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Advanced Reactor for Cogeneration of Heat & Electricity-R&D

Coupled TORT-TD/ATTICA-3D model for pebble bed hot spot/area analysis

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Summary

This document contains a detailed description of the working points to assess the potential for hot spots or hot areas in HTGR with the coupled code system TORT-TD/ATTICA3D.

Approval

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Table of contents

1 Introduction 4
2 Calculation Methods 5
2.1 Pre-processing Codes ZIRKUS and MCNP 5
2.2 Transport and Diffusion Code TORT-TD 5
2.3 Thermal Hydraulics Code ATTICA3D 6
3 Description of Reference Case 10
4 Hot Spots and Areas 16
4.1 Definition and Configuration of Hot Spots and Areas 16
4.2 Definition of Evaluation Cases 16
4.3 Implementation of Evaluation Cases 17
5 Annexes 21
5.1 References 21

1 Introduction

The aim of this task is to assess the potential for hot spots or hot areas in HTGR cores, especially pebble bed cores, which may not have been covered with standard steady state thermal analysis of HTGR cores in the past.
IKE is developing the system TORT-TD/ATTICA3D as a tool for safety analyses based on three-dimensional coupled simulation of neutronics and thermal behaviour HTGRs with pebble and block fuel elements. Special emphasis is on temperature heterogeneity effects (and related reactivity effects) to identify possible thermal issues. Larger area variations of pebble bed porosity can be modelled to investigate their interdependent influence on coolant temperatures, fuel temperatures and power distribution.
The following work steps will be performed:

- Tool and method development to identify possible hot spots/hot areas by coupled neutronic/thermal hydraulic analyses (TORT-TD and ATTICA-3D), consideration of porosity and load variations on cross sections and spectra, feedback with thermal hydraulics.
- Application calculations for reference plants under operational conditions as well as for reactivity transients and loss of cooling accidents (reference plant with pebble or block fuel element as well as scenarios to be jointly defined in the project).

Coupled thermal hydraulic/neutronic analyses are required to identify potentially critical areas/hot spots. The tools applied in the integral coupled analysis usually are not sufficiently accurate to estimate the actual local heat loads (e.g. of structures adjacent to void regions). A more realistic assessment is possible by detailed CFD analyses for local regions, using the results of the integral analyses as boundary conditions. Therefore CFD analyses for potential hot spots/areas identified in the analyses above (e.g. flow in cavities) will be performed with boundary conditions taken from the coupled neutronic/thermal hydraulic analyses.

2 Calculation Methods

2.1 Pre-processing Codes ZIRKUS and MCNP

The code system ZIRKUS/THERMIX [1] is used to calculate the cross sections of the reference case. ZIRKUS is a 2D modular code system, including a pebble flow module, neutron diffusion module and burnup module. Thermal Hydraulic feedback is given by THERMIX/DIREKT. Group cross sections are achieved by the coupled spectral code MICROX2 from the PSI [2]. The ZIRKUS cross sections are also used for the coupled ATTICA3D/TORT-TD calculations.

MICROX2 explicitly considers the double heterogeneous nature of the fuel (fuel particles in a graphite shell, see Figure 6) and its effect on spectral calculations. The simulation chain of cross sections generation, flux and burnup calculation is necessary to achieve the in situ cross sections.

The Monte-Carlo N-Particle Code (MCNP) is a well-known general code for transport problems [3].

The Code allows detailed analysis of various geometries. The geometry of the fuel pebbles, including the fuel particles, can be explicitly modelled in MCNP, as well as different possibilities for their arrangement in the pebble bed. Point wise cross sections and different material compositions of the fuel particles allow the evaluation of different burnup states.

2.2 Transport and Diffusion Code TORT-TD

For other neutronic calculations of this task, especially 3D evaluations, the time-dependent 3-D fine-mesh few-group discrete ordinates (S_N) neutron transport code TORT-TD is used.

The neutron transport code TORT-TD is being developed at GRS [5]. It is based on the DOORS steady-state neutron transport code TORT [4] and solves the steady-state and time-dependent few-group transport equation with an arbitrary number of prompt and delayed neutron precursor groups in both Cartesian and cylindrical (r-φ-z) geometry. Unconditional numerical stability in transient calculations is achieved using a fully implicit time discretization scheme. Scattering anisotropy is treated in terms of a Legendre scattering cross section expansion. Computing time can be saved by extrapolating the angular fluxes to the next time step using the space-energy resolved inverse reactor period. The features of TORT-TD further include:

- 64 bit encoding to meet imposed tight convergence criteria and to enable TORT-TD to be applied to large realistic problems exceeding 32 bit RAM limitations;
- Movements of single control rods or control rod banks;
- Processing of parameterized tabulated cross section libraries for up to 5 state parameters; interpolation either linear or with cubic spline polynomials, thus allowing to study the impact of different interpolation schemes on cross section evaluation;
- Time-dependent anisotropic distributed external source;
- Leakage and buckling calculation over larger spatial regions (e.g. spectral zones) using the neutron current density in discrete ordinates representation;
- Calculation of Xenon/Iodine equilibrium and transient distribution as a prerequisite for operational transients;
- Fully integrated 3-D fine-mesh few-group diffusion solver (steady state and time-dependent) in both Cartesian and cylindrical geometry.

TORT-TD has recently been extended by a 3-D fine-mesh few-group solver for the steady state and time dependent diffusion equation in few energy groups for both Cartesian and cylindrical (r-ϑ-z) geometry. The diffusion solver is fully integrated in TORT-TD and can be invoked by a single parameter in the input data set. Since it operates on the same spatial discretization and the same cross section data, the diffusion solver allows studying the impact of the diffusion approximation by directly comparing with the SN solution. It can also be applied to fast running scoping calculations, especially for transients, or as a preconditioner to accelerate subsequent discrete-ordinates calculations.

