

SCALE 6 ANALYSIS OF HTR-10 PEBBLE-BED REACTOR FOR INITIAL CRITICAL CONFIGURATION

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ABSTRACT

HTR-10 is a high temperature pebble-bed reactor located in China, operated at 10 MW thermal power. The purpose of this study is to create an accurate model of HTR-10 for its initial critical configuration using the ORNL SCALE 6 code system to subsequently validate the methods used in SCALE 6 for treatment of doubly-heterogeneous fuel and the associated data libraries. KENO VI, a three-dimensional Monte Carlo transport code within SCALE 6, is used to create the computational model for HTR-10 based on the benchmark specifications provided in the International Handbook of Evaluated Reactor Physics Benchmark Experiments (IRPhE-Handbook). The results from KENO VI are compared to results obtained with a consistent MCNP model of the same configuration, as provided in the IRPhE-Handbook. The comparison shows a difference in k_{eff} of 73 ± 34 pcm between MCNP and SCALE 6.

Key Words: HTR-10, pebble bed reactor, benchmark, SCALE 6

1. INTRODUCTION

Located in China, HTR-10 is the only operational pebble-bed reactor (PBR) in the world. HTR-10 is a small test reactor, with cylindrical core diameter and height of 180 cm and 197 cm, respectively. It is helium-cooled, graphite-moderated, and operated at 10 MW thermal power. The configuration of the HTR-10 fuel elements and their distribution throughout the core are significantly different from those for conventional light water reactors. The fuel element, referred to as fuel pebble, is spherical with an outer radius of 3 cm. It contains a large number of TRISO fuel particles embedded in a graphite matrix. Each fuel particle has a spherical uranium dioxide kernel with a radius of 0.025 cm that is covered by four carbon-based layers for a total radius of 0.045 cm. In addition to the fuel pebbles, the first critical core consists of graphite moderator pebbles (also known as dummy pebbles) the same size as the fuel pebbles, with a ratio of the fuel to moderator pebbles of 0.57/0.43.

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 actual configuration for the first criticality was different than the pre-experiment specifications, leading to a new set of benchmark specifications that was provided later. Both the initial and an updated set of benchmark specifications along with results obtained with different codes by the participants to the IAEA benchmark exercise were presented in IAEA TECDOC 1382 [2]. The differences between the two sets of benchmark specifications

will be discussed in the next section. The post-experiment benchmark specifications were included and presented in detail in the latest 2009 release of the International Handbook of Evaluated Reactor Physics Benchmark Experiments (IRPhE-Handbook) [3].

This paper discusses the simulation with SCALE 6 of the initial criticality benchmark problem and the results obtained. The purpose of this study is to validate the methodologies used in SCALE 6 for the treatment of double-heterogeneity in the fuel as well as the associated SCALE nuclear data libraries.

2. DESCRIPTION OF BENCHMARK SPECIFICATIONS

The HTR-10 has a cylindrical active core region located above a conical pebble discharge tube and a cylindrical discharge tube. For the initial critical configuration, the conical and cylindrical discharge tubes beneath the active core region are filled with dummy pebbles only, with a packing fraction of 61%. Initial criticality was achieved with a total of 16,890 fuel and dummy pebbles in the active core region [3] out of which 7,263 were dummy pebbles and 9,627 were fuel pebbles, for a 57/43 fuel-to-moderator pebble ratio. The uranium load in each fuel pebble is 5.0 g, with an enrichment of 17 wt% U235. The reflector region surrounding the active core region and the discharge tubes are zones with varying material densities of carbon, natural boron and coolant components. A vertical cutaway view of the KENO VI model for HTR-10 is illustrated in Fig 1.

