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# DEVELOPMENT AND VALIDATION OF SCALE NUCLEAR ANALYSIS METHODS FOR HIGH TEMPERATURE GAS-COOLED REACTORS

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**Abstract –** *In support of the U.S. Nuclear Regulatory Commission, ORNL is updating the nuclear analysis methods and data in the SCALE code system to support modeling of HTGRs. Development activities include methods used for reactor physics, criticality safety, and radiation shielding. This paper focuses on the nuclear methods in support of reactor physics, which primarily include lattice physics for cross-section processing of both prismatic and pebble-bed designs, Monte Carlo depletion methods and efficiency improvements for double heterogeneous fuels, and validation against relevant experiments. These methods enhancements are being validated using available experimental data from the HTTR and HTR-10 startup and initial criticality experiments. Results obtained with three-dimensional Monte Carlo models of the HTTR initial core critical configurations with SCALE6/KENO show excellent agreement between the continuous energy and multigroup methods and the results are consistent with results obtained by others. A three-dimensional multigroup Monte Carlo model for the initial critical core of the HTR-10 has been developed with SCALE6/KENO based on the benchmark specifications included in the IRPhE Handbook. The core eigenvalue obtained with this model is in very good agreement with the corresponding value obtained with a consistent continuous energy MCNP5 core model.*

## I. INTRODUCTION

There are currently several ongoing High Temperature Gas-cooled Reactor (HTGR) development projects underway throughout the world with the U.S. DOE Next Generation Nuclear Plant (NGNP) representing a significant and growing activity in the United States. The NGNP is an HTGR for generating electricity and production of hydrogen and/or high-temperature process heat for industrial applications. The design options are currently being evaluated at this time with prismatic-block or pebble-bed designs considered. Both designs use coated particle fuel, are graphite-moderated, may have both internal and external reflectors, and have a very high exit temperature of greater than 700°C. These specific features represent significant deviations from current commercial light water reactor (LWR) designs, and will therefore have different requirements for computer codes needed for safety analysis.

In support of the U.S. Nuclear Regulatory Commission, Oak Ridge National Laboratory (ORNL) is updating the nuclear analysis methods and data in the SCALE (Standardized Computer Analyses for Licensing Evaluation) code system [1] for modeling of HTGRs. Development activities include methods used for reactor physics, criticality safety, and radiation shielding. This paper focuses on the nuclear methods in the areas of reactor physics, which primarily include lattice physics for cross section processing for both prismatic and pebble-bed designs, Monte Carlo depletion methods and efficiency improvements for double heterogeneous fuels, and validation against relevant experiments, such as the HTTR and HTR-10 startup and initial criticality experiments.

## II. SCALE METHODS DEVELOPMENT FOR HTGRS

The SCALE code system developed by ORNL provides a comprehensive and integrated package of computer codes and nuclear data for a wide range of applications in criticality safety, reactor physics, shielding, isotopic depletion and decay, and sensitivity/uncertainty (S/U) analysis. In order to better support analysis of HTGRs, enhancements and improvements of the methods and data are being performed. Four primary areas of work are described below.

### *II.A. Resonance Processing Methods*

SCALE has had the ability to model double heterogeneous fuels, such as the TRISO fuels used in HTGRs, for several years based on a two-step approach that first performs resonance corrections for the self-shielding of the fuel kernels followed by processing for the pebble-to-pebble or compact-to-compact interactions [2].

SCALE currently treats doubly-heterogeneous (DH) self-shielding using two deterministic point-wise (PW) transport calculations with the one-dimensional discrete ordinates code CENTRM. The first computes space-dependent PW fluxes for an infinite array of spherical fuel grains contained in a graphite matrix. The PW fluxes are typically calculated on an energy mesh of 50,000 – 70,000 points, covering the thermal range to 20 keV (upper limit of the $^{238}$U resolved range). The fine energy mesh allows the spectral fine-structure due to response reactions to be resolved. These fluxes are used to compute PW disadvantage factors for flux weighting the fuel grain/matrix PW cross sections into a homogeneous compact mixture such that the PW reaction rates are preserved. The second PW calculation is performed for the lattice unit cell consisting of the homogenized fuel compact and graphite moderator. PW fluxes from the second CENTRM case are used to average the PW data into self-shielded multigroup (MG) values for the homogenized compact and graphite materials. This method has been shown to agree well with KENO continuous energy (CE) Monte Carlo transport calculations with explicit representation of the individual fuel grains and is the approach that is used in the validation against the HTTR and HTR-10 startup experiments discussed in Sections III and IV.

