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**TORT-TD/ATTICA3D: A COUPLED NEUTRON TRANSPORT AND  
THERMAL HYDRAULICS CODE SYSTEM FOR 3-D TRANSIENT  
ANALYSIS OF GAS COOLED HIGH TEMPERATURE REACTORS**

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**Abstract**

Comprehensive safety studies of high temperature gas cooled reactors (HTR) require full three dimensional coupled treatments of both neutron kinetics and thermal-hydraulics. In a common effort, GRS and IKE developed the coupled code system TORT-TD/ATTICA3D for pebble bed type HTR that connects the 3-D transient discrete-ordinates transport code TORT-TD with the 3-D porous medium thermal-hydraulics code ATTICA3D.

In this paper, the physical models and calculation capabilities of TORT-TD and ATTICA3D are presented, focusing on model improvements in ATTICA3D and extensions made in TORT-TD related to HTR application. For first applications, the OECD/NEA/NSC PBMR-400 benchmark has been chosen. Results obtained with TORT-TD/ATTICA3D will be shown for transient exercises, e.g. control rod withdrawal and a control rod ejection. Results are compared to other benchmark participants' solutions with special focus on fuel temperature modelling features of ATTICA3D. The provided "grey-curtain" nuclear cross section libraries have been used. First results on 3-D effects during a control rod withdrawal transient will be presented.

**Introduction**

Deterministic neutronics, thermal-hydraulics and transient analysis tools and methods available to design and analyse High-Temperature Gas-cooled Reactors (HTGR) have, in many cases, lagged behind the state of the art compared to other reactor technologies, e.g. light water reactors. For comprehensive safety studies of HTGR, full three dimensional coupled treatments of both neutron kinetics and thermal-hydraulics become more important to account for non-symmetric effects. As the neutron transport code TORT-TD [1][2][3] and the thermal-hydraulics code ATTICA3D [4][5][6] are both three dimensional steady-state and transient codes, the coupled code system

TORT-TD/ATTICA3D may provide a basis for high-accuracy full three dimensional coupled neutronics and thermal-hydraulics simulation for HTGRs of pebble bed type.

## 1. The time-dependent 3-dimensional discrete ordinates transport code TORT-TD

TORT-TD [1] is a time-dependent 3-D multi-group discrete ordinates ( $S_N$ ) neutron transport code developed at GRS. It is based on the DOORS steady-state neutron transport code TORT [2][3] and solves the steady-state or time-dependent multi-group transport equation with an arbitrary number of prompt and delayed neutron precursor groups in both Cartesian or cylindrical ( $r$ - $\vartheta$ - $z$ ) geometry. Unconditional stability in transient calculations is achieved using a fully implicit time discretisation scheme. Scattering anisotropy is treated in terms of a  $P_l$  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  $\omega_g(\vec{r})$ . Few-group macroscopic cross sections are fed into TORT-TD in terms of parameterized tabulated cross section libraries where the dependence of up to five parameters (fuel temperature, moderator temperature, xenon density, fast buckling, and thermal buckling) can be considered. Depending on the current thermal-hydraulic state in each spatial mesh cell, appropriate cross sections are interpolated by TORT-TD between given sampling points either linearly or using cubic spline polynomials. For handling buckling dependency of few-group cross sections, TORT-TD calculates the buckling over larger spatial regions, e.g. material zones, by evaluating the net leakages across the surfaces of the corresponding volumes. By implementing steady-state and transient iodine-xenon equations, TORT-TD has been prepared for the simulation of operational transients. In order to test time-dependent capabilities of TORT-TD comparison with results of other code systems were performed and previously presented in [4].

## 2. The time-dependent 3-dimensional thermal hydraulics code ATTICA3D

The Advanced Thermal hydraulics Tool for In-vessel and Core Analysis in 3 Dimensions, abbreviated ATTICA3D, is an IKE in-house code and was developed as a successor of the 2-dimensional thermal hydraulics tool THERMIX/KONVEK. It was previously also referred to TH3D, compare [5][6]. Up to now, ATTICA3D supports cylindrical and Cartesian geometry only, but introduction of hexagonal grids is foreseen for the future.

ATTICA3D applies the porous medium approach leaving aside detailed description of the components. Subdivision between solid and fluid fraction in a considered control volume is done via the porosity parameter  $\varepsilon$ . As there may be significant differences between the fuel surface temperature and the gas temperature during operation, thermal non-equilibrium between the solid and the gas phase is assumed. In each computational step ATTICA3D solves separate energy conservation equations for both, the solid and the fluid fraction. Additionally, the mass conservation and a simplified momentum equation are solved for the fluid only. The simplifications of the momentum equation neglect inertial and time dependent terms and is dominated by friction (Ergun type). For detailed description of the equations, see [4]. The set of partial differential conservation equations is transformed into a set of initial value ordinary differential equations. The staggered grid approach is adopted for calculating parameters of interest, i.e. the velocities are calculated at the interface of the control volumes; all the other parameters are calculated at the centre of the control volume. Time integration is realised using a fully implicit, time adaptive multi-step backward differentiation method. The resulting equations are solved applying sparse matrix techniques in combination with a modified Newton method. Phenomena like heat transfer and effective conductivities are accounted for by a set of empirical constitutive equations.