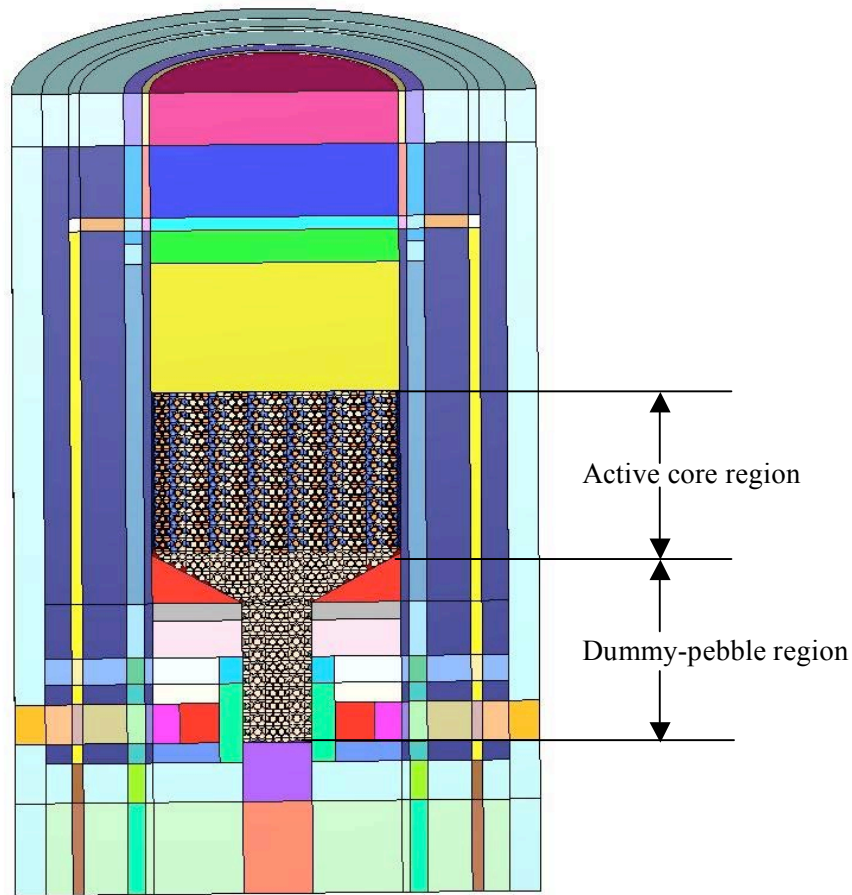


Figure 1. KENO VI model of HTR-10

The original set of benchmark specifications [2] considered that both the graphite in the dummy pebbles and the graphite in the fuel pebble outer shell had the same density of 1.73 g/cm^3 . Later, in the IRPhE benchmark, the graphite density in the moderator (dummy) pebble was modified to 1.84 g/cm^3 . Secondly, the actual boron impurity in the dummy pebbles was much lower than in the pre-experiment specifications and changed from 1.3 ppm [2] to 0.125 ppm [3]. The actual experiment was conducted under atmospheric air at 15°C [3] instead of helium as stated in the pre-experiment benchmark specifications [2].

The IRPhE benchmark specifications [3] were used to develop the SCALE 6 HTR-10 model discussed in this paper. The dimensions of the TRISO particles, fuel and dummy pebbles used in this model are presented in Table I. Table II provides information on the material properties of the TRISO particles, fuel and dummy pebbles used in the initial critical core experiment, as specified in Ref. [3].

Table I: Dimensions of TRISO particles, fuel and dummy pebbles (from Ref. [3])

Parameters	Values
Radius of fuel and dummy pebble	3.0 cm
Radius of fuel zone in fuel pebble	2.5 cm
Packing fraction of pebbles in the core	61%
Radius of fuel kernel (TRISO)	0.250 cm
Buffer layer thickness (TRISO)	0.090 cm
Inner PyC layer thickness (TRISO)	0.040 cm
SiC layer thickness (TRISO)	0.035 cm
Outer PyC layer thickness (TRISO)	0.040 cm

Table II: Material properties of TRISO particles, fuel and dummy pebbles (from Ref. [3])

Material Properties	Values
Density of graphite in matrix (fuel pebble) and fuel pebble outer shell	1.73 g/cm^3
Uranium mass per pebble	5.0 g
Enrichment	17 wt% ^{235}U
Boron content in uranium	4 ppm
Boron content in graphite (assumed in particle coatings)	1.3 ppm
Volumetric filling fraction of pebbles in the core	0.61
Kernel UO_2 density	10.4 g/cm^3
Buffer layer density	1.1 g/cm^3
Inner PyC layer density	1.9 g/cm^3
SiC layer density	3.18 g/cm^3
Outer PyC layer density	1.9 g/cm^3
Density of graphite in dummy pebbles	1.84 g/cm^3
Boron content in dummy-pebble graphite	0.125 ppm
Density of reflector graphite	1.76 g/cm^3
Boron in reflector graphite	4.8366 ppm
Density of boronated carbon bricks that include B_4C	1.59 g/cm^3
Weight percent of B_4C in boronated carbon bricks	5%

Two types of benchmark models called Simplified model and High-Fidelity model for HTR-10 are proposed in Ref. [3]. These models mainly differ in the way ducts and borings in the reflector region are represented. In the High-Fidelity model, 20 coolant flow channels, 13 control rod/irradiations channels, 7 KLAK channels and 1 hot gas duct are explicitly modeled. In the Simplified model, the ducts and borings in the reflector region are homogenized with the reflector material. The dimensions and locations for these regions were modeled according to specifications provided in Table 3.2 of Ref. [3].

