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High-Temperature Reactor Physics and Fuel Cycle Studies
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Analysis of HTR-10 First Criticality with Monte Carlo Code Tripoli-4.3

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1. ABSTRACT

This paper will focus on the calculations of the HTR-10's first criticality. Continuous energy Monte Carlo transport code TRIPOLI-4.3, was used for getting the initial fuel loading of the HTR-10. The calculations have been performed on the basis of different treatment of the particles and the pebbles arrangement. The stochastic distribution of the particles in the fuel zone has been simulated, either using point-wise cross-sections associated with cubic or hexagonal lattices or using multi-group cross-sections provided by 1-D spherical transport calculation (APOLLO2 code). Different types of pebble arrangements have also been compared. Cross comparisons of the different hypotheses have been analysed including the impact of the libraries (JEF2 and ENDF/B-VI) and the estimation of the certain homogenisation effects. Therefore, this paper gives information related to the treatment of stochastic geometry in Pebble Bed Reactor (PBR) with the Monte Carlo method.

INTRODUCTION

The HTR is an advanced reactor concept that can meet the energy and environmental needs of future generations as defined under DOE's Generation IV initiative [1]. There are two major designs of HTR: reactors having prismatic fuel and those having spherical pebbles. HTTR[3] is an example to the first and considered by Japanese; HTR-10 [2] is another example built and operated in Institute of Nuclear Energy and Technology (INET), Tsinghua University, Beijing, China.

To enhance confidence in predictions of neutron physics behaviour, the International Atomic Energy Agency (IAEA) set up a Coordinated Research Project (CRP) on validation of safety related physics calculations for High Temperature Gas Cooled Reactors (HTGRs) [6]. Countries participating in this CRP include China, France, Japan, Switzerland, Germany, Indonesia, the Netherlands, the USA and the Russian Federation. The HTR-10's start-up

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core physics experiment was a good opportunity to fill the gaps in validation of data, code and physics methods used for core design of gas-cooled reactors.

In a HTR, the fuel in a form of dispersed particles, on the one hand and, the treatment of the pebble bed core on the other, impose a **stochastic approach of the geometry** in the Monte Carlo calculations. This may question the principle of the reference that constitutes today the Monte Carlo methods. Such critical experiments like the HTR-10 are particularly well suited for the validation of MC codes, because the composition of the fresh fuel is very well known and room-temperature cross-section libraries are readily available.

The present study deals with the HTR-10's initial loading case. Analyses have been mainly performed with TRIPOLI4 [4], which are based on the well-known Monte Carlo method and partially with the transport code APOLLO2 [8]. The first criticality analysis of the HTR-10 with Monte Carlo codes has already been carried out, but significant discrepancies occurred between the experimental result and coupled calculation scheme APOLLO2/TRIPOLI4 have shown [6]. In this study, we brought forward a new pebble-bed arrangement to achieve the experimentally determined ratio of graphite pebble to fuel pebble in the reactor core as well as respecting the actual filling fraction. At the same time, the fuel particles inside the fuel pebble have been described and modelled in different ways.

