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Prediction calculations for the first criticality of the HTR-PM using the PANGU code

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Abstract The high-temperature reactor pebble-bed module (HTR-PM) is a modular high-temperature gas-cooled reactor demonstration power plant. Its first criticality experiment is scheduled for the latter half of 2021. Before performing the first criticality experiment, a prediction calculation was performed using PANGU code. This paper presents the calculation details for predicting the HTR-PM first criticality using PANGU, including the input model and parameters, numerical results, and uncertainty analysis. The accuracy of the PANGU code was demonstrated by comparing it with the high-fidelity Monte Carlo solution, using the same input configurations. It should be noted that k_{eff} can be significantly affected by uncertainties in nuclear data and certain input parameters, making the criticality calculation challenge. Finally, the PANGU is used to predict the critical loading height of the HTR-PM first criticality under design conditions, which will be evaluated in the upcoming experiment later this year.

Keywords HTR-PM · First criticality · Prediction · PANGU

1 Introduction

The high-temperature reactor pebble-bed module (HTR-PM) [1] is the world's first 200 MWe modular pebble-bed high-temperature gas-cooled reactor (HTGR) in a demonstration power plant with the safety features of fourth-generation nuclear energy systems. It was designed by the Institute of Nuclear and New Energy Technology (INET), Tsinghua University, based on technologies and experiences obtained from the 10 MW high-temperature gas-cooled test reactor (HTR-10) [2].

As one milestone of the HTR-PM project, the first criticality experiment is scheduled for the latter half of 2021. According to the design, the first criticality of the HTR-PM will be reached by loading a mixture of fuel pebbles and graphite pebbles into the core in an air atmosphere at ambient pressure. The critical loading height, or the number of mixed pebbles, will be experimentally obtained.

The HTR-PM first criticality experiment provides a good opportunity to validate computer codes for analyzing the physics of HTGR reactors. At the beginning of the 2000s, prior to the HTR-10 first criticality, INET published the HTR-10 first criticality benchmark and invited the international reactor physics community to submit prediction calculations [3]. Although the result predicted by INET was reportedly very close to the experimental result [4], the overall benchmark exercise yielded a deviation of $\pm$ 4% in the effective multiplication factor (k_{eff}), which indicates that reactor physics analysis in pebble-bed HTGRs is far from a well-established art [5]. Since the HTR-PM is a scaled-up and developed version of the HTR-10, it has particular value for reactor physics analysis in large commercial pebble-bed HTGRs.

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The prediction calculation of the HTR-PM first criticality was recently performed using PANGU [6], a state-of-the-art computer code developed at INET for pebble-bed HTGR neutronics analyses and fuel cycle simulations. PANGU implements a unique two-step calculation flow scheme with an in-line leakage feedback iteration. In addition, it employs some advanced methodologies and capabilities, such as treatment of mixed-type particles and mixed-type pebbles, neutron streaming correction, control rod homogenization, micro-burnup calculation, and iterative searching of the equilibrium cycle. Because of these features, PANGU can be used for the physical design of both traditional and new conceptual pebble-bed HTGRs.

This paper presents the calculation details of the HTR-PM first criticality, including the input data, numerical results, and uncertainty analysis. Moreover, the detailed model for the HTR-PM first criticality is provided so that all interested researchers in the community can participate in this prediction exercise as soon as possible.

The remainder of this paper is organized as follows. Section 2 describes the detailed model and parameters for calculating the first criticality of the HTR-PM. Section 3 presents the calculation results and uncertainty analysis obtained using PANGU. The discussion and conclusions are presented in Sect. 4.

2 Detailed model and parameters for HTR-PM first criticality

The HTR-PM full-core layout is illustrated in Fig. 1. The core equivalent diameter is 150.275 cm, and the equivalent height is 1100 cm in the full loading state. The pebble-bed core is surrounded by the top, bottom, and side graphite reflectors, which are in turn surrounded by carbon bricks. The control rod channels, absorber ball channels, and cold helium channels are located in the graphite reflectors. An *R-Z* axial view with detailed dimensions and materials is shown in Fig. 1(a). It should be noted that materials #19 and #46 are reflectors containing void channels, whose detailed structures are shown in Fig. 1(b). The neutron streaming effect [7] should be considered if these reflectors are treated as a homogeneous medium in deterministic codes. Table 1 provides a detailed description and the composition of the materials illustrated in Fig. 1. The impurities in the materials have been converted to the equivalent boron content (EBC) [8], represented by an equivalent density of natural boron.