3. DESCRIPTION OF SCALE 6 MODELS

The following section covers modeling details for the active core region and the dummy pebble region. Both these regions are common to the Simplified and High-Fidelity models that will be further discussed.

3.1. Active core region

The TRISO particle (illustrated in Fig. 2) is not explicitly modeled with KENO. However, the doubly-heterogeneous nature of the fuel is taken into account through methods implemented to calculate the cross sections for the fuel zone inside the pebble [4]. The fuel and dummy pebbles are explicitly represented in the model using a hexagonal unit cell as a building block. The geometry of the hexagonal unit cell is similar to that used by Seker and Colak [5].

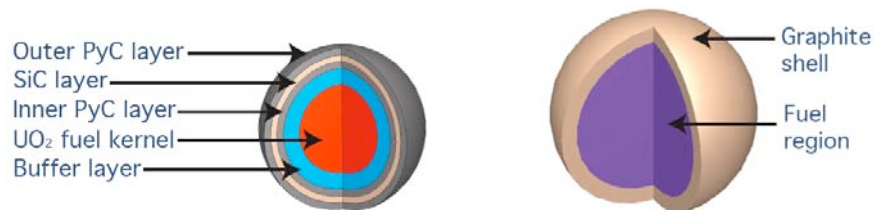


Figure 2. TRISO particle (left) and fuel pebble (right).

As illustrated in Fig. 3, the hexagonal close-packed unit cell ensures that the packing fraction of the pebbles in the active core region is 61% and that the fuel to dummy pebble ratio is conserved at 57:43.

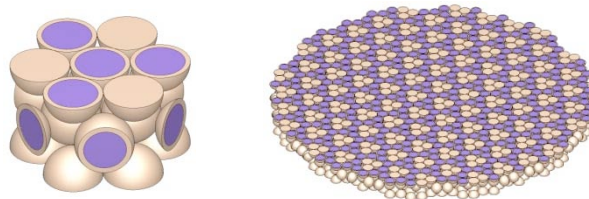


Figure 3. Hexagonal close-packed unit cell (left) and hexagonal unit cells forming a layer (right)

The hexagonal unit cells are packed into layers (Fig. 3), and these layers are stacked vertically to form the detailed active core region. By stacking the layers in this manner, the active core height is brought to 123.574 cm.

Part of the challenge in modeling the detailed fuel region is to preserve the total number of fuel and dummy pebbles as specified in Ref. [3]. In order to achieve this, pebbles have to be added in a manner such that only minimal clipping of fuel and dummy pebbles by the core boundary takes place. This minimal clipping of some fuel pebbles by the core boundary entails slight reduction in graphite in the graphite shell of the fuel pebble. The fuel region within the fuel pebble is not clipped by the boundary, thereby ensuring the total fuel mass is preserved in the core.

A total number of 16,885 fuel and moderator pebbles results when building the KENO VI model, as presented in Table III. There is a difference of 5 fuel pebbles, which would correspond to a reduction of 0.05% in the total mass of uranium in the core compared to the benchmark specifications. A similar number of fuel pebbles in the active core region was reported in Ref [5].

Table III. Inventory of pebbles in active core region

	Total # of Pebbles	Dummy Pebbles	Fuel Pebbles	Fuel:Moderator
KENO VI model	16885	7263	9622	56.99 : 43.01
Benchmark [3]	16890	7263	9627	57.00 : 43.00
Difference	5	0	5	-

The volumes of the fuel and dummy pebbles in the KENO model are calculated using KENO VI to ensure that the number of pebbles anticipated in the fuel region is indeed correct. Both the calculated and actual volumes are presented in Table IV. The comparison shows that the KENO VI volumes have a small uncertainty and the values are consistent to the actual volumes of fuel and dummy pebbles in the active core region.