1. DESCRIPTION OF HTR-10 REACTOR

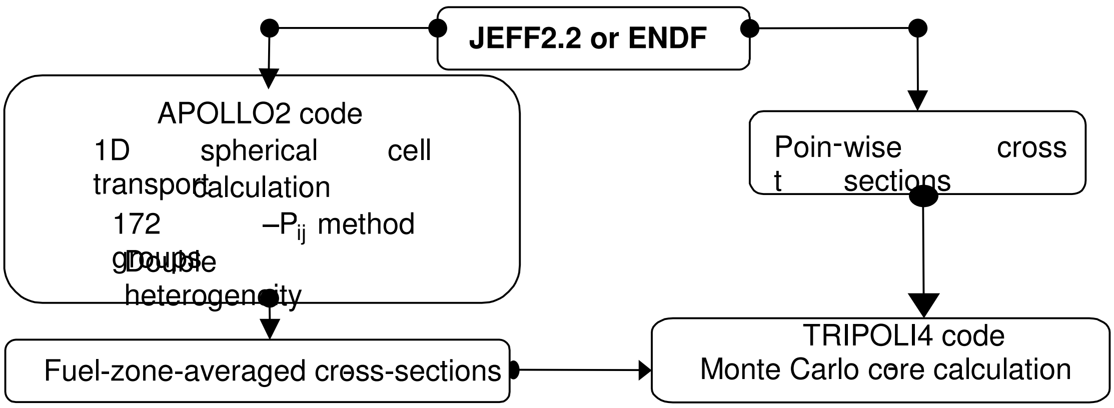
The pebble bed reactor HTR-10 is a test reactor with 10MW thermal power output, which employed spherical fuel elements. These elements are 6 cm in diameter. And they contain coated fuel particles (CFP), TRISO particles, embedded in a graphite matrix. TRISO particles are made of UO_2 kernels coated with two inner pyrolytic carbon layers, an intermediate SiC layer and an external pyrolytic carbon layer. The coating of the particles embedded in the fuel elements is an excellent barrier to retain radioactive gaseous and metallic fission products in the fuel particle up to a temperature of 1600 °C.
The reactor equilibrium core contains about 27,000 fuel elements forming a pebble bed, which is 180 cm in diameter and 197 cm in average height. The thickness of the side reflector is 100 cm and there is a conus region at the low part of the side reflector. There is a fuel discharge tube located at the bottom portion of the core. There are vertical channels in the side reflector. There are ten control rod channels, irradiation channels, and seven absorber ball channels are located near the core. Additionally there are twenty circular channels for helium flow for cooling purposes. These channels are located at near the midsection of the reflector. The reactor core consists of randomly mixed fuel elements and moderator elements. Moderator elements, or dummy balls, are also spherical and made of graphite. The size of these dummy spheres is identical to the fuel elements. The ratio of fuel balls to dummy balls is 57/43, which makes it very difficult to model.

2. COMPUTATIONAL METHOD AND METHODOLOGY

In the following HTR-10 calculations, the French reactor physics transport codes TRIPOLI4.3 and APOLLO2.6 (the data libraries are produced with THEMIS/NJOY) have been used. Figure 1 illustrates the general procedure throughout the study. TRIPOLI4 is a three-dimensional code that uses the Monte-Carlo method. It can be used to simulate the transport of neutrons, photons, electrons and positrons for shielding calculations (long-distance propagation with flux attenuation) and neutronic calculations (criticality and sub-criticality basis). This makes it possible to compute k_{eff}, flux, currents, reaction rate and multi-group cross-section. TRIPOLI4 allows calculations with continuous description in terms of cross-sections energy and multi-group homogenized cross-sections. Both geometrical representations: surface and combinatorial are available. The code uses cross-section libraries in ENDF/B format (such as JEF2.2, ENDF/BVI and JENDL) for point description and cross-sections in APOTRIM format (from the APOLLO2 code) specific to TRIPOLI4 for multi-group descriptions. All the data used in the present work are from JEF2.2.

In this study, APOLLO2.6 has been exploited only for the cell calculation in order to get the 172 groups fuel pebble averaged cross-section. These cross sections have been brought into play by TRIPOLI4 simultaneously with point-wise cross sections for the initial core calculation.

FIG. 1. Calculational method



3. HTR-10 MODELLING WITH TRIPOLI4

According to the initial core loading of the HTR-10 -the inner cone region at the bottom of the core is filled with graphite balls, then, a mixture of fuel and graphite balls in the ratio of 0.57 to 0.43 is loaded gradually to approach first criticality-. The way to describe the mixture of fuel and graphite pebbles in TRIPOLI4 is given below.

3.1 Graphite pebble cell

The graphite pebbles consist of one graphite zone with a radius of 3 cm. According to the core model, they have been either described explicitly in the calculations or homogenised with the air of the core cavity. This is also true for the cone and discharge tube regions (lower reflector). In all cases continuous cross sections have been used with a filling fraction of 0.6046 for the non-homogenised description.

3.2 Fuel pebble models

The stochastic geometries calculations (coated fuel particles -CFP- randomly distributed in the inner zone of the fuel pebble) are not directly possible in TRIPOLI4. Assumptions to model the fuel pebbles have been made. Three different models were adopted to describe the fuel zone of the fuel pebbles: a homogeneous model and two heterogeneous one. However, all the models were based on precise descriptions of the particles with their coatings.