Continued development of the SCALE resonance processing methods has focused on the incorporation of an alternative method to support faster-running calculations and methods that account for resonance upscattering that has been traditionally neglected in lattice physics calculations, but has shown to be significant for high-temperature systems [3].

The intermediate resonance (IR) approximation has been implemented in the SCALE resonance self-shielding module BONAMI as a faster but less rigorous alternative to the CENTRM/PMC self-shielding methodology. The IR method provides a fast-executing approach that can be used for scoping studies and rapid assessment of physics and design issues. In the initial phase of the SCALE IR development, the methodology was implemented for reactor lattices containing typical homogeneous fuel rods. This required modifying the BONAMI code to use the IR method. The modified version of BONAMI is currently referred to as BONAMI-IR. CENTRM and PMC were used to compute IR parameters and to generate Bondarenko self-shielding factors for inclusion in the MG library. The Bondarenko factors were computed from a series of PW transport computations consisting of a homogeneous mixture of graphite and absorber materials, for which the background cross section was varied to span the range of interest for HTGR analysis.

Along with this approach, a new double heterogeneity (DH) method, similar in principle to the current SCALE DH treatment with CENTRM, has been developed. The new approach derives analytical expressions for the energy-dependent flux using the IR approximation and equivalence theory, instead of using CENTRM to compute the PW fluxes numerically. The resulting expressions for the DH self-shielded cross sections in an HTGR lattice are consistent with the Bondarenko method; i.e., they depend only on the value of the background cross section, so that BONAMI-IR can interpolate the shielding factors from the master MG cross-section library. This new approach requires significantly fewer computing resources than the standard approach and is currently in testing and finalization.

Historically, most reactor physics computations have assumed that molecular motion affects the neutron-target scattering kinematics only below some thermal cut-off energy where the neutron kinetic energy is comparable to the molecular-target energy. For example, the thermal cut-off for SCALE MG calculations is 3 eV. In 1991 Ouisloumen and Sanchez showed that it is not the kinetic energy but the momentum that is most significant in determining the impact of molecular motion, and this makes upscattering from heavy nuclei relatively more important at higher neutron energies where large cross section resonances occur for fuel materials [3]. This phenomenon tends to increase resonance absorption and change the calculated Doppler reactivity coefficient. Due to its high concentration and large resonances, $^{238}$U is the most significant nuclide for resonance upscattering in

thermal reactors. Recent work indicates that $^{238}U$ resonance up-scattering may be especially important for HTGR systems [4].

KENO modifications for CE calculations have been completed to simulate $^{238}U$ resonance upscatter with continuous energy Monte Carlo, using a rejection-sampling algorithm similar to that implemented by Dagan [4]. The modified KENO code was used to compute the eigenvalue for an LWR pin cell and results were compared to MCNP results. The two codes predict similar resonance upscattering effects: KENO calculates -321 pcm effect due to $^{238}U$ resonance upscattering, while MCNP calculates -346 pcm.

The updated version of KENO needs more testing, but initial indications show that it can be used for rigorous treatment of resonance upscattering effects with CE Monte Carlo. However, it is also desirable to develop methods to include resonance upscattering effects in MG calculations, since these are typically used for lattice depletion analyses and in producing few-group data for 3D core simulator codes.

Currently work is underway to incorporate resonance upscattering models into the CENTRM PW transport calculation. A routine based on the Ouisloumen and Sanchez expressions has been developed to evaluate PW scattering kernels that include the impact of molecular motion on the differential scatter cross section. This routine allows values for the point-to-point scatter kernel to be evaluated directly on the CENTRM solution mesh.

### *II.B. Lattice Physics Methods*

The SCALE TRITON lattice physics sequence contains a very flexible capability to model neutron transport in general geometries. As the work to date has focused on the analysis of LWR fuel assembly geometry, some additional development is required to support the HTGR geometries. The modeling of fuel pebbles requires a deterministic spherical modeling capability that was not available within TRITON until recently. The XSDRNPM 1-D transport code has been incorporated into TRITON to provide this capability as well as the ability to perform 1-D radial core modeling. For prismatic block designs, the 2-D NEWT discrete ordinates solver has been enhanced to model 30/45/60 degree boundaries. In addition, an improved quadrature set compatible with hexagonal reflection has been added to NEWT.