2.3 Thermal Hydraulics Code ATTICA3D

The ATTICA3D Advanced Thermal Hydraulics Tool for In-vessel and Core Analysis in 3 Dimensions, developed at IKE of Stuttgart University applies the porous medium approach in both cylindrical and Cartesian geometry [6]. Subdivision between solid and fluid fraction in a considered control volume is done via the porosity parameter ε assuming thermal non-equilibrium. Multiple gase phases are foreseen in ATTICA3D.

For the solid structures, the transient energy equation is

$$(1-\varepsilon)\frac{\partial}{\partial t}(\rho_s h_s) = (1-\varepsilon)\nabla\left[\cdot\, \lambda_{s,eff} \cdot \nabla T_s\right] - \dot{q}_{conv} + \dot{q}_{nu}$$

where the index s indicates the solid state, ε, ρ, h, λ_{eff}, Ts, $\dot{q}_{conv}$ and $\dot{q}_{nu}$ denote porosity, density, enthalpy, effective heat conductivity, temperature, convective heat transferred between solids and gases, and the amount of generated nuclear power, respectively.

The time-dependent energy equation for the gas phases is

$$\varepsilon \frac{\partial \rho_g h_g}{\partial t} + \varepsilon\, div\,(\rho_g \vec{u} h_g) = \varepsilon\, div\,(\lambda_{g,eff}\, grad\,(T_{g,i})) + \dot{q}_{conv}$$

where the index g,i indicates gas phase of the gas type i (e.g. Helium, Oxygen), h is the specific gas enthalpy, $\vec{u}$ denotes the velocity vector, $\lambda_{g,i,eff}$ the effective heat conductivity of the gas and Tg,i the gas temperature. The latter is calculated by

$$\dot{q}_{conv} = \alpha(T_s - T_g)$$

where α is the heat transfer coefficient. Heat transfer within the pebble bed is determined according to KTA standards [7] using the Zehner-Schlünder and, for elevated temperature levels, the Robold correlation.

The mass conservation is only solved for the fluid region. The implemented mass conservation equation comes as

$$\varepsilon \frac{\partial \rho_i}{\partial t} + \varepsilon\, div\,(\rho_i \vec{u}_i) = 0$$

with the same declarations as stated above.

The momentum equation has the form of a simplified equation of Ergun type for porous medium. Since the porous medium approach is strongly dominated by pressure loss, fluid-solid friction and body force, the unsteady and convection term on the left hand side, and on the right hand side diffusion of momentum, additional viscous term are neglected, yielding

$$\varepsilon \, grad \, p = -\vec{R} - \varepsilon \rho_i \, \vec{g}$$

with $\vec{R}$ denoting the friction force, and $\vec{g}$ denoting gravitational acceleration.

To capture the feedback of thermal hydraulics on neutronics a quasi-steady-state heterogeneous temperature model (HTM) for the fuel pebble (see Figure 1) is implemented. This consideration is necessary, since fission heat is mainly generated in the uranium kernel and not in the surrounding graphite. In fast transients, the temperature difference between the fuel kernel and graphite can be substantial. This pronounces strong feedback effects from the fuel Doppler temperature.

In the HTM, the fuel is subdivided into an arbitrary number n of spherical shells, see Figure 1, in our example n = 6.

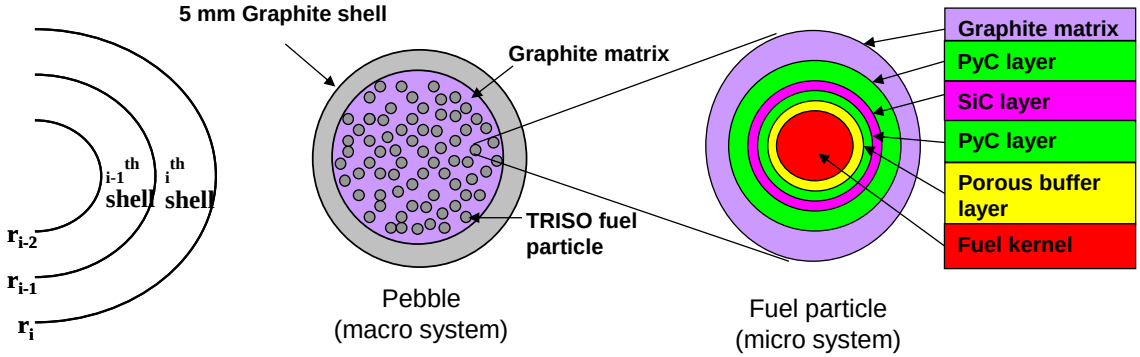


Figure 1 : Subdivision of a fuel element when applying the heterogeneous temperature model

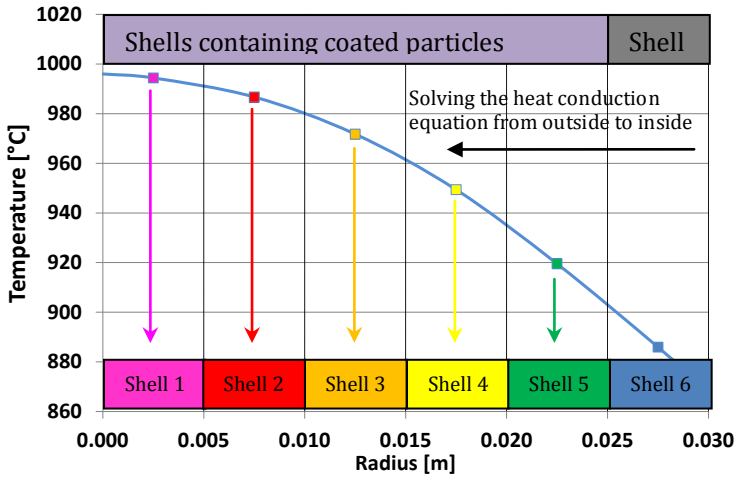


Figure 2 : Temperature distribution after solving the heat conduction equation for the fuel pebble (macro system), delivering boundary conditions for the micro system