3.1.1 Homogeneous model (APOLLO2): multi-groups cross sections for the inner fuel zone

A 1D spherical cell calculation has been performed with the APOLLO2 code accounting for the presence of the CFP fully described. The self-shielding of the uranium isotopes was done during this calculation step. The critical buckling search allows taking into account the neutron leakage by the addition of a homogeneous leakage term in the form of DB^2. The extra region of the spherical cell is representative of the coolant plus the moderator pebbles (dummy balls) loaded into the core together with the fuel pebbles. The volume of the extra-region has been calculated by considering a volumetric filling fraction of pebbles (fuel and dummy balls) of 0.61 in the core and a 57:43 fuel-to-moderator pebble percent ratio. Finally, a white boundary condition was assumed.

This first step provides fuel region averaged cross sections (172 energy groups) for the core calculations with TRIPOLI4. The fuel homogenisation is performed with respect to the pebble bed description in the Monte-Carlo code TRIPOLI4. Therefore, in the core calculations performed by TRIPOLI4, point-wise cross sections are used everywhere in the core except in the fuel region of the fuel pebble where the multi-group cross sections have been generated by APOLLO2.

3.1.2 Heterogeneous models: full description of the CFP in TRIPOLI4

According to the original data available [5], [6], there are about 8335 CFP in the fuel zone of one fuel pebble. These particles are randomly distributed in a graphite matrix. Two different treatments of this inner fuel zone were adopted. The coated fuel particles were uniformly placed according two regular lattices: the first one is a cubic lattice with edge and height of 0.199 cm as shown in Figure 3, the other one is a simple hexagonal column lattice with edge of 0.241 cm and height of 0.209 cm as shown in Figure 2.

FIG.2. Fuel pebble description in TRIPOLI4: hexagonal CFP lattice

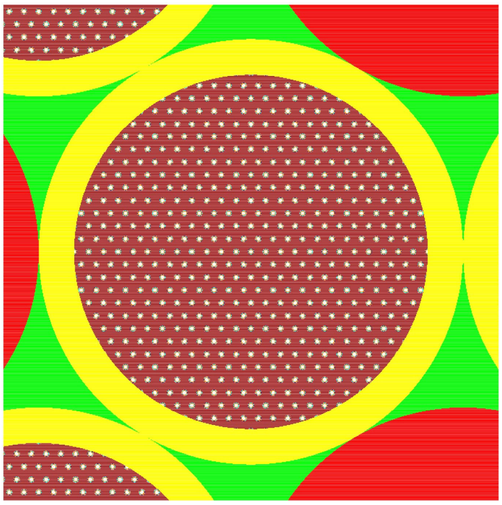
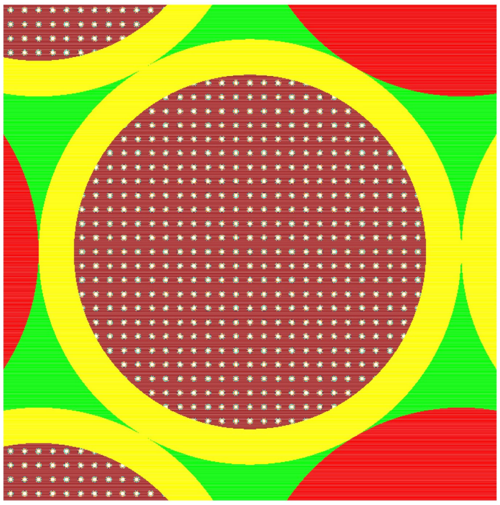


FIG. 3. Fuel pebble description in TRIPOLI4: simple cubic CFP lattice



3.3 Core models

As far as the 3D core model is concerned with TRIPOLI4, the reflector, the main channels in reflector and all the other important components were described in detail except the control rods present in the top reflector (Fig.6 and Fig.7). Nevertheless, according to the stochastic features of the core cavity geometry, different assumptions have been made to describe the arrangement of the spheres in the core.

3.3.1 Exact Core Models

First of all, a column hexagonal point on point (CHPOP) arrangement of the pebble bed has been chosen to describe the core cavity. Indeed, the theoretical CHPOP filling factor of 0.6046 is very close to the one observed experimentally (~ 0.61). This arrangement of balls in the discharge tube, in the bottom conus region and in the cylindrical part of the reactor core, corresponds to a hexagonal prism lattice in x- y plane and is top to top in z – direction.

