite and hydrogen bound in ice. Under the direction of the Collaborative International Evaluated Library Organisation (CIELO) project, the ENDF/B-VIII.0 data contain significant updates to ^1H , ^{16}O , ^{56}Fe , ^{235}U , ^{238}U , and ^{239}Pu [3]. The ENDF/B-VIII.0 data also include important thermal scattering law changes, such as new evaluations for crystalline graphite and two different porosities of reactor grade graphite [4].

There are two new SCALE MG library structures available for the ENDF/B-VIII.0 and ENDF/B-VII.1 data. A new very fine group library was added consisting of a 1,597-group structure based on the Analytical Methods Nuclear Cross-Section Processing Computer Code System (AMPX) 252-group structure and MC²-3 ultra-fine group structures [5]. The energy range from 0.1 keV to 20 MeV was divided into 1,323 groups, each of which has an equivalent lethargy width of $\frac{1}{120}$, to represent broad resonances of intermediate-weight nuclides explicitly. The energy range from 10^{-5} eV to 0.1 keV is represented by 274 groups based on the AMPX 252-group structure. The boundaries of the 1,597-group library were chosen such that the fine groups can be collapsed directly onto the 252-group structure.

In addition, a new 302-group library was added for the analysis of SFR systems. The base weighting function for processing the MG data was taken as the neutron flux of a volume-homogenized SFR fuel assembly computed by the point-wise transport code Continuous Energy Transport Module (CENTRM). The fuel assembly model was generated corresponding to the specifications of the large oxide core (MOX3600), defined within the Organisation for Economic Co-operation and Development (OECD)/ Nuclear Energy Agency (NEA) Benchmark for Uncertainty Analysis in Modelling (UAM) for Design, Operation and Safety Analysis of SFRs [6]. The 302-group structure was developed based on group structures optimized for fast spectrum systems used in the DOE Office of Nuclear Energy (NE) Advanced Reactor Technologies (ART) program, and in particular, the MC²-3 code [5]. Boundaries of the 425-group structure were

added to the 230-group structure to include a finer resolution of resonances in the fast energy range. The group structure below 10 eV has been slightly modified from the original Argonne National Laboratory (Argonne) structures in order to match group boundaries of the 1,597-group library. In contrast to the 252-group library, group-dependent intermediate resonance (IR) parameters (λ) are not included, and Bondarenko factors were exclusively computed using the narrow resonance (NR) approximation for the flux spectrum for all nuclides. The 302-group library was developed and tested with a focus on the models defined within the OECD/NEA UAM SFR benchmark [7]. For the application of this library to other SFR or fast spectrum systems, validation with corresponding CE and 1,597-group calculations is recommended.

The ENDF/B-VIII.0 data were processed to generate both CE and MG libraries for SCALE. The CE data are available for both incident neutrons and gammas and are deployed in HDF5 format rather than the legacy binary format. The new HDF5 directory file for the CE libraries follows the usual SCALE convention: **ce_v8.0_endf**. The MG libraries for incident neutrons were processed analogously to their respective ENDF/B-VII.1 counterparts. Please note that the ENDF/B-VIII.0 versions of the MG libraries have additional isotopes and thermal moderators that are not available in ENDF/B-VII.1. The ENDF/B-VIII.0 MG libraries in SCALE include 1,597-, 302-, and 252-group libraries. Like its ENDF/B-VII.1 counterpart, the ENDF/B-VIII.0 1,597-group library (**v8.0-1597**) is quite large due to the large number of groups. As in the ENDF/B-VII.1 library, the ENDF/B-VIII.0 302-group library (**v8.0-302**) is intended for analysis of SFR systems. Furthermore, as in the ENDF/B-VII.1 library, the ENDF/B-VIII.0 252 group library (**scale.rev01.xn252v8.0**) is best suited for criticality safety and reactor physics applications. As with the ENDF/B-VII.1 library, this library was processed using temperature and Z-dependent fluxes taken from a series of representative lattice cell calculations. The ENDF/B-VIII.0 covariance data (**scale.rev01.56groupcov8.0**) were processed into the same 56-group format as the ENDF/B-VII.1 data. Additionally, the ENDF/B-VIII.0 covariance data contain correlations that are not present in the original ENDF/B-VIII.0 data; these correlations represent our best estimate of integral information

missing from the covariance provided in the released ENDF library [8].

Two coupled MG libraries were added to support coupled (n, γ) reactor physics calculations with Polaris [9]. The **mg_252n_47g** library contains the exact same neutron data as the neutron-only 252 group library (**scale.rev05.xn252v7.1**), with the addition of yield and gamma data to support coupled (n, γ) calculations. The **mg_252n_47g** library uses the usual 47 group gamma structure (identical to the gamma structure of **scale.rev13.xn200g47v7.1**). Similarly, the **mg_56n_19g** library contains the exact same neutron data as the neutron-only 56 group library (**scale.rev04.xn56v7.1**), with the addition of yield and gamma data to support coupled (n, γ) calculations. The **mg_56n_19g** library uses the usual 19 group gamma structure (identical to the gamma structure of **scale.rev12.xn28g19v7.1**). Since the coupled libraries contain identical neutron data as their neutron-only counterparts, neutron transport should be identical when using the coupled or neutron-only version of each library structure.

The most significant change in the ENDF/B-VII.1 data is in the unresolved resonance region. An incorrect assumption in AMPX about the interpretation of the unresolved resonance region data in some ENDF/B data files resulted in a bias of up to ~500 pcm for fast systems in calculations with both CE and MG libraries with the SCALE 6.2 series. AMPX was corrected to interpret the ambiguous ENDF definition as intended, and the latest ENDF/B-VII.1 and ENDF/B-VIII.0 CE and MG libraries to be distributed with SCALE-6.3 were generated with probability tables that were normalized correctly for all isotopes. Due to this change in the probability table treatment, the largest resulting k_{eff} change in the Verified, Archived Library of Inputs and Data (VALID) suite was observed for ICSBEP benchmark cases MCF-005-001 and MCF-006-001, in which the corrected probability tables decrease the predicted k_{eff} by roughly 350 pcm [10]. The impact of this change is negligible for thermal systems.

- [1] D.A. Brown, et al., "ENDF/B-VIII.0: The 8th Major Release of the Nuclear Reaction Data Library with CIELO-project Cross Sections, New Standards and Thermal Scattering Data," *Nuclear Data Sheets* 148, 2018.