For simplicity, the cone shape of the core bottom is converted into a cylindrical shape, while preserving the core volume. Prior to performing the first criticality experiment, the core will be filled with graphite pebbles to a height of 6.05 m. In the first criticality experiment, a mixture of fuel pebbles and graphite pebbles, with a ratio of 7:8, will be continuously loaded into the core until the reactor reaches criticality. The volumetric packing density of the entire pebble bed is 0.61.

As shown in Fig. 2, a fuel pebble consists of an outer graphite shell and an inner fuel region comprising coated fuel particles (CFPs) embedded in a graphite matrix. A CFP consists of a spherical fuel kernel of UO_2 with multi-layer coatings, namely a low-density pyrolytic carbon (PyC) buffer layer, an inner high-density PyC layer, a silicon carbide (SiC) layer, and an outer high-density PyC layer. The detailed physical parameters of the pebbles and CFPs are listed in Table 2.

Because the first criticality experiment will be performed in an air atmosphere, the upper cavity and pebble bed pores should be filled with saturated moist air in the calculation model. The air composition is temperature dependent, as shown in Table 3.

In addition, microscopic pores in graphite can absorb water. Thus, the water content of graphite is usually in the order of several hundreds of ppm. The water content of the graphite in the HTR-PM is estimated to be approximately 600 ppm. However, the reflector and the pre-loaded graphite pebbles have been dehumidified before the first criticality experiment; therefore, it is recommended that only the water content of the mixed pebbles should be considered in the calculation.

The input model and parameters introduced above can be used as preliminary benchmarks for the HTR-PM first criticality. The data provided in this paper will enable readers to perform calculations and conduct comparison studies using their own computer codes. The formal HTR-PM first criticality benchmark will be updated after the experiment and will be published as part of the Computational Methods Validation and Benchmarking (CMVB) project of the Very High-Temperature Reactor (VHTR) system in the Generation-IV International Forum (GIF).

3 Numerical results and uncertainty analysis

3.1 Comparison calculation with base conditions

Before performing the prediction calculation, it is necessary to evaluate the deviation of the PANGU code itself. The "base conditions" of the HTR-PM are assumed to be as follows: the reactor is in an air atmosphere, all components of the reactor are at room temperature (20 °C), and the water content of graphite is neglected. Under these conditions, the PANGU code and the RMC Monte Carlo code [9] were used to calculate the k_{eff} at different loading heights of mixed pebbles. PANGU uses a 2D *R-Z* model based on equivalent homogenization schemes that have