As shown in Figure 5, in the ***exact core model***, the coolant and all the structures of the pebbles (fuel, moderator) loaded into the core have been described explicitly. The fuel-to-moderator pebble ratio of the initial HTR-10 core loading was taken into account. To do that, a specific treatment of a basic regular lattice was done in order to get as well the good filling factor as the good proportion and distribution of the fuel and dummy pebbles. The percentages of fuel balls and dummy balls obtained in the TRIPOLI4 calculations are 56.76% and 43.24% respectively. The filling factor is 60.46%.

3.3.2 Simplified Core Model

In the ***simplified core model***, the pebble bed is represented as fuel spheres embedded in a homogeneous medium (Figure 4). This homogeneous medium is a mixture of air between the pebbles and graphite of the shell and of the moderator pebbles. However, it is noteworthy that as for the ***exact core model*** the lower reflector (conus region and discharge tube) remains described in detail. The homogenisation effect of this lower part of the core will be discussed later. As shown in Figure 4, the adopted fuel pebbles arrangement in the core is based on a simple cubic lattice. Finally, a hexagonal lattice of the CFP was kept in the inner part of the fuel spheres.

FIG.4. Horizontal Cross-section view of the Simpiflied Core Model of HTR-10

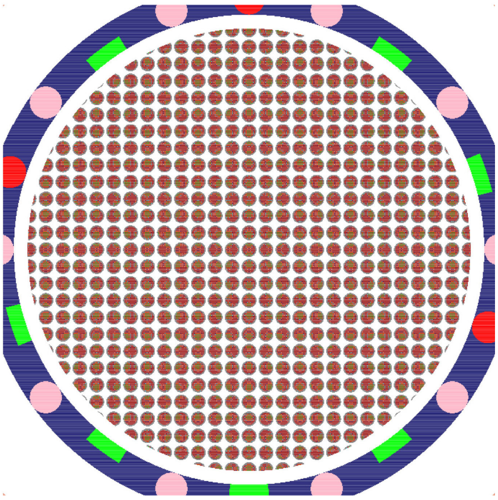
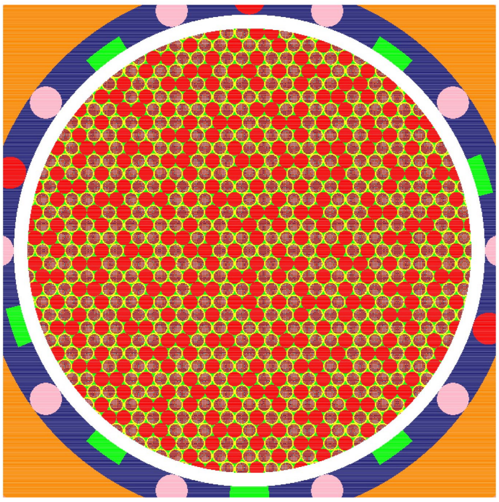


FIG. 5. Horizontal Cross-section view of the Exact Core Model of HTR-10



4. CALCULATIONS AND RESULTS

After the description of these various geometrical models, TRIPOLI4 simulations were done in order to estimate the reactor critical state. The number of the mixed balls required experimentally getting the core critical was 16890 or *123.06* cm in terms of loading height assuming an experimental filling fraction of about *0.61*. Several simulations have been performed for the different nuclear cross-sections libraries and for different geometrical models employed to describe the pebble bed and the fuel zone of each fuel pebbles.

The first criticality experiments of the HTR-10 have been carried out in moist air atmosphere at 15℃, at a pressure of 0.1013 MPa. The conditions of the calculations are the same as those of the experiment except the temperature fixed at 27℃. The relative moisture of the air has been assumed as 100 %. The moist air has been considered in the upper cavity and in the space between the spheres in the core, in other word, the volumetric fraction of moist air in the core was about 39 %. Under the condition of saturation humidity, the density of vapor in the moist air is equal to 2.57×10^{-5} g/cm^3, so the density of the moist air is about 1.175E-

3g/cm^3 and the density of air is about 1.149×10^{-3} g/cm^3. Finally, the weight proportions in air of nitrogen and oxygen were 75.53% and 23.14% respectively.