- [2] Holcomb, A., Wiarda, D., and Marshall, W. J., "ENDF/B-VIII.0 testing with AMPX and SCALE," in ANS NCSD 2017: Nuclear Criticality Safety Division Topical Meeting - Criticality Safety, Pushing Boundaries by Modernizing and Integrating Data, Methods, and Regulations, Carlsbad, NM, 2017.
- [3] M.B. Chadwick, E. Dupont, E. Bauge, et al., "The CIELO Collaboration: Neutron Reactions on ^1H , ^{16}O , ^{56}Fe , $^{235,238}\text{U}$, and ^{239}Pu ," *Nuclear Data Sheets*, 2014.
- [4] A. I. Hawari, "Modern Techniques for Inelastic Thermal Neutron Scattering Analysis," *Nuclear Data Sheets*, 2014.
- [5] C. H. Lee, W. S. Yang, *MC²-3: Multigroup Cross Section Generation Code for Fast Reactor Analysis*, ANL/NE-11-41 Rev.2, Argonne National Laboratory, 2013.
- [6] L. Buiron, G. Rimpault, et al., *Benchmark for Uncertainty Analysis in Modelling (UAM) for Design, Operation and Safety Analysis of SFRs, Core Definitions*, February 10, 2017.
- [7] F. Bostelmann, N. R. Brown, A. Pautz, B. T. Rearden, K. Velkov, W. Zwermann, "SCALE Multi-Group Libraries for Sodium-cooled Fast Reactor Systems," *Proceedings of M&C2017*, Jeju, Korea, April 16–20, 2017.
- [8] Vladimir Sobes, Andrew Holcomb, B.J. Marshall, Travis Greene, Doro Wiarda, Will Wieselquist, "Augmented ENDF/B-VIII.0 Covariance Library for SCALE 6.3," *Annals of Nuclear Energy* 160, 2021.
- [9] Matthew A. Jessee, William A. Wieselquist, et al., "POLARIS: A New Two-Dimensional Lattice Physics Analysis Capability for the SCALE Code System," *Proceedings of PHYSOR 2014 - The Role of Reactor Physics toward a Sustainable Future*, Kyoto, Japan, 2014.
- [10] W. J. Marshall, E. M. Saylor, A. M. Holcomb, D. Wiarda, and T. M. Greene, "Validation of KENO V.a and KENO-VI in SCALE 6.3 Beta 3 Using ENDF/B-VII.1 and ENDF/B-VIII Libraries," *Proceedings of 11th International Conference on Nuclear Criticality Safety 2019*, Paris, France, 2019.

SAMPLER News, SCALE 6.3

New Features: Kinetics Data Perturbations

One of the most important aspects of nuclear safety analysis is the kinetics behavior (e.g., beta-effective analysis). Similar to few-group cross sections, the kinetics parameters used in core calculations include uncertainties that originate from the measured nuclear data. A new SCALE kinetics data library and an associated 1,000 perturbed kinetics data libraries were generated to allow SAMPLER to propagate kinetics data uncertainties to subsequences. A SAMPLER parameter data block was expanded to allow for optional kinetics data perturbations through the new `perturb_kinetics` keyword. The "`perturb_kinetics=yes`" and "`perturb_xs=yes`" should be used together to ensure that all kinetics parameters are perturbed consistently.

Various Bug Fixes

CENTRM-Processed Libraries Cause Inconsistent Variations in TRITON/MG KENO Depletion Results

Using SAMPLER, the TRITON/MG KENO (T6-DEPL) depletion sequence generated MG perturbed libraries that demonstrated a considerably smaller k_{eff} standard deviation compared with k_{eff} standard deviation at time = 0. An investigation showed that the inconsistent results are only observed when CENTRM is used for cross section processing. In addition to perturbed MG libraries, SAMPLER also generates consistent CENTRM-specific perturbed libraries. The sudden reduction in the variation of depletion results is caused by erroneously deleted CENTRM-specific perturbed libraries after the first set of calculations at time = 0. This behavior is specific to TRITON/MG KENO realizations under SAMPLER and was resolved by implementing more robust file handling. This has been fixed in SCALE 6.3.0.

Variable Response Table Reports Wrong Dependent Variable Values for Parametric Studies

In one parametric study, the response table displayed different values than those used in the perturbed input files if users requested a dependent variable as a response. Although the correct variables are used in the perturbed input files, the incorrect response table entries can affect analysis results unless the user globally searches for a regular expression and prints (i.e., `greps`)

the matching lines for the correct values from the input files.

The discrepancies in the response table for dependent variables are caused by inconsistently sampling variables during response generation. Because SAMPLER can be run in two independent executions—input generation and output processing—the perturbed variables used in input generation are not preserved. These variables are sampled when requested by users as a response during postprocessing. However, the resampling of variables was inconsistent with the parametric study, and incorrect values were generated. This has been fixed in SCALE 6.3.0.

SCALE Multithreading Does Not Work with SAMPLER on Mac or Windows

Certain applications within SCALE support multithreading, which is enabled by using the -l option when launching jobs from the command line. SAMPLER is one of those applications, and the capability is functional on the Linux operating system. However, despite the appearance of launching simultaneous jobs, each job is run sequentially on Mac and Windows. This has been fixed so that threading works on all platforms in v6.3.0.

HALEU

Commercial LWR operators and fuel vendors in the United States are pursuing changes to reactor fuel, such as increased enrichment and ATF designs. The enrichments under consideration are between 5 and 10% ^{235}U , a range which is a subset of HALEU fuels. ATF features—including coated clad, doped UO_2 , and FeCrAl clad—are designed to improve fuel system performance under accident conditions. With extended enrichment (EE), fuel cycle economics can be improved if fuel can be licensed for higher burnup than typical current limits (e.g., 62 GWd/MTU maximum for fuel pin). The adoption of EE fuels, ATFs, and high-burnup fuels in the US commercial fleet requires a clear understanding of the effects on core physics parameters and used fuel isotopic content, as well as confidence in the accuracy of computer code predictions over an expanded range of materials, enrichment, and burnup. Studies are ongoing at ORNL to address these challenges. Phase 1 of these studies was completed for lattice physics parameters and used fuel isotopic changes for a conventional 17×17 pressurized water reactor (PWR) design and a conventional 10×10

boiling water reactor (BWR) design. In addition to conventional UO_2 fuel with Zircaloy clad, new ATF concepts were also investigated. Key quantities of interest include (1) lattice physics parameters (reactivity, reactivity coefficients, power and distributions, cross sections, and kinetics parameters), (2) isotopic inventory at various decay times, (3) neutronic similarity in spent fuel pool storage, and (4) uncertainty in k_{inf} that arises directly from cross section uncertainties and indirectly from uncertainties in the discharged isotopic content. Calculations were performed using the pre-release of SCALE 6.3 Polaris and ORIGEN computer codes. As examples from these studies, Figure 10 shows a reactivity difference for Cr-coated BWR ATF compared to the conventional BWR design for both dominant (DOM) and vanished (VAN) lattices, and Figure 11 shows the decay heat difference compared to 60 GWd/MTU 5 wt % PWR fuel when higher enrichment and burnup are used.

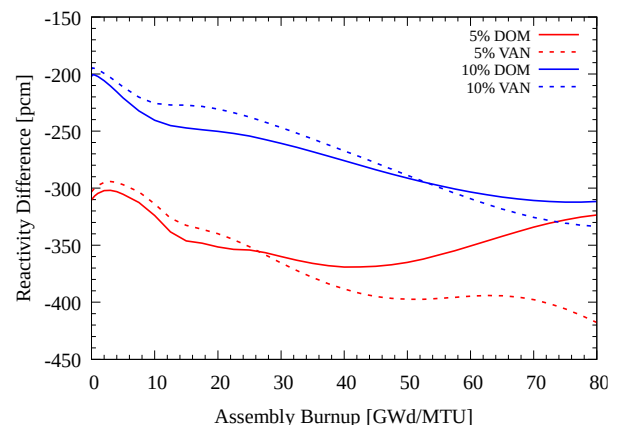


Figure 10. Reactivity difference for Cr-coated BWR ATF.

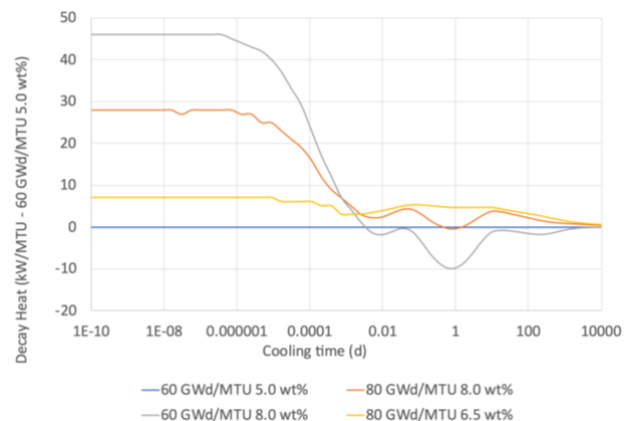


Figure 11. Decay heat difference from 60 GWd/MTU 5 wt % PWR case.

