

# MODELING OF THE THERMAL HYDRAULICS OF VERY-HIGH-TEMPERATURE REACTORS WITH THE SYSTEM CODE ATHLET

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## ABSTRACT

Gas-cooled, graphite-moderated very-high-temperature reactors (VHTRs) are one design concept of Generation VI reactors. To examine the ability of the thermal hydraulics system code ATHLET for the safety assessment of these reactors, we performed simulations of the cores of both pebble bed and prismatic block VHTRs. Besides creating the reactor models, some VHTR specific code development had to be done. The simulation results of both reactor types showed a good general agreement with our qualitative expectations and, in the case of the prismatic block reactor, also with the predictions of other codes. Based on the experience gained with the core simulations, the creation of a model for the whole primary circuit of a pebble bed reactor is planned to be a next step. For the more distant future coupled neutronics/thermal hydraulics calculations are conceivable.

## KEYWORDS

VHTR, pebble bed, prism, ATHLET, heat conduction

## 1. INTRODUCTION

Within the context of research and development regarding Generation IV reactors, very-high-temperature reactors (VHTRs) are an important concept under consideration. Although several units of both VHTR types—the Prismatic Modular Reactor as well as the Pebble Bed Modular Reactor—have been or still are under operation (e.g. Fort St. Vrain, HTTR, Peach Bottom or THTR-300 and HTR-10), the neutronics and thermal hydraulics analysis tools have often lagged behind the state of the art compared to other reactor technologies [1,2]. For this reason, two OECD code benchmarks were organized to compare simulation methods and tools and to test their capabilities to predict the behavior of VHTRs. The benchmark with regard to the pebble bed reactor type covered the PBMR-400 core design [1] and the benchmark concerning the prismatic core reactor type is addressing the MHTGR-350 [2]. This paper presents code developments, modeling challenges and simulation results of the thermal hydraulics system code ATHLET (Analysis of the Thermal Hydraulics of LEaks and Transients) which were obtained within the framework of the aforementioned benchmark cases.

## 2. ATHLET SIMULATION OF A PEBBLE BED MODULAR REACTOR

This section describes first the code developments which were necessary to simulate a pebble bed reactor core with ATHLET and gives then a brief description of the conducted simulation and their results.

## 2.1. Code extensions

The developments had the code version ATHLET 2.2.B as their starting point. Since ATHLET has been initially developed as a best-estimate code for the thermal-hydraulic simulation of light water reactors, VVERs and RBMKs, version 2.2B already contained geometry data and specific correlations for heat transfer and pressure losses on cylindrical or plate-shaped objects, but it lacked those correlations for spheres and pebble beds. The following extensions were implemented and made available for the user in ATHLET version 3.0A. More details about the models and their derivation can be found in [3,4].

### 2.1.1. Heat conduction in spheres

In ATHLET, a solid structure that conducts or generates heat—a so-called heat conducting object (HCO)—consists of several layers for each of which the energy balance is solved in order to derive temperatures and heat fluxes. If desired, the user can assign various material properties to the layers; an HCO can consist of up to three different materials together with an arbitrary number of layers.

The general energy balance of a layer—arranged for the time derivative of the temperature—is shown in equation (1).

$$\frac{dT_{\text{layer}}}{dt} = \frac{1}{\rho \cdot c_v \cdot V} \cdot (\dot{Q}_{\text{in}} - \dot{Q}_{\text{out}} + \dot{\phi}''' \cdot V) \quad (1)$$

Here,  $\dot{Q}_{\text{in}}$  and  $\dot{Q}_{\text{out}}$  are the rates of the heat flows entering resp. leaving the layer volume  $V$  and  $\dot{\phi}'''$  is the volumetric source term of heat generation in  $[\text{W}/\text{m}^3]$ .

The rate of heat flow from layer  $(j-1)$  to layer  $j$  can be expressed as a function of the layer temperatures and a thermal resistance  $R_j$ :

$$\dot{Q}_j = \frac{1}{R_j} (T_{j-1} - T_j) \quad (2)$$

In ATHLET, the thermal resistance is calculated based on the thermal conductivities of both layers, the geometry of the HCO (plate, cylinder or sphere) and—in the case of gaps between the layers or in the case of layers at the boundary of a HCO which are in contact with a fluid—the heat transfer coefficient. For a spherical HCO, the following was derived and implemented:

$$R_j = \frac{1}{4\pi \cdot h_{tcj} \cdot r_{j-1}^2} + \frac{\frac{1}{r_{j-1} \cdot \Delta r_{j-1}} - \frac{1}{r_{j-1}}}{4\pi \cdot \lambda_{j-1}} + \frac{\frac{1}{r_{j-1}} - \frac{1}{r_j \cdot \Delta r_j}}{4\pi \cdot \lambda_j} \quad (3)$$

### 2.1.2. Fuel particle temperature

The heat generation inside a layer volume in ATHLET is considered to be uniformly distributed. Actually, the fuel pebbles of reactor concepts like the PBMR-400 consist of a graphite matrix with embedded fuel particles, i.e. heat generation is localized. The fuel particles themselves have a heat generating kernel and several coating layers. For coupled neutronics/thermal hydraulics calculations, the fuel kernel temperature is necessary to know to compute the nuclear Doppler effect. For this reason, in each HCO layer where heat is generated, an average fuel kernel temperature is calculated based on the layer temperature for a representative fuel particle in this layer. This average fuel kernel temperature can be passed to the coupled neutronics module.

Based on a stationary energy balance for the fuel particles and volumetric averaging of the thermal energy, the following expression for the average fuel kernel temperature in a layer as a function of the layer temperature can be obtained:

$$T_{\text{fuel,avg}} = T_{\text{layer}} + \frac{\dot{\phi}''' \cdot D}{6} \cdot \left( \frac{1}{\text{htc}} + \frac{D}{10 \cdot \lambda_{\text{fuel}}} \right) \quad (4)$$

$\dot{\phi}'''$  is the volumetric heat source,  $\lambda_{\text{fuel}}$  is the thermal conductivity of the fuel kernel,  $D$  is the fuel kernel diameter and  $\text{htc}$  is a heat transfer coefficient taking into account the thermal resistance of the coating.