4.1 Impact of different core models

Based on the core cavity descriptions mentioned above (Figure 4 and Figure 5) a comparison of the results has been done. In the first ***simplified core model***, it is reminded that only the fuel zone of the fuel pebble is described exactly (hexagonal CFP lattice), the rest of the core cavity being homogenized. A vertical cross-section view of this HTR-10 model is shown Figure 6.

In the second ***exact core model*** (based on Figure 5), all the fuel pebble and graphite pebbles are described exactly with the same hexagonal CFP lattice inside the fuel spheres. Moreover, it is worth to mention that each layer is radially shifted one by one of a half pebble along the axial direction as shown in Figure 7. With the shifted arrangement, the “artificial streaming” is avoided, which is induced in the CHPOP model with the inter-pebble void between pebbles.

FIG.6. Vertical Cross-section view of the Simplified Core Model of HTR-10

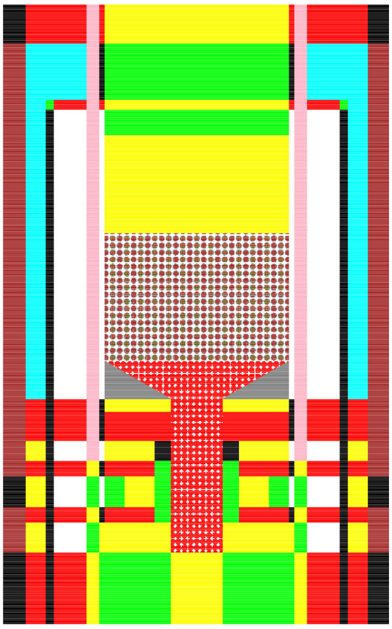


FIG. 7. Vertical Cross-section view of the Exact Core Model of HTR-10

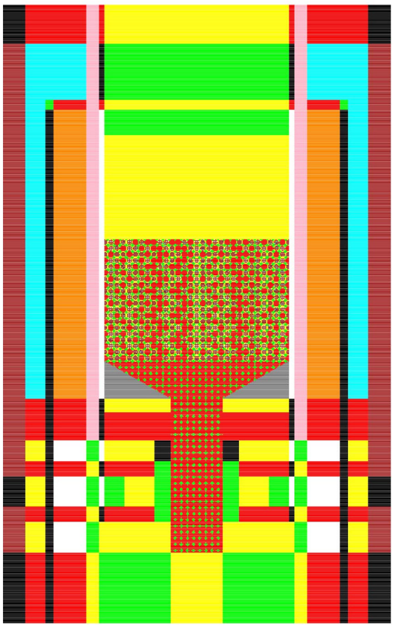


Table I gathers the results obtained for those two different core models calculated with the same JEF2.2 library. It turns out that the obtained results with the ***exact core model*** are quite good compared with the experiment. By comparing with the previous calculations performed with TRIPOLI4 on that HTR-10 reactor [6] based on a different approach of the treatment of the core cavity, it underscores and confirms that the adopted manner to describe the **pebbles arrangement in a PBR is of importance with the Monte Carlo method**. In those previous calculations, all the pebbles (fuel and moderator pebbles) loaded into the core had been described explicitly considering a Face-Centred-Cubic -*FCC*- lattice (theoretical filling fraction of 74%), then some fuel and dummy pebbles had been randomly removed to achieve an average filling fraction of 61%. The discrepancies with the experiment corresponded to an overestimation of about 1500 pcm (~ 1.5 % $\Delta k/k$) or 16108 pebbles for k_{eff} =1.

Moreover, it is noteworthy that according to the Table I, a mixed heterogeneous description of the fuel and graphite spheres in the core cavity is necessary to predict the good results. Indeed, the air and graphite homogenisation leads to an overestimation of the core reactivity of about 1700 pcm (~ 1.7 % $\Delta k/k$).