No unexpected or anomalous trends were found, ensuring the adequacy of the Polaris code when using SCALE 56-group ENDF/B-VII.1 cross sections for depletion, lattice physics, and isotopic content calculations of the analyzed fuel type and lattice designs.

Assessment of Existing Transportation Packages for Use with HALEU (ORNL/TM-2020/1725)

Commercial LWR operators and fuel vendors in the United States are pursuing changes to fuel, including increased ^{235}U enrichment. Economic studies generally anticipate maximum near-term fuel assembly designs with up to 8 wt% ^{235}U . Many next-generation nuclear reactor designs require HALEU (19.75 wt% ^{235}U > 5 wt%) fuel. One necessary element for the commercial-scale use of HALEU is the ability to safely transport large quantities of enriched fuel material in multiple forms, but it is uncertain whether subcriticality requirements can be satisfied with existing package designs and whether existing critical benchmark experiment data are sufficient to support criticality safety code validation for HALEU transportation applications.

The study assesses the potential to use currently licensed transportation packages for the transportation of increased enrichment, unirradiated U fuel forms. The assessment analyzed selected package designs representing five categories of fuel form—BWR pins and assemblies, pressurized water reactor pins and assemblies, UF_6 , U-metal and TRISO particles, and UO_2 pellets or powder. The analysis focused on demonstrating subcriticality and identifying the benchmark critical experiments appropriate for use in criticality computer code validation.

Key quantities of interest for subcriticality are limiting conditions (e.g., optimum moderation), package or package array k_{eff} , package capacity, and package transportation array size. A KENO-VI model for a cube-shaped package designed to transport uranium oxide in powder or pellet form is illustrated in Figure 12. The SCALE TSUNAMI-3D and TSUNAMI-IP codes were used to perform sensitivity and uncertainty calculations and to identify candidate critical benchmark experiments for code validation. The similarity coefficient c_k was the

metric used to identify candidate benchmarks. The c_k for a Traveller package is shown in Figure 13.

A representative package was evaluated for each fuel form category. The results for each package evaluation include enrichment and packaging limits (e.g., maximum transportation array size as a function of enrichment) and benchmark critical experiment similarity coefficients. The results show that there are viable means for increasing enrichments into the HALEU range across the spectrum of fuel forms with differing amounts available for different packages. Sources of subcriticality margin to offset increased enrichment reactivity include reduced transportation array size, reduced fissile mass, burnable absorber credit, and safety analysis margin harvesting. Numerous critical benchmark experiment candidates for validation were identified for all packages except the DN-30.

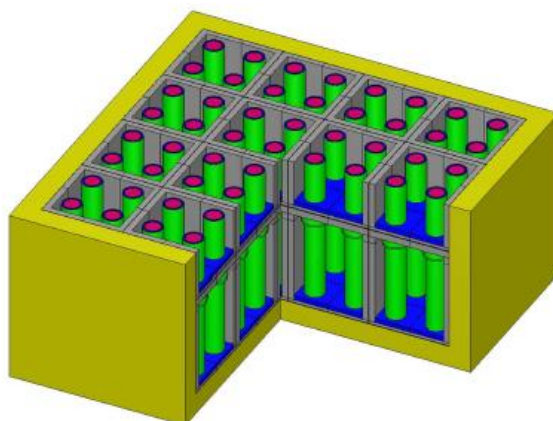


Figure 12. KENO-VI model of CHT-OP-TU array.

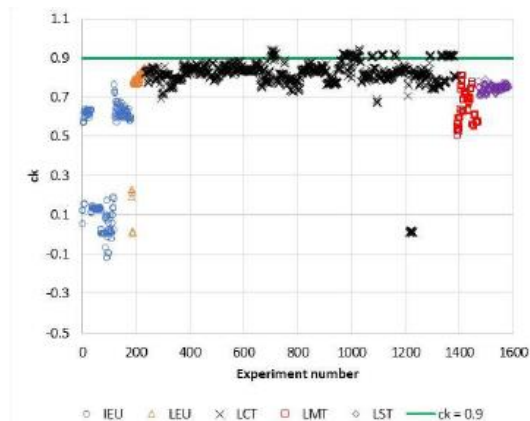


Figure 13. c_k for TN-B1 with 8 wt% UO_2 and 24 Gd rods /assembly

Criticality Safety Validation with VADER

Validation and Data Evaluation Resource (VADER) is the successor code to USLSTATS, an upper subcritical limit (USL) statistical program. It maintains all of the functionality of the USLSTATS software and adds new features, methods, and tests.

VADER's main user-facing change is the implementation of the new input format available with SCALE object notation (SON). The SON format is free form and can be checked easily on the fly with the SCALE graphical user interface (GUI) Fulcrum. Using SON-formatted input makes it much easier to add new features while preserving backwards compatibility in the future. An example of the VADER input in Fulcrum is shown in Figure 14 below.

```
1 =vader
2
3 data=[
4 1.9947003 0.97978 0.00666
5 2.3125354 0.97862 0.00519
6 2.0489823 0.98018 0.00559
7 1.4951488 0.98123 0.00893
8 1.6272778 0.98207 0.00697
9 1.6992786 0.98000 0.00735
10 0.9360934 0.98848 0.00544
11 1.7664417 0.97843 0.00558
12 1.8082888 0.97523 0.00810
13 1.1019401 0.97965 0.00549
14 1.8500284 0.97295 0.00487
15 1.8733395 0.97805 0.00479
16 ]
17
18 trend_values=[-2.995732274 0 3.912023005]
19
20 methods {
21   USL=[confidence=0.95 proportion=0.95
22     extrapolate=Yes]
23   LTB=[confidence=0.95 proportion=0.95]
24   LTL=[confidence=0.95 proportion=0.95]
25 }
26
27 tests{
28   trend_significance[confidence=0.95]
29   shapiro_wilk[confidence=0.95]
30 }
31 end
```

Figure 14. Vader input.

In addition to the methods and tests supported in USLSTATS, VADER adds several new methods, including single-sided lower tolerance band, historical nonparametric/parametric, and weighted versions of all tests.

Like ULSTATS, VADER also supports the chi-squared normality test, and it also allows users to change the test parameters. Furthermore, the development team plans to implement a variety of new normality tests, including trend significance testing. Well-known tests such as the Anderson–Darling and the Shapiro–Wilk tests are being implemented.

VADER supports reading the USLSTATS legacy input format, allowing users to execute their existing USLSTATS inputs. However, new functionality is only available through the VADER sequence. Furthermore, VADER generates the plot files (see Figure 15), which is a familiar feature for USLSTATS users. These types of plots show the trend lines, in addition to the user data used to construct the model.

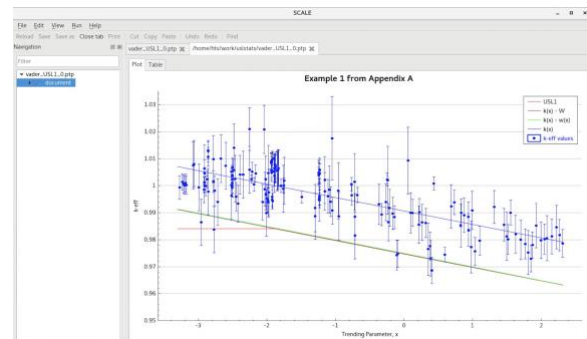


Figure 15. VADER plot.