It is emphasized that  $T_{\text{fuel,avg}}$  is only calculated as a transfer parameter in coupled calculations and is not considered in the energy balance.

### 2.1.3. New thermophysical properties

As part of the ATHLET code developments concerning pebble bed reactor types, correlations for the specific heat capacity and thermal conductivity of graphite and silicon carbide were implemented. The correlations are functions of the material temperature and, in the case of the thermal conductivity of graphite, of the neutron fluence.

### 2.1.4. Pressure loss and heat transfer correlations for pebble beds

The correlations for pressure loss and heat transfer which are used in ATHLET are based on the KTA design rules\* for high-temperature gas-cooled reactors [5,6]. The pressure loss coefficient can also be derived from the Ergun equation for flow through a packed bed, which yields the same equation as starting from the KTA rule.

The following correlation for pressure loss has been implemented into ATHLET:

$$\lambda_{\text{pebble bed}} = 213,3 \cdot \frac{\eta_{\text{fluid}}}{d_{\text{pebble}} \cdot u_0 \cdot \rho_{\text{fluid}}} \cdot (1 - \psi) + 4 \cdot \left( \frac{1 - \psi}{\text{Re}} \right)^{0,1} \quad (5)$$

with

$d_{\text{pebble}}$ : pebble diameter  
 $\psi$ : porosity of the pebble bed  
 $u_0$ : superficial velocity of the fluid  
 $\text{Re}$ : Reynolds number as defined in eq. (6)

$$\text{Re} = \frac{\left( \frac{\dot{m}}{A_{\text{core}}} \right) \cdot d_{\text{pebble}}}{\eta_{\text{fluid}}} \quad (6)$$

with  $A_{\text{core}}$  being the cross sectional area of the core barrel.

The heat transfer coefficient is computed according to the following equations with the Reynolds number defined as in eq. (6).

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\* KTA (Kerntechnischer Ausschuss) is the German nuclear safety standards commission with the task to issue nuclear safety standards and support their application.

$$htc_{\text{pebble bed}} = \frac{Nu_{\text{pebble bed}} \cdot \lambda_{\text{fluid}}}{d_{\text{pebble}}} \quad (7)$$

$$Nu_{\text{pebble bed}} = 1,27 \cdot \frac{1}{\psi^{1,18}} \cdot Re^{0,36} + 0,033 \cdot \frac{1}{\psi^{1,07}} \cdot Re^{0,86} \quad (8)$$

The geometric and fluid dynamic ranges of validity for eqs. (5) and (8) can be found in [5,6]. Under usual operational conditions of pebble bed reactors these limits are observed.

## 2.2. Data Set and Simulation

The ATHLET simulation model of the PBMR-400 reactor core was developed based on the benchmark descriptions in [1]. A schematic representation can be seen in Fig. 1. At the inlet plenum a mass flow boundary condition was imposed (ca. 193 kg/s helium mass flow at 500°C). The helium flow was directed upwards into the upper plenum and from here downwards through the reactor core (i.e. the pebble bed) into the outlet plenum which acted as a pressure boundary condition (90 bar at 900°C). The core consisted of ca. 452000 pebbles with a thermal power of 885 W per pebble, resulting in a total thermal power of 400 MW. The heat generation in the pebbles was controlled by a signal, neutron kinetics was not considered. As can be seen from Fig. 1, the annular core was subdivided into 17 (16+1) interconnected channels with an axial subdivision of 11 zones. Heat losses to the environment were considered in radial direction only. Starting from the core, heat flow is outwards through the graphite moderator and the riser channel, then through a gap filled with stagnant helium, the core barrel wall, again a stagnant helium gap, the reactor pressure vessel (RPV) wall and finally through a layer of stagnant air with a specified constant temperature of 20°C at its outside.