Table IV. Calculated volumes of fuel and dummy pebbles

Parameters	Theoretical value	KENO VI value	Uncertainty (1 σ) in KENO VI value
Volume of air (10^5 cm^3)		12.3694	0.0003
Volume of 7,263 dummy pebbles (10^5 cm^3)	8.2061	8.2061	0.0002
Volume of 9,622 fuel pebbles (10^5 cm^3)	10.8713	10.8702	0.0001
Total volume of fuel and dummy pebbles (10^5 cm^3)	19.0774	19.0763	0.0003
Total volume of fuel region (10^5 cm^3)	31.4458	31.4457	<0.00005
Packing fraction	0.606676	0.606643	0.000008

3.2. Dummy pebble region

Dummy pebble regions below the active core are also modeled explicitly. In order to conserve a packing fraction of 61%, dummy pebble clipping is inevitable when modeling these two regions: conical and

cylindrical, respectively. KENO VI is used as a tool to calculate dummy pebble volumes to ensure that the packing fraction is being conserved when modeling these regions. The KENO VI-computed volumes for the dummy pebble regions are presented in Table V. The computed volumes indicate that the packing fraction in the dummy pebble region is 60.5%.

Table V. Computed volumes of dummy pebble regions below active core

Parameter	KENO VI Value	Uncertainty (1σ) in KENO VI value
Dummy pebbles volume (10^5 cm^3)	3.83226	0.00004
Air volume (10^5 cm^3)	2.50001	0.00012
Total Volume (10^5 cm^3)	6.33227	0.00016
Packing Fraction	0.605195	0.000017

The detailed models of the fuel and dummy pebble regions, which are present in both Simplified and High-Fidelity models, are shown in Fig. 4. The blue color in Fig. 4 represent fuel pebbles and the gold pebbles signify dummy pebbles. The vertical cutaway view of the regions show the distribution of the fuel and dummy pebbles throughout the core. The orange-colored region in the center of the fuel pebble signifies the fuel zone, which is surrounded by the fuel pebble graphite shell.

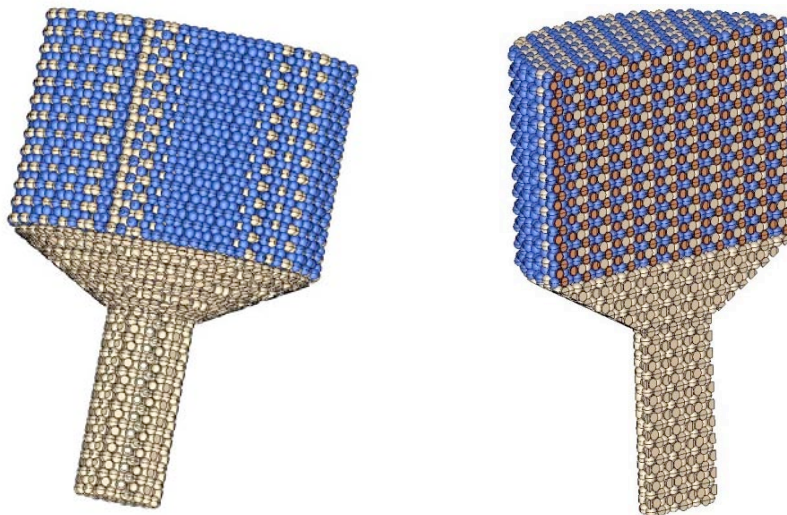
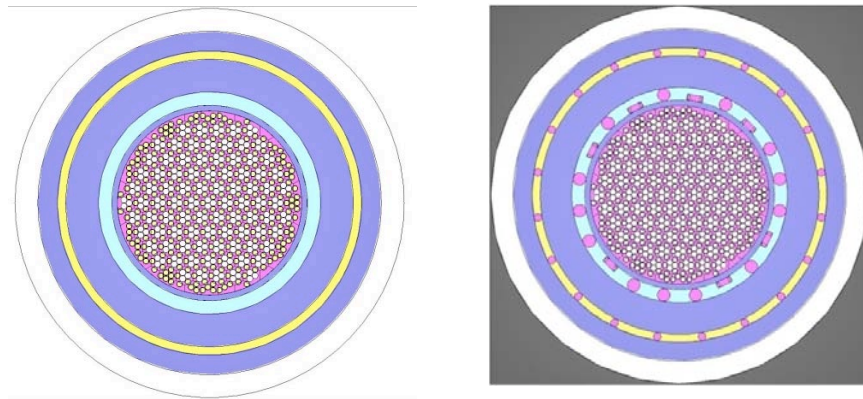


Figure 4. Detailed Active Core and Dummy Pebble regions.