VADER development tasks are in progress to implement new features. In addition to the new tests to be added, planned features include histogram and Q–Q plots for graphical normality assessment, extreme value theorem methods, correlated trending and non-trending methods, and single-sided statistics for reactor physics validation.

SCALE 6.2.4 Validation for Criticality Safety Analysis

The SCALE 6.2.4 validation report on criticality safety was generated based on high-quality models that cover a broad range of systems. These models were developed using the KENO V.a and KENO-VI codes. The report contains over 600 configurations based on 15 system categories from the ICSBEP Handbook [3]. These configurations are part of the SCALE validation suite, VALID, maintained at ORNL. Nuclear data used for this report include three MG libraries—56-group neutron,

200-neutron/47-gamma group, and 252-group neutron libraries—and a CE library based on ENDF/B-VII.1.

The average calculated-to-evaluation (C/E) values (Figure 16) indicate that the code bias for a wide range of systems is fairly small, and when considering all the categories of the examined systems, the bias is less than 2.2% Δk . After removing the intermediate spectrum systems that are fueled with ^{233}U due to suspected nuclear data problems, the bias for KENO V.a is less than 1% Δk , whereas the bias is less than 0.5% Δk for most categories. The biases in KENO-VI appear to be larger, but they are still less than 0.9% Δk . These biases may be the result of the increased geometric complexity of the benchmark experiments and the associated difficulties in accurately describing the complex configurations.

Trends identified in several experiment series may provide insights into the nuclides and energy ranges, meriting further investigation. The ^{233}U -fueled solution systems can be used to identify potential cross section issues. Thick iron-reflected fast-spectrum cases, which exhibit unusual disagreements between MG and CE results, allow quantification of methodology limitations

on resonance self-shielding calculations and are useful when developing improvements.

The overall cross section uncertainty as quantified through the SCALE covariance library is probably overestimated, which is consistent with previous research. All categories of experiments in KENO V.a and KENO-VI show significantly less variability than expected based on the cross section uncertainties. The cause of this overestimation is believed to be the inconsistent treatment of cross sections and their uncertainties during the evaluation process.

Overall, the KENO V.a and KENO-VI codes have been shown to provide consistent, low-bias results across a range of systems commonly encountered in criticality safety applications. The data presented in the report are valuable because the results are based on the models included and have undergone the quality checks recommended in VALID. The associated report is in press and will become available in 2021.

[T. M. Greene and W. J. Marshall. 2021. “SCALE 6.2.4 Validation – Volume 2: Nuclear Criticality Safety,” ORNL/TM-2020/1500, Oak Ridge National Laboratory]

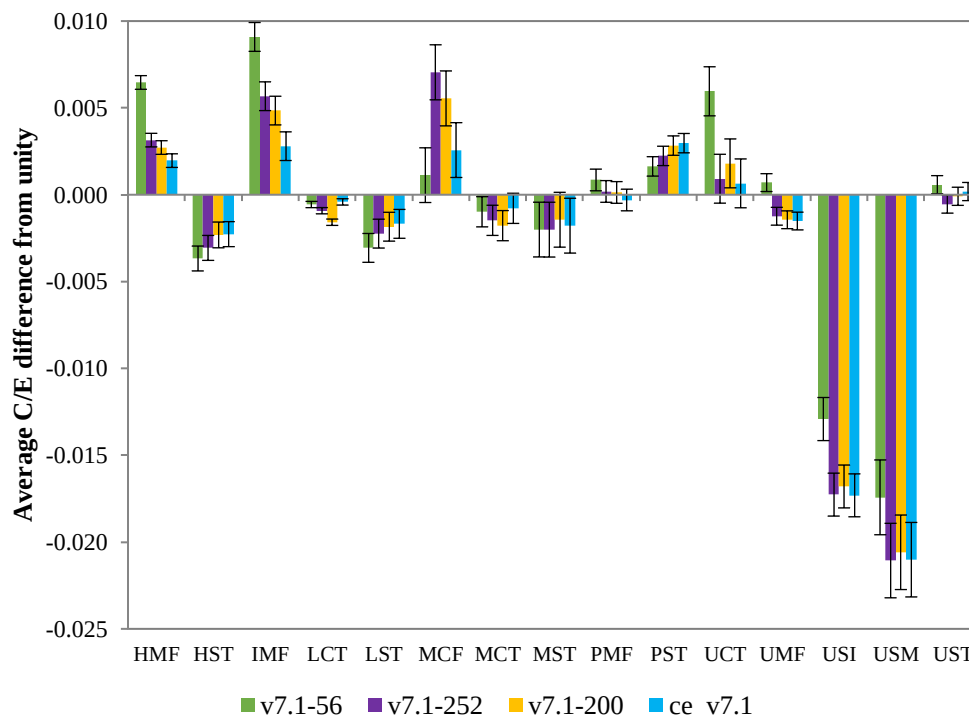


Figure 16. Absolute bias for all 4 libraries for each of the 15 categories of experiments.

SCALE 6.2.4 Validation for Reactor Physics Applications

A validation report on SCALE version 6.2.4 for reactor physics applications *SCALE 6.2.4 Validation – Volume 3: Reactor Physics Applications*, is pending publication [G. Ilas, J.R. Burns, B. Hiscox, U. Mertzyurek. 2021, ORNL/TM-2020/1500, Oak Ridge National Laboratory]. The validation basis includes a number of relevant cases for each group of key metrics considered, including nuclide inventory, decay heat, and full-core criticality. All SCALE simulations were performed using ENDF/B-VII.1 libraries.

The accuracy of predicting nuclide inventories in spent nuclear fuel is generally assessed via C/E nuclide concentration ratios for nuclides of interest using experimental radiochemical assay (RCA) data as a basis. The RCA data used for validation in the study include 92 PWR samples which cover an approximate burnup range of 7–70 GWd/MTU, as well as 76 BWR samples characterized by burnups of 4.2–68.4 GWd/MTU and average void fractions during irradiation at the sample location in the range of 0–74%.

The decay heat validation basis includes full-assembly decay heat experimental data: 91 decay heat measurements for 52 PWR assemblies, and 145 measurements for 83 BWR assemblies. These measurements cover a large range of assembly burnups (5.3–51.0 GWd/MTU) and cooling times after discharge from the reactor (2.3–26.7 years). Validation for very short cooling times up to approximately 10^5 s that are of interest for evaluating postulated loss-of-coolant-accident scenarios are usually based on pulse fission experiments, which involve irradiation of fissile nuclides to determine the energy release from fission. The experimental data used for validation in this research include energy following fission of ^{233}U , ^{235}U , ^{238}U , ^{239}Pu , ^{241}Pu , and ^{232}Th .

The validation basis for full-core analyses includes criticality measurements for both Watts Bar and AP1000 LWRs. The non-LWR examples include the HTR-10 and the High-Temperature Engineering Test Reactor (HTTR) HTGR benchmarks from the International Reactor Physics Benchmark Experiments (IRPhE) Handbook.

The results obtained with SCALE 6.2.4 and ENDF/B-VII.1 for nuclide inventories show improved prediction accuracy for a series of actinides and fission products—particularly plutonium nuclides—with the new SCALE version and nuclear data. For example, the SCALE 6.2.4 ENDF/B-VII.1 prediction of the major actinide ^{239}Pu (important for burnup credit, decay heat, and nuclear safeguards) improved by approximately 2% on average compared with the SCALE 6.1 ENDF/B-VII.0 results for the considered 92 PWR samples. The comparison of ^{235}U and ^{239}Pu in PWR fuel samples is presented in Figure 17. Comparison of the calculated and experimental decay heat for full assemblies showed very good agreement, as illustrated by the C/E histograms in Figure 18.