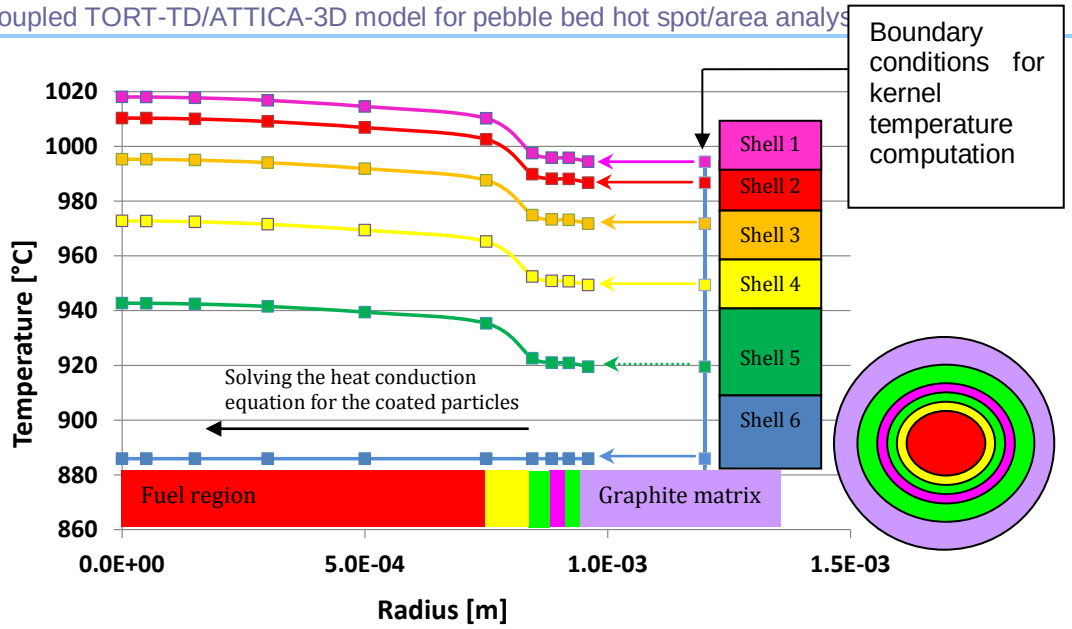


Figure 3 : Temperature distribution for the representative kernels per shell (micro system). The blue bar on the right side visualises the boundary condition after solving the heat conduction equation and is coloured as in the macro system. The colouring at the bottom display the different coatings according to Figure 2

Starting from the surface of the fuel element (kth shell or graphite matrix, here k = 6), the steady-state heat conduction equation for each shell is solved towards the fuel element centre (k-1st shell, then k-2nd shell and so on). The surface temperature of the fuel element is taken as the boundary condition. Mean temperatures are calculated for successive fuel shells, until the innermost shell. These temperatures, however, only apply to the graphite shells (macro system), not the fuel kernels (micro system).

For the average temperature of the fuel particles contained in a considered shell, a representative particle is determined that gets appointed the mean temperature for all the fuel kernels contained within. In order to determine the representative particle temperature, the respective shell temperature of the surrounding graphite serves as boundary condition.

Here, the heat conduction equation is solved for the micro system once more, taking into account the different heat conductivities of the coatings of the particles. After fuel and moderator temperatures are determined, the temperature values are averaged and one fuel temperature and moderator temperature per thermal hydraulic mesh is obtained to process nuclear cross sections. Thus, fuel temperature feedback is much more pronounced than it is without HTM. In Figure 2 and Figure 3, typical temperature profiles during steady-state are presented for a pebble in the central bottom part of the reference plant.

In order to correctly account for variation of material properties, ATTICA3D comes with a large material properties library. For the description of other phenomena like heat transfer outside the pebble bed, pressure losses due to changing diameters in the flow path, thermal radiation and so on, a set of constitutive equations are provided within ATTICA3D.

Technically, the coupled code system TORT-TD/ATTICA3D is represented by a single executable in which ATTICA3D acts as the main program and calls TORT-TD in terms of a subroutine whenever an update calculation of the power distribution is requested. For the data exchange between TORT-TD and ATTICA3D, already existing TORT-TD interface routines have been utilized in combination with the ATTICA3D mesh overlay feature that transfers 3-D distributions from its thermal-hydraulic mesh to a superimposed neutron-kinetics mesh and vice versa. This allows for efficient data transfer via direct memory access of array elements.

A TORT-TD/ATTICA3D transient simulation consists of a three-step procedure. First, a coupled steady state calculation is performed. ATTICA3D and TORT-TD are called repeatedly, followed by

exchange of thermal-hydraulic and neutron kinetics data, until convergence of the 3-D temperature and power distributions are achieved. At the beginning of the iteration process, TORT-TD calculates for a given thermal-hydraulic initial distribution the corresponding power distribution that is transferred to ATTICA3D as first estimate. Second, a zero transient follows based on the converged steady state with no changes being imposed on the system. A few seconds zero transient may help verify the stability of TORT-TD and ATTICA3D when both codes switch to their respective time-dependent mode of operation. In the last step, the actual transient is being initiated.