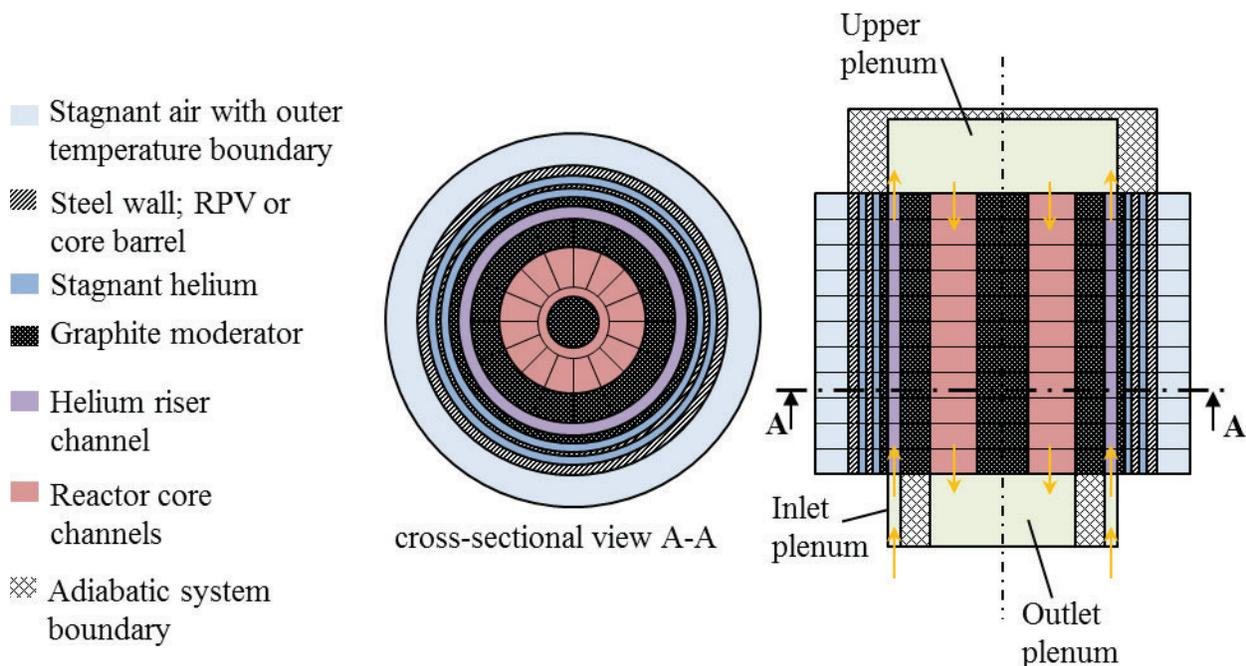


Fig. 1. Scheme of the ATHLET model of the PBMR-400 reactor core

In the simulation a turbine/compressor trip with simultaneous SCRAM was assumed. The full simulation time was 8000 seconds. After 1000 s of normal plant operation, the trip should take place, i.e. the helium mass flow at the inlet was reduced to 0 kg/s. The plunge of the mass flow from 193 kg/s to zero was set to happen within 3 seconds. Simultaneously to the trip, the reactor protection system performed SCRAM for which it was assumed that 5 seconds were required for the complete insertion of the control rods. Afterwards, the heat generated by the fuel elements followed the decay heat curve starting from about 6.4% of nominal power (detailed specification in [1]).

Some results of the simulation can be seen in Fig. 2. Here, the temporal evolutions of some structural and fluid temperatures at chosen positions of the core are shown. The red curves show the central temperatures of the fuel pebbles at the top resp. bottom of the core. Within the first 1000 s, these curves are clearly above the yellow curves which represent the surface temperatures of the pebbles. The green curves represent the coolant temperatures which are again a bit lower. Since the coolant flows downwards through the core, the temperatures at the bottom are higher than those at the top. After the turbine/compressor trip and SCRAM take place, the pebble and helium temperatures at each position coincide which is due to the now missing forced convective cooling in the core (thermal radiation is not simulated). The drop of the central temperature of the pebbles is a consequence of the decreased thermal power because of the SCRAM. Because heat is generated uniformly in the pebbles and forced convection is stopped, the temperatures in the upper and lower core are expected to approach each other in the long run. This tendency can be observed since the slope of the temperature curves of the upper core in Fig. 2 is steeper than that of the temperature curves of the lower core. However, because of the large heat capacity of the graphite, the system reacts very slowly.

The blue curve represents the inner wall temperature of the reactor pressure vessel. The position (upper or lower core) does not matter here because the temperatures were found to be almost the same across the inner RPV wall, i.e. ATHLET did not calculate a distinct axial temperature profile. The reason for this is the thermal insulation by the two gaps of stagnant helium. Because of this insulation, there is also no effect of the trip or the SCRAM on the RPV temperature observable in Fig. 2. It has to be mentioned that this behavior is not realistic and is owed to the ATHLET input model in which effects like thermal radiation and natural convection in the helium gaps were neglected.

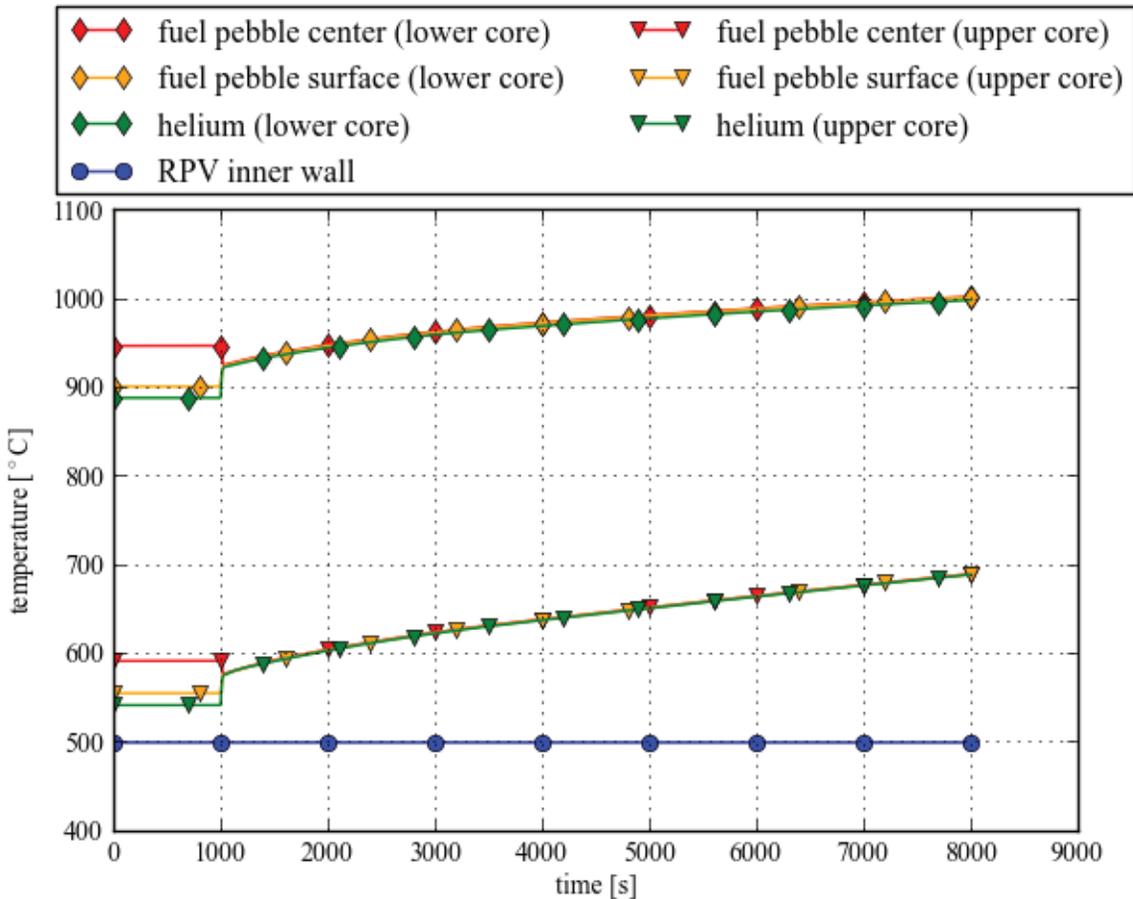


Fig. 2. Results of the ATHLET PBMR-400 simulation

### 3. ATHLET SIMULATION OF A PRISMATIC BLOCK REACTOR

This section describes the simulation of a MHTGR-350 reactor within the ongoing OECD benchmark program [2].