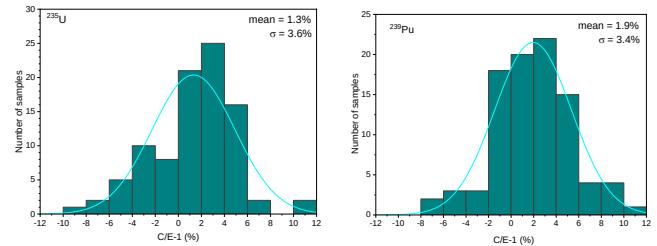


Figure 17. Histogram plots for ^{235}U and ^{239}Pu C/E comparison for PWR samples.

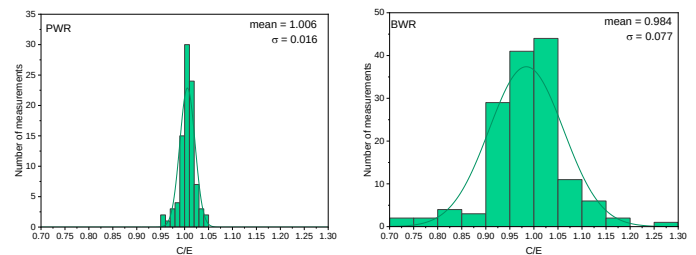


Figure 18. Histogram plots of C/E decay heat ratios for PWRs and BWRs.

SCALE 6.2.4 Shielding Validation

The goal of modeling is to accurately conceptualize and predict physical phenomena. In nuclear engineering, and particularly in radiation shielding, modeling can be used in important projects for which accuracy is key, such as nuclear reactor licensing and radiation safety. Thus, existing data from real-life operation must be compared with code predictions to judge data accuracy. A validation report demonstrating the accuracy of MAVRIC, the shielding module in SCALE 6.2.4, is pending publication.

In the past, MAVRIC was validated against existing benchmarks, but this is the first time that all the data have been compiled into a single document; the report regroups all types of experiments, materials, and quantities of interest. In the 6.2.4 shielding validation report, results are given for MAVRIC tests compared against eight different benchmarks from reliable sources, such as the ICSBEP Handbook, the Shielding Integral Benchmark Archive and Database (SINBAD), and other peer-reviewed shielding validation studies presented in the literature. Thousands of points of comparison between calculation and experiment are presented.

Experimental results analyzed from these benchmarks include neutron fluxes, detector count rates, detector energy response functions, neutron and gamma doses, foil neutron activation rates and activities, neutron leakage fluxes, and skyshine dose rates from interaction with various materials (e.g., iron, polyethylene, water, cadmium, lead, air, and soil). The SCALE models used were either obtained from previous published work or were created or modified specifically for this effort. Table 1 provides an overview of the eight benchmarks under consideration. Figure 19 through Figure 21 provide illustrations of the three selected models.

Table 1. Overview of the SCALE 6.2.4 shielding validation report benchmarks characteristics

Benchmark	Radiation of interest	Source	Material interaction of interest	Quantity of interest
Neutron transmission through an iron sphere	Neutron	^{252}Cf	Fe	Neutron flux spectrum
Neutrons through a heavy water sphere	Neutron	^{252}Cf	Heavy water	Neutron flux spectrum
Concrete labyrinth (Figure 19)	Neutron	^{252}Cf	Concrete (borated), polyethylene, Cd	Counts per second in Bonner sphere
Am-Be neutrons leakage through several materials	Neutron	Am-Be	Polyethylene, Be, Pb, Nb, Mo, Ta, W	Neutron flux spectrum
D-T neutrons through an iron sphere	Neutron	Deuterium-tritium	Fe	Neutron flux spectrum
Graphite shielding measurements	Neutron	^{252}Cf	Paraffin, steel, polyethylene	Neutron dose rate
Skyshine benchmark (Figure 20)	Gamma	^{60}Co	Air, soil	Gamma dose rate skyshine
SILENE critical assembly benchmark (Figure 21)	Neutron	Uranyl nitrate solution	Foils (Co, Au, In, Fe, Mn, Mg, Ni)	Neutron activation

Other than rare outliers typically explained by either a lack of information or large uncertainties in the experiment conditions, material, or dimensions, results obtained by MAVRIC agree well with the experimental results, within the estimated measurement uncertainties. MAVRIC was also compared to MCNP calculations where available, and both codes generally produce good agreements. The team plans to update this validation analysis for each new SCALE release, to include updates for new cases, benchmarks, and other useful items. In 2021, a new shielding validation report will be published for the upcoming SCALE 6.3 release.

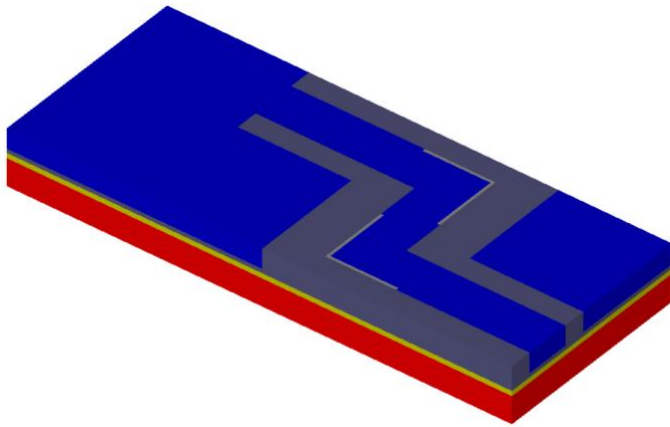


Figure 19. Concrete labyrinth SCALE model overview.

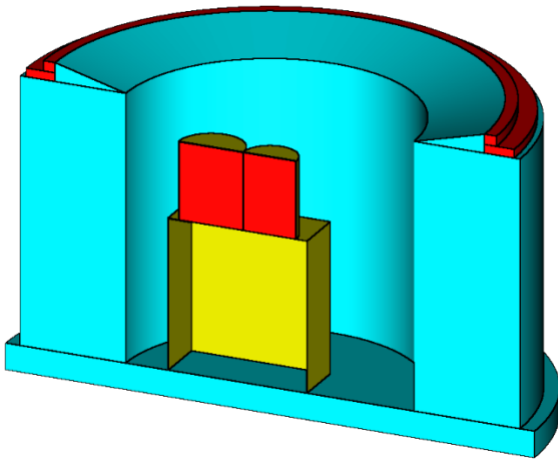


Figure 20. Photon skyshine SCALE model overview.

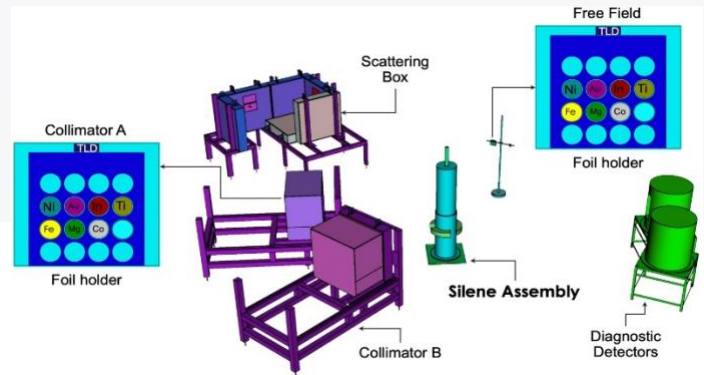


Figure 21. SILENE critical assembly SCALE model overview.