3.3. Simplified and High-Fidelity core models

Both models for HTR-10, a Simplified and a High-Fidelity model were developed using the 3-D Monte Carlo code KENO VI in the SCALE 6 package, based on the IRPhE benchmark specifications. Both models contain detailed fuel and dummy pebble regions as discussed in the previous section. However,

the High-Fidelity model contains a detailed reflector region where the ducts and borings are explicitly modeled. Differences between the two models are illustrated in Fig. 5.



(a) Simplified model (b) High-Fidelity model
Figure 5. Horizontal cross-sectional view of the core

The High-Fidelity model contains a detailed reflector region, which includes KLAK channels, coolant channels, control rod and irradiation channels, and the hot gas duct. These details are illustrated using light blue color in Fig 6.

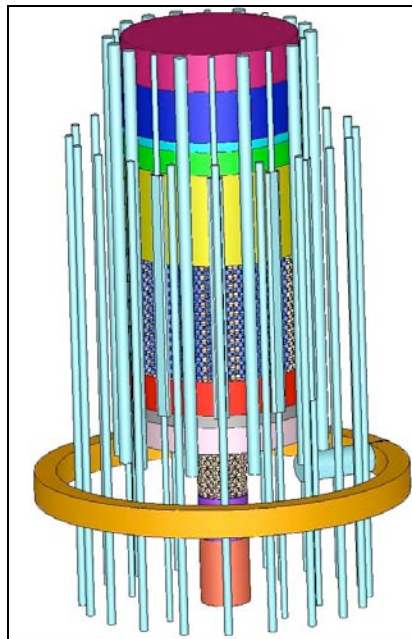


Figure 6. Detailed Reflector Region in High-Fidelity Model

Actual volumes for borings and ducts in the reflector region are compared to KENO VI-calculated volumes for these regions in Table VI. This is to ensure that the geometry representation in KENO VI is consistent with the actual specifications provided for these regions [3].

Table VI. Computed values of void regions in reflector using KENO VI

	Actual Volume (10^5 cm^3)	KENO VI Calculated Volume (10^5 cm^3)	KENO VI Volume Uncertainty (1σ) (%)
Coolant channels	5.07681	5.07724	0.041
Control rod/irradiation channels	7.76484	7.76456	0.027
KLAK channels	2.29410	2.29295	0.034
Hot gas duct	0.70686	0.70664	0.113

3.4. Variation in KENO VI model from IRPhE handbook specifications

The High-Fidelity model specified in Ref. [3] involves a conical fuel arrangement at the top of the fuel region, which is not modeled in the KENO VI High-Fidelity model. Instead of modeling the conical fuel arrangement, the pebbles are arranged in a manner such that the equivalent core height is maintained while conserving the total number of fuel and dummy pebbles.

Ref. [3] also specifies the standard boron concentrations to be 19.9% ^{10}B and 80.1% ^{11}B . The values used in the KENO VI models are based on the following isotopic compositions for natural boron as provided in the National Nuclear Data Center's Nuclear Waller Cards [6]: 19.8% ^{10}B and 80.2% ^{11}B .

4. RESULTS

Both KENO VI models use 238-group cross sections based on ENDF/B-VII.0 data with thermal scattering law evaluation provided for most isotopes in SCALE, which includes graphite. The k_{eff} values obtained with KENO-VI were compared to the corresponding values provided in the IRPhE benchmark [3]. No information was available in the IRPhE benchmark on the actual nuclear cross section libraries used for calculating the reported k_{eff} values. However, it was noted that the MCNP input file included in the IRPhE shows ENDF/B-V (release unknown) data as being used in the model. MCNP calculations were repeated at ORNL using the MCNP High-Fidelity model input deck provided in Ref. [3] with both continuous energy ENDF/B-V.0 and ENDF/B-VII.0 data libraries. The thermal scattering data $S(\alpha, \beta)$ for the graphite used in the MCNP calculations were from data set "endf70sab" for ENDF/B-VII.0 and from data set "tmccs" for ENDF/B.V.0. It was observed that in the MCNP input deck provided, the values for material densities in the input deck were slightly different from the benchmark specifications in Tables 3.5a, 3.5b, and 3.7 in Ref. [3]. Those values were modified wherever necessary in the MCNP input deck to ensure consistency with the benchmark specifications and calculations were repeated. The MCNP calculations were also repeated for two sets of boron content specifications to assess the effect on k_{eff} of using a slightly different boron isotopic composition. The results obtained for the modified MCNP deck for both ENDF/B-V.0 and ENDF/B-VII.0 data libraries, and boron isotopic compositions are provided in Table VII. They indicate that the specified change in boron isotopic composition has a very small effect on k_{eff} when using either ENDF/B-V.0 or ENDF/B-VII.0 data