To capture the feedback of thermal hydraulics on neutronics a quasi steady-state heterogeneous temperature model (HTM) for the fuel element is available. This consideration is necessary, since fission heat is generated in the uranium kernel and not in the graphite. In fast transients, the temperature difference between the fuel kernel and its surrounding 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  $n = 6$ . The surface temperature of the fuel element is taken as the boundary condition. Starting from the surface of the fuel element ( $i^{th}$  shell or graphite matrix) the steady-state heat conduction equation is solved towards the fuel element centre ( $i-1^{th}$  shell, then  $i-2^{th}$  shell). Proceeding like this, one shell after another gets appointed a mean temperature until the innermost shell is reached. These temperatures, however, only apply to the graphite shells, not the fuel (macro system).

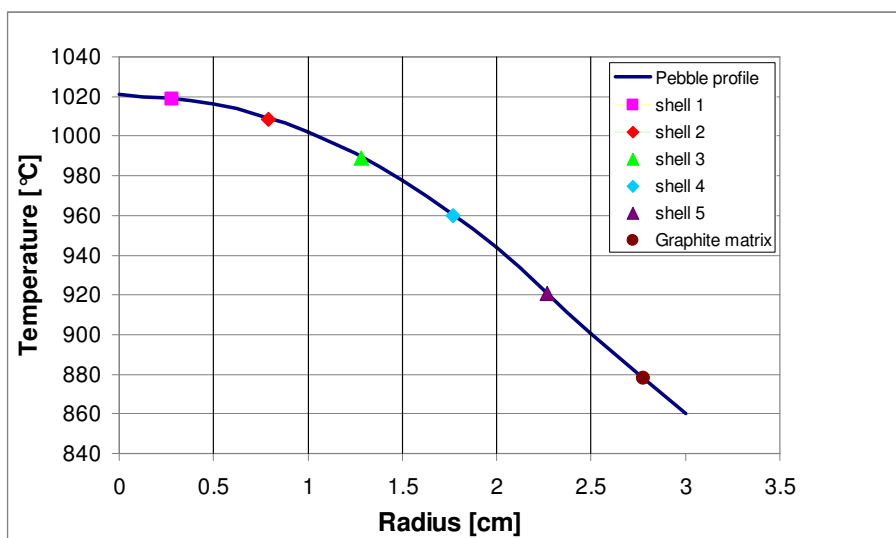


Figure 1: The temperature distribution within a fuel pebble (macro system)

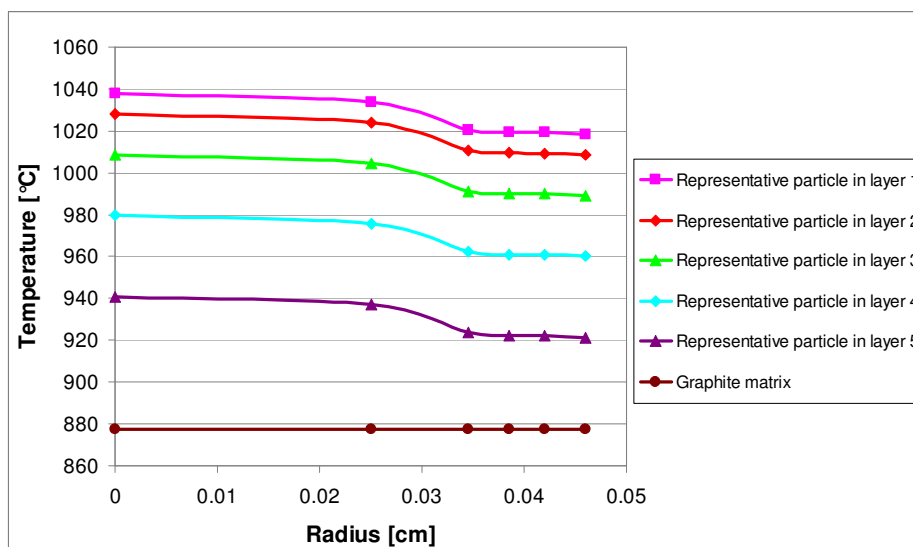


Figure 2: Temperature distribution of the representative particles in a fuel pebble (micro system)

For the average temperature of the fuel particles contained in a considered shell, a representative particle is determined that has the volume-averaged mean temperature for all the fuel kernels contained. For the determination of the representative particle temperature, the respective shell temperature of the surrounding graphite serves as boundary condition, see Figure 2.