SCALE User Support and Training

Requesting SCALE

Distribution

SCALE is distributed to end users subject to US export control regulations. Each user must be individually licensed through an authorized distribution center. SCALE licenses are issued through the [Radiation Safety Information Computational Center \(RSICC\)](#) at ORNL, the OECD NEA [Data Bank](#) in Paris, France, and the Research Organization for Information Science and Technology (RIST) [Nuclear Code Information Services](#) in Japan. Any license fees collected for the distribution of SCALE are retained by these organizations to offset the costs of background checks and media duplication. No part of the license revenue is used to support SCALE activities.

Requesting SCALE from RSICC

When completing the required end-use statement in the RSICC request form, requestors should include a complete description of how they will use the software in their work as an employee or in their academic studies as a student. Specific information is recommended, and general statements such as “to solve work/homework problems,” or “for a class” should be avoided. A thorough description of the types of problems to be solved using SCALE is required.

The RSICC software selection list only includes the executable SCALE/EXE version. If you need the *source* version, you may select the available executable version and include a justification in the end use statement or the comments of the request to explain why the source version is needed.

SCALE Technical Support

The SCALE Team is dedicated to supporting all SCALE users. The team provides limited complimentary technical support for inquiries submitted to scalehelp@ornl.gov.

The SCALE Team has a Google Group to facilitate discussions among SCALE users and developers, and it can be found here: <https://groups.google.com/g/scale-users-group>. Anyone visiting the site can browse the discussion topics and responses, but an authorized user account—which requires a Google account and a SCALE license (any version of SCALE)—is required to post to the forum. The forum is monitored by the SCALE development team. Some basic instructions for accessing and registering for this group are provided [at this link](#). Please do not post export-controlled, sensitive, or proprietary information to this forum. For inquiries that include these kinds of information, please contact the SCALE Team directly at scalehelp@ornl.gov.

A scalenews mailman list is maintained to distribute news announcements. It is updated each month with the email addresses of those who have obtained a new SCALE license from RSICC, RIST, or the NEA Data Bank.

- If your email address has changed since you last obtained a SCALE license, please send an email to scalehelp@ornl.gov, and include your old and new email addresses.
- If you would like your email address removed from the scalenews mailman list, please send an email to scalehelp@ornl.gov and include the email address that you would like to have removed.

How to Request a Patch or Beta Release

If any minor bug fixes are found in the current version of SCALE, a patch will be created that users may obtain by sending a request to scalehelp@ornl.gov. The patches are free, but to obtain them, you must be licensed for the current version of SCALE.

Information about SCALE releases can be found at <https://www.ornl.gov/scale/releases>, along with details on how to request a beta version.

SCALE Documentation

The SCALE manual, primers, and other helpful documentation are available on the SCALE user documentation web page at <https://www.ornl.gov/content/user-documentation>.

Links to previous SCALE newsletters, annual reports, and quality assurance documents are found on the SCALE support web page: <https://www.ornl.gov/scale/support>.

Publications related to the following categories can be found on the SCALE references web page: <https://www.ornl.gov/scale/references>.

- Advanced Reactors
- Criticality Safety
- Depletion and Decay
- Nuclear Data
- Radiation Shielding
- Reactor Physics
- Sensitivity and Uncertainty Analysis
- User Documentation

SCALE Training

Training courses are presented by developers and expert users from the SCALE Team. These courses include reviews of theory, as well as descriptions of capabilities and software limitations. Hands-on exercises at varying levels of complexity are included.

All SCALE training course attendees must be licensed for the SCALE version used in the training. If you are not a licensed user of SCALE and would like to order the software, please visit <https://www.ornl.gov/content/how-order-scale>. Please request the software at least **two months** prior to the start of the training course.

The next SCALE training block to be held by ORNL will be October–November of 2021. It is currently not certain whether the training will be in person, virtual, or hybrid. Course descriptions are provided on the training page of the SCALE website: <https://www.ornl.gov/scale/training>. The following courses are planned:

- October 11–15, 2021: SCALE/TRITON Lattice Physics and Depletion
- October 18–22, 2021: SCALE/ORIGEN Standalone Fuel Depletion, Activation, and Source Term Analysis
- October 25–29, 2021: SCALE Computational Methods for Burnup Credit
- November 1–5, 2021: Nuclear Data Fundamentals and AMPX Libraries Generation

The SCALE Team can provide direct virtual support or a visit to your site to present customized, hands-on courses to share the expertise needed to solve challenging application scenarios. Please contact scalehelp@ornl.gov for more information.

SCALE Users' Group Workshop

The fourth annual meeting of the SCALE Users' Group Workshop was hosted virtually from ORNL July 27–29, 2020. The full agenda and links to the presentations from the meeting are available at <https://www.ornl.gov/content/2020-scale-users-group-workshop>.

Save the Dates for the 2021 SCALE Users' Group Workshop!

Please save the dates for the [5th SCALE Users' Group Workshop](#), to be hosted by ORNL August 4–6, 2021. Like the 2020 workshop, this year's workshop will be a virtual-only event.

The workshop will provide a highly interactive forum for a fruitful exchange between SCALE users and developers and will include a mix of presentations, open discussions, and tutorial sessions. End users are invited to participate in the meeting and may contribute with presentations on impactful and innovative applications of SCALE. The meeting will be free of charge to all participants. Participation will be limited to 200 attendees.

SCALE Publications, April 2020–April 2021

Journal Articles

G. Ilas and J. Burns, "SCALE 6.2.4 Validation for Light Water Reactor Decay Heat Analysis," *Nuclear Technology*, (2021) (in press).

A. Shaw, F. Rahnema, A. Holcomb, and D. Bowen, "Validation of Continuous-Energy ENDF/B-VIII.0 ^{16}O , ^{56}Fe , and $^{63,65}\text{Cu}$ Cross Sections for Nuclear Criticality Safety Applications," *Nuclear Science and Engineering*, **195**(4), 412–436 (April 2021).

DOI: [10.1080/00295639.2020.1830621](https://doi.org/10.1080/00295639.2020.1830621)

R. A. Hall, W. J. Marshall, E. Eidelpes, and B. M. Hom, "Assessment of Critical Experiment Benchmark Applicability to a Large-Capacity HALEU Transportation Package Concept," *Nuclear Science and Engineering*, **195**(3), 310–319 (March 2021).

DOI: [10.1080/00295639.2020.1801319](https://doi.org/10.1080/00295639.2020.1801319)

C. Gentry, B. Collins, E. Davidson, G. Davidson, T. Evans, A. Godfrey, S. Hart, G. Ilas, S. Johnson, K. S. Kim, S. Palmtag, T. Pandya, K. Royston, W. Wieselquist, and G. Wolfram, "Secondary-Source Core Reload Modeling with VERA," *Nuclear Science and Engineering*, **195**(3), 320–337 (March 2021).

DOI: [10.1080/00295639.2020.1820797](https://doi.org/10.1080/00295639.2020.1820797)

G. Radulescu, K. Banerjee, T. M. Miller, and D. E. Peplow, "Skyshine Calculations for a Large Spent Nuclear Fuel Storage Facility with SCALE 6.2.3," *Nuclear Technology* (February 2021).

DOI: [10.1080/00295450.2020.1842702](https://doi.org/10.1080/00295450.2020.1842702)

U. Mertyurek, M. A. Jessee, and B. R. Betzler, "Lattice Physics Calculations Using the Embedded Self-Shielding Method in Polaris, Part II: Benchmark Assessment," *Annals of Nuclear Energy*, **150**, 107829 (January 2021).