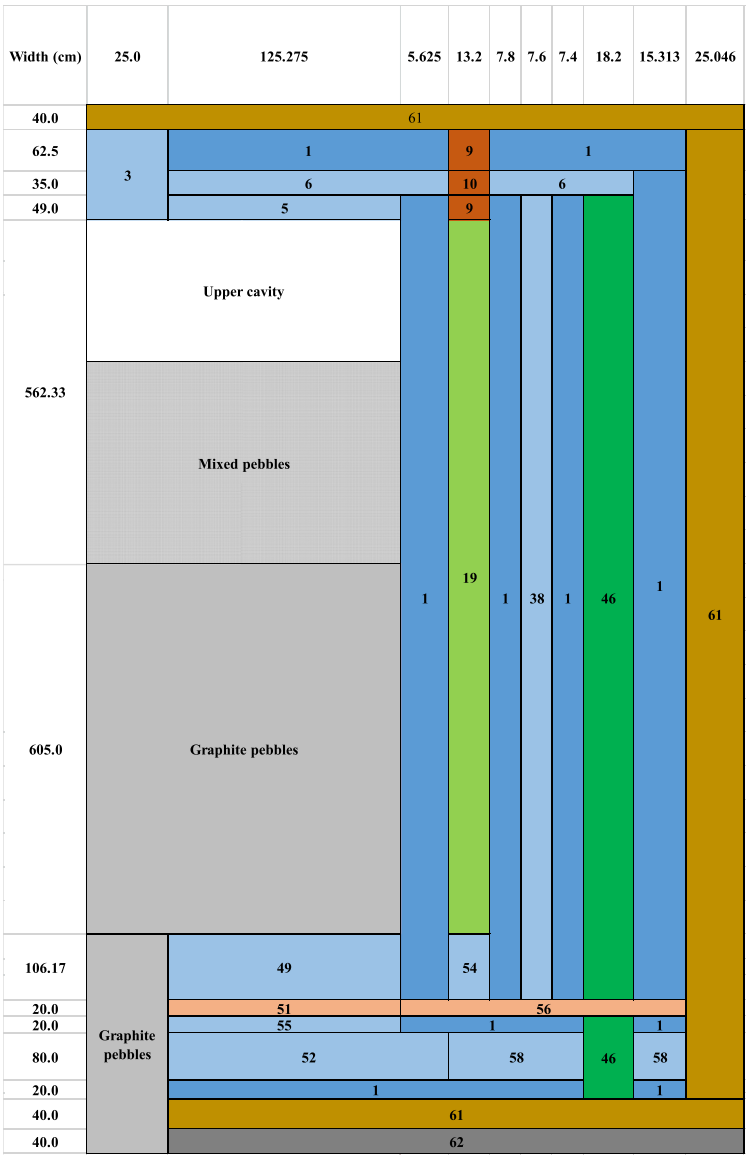

Fig. 1 (Color online) Full core layout of the HTR-PM. **a** Axial view; **b** Cross-sectional view

Table 1 Material description and composition

ID	Description	Composition (n/barn/cm)	
		C12	Boron
1	Standard reflector material (IG110, 1.781 g/cm^3, 0.445 ppm EBC)	8.92947×10^{-2}	4.41429×10^{-8}
3	Top reflector with charge tube	0.91 × IG110	
5	Top reflector with cold helium channel	0.84 × IG110	
6	Top reflector with cold helium chamber	0.6286 × IG110	
19	Side reflector with control rod channel	0.719 × IG110	
38	Side reflector with gap	0.99 × IG110	
46	Side reflector with cold helium channel	0.6679 × IG110	
49	Bottom reflector with hot helium channel	0.7135 × IG110	
52	Bottom reflector with hot helium chamber	0.5079 × IG110	
54	Bottom reflector with control rod channel	0.8315 × IG110	
55	Bottom reflector with hot helium channel	0.8741 × IG110	
58	Bottom reflector with hot helium guide tube	0.9317 × IG110	
9	Top reflector with control rod structure	5.62021×10^{-2}	3.69779×10^{-6}
10	Top reflector with control rod structure	2.30380×10^{-2}	3.68139×10^{-6}
51	Bottom reflector with B_4C	7.49075×10^{-2}	1.26898×10^{-4}
56	Bottom reflector with B_4C	8.14783×10^{-2}	1.22899×10^{-4}
61	Borated carbon bricks	8.39217×10^{-2}	3.79675×10^{-3}
62	Non-borated carbon bricks	8.53015×10^{-2}	3.79190×10^{-5}

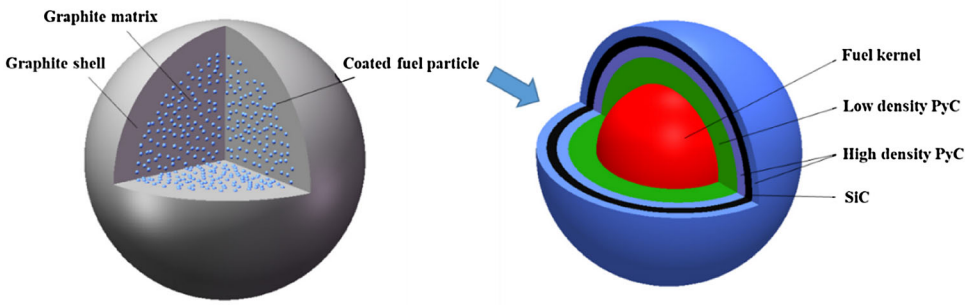

Fig. 2 (Color online) Geometric structure of a fuel pebble

been thoroughly validated by our previous studies [10, 11]. RMC uses a high-fidelity 3D model with explicit modeling of the detailed geometric structures of the coated fuel particles, pebble beds, and reflector channels. The most recent ENDF/B-VIII.0 nuclear data library [12] was adopted by both codes.