TRITON provides a rigorous transport solution, resonance processing methods, and detailed isotopic depletion capability at the cost of large execution times. Improvements in the execution times are needed to support the large number of calculations that are required for cross-section processing for core-level analysis. This will be particularly important in the case of on-line cross-section processing during the core-level calculation. In the near-term, significant gains can be obtained by implementing the ability to perform an initial problem-specific energy collapse so that the transport calculations may be performed with a smaller number of groups. Additionally, enhancements to the CMFD acceleration methods have been performed to support the HTGR geometries with more robust methods. Finally, the simplified BONAMI-IR resonance processing method, discussed above, provides a quicker, albeit more approximate, approach than CENTRM/PMC. A combination of the IR and PW transport methods also is being considered, whereby the PW CENTRM transport calculation is performed over the energy range below ~100 eV, while the fast running Bondarenko approach is applied elsewhere. This combination will significantly reduce the size of the CENTRM solution energy mesh.

### *II.C. Monte Carlo Methods*

Due to the dearth of measured benchmark-quality data for HTGRs, CE Monte Carlo depletion is needed for benchmarking SCALE MG lattice physics depletion models of HTGRs with TRITON. SCALE version 6 includes a CE Monte Carlo neutron transport capability in KENO, but it does not have the ability to perform depletion calculations using the CE results.

To efficiently perform CE Monte Carlo-based depletion calculations, accurate few-group cross sections must be calculated for use with the isotopic depletion and decay solver. The few-group microscopic reaction cross-section calculation capability has been added to KENO as part of this development. Instead of using the TRITON/KENO region-wise neutron spectra for collapsing MG cross sections in a post-processing stage, the new calculation method produces the transmutation cross sections directly and stores the data. Although the capability was developed specifically for CE mode calculations, it may also be used in MG mode. When the few-group cross sections are computed during or after a CE mode calculation, they do not suffer from inadequacies of the MG approximations such as inadequate group structure or inability to properly shield the cross sections for the problem using one-dimensional resonance self-shielding modules. Although tallies in CE mode are more expensive in terms of CPU time, the gain in accuracy makes it a viable choice.

### *II.D. Integration with the PARCS Core Simulator*

TRITON represents only a portion of the capabilities needed for HTGR core analysis. Although the methods and data available within TRITON provide the necessary rigor to capture the detailed physics of advanced reactor concepts, TRITON is not practical to perform full-core calculations for commercial-scale reactors. Linkage between TRITON and the nodal core analysis code PARCS [5] has been used to apply TRITON-generated assembly cross sections in LWR core calculations.

Updates to the lattice physics capability have been performed to support generation of additional homogenization parameters for boundaries corresponding to hexagonal geometries and for the six equilateral triangular regions that make up the prismatic fuel blocks. The interface cross section file used for linkage between TRITON and PARCS has been updated to include these additional parameters and expanded to support an arbitrary number of energy groups.

Extensive testing is being performed to generate cross sections for HTTR and their transfer to PARCS for the development of a benchmarking model for the complete TRITON-PARCS system. The results obtained with TRITON-PARCS will be compared with the experimental results as well as the CE and MG KENO Monte Carlo results to assess the accuracy of the cross-section processing methods and the full-core methods used in PARCS.

## III. SCALE VALIDATION WITH HTTR STARTUP CORE PHYSICS TESTS

The available experimental data necessary to benchmark computational methods on prismatic designs are currently limited. One such set of experimental data is provided by startup measurements on the High Temperature Engineering Test Reactor (HTTR) [6]. This 30 $MW_t$, prismatic design, graphite-moderated, helium-cooled reactor was built by the Japan Atomic Energy Agency (JAEA), with the first criticality achieved with an annular core on November 10, 1998, and with full-core criticality attained on December 16, 1998. The core of this reactor consists of fuel blocks with different fuel enrichments of up to 10 wt% $^{235}U$. These blocks are arranged in five-block columns that are intermixed with control rod columns and surrounded by reflector blocks. The fuel blocks are regular hexagonal prisms with a height of 58 cm and an apothem (center-to-side distance) of 18 cm. Each fuel block contains either 33 fuel pins of constant enrichment arranged in a triangular pitch or 31 constant enrichment fuel pins and two burnable poison (BP) pins in two corners of the hexagon at 120° with respect to the center of the hexagon. One characteristic of the fuel pins that distinguishes them from the proposed NGNP design is their annular shape. The fuel is made of TRISO particles with a $UO_2$ kernel that is embedded in a graphite matrix in the form of an annular cylinder.