#### 3.1. Code extensions

The developments had the code version ATHLET 3.0A as their starting point and are available now with version ATHLET 3.0B. Unlike the developments regarding the pebble bed reactor, these code extensions were not specifically tailored to the new fuel element geometry. The developments which affected the MHTGR-350 simulation are mentioned very briefly below. A thorough description can be found in [4].

One relevant development is the model for axial (or two-dimensional) heat transfer in HCOs. Since the conductive heat transfer within the graphite blocks is expected to be significant not only in radial, but also in axial direction, the original one-dimensional (radial) heat transfer model was enhanced to also allow for thermal conduction in axial core direction. The consequence should be a more realistic axial temperature profile of the reactor.

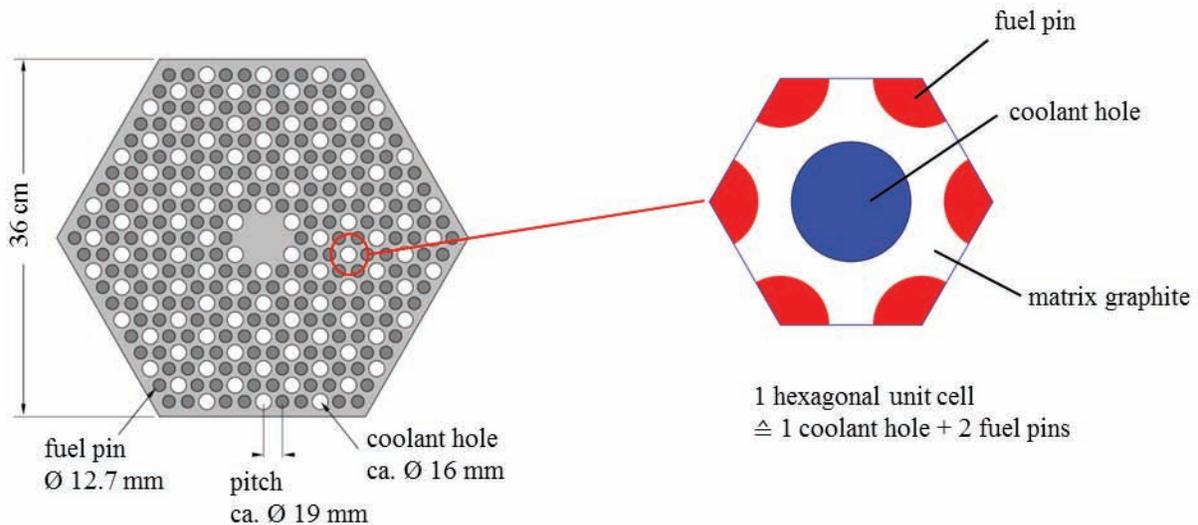
Besides, the user input of the thermal radiation model was facilitated while the model itself was not revised. This smaller modification made it possible to generate an ATHLET input deck with much less

HCOs to be defined than before. For example, the later discussed MHTGR-350 data set could be built up with 21 HCOs when applying the modified radiation model, compared to 60 HCOs when using the old model, with both data sets yielding the same computational results. Moreover, the modified radiation model can be utilized together with the above mentioned model for axial heat transfer, which was not feasible with the old model.

### 3.2. Data Set and Simulation

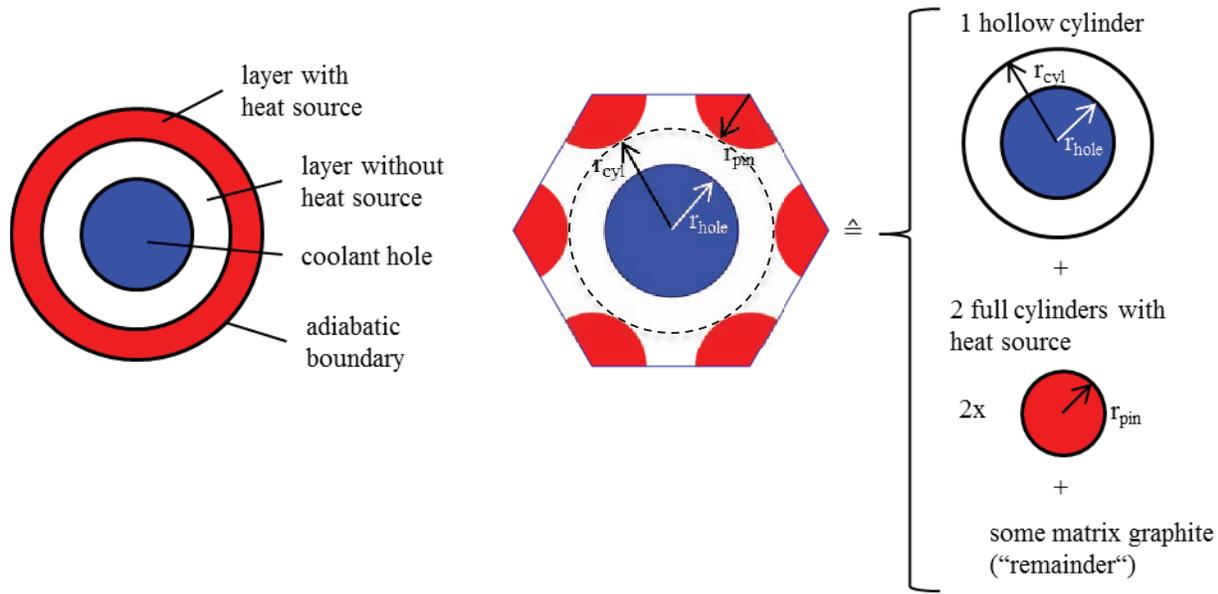
#### 3.2.1. Modeling of the fuel blocks

The major challenge in simulating the MHTGR-350 was the computation of the temperature distribution within the prismatic fuel blocks by using standard ATHLET HCO geometries (i.e. plates, cylinders or spheres). Even if one neglects the axial heat conduction, the thermal conduction problem in a fuel block is two-dimensional, while the standard HCO geometries only allow for one-dimensional heat transfer calculations. In Fig. 3 a prismatic fuel block together with a hexagonal unit cell is shown. A fuel block consists of 108 coolant holes and 210 fuel pins so that it can be represented by about 105 to 108 unit cells.