DOI: [10.1016/j.anucene.2020.107829](https://doi.org/10.1016/j.anucene.2020.107829)

M. A. Jessee, W. A. Wieselquist, U. Mertyurek, K. S. Kim, T. M. Evans, S. P. Hamilton, and C. Gentry, "Lattice Physics Calculations Using the Embedded Self-Shielding Method in Polaris, Part I: Methods and Implementation," *Annals of Nuclear Energy*, **150**, 017830 (January 2021).

DOI: [10.1016/j.anucene.2020.107830](https://doi.org/10.1016/j.anucene.2020.107830)

F. Bostelmann, C. Celik, M. L. Williams, R. J. Ellis, G. Ilas, W. A. Wieselquist, "SCALE Capabilities for High Temperature Gas-Cooled Reactor Analysis," *Annals of Nuclear Energy*, **147**, 107673 (November 2020).

DOI: [10.1016/j.anucene.2020.107673](https://doi.org/10.1016/j.anucene.2020.107673)

B. R. Betzler, B. J. Ade, A. J. Wysocki, P. K. Jain, P. C. Chesser, M. S. Greenwood, and K. A. Terrani, "Transformational Challenge Reactor Preconceptual Core Design Studies," *Nuclear Engineering and Design*, **367**, 110781 (October 2020).

DOI: [10.1016/j.nucengdes.2020.110781](https://doi.org/10.1016/j.nucengdes.2020.110781)

J. M. Ghawaly Jr., A. D. Nicholson, D. E. Peplow, C. M. Anderson-Cook, K. L. Myers, D. E. Archer, M. J. Willis, and B. J. Quiter, "Data for Training and Testing Radiation Detection Algorithms in an Urban Environment," *Scientific Data*, **7**, 328 (October 2020).

DOI: [10.1038/s41597-020-00672-2](https://doi.org/10.1038/s41597-020-00672-2)

D. Chandler, B. R. Betzler, E. E. Davidson, and G. Ilas, "Modeling and Simulation of a High Flux Isotope Reactor Representative Core Model for Updated Performance and Safety Basis Assessments," *Nuclear Engineering and Design*, **366**, 110752 (September 2020).

DOI: [10.1016/j.nucengdes.2020.110752](https://doi.org/10.1016/j.nucengdes.2020.110752)

J. Hu, I. C. Gauld, S. Vaccaro, T. Honkamaa, and G. Ilas, "Validation of ORIGEN for VVER-440 Spent Fuel with Application to Fork Detector Safeguards Measurements," *ESARDA Bulletin*, **No. 60**, 28–43 (June 2020).

DOI: [10.2760/217080](https://doi.org/10.2760/217080)

D. Huang, U. Mertyurek, and H. Abdel-Khalik, "Verification of the Sensitivity and Uncertainty-Based Criticality Safety Validation Techniques: ORNL's SCALE Case Study," *Nuclear Engineering and Design*, **361**, 110571 (May 2020).

DOI: [10.1016/j.nucengdes.2020.110571](https://doi.org/10.1016/j.nucengdes.2020.110571)

Conference Papers

F. Bostelmann, A. M. Holcomb, D. Wiarda, and W. A. Wieselquist, "On the Creation of the New ENDF/B-VIII.0 Covariance Library for SCALE Applications with AMPX," in *Proceedings of the International Conference on Mathematics and Computational Methods Applied to Nuclear Science and Engineering (M&C 2021)*, Charlotte, NC, USA, October 3–7, 2021 (accepted).

J. Seo, D. Huang, U. Mertyurek, and H. S. Abdel-Khalik, "Non-Intrusive Alternative to Generalized Linear Least-Squares Methodology for Criticality Safety Applications," in *Proceedings of the International Conference on Mathematics and Computational Methods Applied to Nuclear Science and Engineering (M&C 2021)*, Charlotte, NC, USA, October 3–7, 2021 (accepted).

J. Li, S. Kinast, V. Seker, J. Wang, A. Ward, B. Kochunas, T. Downar, and U. Mertyurek, "Neutronics Simulation of the Molten Salt Reactor Experiment With SCALE/Shift and Serpent/PARCS," in *Proceedings of the International Conference on Mathematics and Computational Methods Applied to Nuclear Science and Engineering (M&C 2021)*, Charlotte, NC, USA, October 3–7, 2021 (accepted).

K. S. Kim, A. M. Holcomb, and W. A. Wieselquist, "Spatially Dependent Resonance Self-Shielding Capability for Non-Uniform Temperature Profile in SCALE-6.3 XSPROC-BONAMI," in *Proceedings of the International Conference on Mathematics and Computational Methods Applied to Nuclear Science and Engineering (M&C 2021)*, Charlotte, NC, USA, October 3–7, 2021 (accepted).

K. S. Kim, A. M. Holcomb, F. Bostelmann, D. Wiarda, B. R. Langley, and W. A. Wieselquist, "Improvement of the SCALE-XSPROC Capabilities for High-Temperature Gas-Cooled Reactor Analysis," in *Proceedings of the International Conference on Mathematics and Computational Methods Applied to Nuclear Science and Engineering (M&C 2021)*, Charlotte, NC, USA, October 3–7, 2021 (accepted).

K. S. Kim and W. A. Wieselquist, "Reactivity Underestimation of ENDF/B-VIII.0 Compared with ENDF/B-VII.1 for the Pressurized Water Reactor Depletion Analysis," in *Transactions of the American Nuclear Society*, **124** (June 2021).

M. N. Dupont, D. E. Peplow, C. Celik, G. Radulescu, and W. A. Wieselquist, "Overview of the 2020 SCALE 6.2.4 Validation Report for Radiation Shielding Applications," in *Transactions of the American Nuclear Society*, **124** (June 2021).

C. Chapman, A. Lang, and B. J. Marshall, "Discovery of AMPX Thermal Scattering Law Processing Issue for Solid Moderators," *Transactions of the American Nuclear Society*, **124** (June 2021).

G. Ilas and B. Hiscox, "Validation of SCALE 6.2.4 and ENDF/B-VII.1 Data Libraries for Nuclide Inventory Analysis in PWR Used Fuel," *Transactions of the American Nuclear Society*, **124** (June 2021).

J. Alwin, F. Brown, J. Clarity, I. Duhamel, F. Fernex, L. Leal, R. Little, B. J. Marshall, M. Rising, E. Saylor, and K. Spencer, "S/U Comparison Study with a Focus on USLs," *Transactions of the American Nuclear Society*, **123**, 780–783 (November 2020). DOI: [10.13182/T123-33156](https://doi.org/10.13182/T123-33156)

W. J. Marshall, J. B. Clarity, and B. T. Rearden, "A Review of TSUNAMI Applications," *Transactions of the American Nuclear Society*, **123**, 795–798 (November 2020). <https://www.osti.gov/servlets/purl/1731033>

B. T. Rearden, W. J. Marshall, and W. A. Wieselquist, "Development of SCALE Tools for Sensitivity and Uncertainty Analysis Methodology Implementation (TSUNAMI) from SCALE 5 through SCALE 6.2," *Transactions of the American Nuclear Society*, **123**, 799–803 (November 2020). DOI: [10.13182/T123-33078](https://doi.org/10.13182/T123-33078)

J. B. Clarity, W. J. Marshall, B. T. Rearden, and I. Duhamel, "Selected Uses of TSUNAMI in Critical Experiment Design and Analysis," *Transactions of the American Nuclear Society*, **123**, 804–807 (November 2020). <https://www.osti.gov/servlets/purl/1760136>