### *III.A. Comparison of Results for HTTR Fuel Blocks*

A recent study was performed involving 3-D modeling of an HTTR fuel block with the SCALE code system [7]. Calculations have been performed with ENDF/B-VII MG cross sections processed with the "double heterogeneity" option and with CE ENDF/B-VII cross section data. The multiplication constant and the fission density distributions have been analyzed and compared to the results obtained with the MCNP5 code [8].

The fuel block that was analyzed contains 33 pins, with the fuel kernels at 6.3% enrichment and the burnable poison (BP) rods with 2.5% $^{10}B$ content, based on the specifications provided in reference [7]. Figure 1 shows cross-sectional (Fig. 1a) and vertical (Fig. 1b) views of the fuel block considered. Each annular fuel pin (with an inner radius of 0.5 cm, an outer radius of 1.3 cm, a height of 54.6 cm, and a pitch between pins of 5.15 cm) is made of 14 fuel compacts, each 3.9 cm in height. The $UO_2$ fuel pins are enclosed in a graphite sleeve outside of which helium is circulated. The annular fuel pin contains 12987 TRISO fuel particles (Fig. 1c) embedded in a graphite matrix for a total mass of 188.58 grams of uranium. The TRISO grain is made of a spherical 0.03 cm-radius fuel kernel surrounded by four layers of carbon or silicon carbide.

The BP pin consists of two 20-cm-long sections of absorber material at the top and bottom separated by a 10-cm thick section made of graphite discs. Only two of the three available BP positions in the fuel block are filled with the boron pin, while the third one is left empty. A hole is provided at the center of the fuel block for handling purposes. Detailed material description and additional geometry details are given in reference [6].

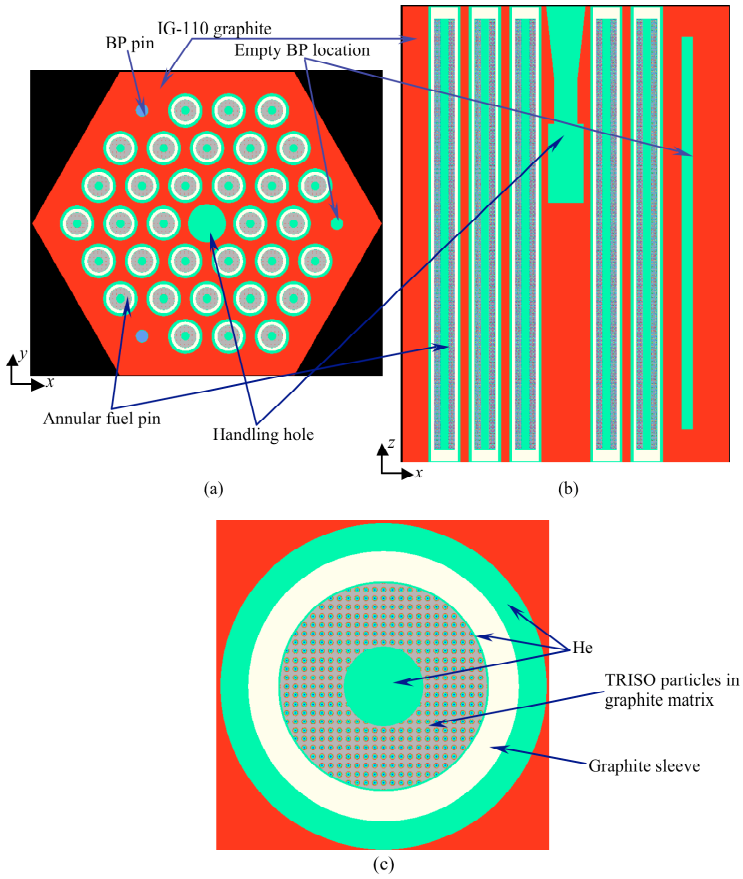


Fig. 1. Cross-sectional (a), vertical (b) views of the HTTR fuel block and fuel pin detail with explicit TRISO particles modeling (c) for the SCALE/KENO CE model.