3 Description of Reference Case

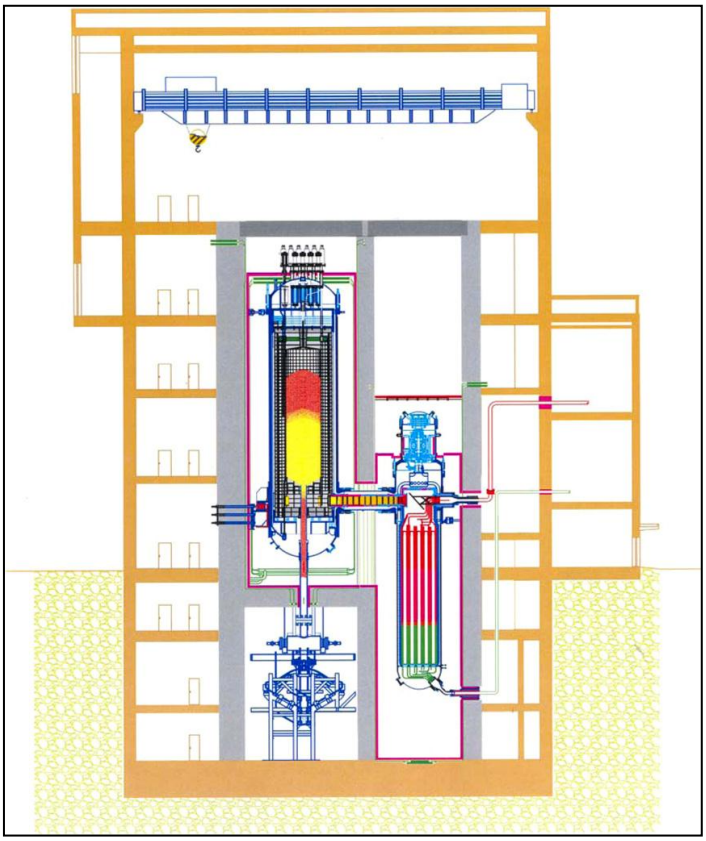


Figure 4 : Cross section of HTR-PM building with primary cavity (reactor pressure vessel, steam generator)

The only HTR concept at the brink of finalization at the moment is the Chinese HTR-PM (Figure 4), which stands for High Temperature Reactor – Pebble Bed Modular. It was developed after the successful test with the HTR-10 test reactor and is based on HTR-Modul designed in Germany by Siemens-Interatom in the 1980s [8]. It was decided that a pebble bed reactor based on the HTR-PM the ***ARCHER Reference Plant*** (ARP) will be selected as a reference case for further calculations.

The layout of the ARP is therefore a one zone cylindrical core consisting of a pebble bed (Figure 4, Figure 5). To compete economically with current Light Water Reactor (LWR) designs, two or more reactor cores should be coupled to one power conversion unit (turbine). To benefit from existing equipment, the power conversion is a Rankine Process (steam turbine) which includes a steam generator at the reactor.

A central graphite structure consisting of a fixed structure or moderator pebbles is not foreseen. The core has a diameter of 3 m which is the same as the HTR-Modul (Table 1). The height of the flattened core is 11m. With an estimated average porosity of 0.39 of the pebble bed there are approximately 420,000 pebbles in the reactor. The Helium pressure in the primary loop is 7 MPa. The Helium in the primary loop flows from the steam generator with a temperature of 250°C and a rate of 96.3 kg/s through a coaxial pipe, through the helium risers to the top of the core, from there through the pebble bed downwards and the porous bottom reflector with a temperature of 750°C back to the steam generator. The control rods (CRs) consist of multiple B4C rings hanging from the top of the reactor (Figure 7). Each CR can be driven independently. In case of a station blackout, the control rods fall into their shut-down position by gravity. As secondary and additional shut-down system, small absorber spheres (SAS) with a diameter of 1cm can fall by gravity (withheld by electrical valves) into long holes in the side reflector (Figure 8). The side reflector has a thickness

of 75cm (this includes borated carbon bricks with a thickness of 5cm to protect the outer components of the reactor). The side reflector is dived into 30 azimuthal sections, each with either a CR-hole or two long holes for the SAS (hole circle diameter for both 162.5cm).