W. Wieselquist, J. Bess, D. Bowen, I. Duhamel, I. Hill, N. Leclaire, W. Marshall, C. Percher, E. Saylor, and S. Tsuda, "Initial Efforts Organizing WPNCs SG-8: Preservation of Expert Knowledge and Judgement Applied to Criticality Benchmarks," *Transactions of the American Nuclear Society*, **123**, 895–897 (November 2020). DOI: [10.13182/T123-32977](https://doi.org/10.13182/T123-32977)

J. B. Clarity, S. W. D. Hart, W. A. Wieselquist, and W. J. Marshall, "VADER: A Tool for Criticality Safety Validation," *Transactions of the American Nuclear Society*, **123**, 931–933 (November 2020). <https://www.osti.gov/servlets/purl/1760137>

K. B. Bekar, J. B. Clarity, M. N. Dupont, R. A. Lefebvre, W. J. Marshall, and E. M. Saylor, "Updated Primers Generated for SCALE 6.2 for KENO V.a and KENO-VI," *Transactions of the American Nuclear Society*, **123**, 934–936 (November 2020). DOI: [10.13182/T123-33125](https://doi.org/10.13182/T123-33125)

W. J. Marshall and B. D. Brickner, "Improved Runtime Performance in KENO-VI Models Using Arrays and Holes," *Transactions of the American Nuclear Society*, **123**, 937–940 (November 2020). DOI: [10.13182/T123-33121](https://doi.org/10.13182/T123-33121)

A. Rivas, J. Hou, and G. Ilas, "Preliminary Benchmark Calculations of Spent Nuclear Fuel Isotopic Compositions Using BWR Assay Data," *Transactions of the American Nuclear Society*, **123**, 1365–1368 (November 2020).

W. J. Marshall, T. M. Greene, B. D. Brickner, and R. A. Hall, "Description and Use of SCALE Sampler Parametric Capability for Engineering Analysis and Optimization," *Transactions of the American Nuclear Society*, **122**, 471–474 (June 2020). <https://www.osti.gov/servlets/purl/1649393>

W. J. Marshall, J. B. Clarity, and K. Banerjee, "Performing k_{eff} Validation of As-Loaded Criticality Safety Calculations using UNF-ST&DARDS: Sensitivity Calculations," *Transactions of the American Nuclear Society*, **122**, 479–482 (June 2020). <https://www.osti.gov/servlets/purl/1649369>

B. R. Betzler, B. J. Ade, A. J. Wysocki, P. C. Chesser, M. S. Greenwood, P. L. Wang, N. D. See, X. Hu, and K. A. Terrani, "Design Downselection for the Transformational Challenge Reactor," *Transactions of the American Nuclear Society*, **122**, 769–772 (June 2020). <https://www.osti.gov/servlets/purl/1633160>

B. R. Betzler, B. J. Ade, A. J. Wysocki, P. K. Jain, M. S. Greenwood, J. D. Rader, J. J. W. Heineman, R. F. Kile, N. R. Brown, and K. A. Terrani, "Power Level Downselection Analyses for the Transformational Challenge Reactor," *Transactions of the American Nuclear Society*, **122**, 773–776 (June 2020). <https://www.osti.gov/servlets/purl/1633159>

A. D. Nicholson, D. E. Peplow, J. M. Ghawaly, M. J. Willis, and D. E. Archer, "Generation of Synthetic Data for a Radiation Detection Algorithm Competition," *IEEE Transactions on Nuclear Science*, **67**, 1968–1975 (June 2020). DOI: [10.1109/TNS.2020.3001754](https://doi.org/10.1109/TNS.2020.3001754)

K.S. Kim, A. M. Holcomb, F. Bostelmann, D. Wiarda, and W.A. Wieselquist, "Improvement of the SCALE-XSProc Multigroup Cross Section Processing Based on the CENTRM Pointwise Slowing Calculation," 1329–1336 in *Proceedings of PHYSOR 2020 – Transition to a Scalable Nuclear Future*, Cambridge, United Kingdom (March 29–April 2, 2020). DOI: [10.1051/epjconf/202124702011](https://doi.org/10.1051/epjconf/202124702011)

U. Mertzyurek, H. S. Abdel-Khalik, and W. J. Marshall, "MAPPER – A Novel Capability to Support Nuclear Model Validation and Mapping of Biases and Uncertainties," 1615–1615 in *Proc. of PHYSOR 2020 – Transition to a Scalable Nuclear Future*, Cambridge, United Kingdom (March 29–April 2, 2020). DOI: [10.1051/epjconf/202124715018](https://doi.org/10.1051/epjconf/202124715018)

B. D. Hiscox, B. R. Betzler, V. Sobes, and W. J. Marshall, "Neutronic Benchmarking of Small Gas-Cooled Systems," in *Proceedings of PHYSOR 2020 – Transition to a Scalable Nuclear Future*, Cambridge, United Kingdom (March 29–April 2, 2020). DOI: [10.1051/epjconf/202124710033](https://doi.org/10.1051/epjconf/202124710033)

A. Shaw, F. Rahnema, A. Holcomb, and D. Bowen, "ENDF/B-VIII.0 Cross Section Testing for Copper Nuclear Criticality Safety Applications," in *Proceedings of PHYSOR 2020 – Transition to a Scalable Nuclear Future*, Cambridge, United Kingdom (March 29–April 2, 2020). DOI: [10.1051/epjconf/202124710007](https://doi.org/10.1051/epjconf/202124710007)

Technical Reports

K. Bekar, J. Clarity, M. Dupont, R. Lefebvre, W. Marshall, and E. Saylor, "KENO V.a Primer: Performing Calculations using SCALE's Criticality Safety Analysis Sequence (CSAS5) with Fulcrum," ORNL/TM-2020/1664, UT-Battelle, LLC, Oak Ridge National Laboratory (December 2020). DOI: [10.2172/1760121](https://doi.org/10.2172/1760121)

K. Bekar, J. Clarity, M. Dupont, R. Lefebvre, W. Marshall, and E. Saylor, "KENO-VI Primer: Performing Calculations using SCALE's Criticality Safety Analysis Sequence (CSAS5) with Fulcrum," ORNL/TM-2020/1601, UT-Battelle, LLC, Oak Ridge National Laboratory (December 2020). DOI: [10.2172/1760129](https://doi.org/10.2172/1760129)

B. Bevard, J. Giaquinto, C. Hexel, G. Ilas, R. Montgomery, R. N. Morris, and B. Roach, "Sister Rod Destructive Examinations (FY20) Appendix D: Fission Gas, Fuel Burnup and Fuel Isotopic Measurements," ORNL/SPR-2020/1770, UT-Battelle, LLC, Oak Ridge National Laboratory (November 2020). DOI: [10.2172/1764471](https://doi.org/10.2172/1764471)

M. N. Dupont and E. M. Saylor, "Sulfur Pellets Responses to a Bare and Steel-Reflected Pulse of the Oak Ridge National Laboratory Health Physics Research Reactor," ORNL/TM-2020/1731, UT-Battelle, LLC, Oak Ridge National Laboratory (September 2020). DOI: [10.2172/1765486](https://doi.org/10.2172/1765486)

H. Akkurt, H. Liljenfeldt, G. Ilas, S. Baker, and K. Fuhr, "Phenomena Identification and Ranking Table (PIRT) for Decay Heat: Review of Current Status and Recommendations for Future Needs," EPRI Report 3002018440 (July 2020). <https://www.epri.com/research/products/000000003002018440>

F. Bostelmann, G. Ilas, and W. A. Wieselquist, "Key Nuclear Data Impacting Reactivity in Advanced Reactors," ORNL/TM-2020/1557, UT-Battelle, LLC, Oak Ridge National Laboratory (June 2020). DOI: [10.2172/1649145](https://doi.org/10.2172/1649145)