Table I. HTR-10's First Criticality results. Simplified and exact core model with hexagonal CFP lattice

Cases	Loaded height	$k_{eff} \pm \sigma$	Needed number of pebbles for k_{eff} =1	**Experimental result**
Simple model	120 cm	1.01016 ± 0.00056	15 988	**$N_{pebbles}$ = 16890**
	126 cm	1.02753 ± 0.00062		**N_{fuel} = 9627**
Exact model	120 cm	0.99194 ± 0.00070	16 681	**$N_{graphite}$ = 7263**
	126 cm	1.01040 ± 0.00070		

4.2 impact of the different library

The ***exact core model*** has been used to compare the impact of the different libraries. Two different libraries JEF2.2 and ENDF6 have been considered. Table II shows the sensitivity of k_{eff} to both libraries. It is worth to mention that no significant change in k_{eff} can be observed.

Table II. HTR-10's First Criticality results for different libraries: exact core model

Library	Loaded height	$k_{eff} \pm \sigma$	Needed number of pebbles for k_{eff} =1	**Experimental result**
JEF-2.2	120 cm	0.99194 ± 0.00070	16 681	**$N_{pebbles}$ = 1689**
	126 cm	1.01040 ± 0.00070		**N_{fuel} = 962**
ENDF/B6	120 cm	0.99257 ± 0.00062	16 701	**$N_{graphite}$ = 726**
	126 cm	1.00965 ± 0.00067		

4.3 Impact of different models of the fuel zones of the fuel pebbles

In the Table III the ***exact core model*** has been exploited to compare different ways of modelling the CFP in the inner region of the fuel pebbles. Three models mentioned above can be compared with each other: two regular lattices based on point-wise cross sections and an homogeneous model using 172-groups cross sections coming from a heterogeneous transport calculations performed previously (it is reminded that point-wise cross sections have been used everywhere else in the core simultaneously with this APOLLO2 library).

Table III. Impact of the fuel zone modeling: exact core model

Fuel zone model	Loaded height	$k_{eff} \pm \sigma$	Needed number of pebbles for k_{eff} =1	Experimental result
Hexgonal model	120 cm	0.99194 ± 0.00070	16 681	**$N_{pebbles}$ = 16890**
	126 cm	1.01040 ± 0.00070		
Cubic model	120 cm	0.99318 ± 0.00060	16 637	**N_{fuel} = 9627**
	126 cm	1.01114 ± 0.00061		
APOLLO2 library	120 cm	0.99050 ± 0.00088	16 691	**$N_{graphite}$ = 7263**
	126 cm	1.01166 ± 0.00082		

The obtained k_{eff} value with the APOLLO2 library is very close to the others results using detailed CFP description in a regular lattice associated with continuous energy cross sections. Bearing in mind that the statistical uncertainty (1 σ) is always lower than 100 pcm, the relative small effect on k_{eff} confirms on the one hand the appropriate treatment of the double heterogeneity in APOLLO2 and on the other hand, that the calculation scheme using multi-group cross sections in the fuel element appears as a good approach.

4.4 Homogenisation effect of the lower reflector

To study the impact on the reactivity of the different models adopted for the conus region and the discharge tube, the ***simple core model*** described before has been used. The only change in this ***simple core model*** concerns the CFP, arranged according a cubic lattice instead of a hexagonal lattice. From this configuration, two calculations have been carried out with and without homogenized lower reflector. The homogenised reflector has been described with averaged concentrations of graphite plus air and continuous cross sections. Table IV gathers the obtained results.

Table IV. Lower reflector homogenisation effect: simple core model

Lower reflector & discharge tube model	Loaded height	$k_{eff} \pm \sigma$	Needed number of pebbles for k_{eff} =1	Experimental result
Detailed (CHPOP lattice)	120 cm	1.008799 ± 0.00058	16 090	**$N_{pebbles}$ = 16890**
	126 cm	1.027889 ± 0.00050		**N_{fuel} = 9627**
Homogenized	120 cm	1.013758 ± 0.00074	15 590	**$N_{graphite}$ = 7263**
	126 cm	1.029039 ± 0.00075		

A non-constant discrepancy can be observed as a function of the loading height. The results underscore that the greater is the number of loaded pebbles the smaller is this reflector homogenisation effect on the reactivity. Nevertheless, as far as the first criticality configuration is concerned, this homogenisation effect is significant and amounts to 800 pcm according the TRIPOLI4 simulations.