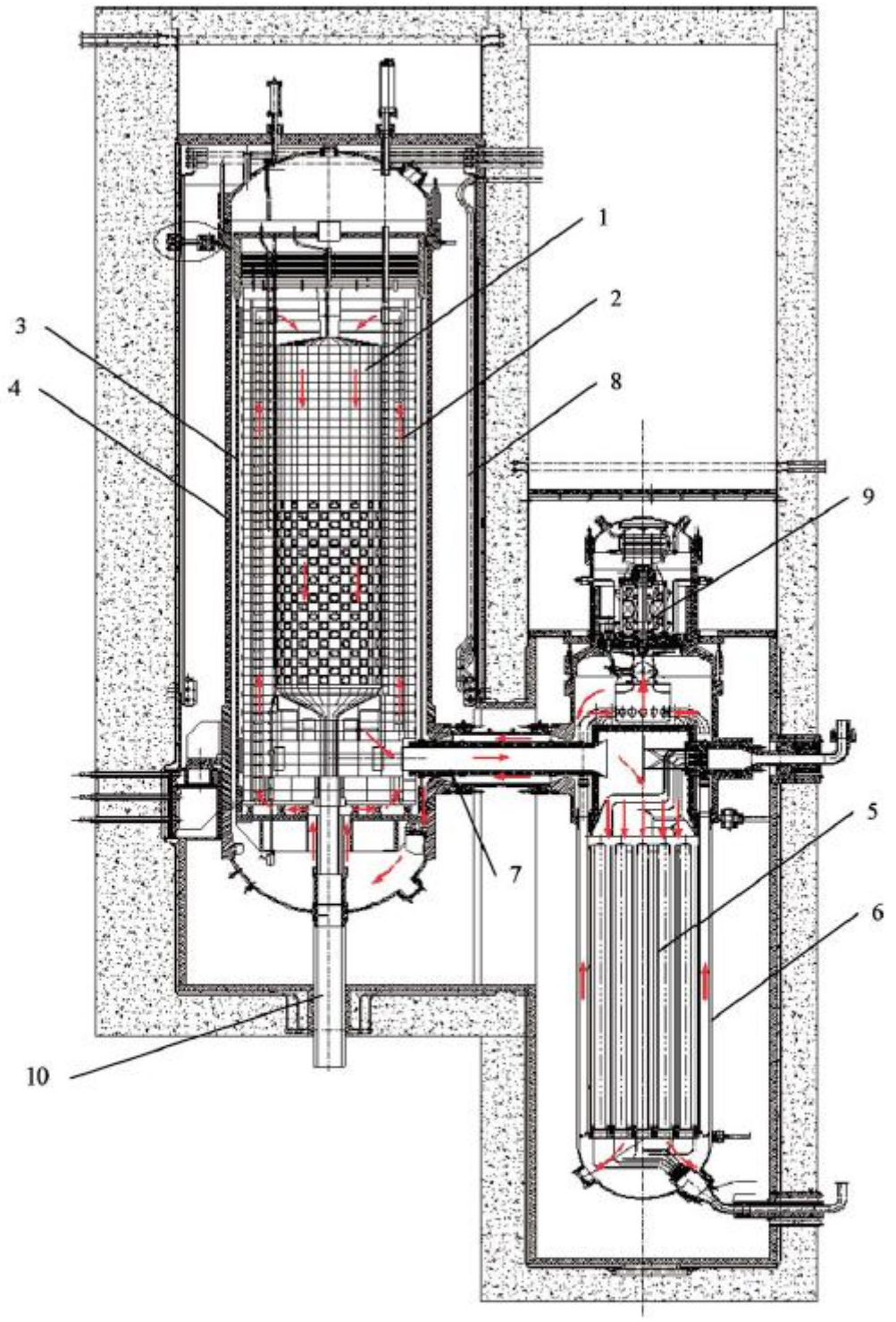


Fig. 1 Cross-section of the HTR-PM reactor: (1) reactor core, (2) side reflector and carbon thermal shield, (3) core barrel, (4) reactor pressure vessel, (5) steam generator, (6) steam generator vessel, (7) coaxial gas duct, (8) water-cooling panel, (9) blower, (10) fuel discharging tube, (11) control rod driving system, and (12) small absorber sphere unit

Figure 5 : Cross section of HTR-PM

The graphite components are kept in shape by a core barrel made of steel, which is then surrounded by a carbon structure. The whole setup is situated inside a Reactor Pressure Vessel (RPV) made of steel. At the outside of the RPV the Reactor Cavity Cooling System (RCCS) is installed, which protects the reactor structures from temperature induced damage during accidents by transporting the expected excessive heating power.

The fuel of the reactor consists of fuel pebbles made from graphite, which include fuel particles with a diameter of 500µm (Figure 6). The particles have different coatings, namely a buffer graphite coating to absorb gaseous fission products, a binder coating to the Silicon-Carbide coating and another binding layer (TRISO). The Silicon carbide coating is intended to sustain the fission products during an accident with a assumed heating up of the core. The main fuel parameters can be found in Table 2.

Table 1 : Main design parameters

Parameter	Unit	Value
Rated electrical power	MW	110
ReactorThermal Power	MW	250
Average core power density	MW/m^3	3.22
Eletrical Efficency	%	42
Primary helium pressure	MPa	7
Helium temperature at reactor inlet/outlet	°C	250/750
Helium flow rate	kg/s	96.3
Numer of Helium riser channels	-	30
Active core diameter	m	3
Equivalent core height	m	11
Height upper void	m	0.57
Number of control rods	-	8
Diameter of control rod holes	cm	65
Number of SAS	-	2x22
Type of steam generator	-	Once through helical coil
Main steam pressure	MPa	13.24
Main steam temperature	°C	566
Main feed-water temperature	°C	205
Main steam flow rate at the inlet of turbine	t/h	673

Table 2 : Main fuel element parameters

Parameter	Unit	Value
Fuel Type	-	TRISO
Heavy Metal (HM)	-	UO2
Radius of U- Kernel	µm	250
Thickness of the 4 Kernel Layers	µm	95 / 40 / 35 / 35
Density of HM-Oxide	g/cm3	10.4
Density of the 4 Coatings	g/cm3	1.05 / 1.9 / 3.18 / 1.9
Radius of Fuel Matrix	cm	2.5
Radius of Fuel Element	cm	3.0
Graphite Density of Matrix	g/cm3	1.74
HM per fuel element	g	7
Enrichment of fresh fuel	%	8.9
Thermal absorption cross section of Graphite [Fuel and Reflector]	mbarn	4
Number of fuel elements in reactor core	-	420,000