**Fig. 3. Prismatic fuel block (taken from [7] and modified) and hexagonal unit cell**

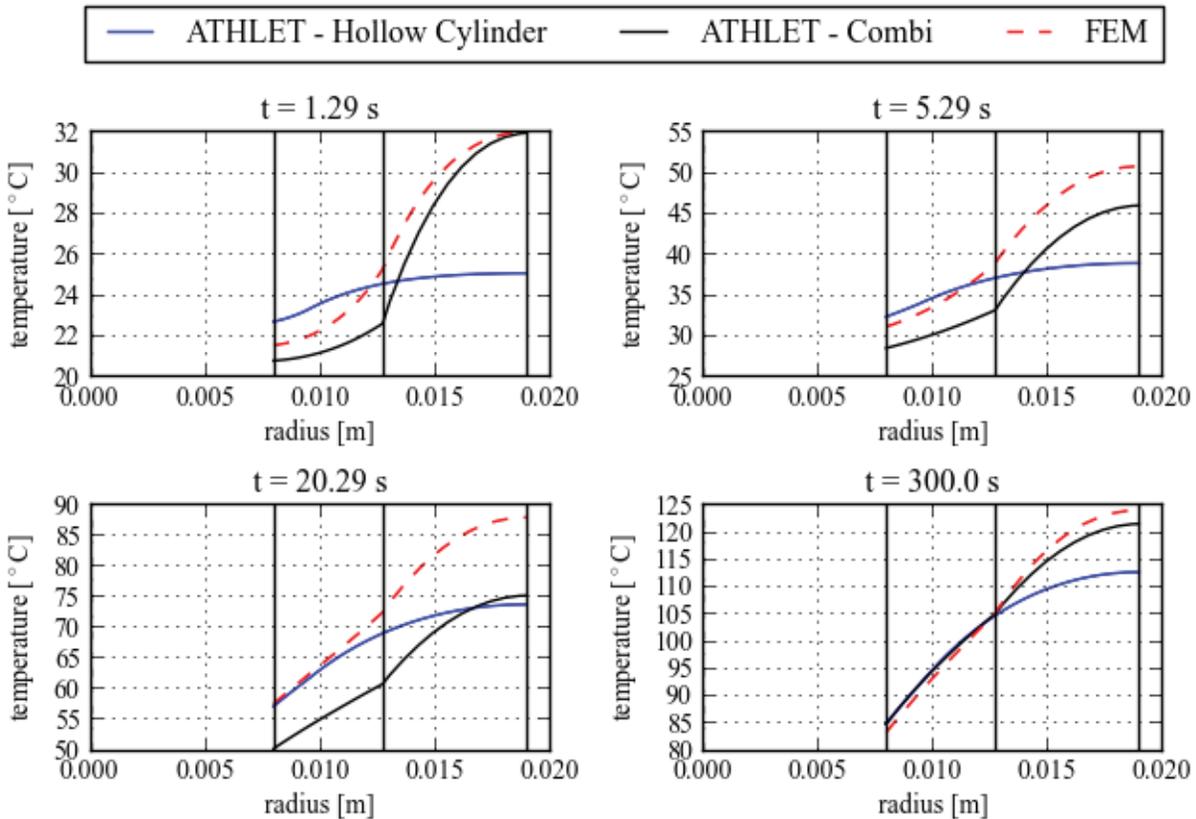
One option to model a unit cell is to use a hollow cylinder with a coolant hole in its center and a spread heat source in the surrounding material, see Fig. 4 on the left. At the cell boundary, an adiabatic boundary condition is assumed. As will be shown below, using this approach did not yield a reasonable temperature profile because the maximum temperature in the fuel pin was underestimated.



**Fig. 4. Approximation of a unit cell by a hollow cylinder (left) or a combination of hollow and full cylinders (right)**

For this reason, another approach was chosen, cf. Fig. 4 on the right. The coolant hole and some matrix graphite were modeled as a hollow cylinder without heat source. The fuel pins were modeled as full cylinders with internal heat generation. In order to simulate a unit cell, one hollow cylinder was coupled with two full cylinders by means of a fluid which thermal properties were chosen to represent the thermal behavior of the matrix graphite of the prismatic blocks. This fluid represented the “remainder” in Fig. 4 on the right, i.e. the remaining matrix graphite not covered by the hollow cylinder. For modeling a whole fuel block, simply 108 hollow cylinders had to be coupled to 210 full cylinders together with the correct amount of the “graphite fluid”.