libraries. However, the choice of ENDF/B library influences k_{eff} significantly: difference in k_{eff} between Case 1a and Case 1b in Table VII is 307 ± 30 pcm ($1 \text{ pcm} = 10^{-5}$) if the boron isotopic composition is used as 19.9% ^{10}B and 80.1% ^{11}B . The difference in k_{eff} for Case 2a and Case 2b, when a slightly different boron isotopic composition is used, is similar, of 285 ± 30 pcm.

Table VII. Results for modified MCNP input deck (High-Fidelity model)

Case #	Boron Isotopic Composition	Data Library	k_{eff}	Standard deviation	Difference in k_{eff} (pcm)
1a	19.9% ^{10}B 80.1% ^{11}B	ENDF/B-V.0	1.01166	0.00021	307 \pm 30
1b	19.9% ^{10}B 80.1% ^{11}B	ENDF/B-VII.0	1.01473	0.00021	
2a	19.8% ^{10}B 80.2% ^{11}B	ENDF/B-V.0	1.01187	0.00022	285 \pm 30
2b	19.8% ^{10}B 80.2% ^{11}B	ENDF/B-VII.0	1.01472	0.00021	

A comparison of the results obtained with the KENO VI and MCNP models is presented in Tables VIII and IX for the Simplified and High-Fidelity models. Since no MCNP input deck was included in Ref [3] for the Simplified model, the MCNP k_{eff} value in Table VII is the same value as reported in the IRPhE-Handbook; it was not possible in this case to check the consistency of the MCNP input deck with the KENO VI Simplified model.

When using ENDF/B-VII.0 data library, the difference in k_{eff} between the KENO VI high-fidelity model and the corresponding, consistent MCNP model is -73 ± 34 pcm. This close agreement between SCALE 6 and MCNP results is an indication of the SCALE 6 capabilities to accurately model the HTR-10 configuration. Note however that the experimental k_{eff} provided in Ref. [3] is 1.0000 ± 0.0037 . The difference between the experimental k_{eff} and the Monte Carlo results from MCNP and SCALE 6 is 1.4%. One of the possible sources for this difference may arise from uncertainties in the benchmark specifications that were not included in Ref. [3] and therefore cannot be accounted for in the computational models. As specified in Ref. [3], the sources of information used to develop the benchmark specifications do not contain a complete set of data on the uncertainties or tolerances of all relevant parameters. Sensitivity studies on various parameters such as variations in boron concentration in the fuel element, density of graphite matrix in the fuel pebble, dimensions of the core and fuel were evaluated and presented in Ref. [3].

Table VIII. Results for Simplified Model

Code	Data Library	k_{eff}	Standard deviation	k_{eff} difference (pcm)
MCNP (from Ref. [5])	N/A	1.02500	0.00021	304 \pm 34
KENO VI	ENDF/B-VII	1.02804	0.00027	

Table IX. Results for High-Fidelity Model

Code	Data Library	k_{eff}	Standard deviation	Difference in k_{eff} (pcm)
MCNP (from Ref. [5])	ENDF/B-V	1.01190	0.00021	-
KENO VI	ENDF/B-VII	1.01399	0.00027	-73 ± 34
MCNP	ENDF/B-VII	1.01473	0.00021	

5. CONCLUSION

Code-to-code comparison of KENO VI and MCNP high-fidelity models for the HTR-10 initial critical core configuration show an excellent agreement of the k_{eff} results obtained with the two codes. Both codes 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 uncertainty datasets 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. A full power SCALE 6 core model will be built based on the model for the initial critical core, with the purpose of developing burnup-dependent cross section libraries for HTR-10 spent fuel studies.

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