Table 4 lists the k_{eff} results calculated by PANGU and RMC; the latter was used as the reference solution. It was found that the PANGU results agree well with the high-fidelity RMC Monte Carlo solution. The differences in k_{eff} are generally below 0.15% over a wide range of loading heights. This demonstrates the accuracy of the PANGU code.

3.2 Uncertainty analysis

The HTR-10 first criticality benchmark [5] revealed that there are many uncertainties when analyzing the reactor physics of a pebble-bed HTGR. Consequently, the uncertainty of the HTR-PM criticality calculation, caused by uncertainties in the input data, was investigated.

Starting from the base condition at a loading height of 275 cm, the variation of k_{eff} with the change in a single input variable was calculated using the PANGU code. The sensitivity of k_{eff} with regard to particular key input variables is summarized in Table 5.

Noticeably, ENDF/B-VIII.0 was found to underestimate k_{eff} by approximately 1.3% compared with ENDF/B-VII.0. Further analysis suggests that this is mainly due to the update of the graphite thermal scattering cross section and

Table 2 Physical parameters of the fuel pebble and the coated fuel particle

Physical parameter	Value
Fuel pebble	
Uranium weight in single fuel pebble (g)	7
Enrichment of ^{235}U (weight) (%)	4.2
Diameter of the fuel pebble (cm)	6
Diameter of fuel zone in the fuel pebble (cm)	5
Density of graphite (including matrix and outer shell) (g/cm^3)	1.74
Impurities represented by EBC in uranium (ppm)	4
Impurities represented by EBC in graphite (ppm)	0.795
Coated fuel particle	
Radius of the kernel (μm)	250
Thickness of low density PyC (μm)	95
Thickness of inner high density PyC (μm)	40
Thickness of SiC (μm)	35
Thickness of outer high density PyC (μm)	40
Density of UO_2 (g/cm^3)	10.4
Density of low density PyC (g/cm^3)	1.05
Density of high density PyC (g/cm^3)	1.9
Density of SiC (g/cm^3)	3.18
Impurities represented by EBC in coatings (ppm)	0.795
Graphite pebble	
Diameter of the graphite pebble (cm)	6
Density of graphite (g/cm^3)	1.74
Impurities represented by EBC in graphite (ppm)	1.0

Table 3 Composition of saturated moist air at different temperatures

Temperature (°C)	Density (g/cm^3)	Composition (n/barn/cm)		
		O	N	H
20	1.19500×10^{-3}	1.10074×10^{-5}	3.87347×10^{-5}	1.15773×10^{-6}
30	1.14600×10^{-3}	1.08939×10^{-5}	3.66943×10^{-5}	2.02935×10^{-6}
40	1.09700×10^{-3}	1.09688×10^{-5}	3.44020×10^{-5}	3.41344×10^{-6}

Table 4 Variation of k_{eff} with different loading heights under base conditions

Loading height of mixed pebbles (cm)	k_{eff}		$\Delta\rho$* (%)
	Monte Carlo	PANGU	
220	0.94760	0.94648	− 0.12
250	0.98130	0.98083	− 0.05
275	1.00432	1.00358	− 0.07
300	1.02293	1.02232	− 0.06
330	1.04095	1.04075	− 0.02
385	1.06638	1.06634	0.00
440	1.08496	1.08485	− 0.01

*$\Delta\rho = \Delta(1–1/k_{eff})$

the nuclear data of ^{235}U and ^{238}U in ENDF/B-VIII.0. Nevertheless, nuclear data uncertainty does have a significant influence on the criticality calculation of pebbled-bed HTGRs, which conforms to some previous studies [13, 14].