The configuration in Fig. 1 was modeled in SCALE/KENO with the CE option and in MCNP5. Because the double-heterogeneity procedure for cross-section processing does not support annular pins at this time, the annular fuel was homogenized with the central hole to form a solid cylindrical pin for the MG option in SCALE/KENO and the DH procedure was applied. A similar procedure was used with the CE option of SCALE/KENO to assess the error introduced by this homogenization.

Table 1 shows the multiplication constant obtained in each case consisting of the CE vs MG calculations (cases 1 & 2), an MCNP5 calculation (case 3), and the different methods of treating the annual fuel compacts (cases 4 & 5). From the comparison between cases 1 and 3, it can be seen that the SCALE/KENO CE and MCNP5 have an excellent agreement. The eigenvalue predicted by the SCALE/KENO CE model is 85 ± 35 pcm higher than the MCNP5 result. The SCALE/KENO multigroup result is 336 ± 37 pcm lower than the continuous energy SCALE/KENO result.

As observed from cases 1 and 4, the homogenization of the fuel pins with their central holes leads to an overestimation of the result by 68 ± 37 pcm. Although small, the error introduced by the homogenization of the central hole into the fuel pin is statistically significant. The axial homogenization of the central handling hole has virtually no effect on the multiplication constant, as observed for case 5 in Table 1.

| Case | Description | $k_{eff}$ |
|---|---|---|
| 1 | SCALE/KENO CE | 1.3319 ± 0.0003 |
| 2 | SCALE/KENO MG | 1.3285 ± 0.0003 |
| 3 | MCNP5 | 1.3310 ± 0.0002 |
| 4 | SCALE/KENO CE with homogenized pins | 1.3325 ± 0.0003 |
| 5 | SCALE/KENO CE with homogenized handling hole | 1.3316 ± 0.0002 |

Table 1. HTTR fuel block multiplication factors for continuous energy (CE) and multigroup (MG) models.

### *III.B. Continuous Energy and Multigroup Monte Carlo Results for Critical Configurations*

During the startup testing of the HTTR, critical configurations were measured for several different fuel configurations representative of annular and cylindrical cores [9]. These startup experiments provide a means of validation for the SCALE CE KENO Monte Carlo code and data libraries. Additionally, these experiments have been analyzed with the SCALE KENO Monte Carlo code in MG mode, which additionally validates the MG libraries and resonance processing methods.

HTTR critical configurations with 19, 21, 24, 27 and 30 columns (a column being a stack of fuel blocks), which is the full core configuration, were modeled. A comparison of the critical multiplication factors for these calculations is summarized in Table 2, which shows an excellent level of agreement between the continuous energy and multigroup calculations. There appears to be a consistent bias of about 1.8% in multiplication factor in comparison with the experimental critical configuration, which has not been fully evaluated. It is worth noting that calculations performed with MCNP in the evaluation of the experiments for the International Handbook of Evaluated Reactor Physics Benchmark Experiments (IRPhE Handbook) [6] show a similar level of bias from the experimental critical configuration of about 2.5%.

Modeling and analysis of the HTTR experimental configurations and measurements are ongoing to support the validation of the SCALE methods and data being developed for HTGRs.

## IV. SCALE VALIDATION WITH HTR-10 STARTUP CORE PHYSICS TESTS

The HTR-10 pebble bed reactor startup core configuration has been used to validate the SCALE methods for pebble bed reactor designs [10]. The HTR-10 is a small test reactor with cylindrical core with a 180-cm diameter and a 197-cm height.

| Configuration | SCALE6 CE | SCALE6 MG |
|---|---|---|
| 19 columns | 1.0185 ± 0.0003 | 1.0172 ± 0.0003 |
| 21 columns | 1.0227 ± 0.0003 | 1.0216 ± 0.0002 |
| 24 columns, FS config. | 1.0178 ± 0.0003 | 1.0167 ± 0.0003 |
| 24 columns, F23 config. | 1.0198 ± 0.0003 | 1.0172 ± 0.0002 |
| 27 columns | 1.0139 ± 0.0002 | 1.0118 ± 0.0003 |
| 30 columns (fully loaded) | 1.0152 ± 0.0004 | 1.0132 ± 0.0002 |

Table 2. Multiplication factors for HTTR core configurations based on SCALE 6 continuous energy (CE) and multigroup (MG) models.