Average burn-up	GWd/tU	90
Pebble-bed porosity	-	0.39
Fueling mode	Multipass	15

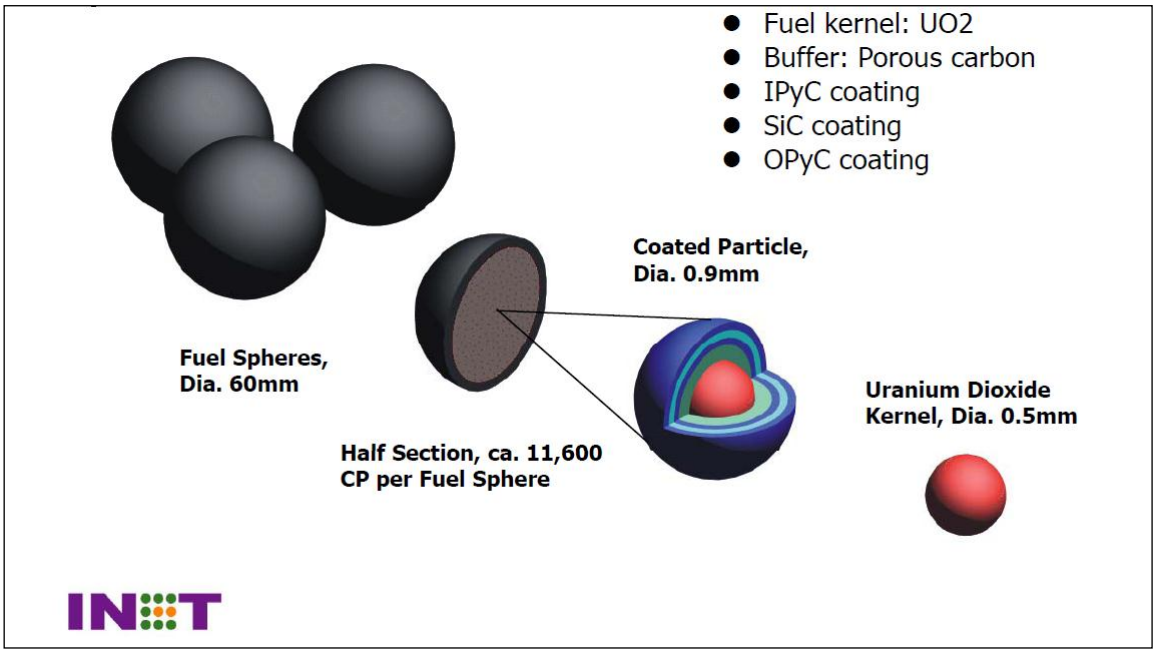


Figure 6 : Layout of fuel Elements

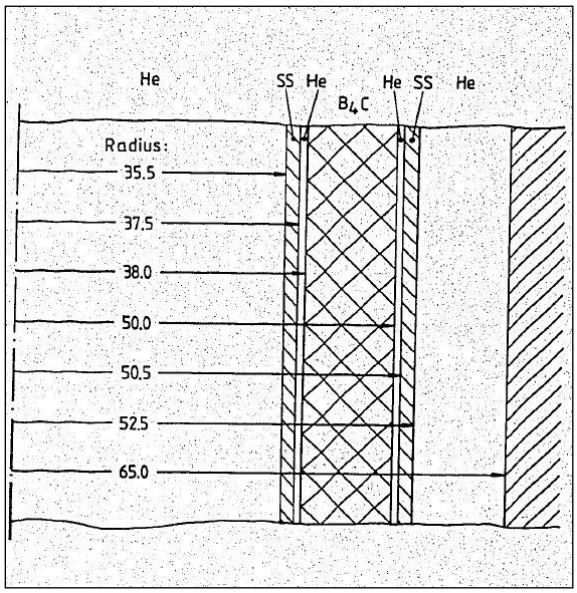


Figure 7 : Control Rod layout (SS : Stainless Steel)

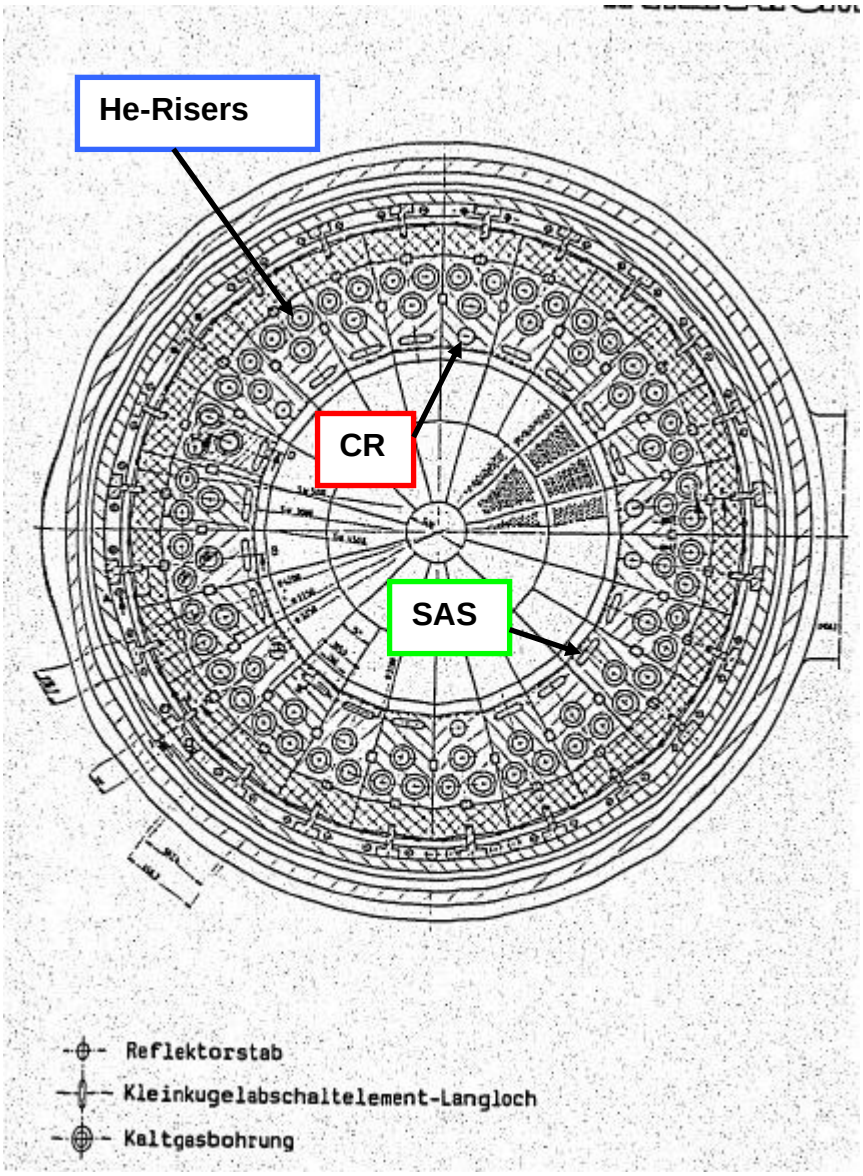


Figure 8 : Horizontal cross section of HTR-Modul with Helium risers, control rod holes and small absorber sphere holes

4 Hot Spots and Areas

4.1 Definition and Configuration of Hot Spots and Areas

Hot spots and areas in pebble bed cores occur as a consequence of unexpected fuel loading patterns and fuel handling inside the reactor.
A variation of the flow velocity of one of the flow channels mentioned above might lead to a higher or smaller burnup of the specific zones and therefore to a more unbalanced power distribution. The highest effect is expected at the radial outermost flow channel since the highest flow velocity occurs here.

Hot spots in Pebble Beds might be triggered through a densification of the fuel pebbles [11] [12].
At first hand, this may lead to the thermal hydraulic effect that the coolability of the densification may be insufficient.
A higher density of the fuel pebbles may also lead to a local increase of the moderator density.
If the densification migrates through the core as part of the normal fuel cycle, the change in moderator to fuel ratio may lead to spectral changes and as a consequence, to burnup and power density changes which could be determined.
The densification might also occur spontaneous during normal operations, which leads to a cluster of pebbles with an unaffected nuclide vector of previous burnup.