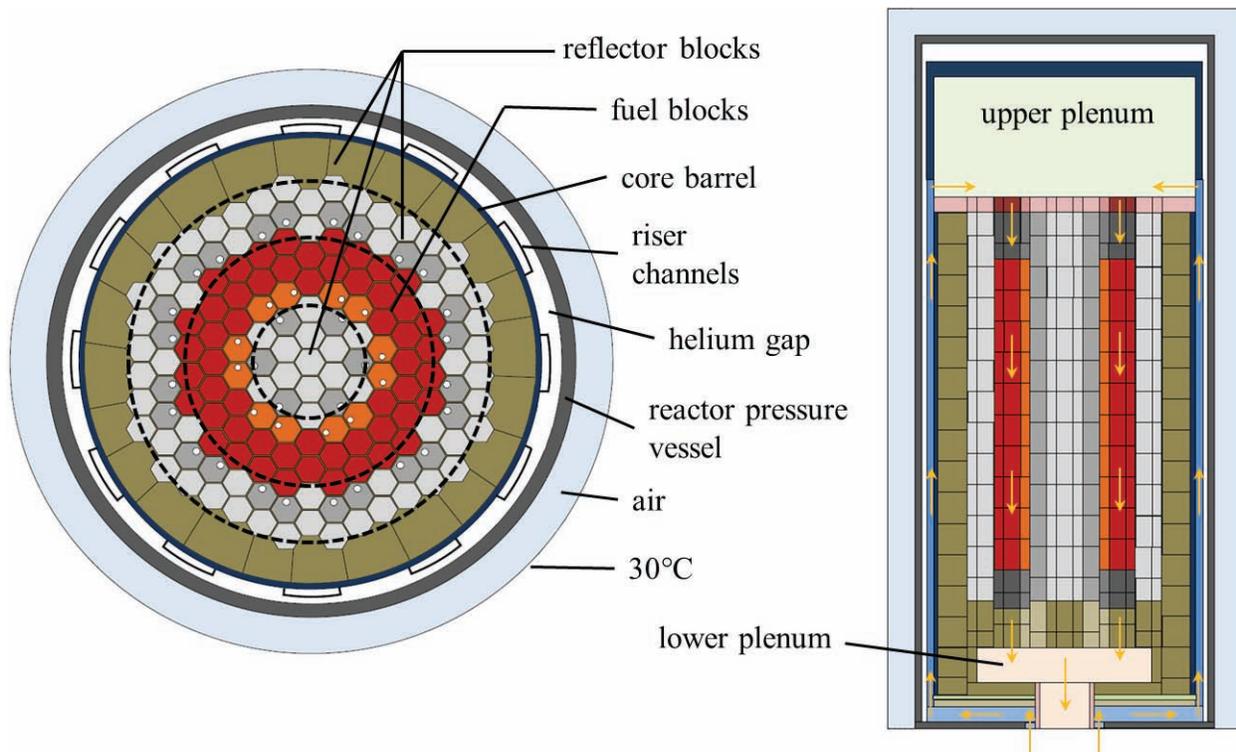
Fig. 5 shows the evolution of a temperature profile in a unit cell, starting from a flat profile at 20°C. The x-axis shows the radial coordinate originating from the center of a coolant hole and pointing to a vertex of the hexagon (= the center of a fuel pin). The vertical solid lines in the plots mark the radii of the coolant hole and the fuel pin. Each time plot shows three temperature curves: the dashed red curve is the result of a FEM calculation and is taken from [7]; this is the reference value. The blue curve is the result of an ATHLET calculation using the cylindrical model shown in Fig. 4 (left) and the black curve stems from an ATHLET calculation with the model shown in Fig. 4 on the right. One can see the good agreement of the black and the red curve at steady state. Since the MHTGR-350 simulation described below was performed for a steady state case, the application of this model is acceptable. Another advantage is that the model can easily be adapted to fuel elements with another configuration than 108 holes/210 pins per block, as the MHTGR-350 design also contains so-called shutdown control (RSC) fuel elements with 95 holes/186 pins [2].



**Fig. 5. Calculated temperatures with the hollow-cylinder and the combination model explained in Fig. 4 compared to FEM predictions. Within 300 s steady state is reached**

### 3.2.2. MHTGR-350 simulation

The simulation model of the MHTGR-350 is described in [2] in detail. Fig. 6 shows the radial and axial core layout which was the basis for the ATHLET input data set. As indicated by the dashed lines in Fig. 6, the ATHLET model of the core was composed of concentric rings, representing the reflector and active core regions, respectively. The model bears resemblance to the PBMR-400 model shown in Fig. 1: At the inlet, a defined helium mass flow was imposed (ca. 157 kg/s at 259°C) from where the helium went upwards into the upper plenum. From here, it had to flow downwards through the annular core into the lower plenum and the outlet where a pressure boundary condition was defined (6.39 MPa and 687°C). The core was made up by hexagonal fuel blocks with a total power of 350 MW. At the radial outside of the model, a fixed temperature of 30°C was defined as a boundary condition, while top and bottom of the reactor were modeled to be adiabatic. Neutron kinetics was not considered in the simulation, instead a fixed spatial power density distribution was provided according to the benchmark specification.



**Fig. 6. MHTGR-350 core layout (taken from [2] and modified)**

The performed simulation was a steady state case using the given fixed power density distribution with the boundary conditions mentioned above and fixed thermophysical properties without bypass flow (see exercise 2a in [2]). Its purpose was to compare the computational results obtained by various codes\* and to look for striking differences.

Figures 7 to 10 show selected preliminary results calculated by ATHLET. For confidentiality reasons, the results obtained by the other benchmark participants, using different codes and models, are not presented. All of the figures below show pressure or temperatures plotted against axial layers of the core. The range between upper and lower plenum in Fig. 6 was subdivided into 16 axial layers, 10 of which belonging to the active core (for this reason, the fuel temperature in Fig. 10 is plotted against only 10 layers). The layers are numbered from the lower to the upper plenum, therefore the pressure in Fig. 7 increases with growing layer numbers. The curves shown in Figs. 7 to 9 are in good agreement with the results of the other codes, which are not presented here. This is also representative for further curves, which are not shown in this paper. The graph in Fig. 10 deviates from the average fuel temperatures calculated by the other codes; ATHLET underestimates the temperature by about 20°C to 30°C. Recently, it has been found out that this difference is due to a small gap between the fuel pins and the matrix graphite (not shown in Fig. 3), which is specified in [2], but was neglected in the ATHLET MHTGR-350 model. By including this gap in the simulation model and recalculating the exercise, better results have been obtained. Since these are not yet submitted to the OECD benchmark committee, the older graph is presented in Fig. 10.

\* Not only the codes were different, but also the input models varied in their nodalization.