HTR-10 reached initial criticality in 2000. A set of benchmark specifications for the HTR-10 initial critical core experiment was released before the actual experiment took place for a benchmark exercise coordinated by the International Atomic Energy Agency (IAEA). The post-experiment benchmark specifications were included and presented in detail in the latest release of the IRPhE Handbook. These IRPhE specifications were used to develop a SCALE model of the startup core.

A multigroup SCALE/KENO model was developed of the startup core based on an explicit representation of the fuel and moderator (graphite) pebbles present in the core (Fig. 2). The standard SCALE double-heterogeneity approach, as discussed in Section II, was applied to obtain the MG cross sections for the calculation. When building the SCALE/KENO model in a manner that preserves the overall fuel to moderator ratio the loading consists of a total of 16,885 fuel and moderator pebbles.

Code-to-code comparison of SCALE/KENO and MCNP high-fidelity models for the HTR-10 initial critical core configuration presented in Table 3 shows an excellent agreement of the calculated $k_{eff}$ results obtained with the two codes. Both results show a bias of 1.4 ± 0.4% compared to the experimental $k_{eff}$ value. Part of this bias could be due to incomplete data in the benchmark specifications. Though the bias with respect to the experimental data is yet to be resolved, the present study demonstrates that SCALE 6 provides the same level of accuracy as the widely used MCNP code for modeling the full core of HTR-10.

## V. SUMMARY

The SCALE code system is widely used to perform reactor physics, criticality safety, and

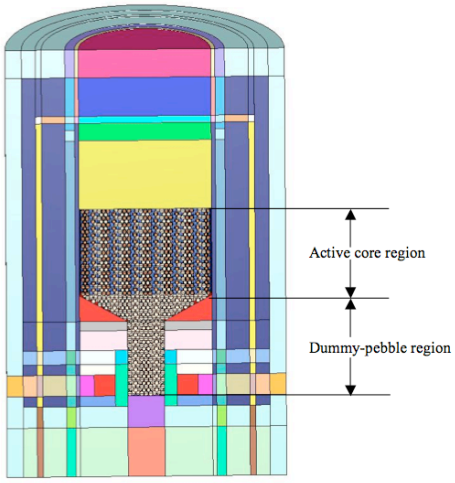


Fig. 2: SCALE/KENO geometric model of the HTR-10 startup core configuration.

| Code | Data Library | $k_{eff}$ |
|---|---|---|
| MCNP (from Ref. [11] | ENDF/B-V | 1.0119 ± 0.0002 |
| SCALE/KENO | ENDF/B-VII | 1.0153 ± 0.0003 |
| MCNP | ENDF/B-VII | 1.0147 ± 0.0002 |

Table 3. Multiplication factors for HTR-10 startup core configuration.

radiation shielding analysis for a wide range of nuclear systems. Currently ORNL is working to extend and improve this analysis capability for modeling prismatic and pebble-bed high temperature reactors. The development of analysis methods at ORNL has been an ongoing process building upon the past developments incorporated in the SCALE code system to support LWR and non-LWR nuclear reactor analysis. Recent developments in support of HTGR analysis include improvements in the SCALE resonance processing methods, lattice physics methods, Monte Carlo developments to support high-fidelity depletion analysis, and improved integration with the PARCS reactor core simulator. In addition to these areas, future enhancements will include the development of parallel computing methods and the extension of the current SCALE sensitivity/uncertainty methods to address double-heterogeneous fuels for applications to both pebble-bed and prismatic HTGRs.

The SCALE system is also being validated for HTGR applications based on available specifications for the HTTR prismatic and the HTR-10 pebble bed reactors. Results obtained with three-dimensional SCALE6/KENO Monte Carlo models of the HTTR initial core critical configurations show excellent agreement between the continuous energy and multigroup methods and the results are consistent with results obtained by others. A three-dimensional multigroup Monte Carlo model for the initial critical core of the HTR-10 has been developed with SCALE6/KENO based on the benchmark specifications included in the IRPhE Handbook. The core eigenvalue obtained with this model is in very good agreement with the corresponding value obtained with a consistent continuous energy MCNP5 core model. Additional work will be performed to analyze other parameters available for the startup core configurations as well as analyzing additional experiments to support the validation of SCALE for HTGRs.

## ACKNOWLEDGEMENTS

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