The consequences of these considerations during accident conditions have also to be determined.

The affects described above may also occur with some fresh fuel pebbles (after the run-in phase, a mixture of fuel pebbles from every fuel cycle is loaded into the core) may be formed, which may lead to different results of the evaluation.

4.2 Definition of Evaluation Cases

One working point would be the modification of the flow channel velocity. A variation of +-20% of the velocity during normal steady state will be accomplished and compared to the previous steady state.

Another study will be the influence of a wrong fuel loading pattern. It will be assumed that, after the run-in phase to the equilibrium core, only fresh fuel pebbles will be loaded to a pebble flow channel. The effect is expected to be greatest at the innermost flow channel resulting from the highest neutron flux. A test case loading fresh fuel in the innermost zone will be investigated and compared to the previous steady state results.

For the following considerations for the TORT-TD/ATTICA3D, it is assumed that the densification occurs after the run-in phase of the core.

A small zone with a modified cross section set is to be defined with the following modifications:

The densification forms an area with a smaller porosity, additional influence may be the fuel loading pattern where a series of fresh fuel is introduced into the core and forms a densification.

Stationary results are to be achieved for the following different cases:

- Densification in the maximum of neutron flux
- Densification in the maximum of neutron flux with a bulk of fresh loaded fuel elements
- Densification at the temperature maximum (near the lower end of the core)
- Densification at the temperature maximum (near the lower end of the core) flux with a bulk of fresh loaded fuel elements

To gather reference information about local densifications, MCNP calculations will investigate the influence of the lower porosity of the pebble bed as a reference for the following simulations. The

MCNP calculations will be done without consideration of burnup. The results will be compared to the normal pebble bed results.

Transient calculations are intended for the following cases:

- Control rod ejection: The ejection of one control rod leads to a power excursion. The influence on temperature and power distribution will be investigated.
- PLOFCA (pressurized loss of forced cooing accident): The influence on temperature will be investigated.
- DLOFCA (depressurized loss of forced cooling accident): The influence on temperature will be investigated.

4.3 Implementation of Evaluation Cases

With the transport code MCNP, it is possible to simulate every single fuel particle inside the pebble. In this example, the distribution of the fuel particles are achieved by using a regular lattice of cubes, each consisting of the fuel particle with a diameter of 500 µm and a surrounding mixture of fuel matrix graphite with the coating materials (Figure 9). The MCNP built-in uranium card can provide additional information by randomly distributing the fuel particles inside the graphite matrix.
It is foreseen to do MCNP calculations with some fuel pebbles in different assemblies, thereby simulating different porosities of the pebble bed. Fuel compositions from the run-in stationary case will be used. The calculations results are intended to be used as reference for the influence on neutron flux of the densification for the following TORT-TD/ATTICA3D calculations.

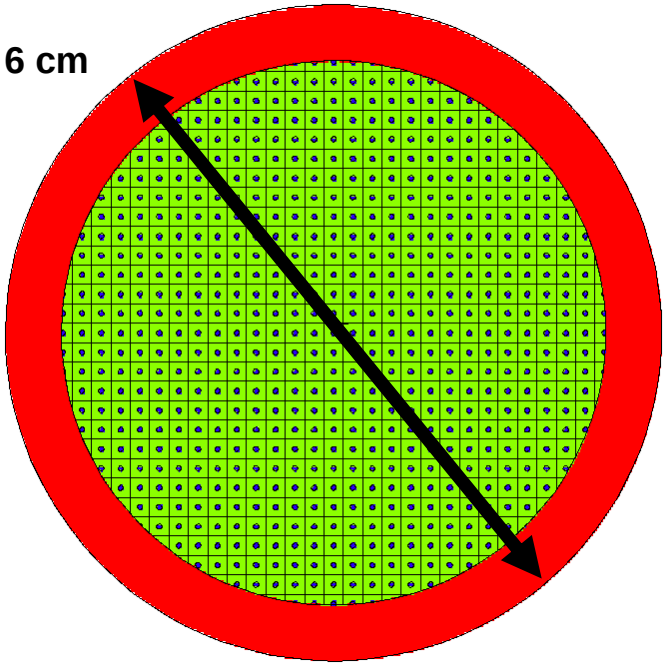


Figure 9 : Representation of a fuel pebble in MCNP

For pre-processing, a ZIRKUS calculation of the implemented ARP layout is done to achieve the nuclide densities and cross sections of the run-in steady state. For this purpose, the core is divided into 8 flow zones of equal area (and therefore volume) to model adequately the pebble flow. The control rods are inserted as a grey curtain to achieve a critical reactor (Figure 10, zone 199). The reflectors and other core structures are divided into different zones to provide detailed consideration of thermal and material for the cross sections. Different pebble flow velocities and their influence can be investigated with analysis of ZIRKUS results. It will be assumed that the densification occurs after the formation of the equilibrium state of the core.

Since ZIRKUS is a 2D-code, the cross sections represent a 2D reactor model. Therefore, it is only safe to say that only densifications on the symmetry axis can be correctly implemented on ZIRKUS. The densification leads also to a decrease of pebbles in the surrounding channel areas. Since it is assumed that the pebbles move in flow channels, the decrease is only suspected to only occur in the surrounding flow channel cells. The unintended loading of fresh fuel can also be simulated.



Figure 10 : Representation of neutronic zones in ZIRKUS

For the calculation in TORT-TD/ATTICA3D, the achieved cross sections from ZIRKUS are used. Figure 11 and Figure 12 show a 180° representation of the ARP in ATTICA3D.
The neutronics discretisation model of TOR-TD is similar with the ZIRKUS model, but expanded azimuthally to 180 into 13 zones, also representing the control rods. The ATTICA3D-model is divided into similar azimuthal zones. The control rods can be driven individually by TORT-TD input options. The flux and spectra are calculated by TORT-TD model. Additional probe points can be

added to the ATTICA3D input for additional information. The zonal structure in the densification has to be more detailed to gather the desired information.