5. COMPARISON WITH OTHERS RESULTS

Based on the IAEA documents [7], a tentatively comparison of all the others Monte Carlo calculations on the revised HTR-10 physics benchmark has been done. Table V summarizes those results presenting some significant variations. First of all, one should keep in mind that the actual experimental known value for the first criticality is the number of pebbles (16890) loaded into the core with a 0.43/0.57 graphite-to-fuel ratio. Assuming a filling factor of about 0.61 a critical height can be deducted (123.06 cm). That is the reason why the critical heights mentioned in the Table V must not be considered as a final result since they might be evaluated either from the given 0.61 value or from the actual filling fraction used in the simulation (for example 0.6046 with TRIPOLI4).

This Table highlights the progress between both first criticality predictions by using TRIPOLI4. The present study allowed understanding that the reason for this discrepancy with the previous TRIPOLI4 results is essentially the adopted method to describe the pebbles inside the core cavity and not the method used to model the particles inside the fuel pebbles.

Besides, it is worth to mention that there is a good agreement between the results of the present study (CHPOP with TRIPOLI4) and the results of INET (China) calculations using MCNP4B with the nuclear database of ENDF/B-V. Considering that the impact of the library is small, one can say that both results are in good agreement and quite acceptable compared to the experiment. Both calculations used detailed models with little differences on the graphite-to-fuel pebbles ratio, which is not the case for the other models and might partially explain the discrepancies.

Table V. Results for Critical Height and Total Number of Mixed Balls of HTR-10[5], [6], [7]

	China (INET)	France (CEA)		USA# (MIT)	Turkey		
Code	MCNP4B	TRIPOLI4.3		MCNP4A	MCNP4B		
CFP description	Cubic lattice	Homog. (172 gr)	Hexag. lattice	Cubic lattice	Random	Cubic lattice	**Experiment**
Pebble bed description	CHPOP	adapted FCC	CHPOP	CC	N/A		**$N_{pebbles}$ = 16 890**
Critical height (cm)	*122.87 (0.61)*	*117.37 (0.61)*	*122.62 (0.6046)*	*127.5 (0.61)*	*125.22 (0.6073)*	*125.54*	**N_{fuel} = 9 627**
Number of pebbles	**16 865**	**16 108**	**16681***	**17 499**	**17 111**	**17 154**	**$N_{graphite}$ = 7 263**

In this calculation, the coolant is helium, and the temperature is 20 °C, reference [6]
* *Result present in our calculation.*

Without taken into account the presence of the control rod in the top reflector (very small effect) and by considering a little bit higher temperature (27 °C) in the calculation (evaluated to 62 pebbles in[10]) the TRIPOLI4 results are comprised within the 3σ standard deviation which corresponds to about 150 pcm of discrepancy with the experiment.

CONCLUSIONS

The HTR-10's core physics benchmark has been treated with the Monte-Carlo code TRIPOLI4 by considering two different models for the pebble bed geometrical description and three different models of the CFP arrangement inside the fuel pebbles. These calculations followed the previous attempt that had been made earlier before with TRIPOLI4 [6] assuming a FCC pebble lattice in the core cavity with randomly removed pebbles in order to get the actual filling fraction.

The present study has shown that the pebble arrangement in a PBR is important for Monte Carlo methods. On the opposite, it has been shown that the system reactivity is insensitive to the type of arrangement of fuel particles in the fuel pebble. Moreover, the use of multi-group cross sections (provided by the transport code APOLLO2) only in the fuel region with point-wise cross sections elsewhere seems to be sufficient. This confirms the APOLLO2/TRIPOLI4 calculations performed previously on the HTTR benchmark [6] and on the PROTEUS experiment [10]. This makes easier the geometry description and has the advantage to reduce the global CPU time.

Finally, this work allowed quantifying the impact on the reactivity of different homogenisations of certain materials and regions of the reactor. It turns out that a homogenised reflector has a strong influence on the reactivity for small heights of core loading. The homogenization of the graphite pebbles with the inter-pebble void has also an important impact on the core reactivity.

The present HTR-10 study provides preliminary information concerning what would be an appropriate manner to model particles and pebbles in PBR with MC codes. This analysis might then be extended to others core configurations before to propose some final recommendations (compromise between acceptable results, mastered discrepancies with the actual configurations and easiness of input data description, CPU time consuming, ...).

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