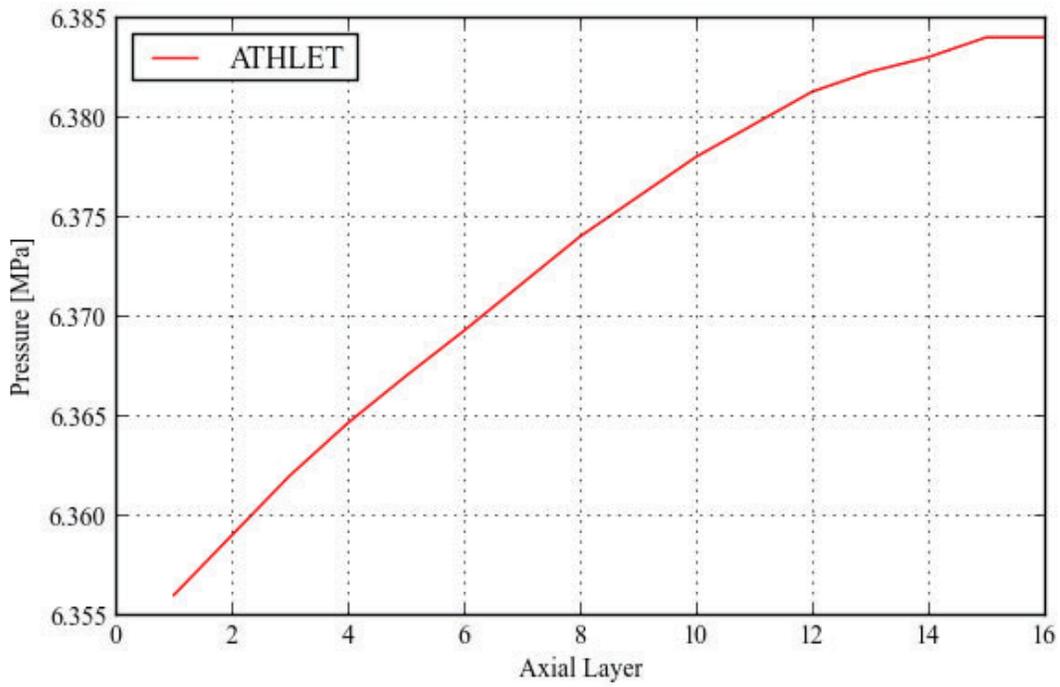


Fig. 7. Axial pressure distribution

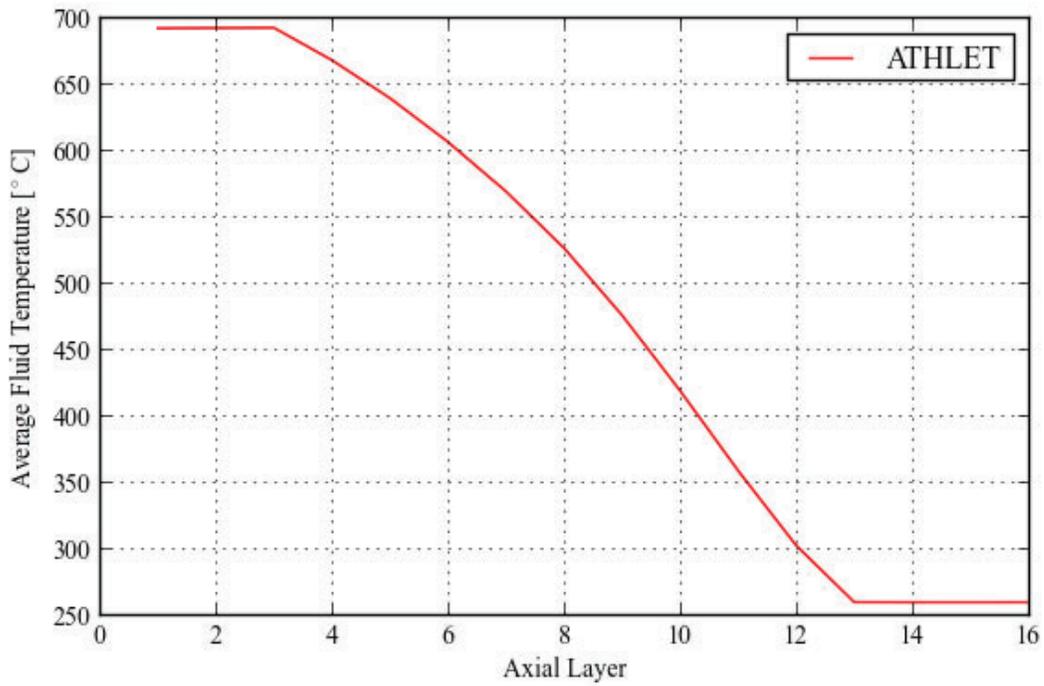


Fig. 8. Axial distribution of the average helium temperature

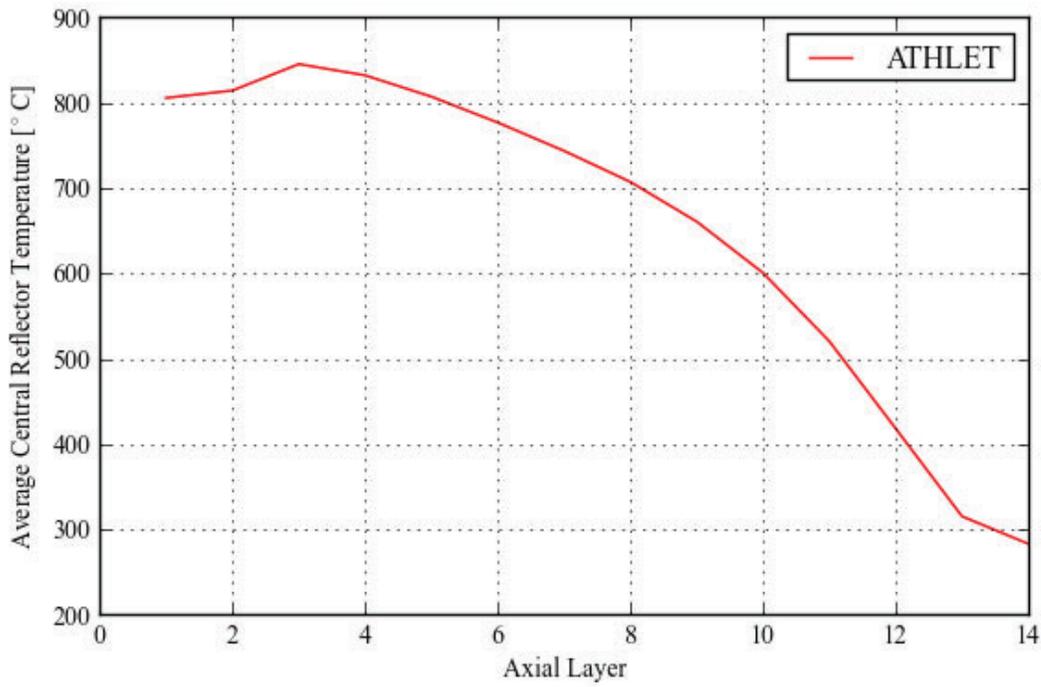


Fig. 9. Axial distribution of the average central reflector temperature

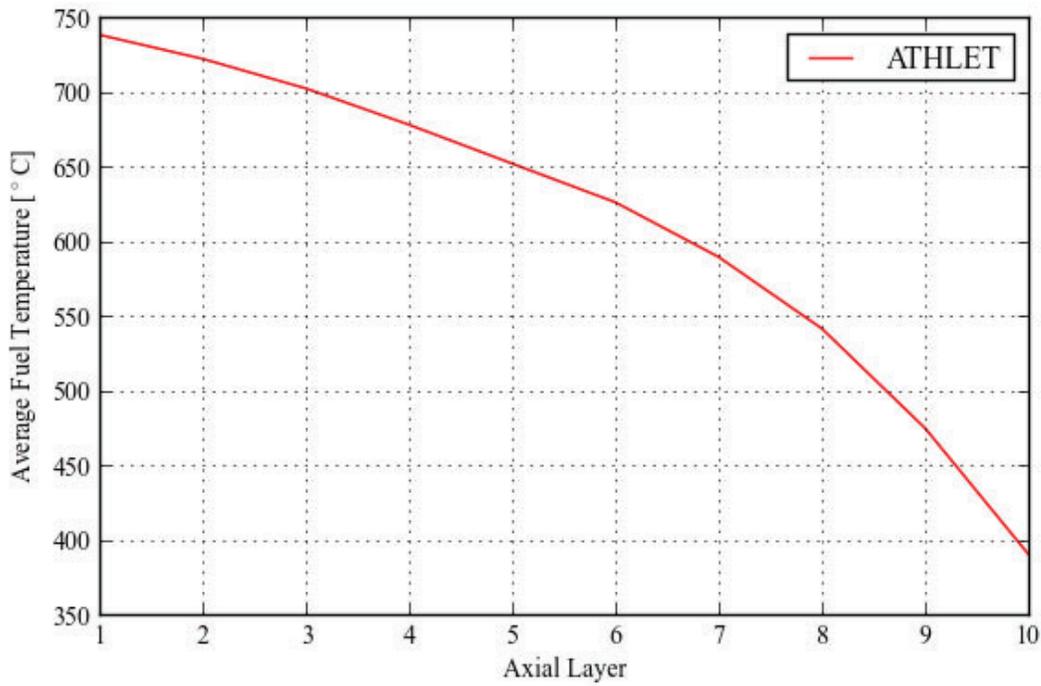


Fig 10. Axial distribution of the average fuel temperature

## 4. CONCLUSIONS

Simulations of both types of VHTR—the pebble bed and the prismatic block reactor—were performed with the thermal hydraulics system code ATHLET. Because of their distinct fuel element geometries and the usage of graphite as moderator material, some code developments had to be done regarding e.g. heat transfer correlations and material properties. While, from an ATHLET user’s point of view, after the code developments the pebble bed reactor could be modeled as straightforwardly as common PWRs, the prismatic fuel of the block-type reactor required a more elaborate input model in order to handle the two-dimensional heat conduction problem.

Regarding the pebble bed reactor, a transient calculation of the core was performed (turbine/compressor trip with SCRAM). Since there was no data for comparison available, the simulation results were assessed only qualitatively. From this point of view, ATHLET was able to compute realistic temperatures in the core and to capture the large thermal inertia of the core structures which is typical of this reactor type.