In addition, k_{eff} is sensitive to the water content and EBC of graphite. Because the measurement of water content and EBC tends to involve large degrees of uncertainty, these datasets are expected to cause considerable

Table 5 Sensitivity of k_{eff} to changes in input data

Input data	Change of input	Δρ (%)
Nuclear data	ENDF/B-VIII.0, ENDF/B-VII.0	1.32
Water content in graphite (ppm)	0, 600	− 0.28
Graphite EBC in fuel pebble (ppm)	0.795, 1.095	− 0.30
Graphite EBC in graphite pebble (ppm)	1.0, 0.6	0.56
Graphitization degree (%)	100, 90	0.17
Radius of the fuel zone in fuel pebble (cm)	2.5, 2.3	0.2
Reactor global temperature (°C)	20, 30	− 0.25

Table 6 k_{eff} at different loading heights under design conditions

Loading height of mixed pebbles (cm)	Number of mixed pebbles	k_{eff}
220	84,183	0.94214
250	95,662	0.97625
275	105,229	0.99885
300	114,795	1.01745
330	126,274	1.03575
385	147,320	1.06115
440	168,366	1.07951

uncertainty in the criticality calculation. In addition, the degree of graphitization can also influence the k_{eff} value, which has been studied in our previous work [15].

X-ray photographs show that the actual fuel-zone radius of the fuel pebble is slightly smaller than the nominal value of 2.5 cm, which can lead to a somewhat higher k_{eff} in the HTR-PM criticality calculation.

The influence of the reactor temperature on k_{eff} was found to be approximately 25 pcm/°C. There are several detectors in the HTR-PM reflector for measuring the temperatures during the first criticality experiment, so that the prediction results can be corrected according to the actual temperatures.

In summary, k_{eff} is largely affected by the uncertainties of the input data. For this reason, it is quite challenging, in practice, to perform an accurate criticality prediction for the HTR-PM.

3.3 Predicted critical loading height under design conditions

In this section, PANGU is used to predict the critical loading height of the HTR-PM first criticality using the following "design conditions": all components of the reactor temperature are assumed to have a temperature of 30 °C, the water content of the mixed pebbles was assumed to be 600 ppm, and the nominal values were used for all input parameters.

The ENDF/B-VIII.0 nuclear data library was adopted for this prediction calculation, although there is no particular reason for choosing ENDF/B-VIII.0 over ENDF/B-VII.0 or some other nuclear data. According to the authors' experience, using PANGU with ENDF/B-VIII.0 seems to provide better results in simulating the HTR-10 initial criticality and power operation history [16], but it is not certain whether this will hold true for the HTR-PM case.

Table 6 presents the resulting k_{eff} values obtained at different loading heights under the design conditions. By interpolating between the heights of 275 cm and 300 cm, a critical loading height of 276.5 cm, corresponding to 105,821 mixed pebbles, can be obtained. Note that there may be differences between the experimental and design conditions. For example, the actual temperature may deviate from the assumed temperature of 30 °C; In such cases, the prediction results will be corrected according to the experimental conditions.

4 Conclusion

This work presents the prediction calculations of the HTR-PM first criticality obtained with the PANGU code and provides a preliminary benchmark model with detailed input parameters for the calculation of the first criticality in the HTR-PM.

By using the same input configurations, PANGU exhibits excellent consistency with the high-fidelity Monte Carlo solution, which demonstrates the accuracy of the PANGU code itself.

However, it is clear that the calculated k_{eff} is sensitive to the nuclear data and certain key input parameters, and therefore, it is challenging in practice to obtain an

"accurate" prediction result that agrees well with the experimental results. This could explain why there were large deviations among the results of different participants in the benchmark exercise of the HTR-10 first criticality.

Under the design conditions of the HTR-PM first criticality and using the ENDF/B VIII.0 nuclear data library, PANGU predicted a critical loading height of 276.5 cm. Considering the uncertainties resulting from the input data, as well as the variations in the actual experimental conditions, some luck is required to achieve a good consistency between the predicted and experimental results.

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Author contributions All authors contributed to the study's conception and design. Material preparation, data collection, and analysis were performed by Ding She, Jiong Guo, Chun-Lin Wei, Jian Zhang, and Bing Xia. The first draft of the manuscript was written by Ding She and all authors commented on previous versions of the manuscript. All authors read and approved the final manuscript.

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