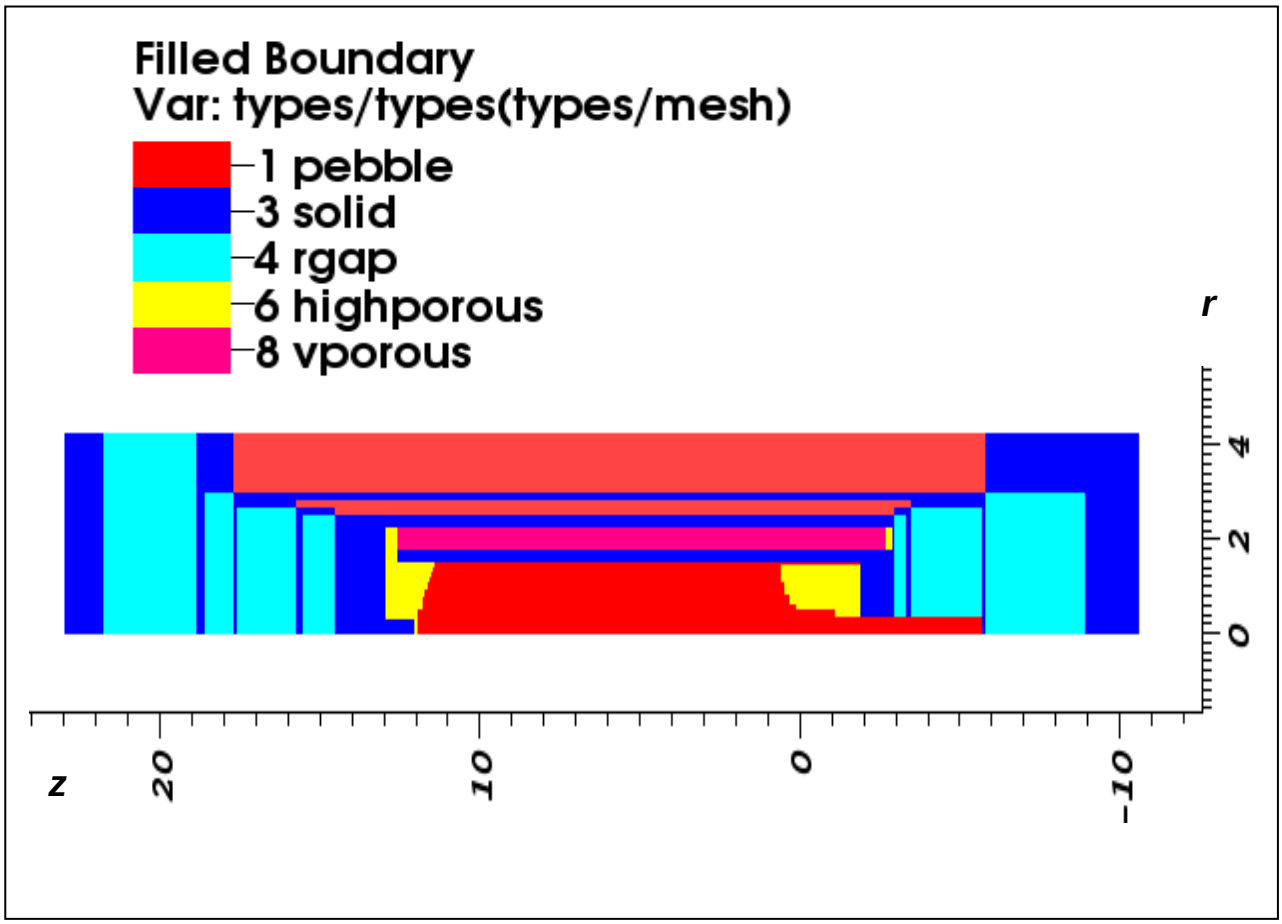


Figure 11 : Cross section of representation of thermal hydraulic zones in ATTICA3D

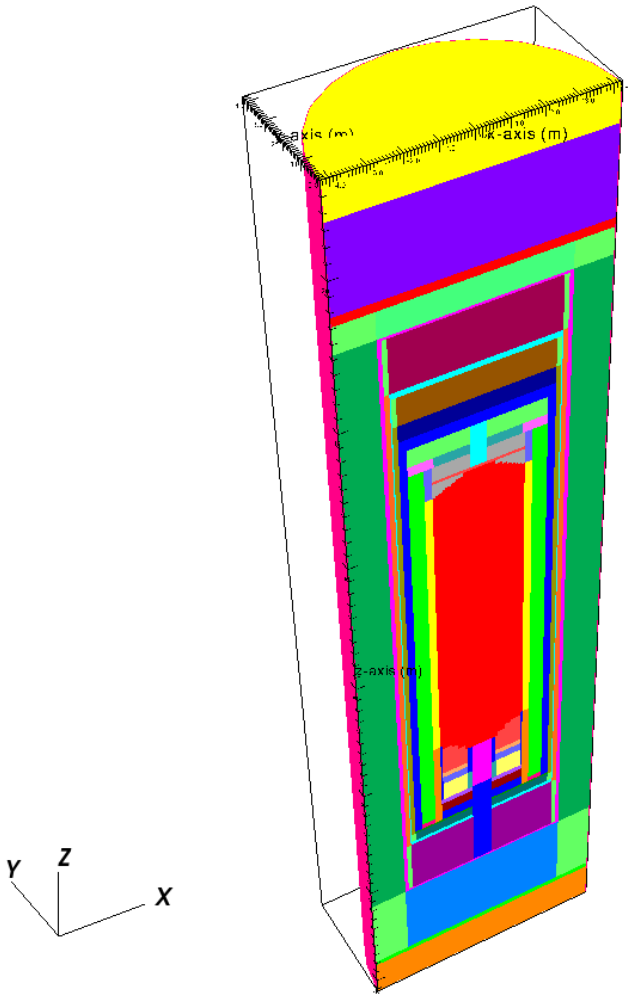


Figure 12 : 180° ATTICA3D model

5 Annexes

5.1 References

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