As for the prismatic block reactor, a steady state simulation of the core was performed according to Phase I, Exercise 2a of the ongoing OECD MHTGR-350 benchmark. The simulation results were assessed in a code-to-code comparison with other thermal hydraulics codes. In general, ATHLET as well as the other programs led to conformable results. Due to a simplification in the input model, ATHLET underestimated the fuel temperatures at first. After a revision of the model and a recalculation of the exercise, the fuel temperatures predicted by ATHLET match the results of the other codes.

For the near future it is planned to build up an ATHLET model of the primary circuit of the pebble bed VHTR, utilizing the existing core model described in this paper. Looking further ahead, a primary circuit model of the prismatic block reactor as well as coupled neutronics/thermal hydraulics calculations are conceivable.

## ABBREVIATIONS

ATHLET	Analysis of the Thermal Hydraulics of Leaks and Transients
FEM	Finite Element Method
HCO	Heat Conducting Object
KTA	Kerntechnischer Ausschuss
MHTGR	Modular High Temperature Gas Reactor
OECD	Organisation for Economic Co-operation and Development
PBMR	Pebble Bed Modular Reactor
PWR	Pressurized Water Reactor
RBMK	Reaktor Bol’shoy Moshchnosti Kanal’nyy
RPV	Reactor Pressure Vessel
VHTR	Very-High-Temperature Reactor
VVER	Voda-Vodyanoy Energeticheskiy Reaktor

## ACKNOWLEDGMENTS

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