Here, again, the heat conduction equation is solved taking into account the different heat conductivities of the coatings of the particles (micro system). After fuel and moderator temperatures are determined, the temperature values are averaged and one fuel temperature and moderator temperature is obtained to process nuclear cross section. Thus, fuel temperature feedback is much more pronounced than it is without HTM. This can also be observed in the comparison of homogeneous and heterogeneous calculations, see Figure 4 and Figure 6.

With ATTICA3D, a validation calculation of the OECD/NEA/NSC PBMR-400 benchmark was already performed in the stand-alone version yielding good agreement with other benchmark participants [4].

### **3. Coupling of TORT-TD to ATTICA3D**

For coupling a neutronics code to a thermal hydraulics code, in general, one has to establish an interface between the codes that allows for data transfer. Neutronics usually provide information about the spatial power density distribution and transfers this to the thermal hydraulics code. The thermal hydraulics code uses provided power density to calculate the corresponding temperature distribution and transfers obtained temperatures back to the neutronics code to process cross sections. For the steady state calculation, 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.

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.

### **4. Analysis of the PBMR-400 Benchmark with TORT-TD/ATTICA3D**

For first test calculations with the coupled tool TORT-TD/ATTICA3D the PBMR-400 design was selected. This benchmark was initiated by the OECD/NEA/NSC as an international effort for code to code comparison [8]. It was selected since it offers both, stand-alone neutronics and stand-alone thermal hydraulics as well as coupled analysis. It provides a thoroughly defined data base for cross sections, geometry and material specifications along with a guide to process cross sections suitable for the benchmark and subsequent comparison to other code systems.

The TORT-TD/ATTICA3D model is based on the simplified geometry depicted in Figure 3 according to the benchmark specification. The main design parameters used are listed in Table 1 below.

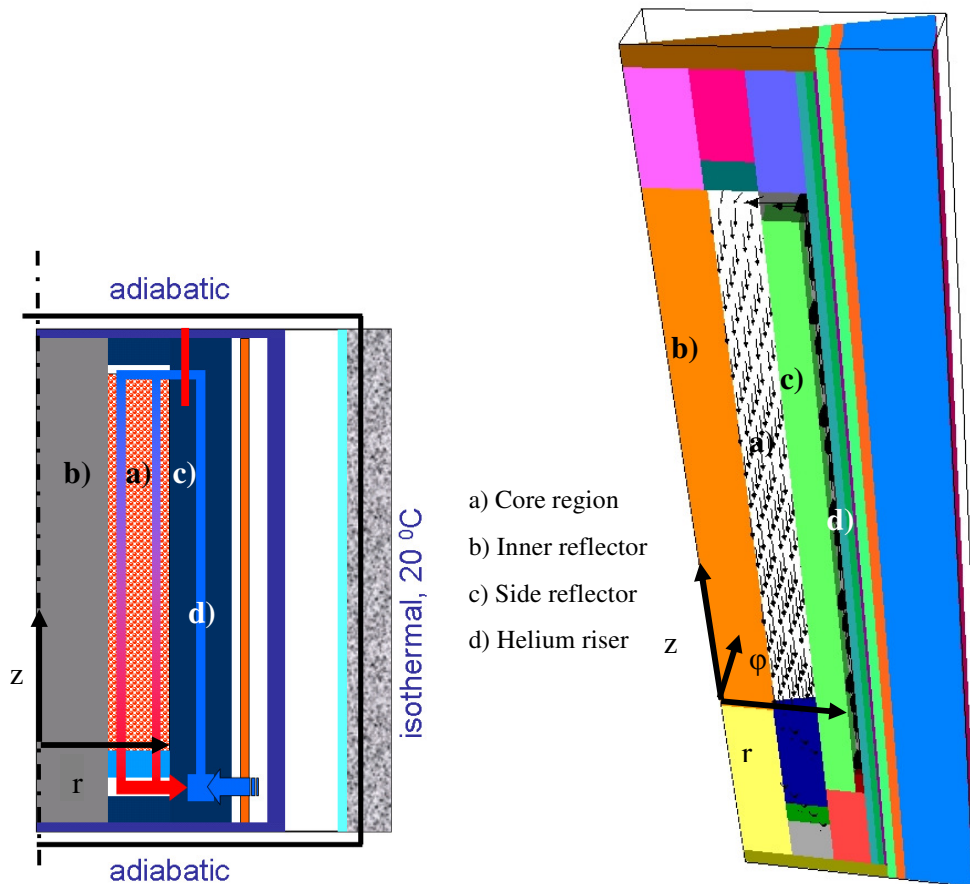


Figure 3: Left side: Simplified geometry for the PBMR-400 benchmark with thermal boundary conditions, control rods enter from top reflector (red bar in blue side reflector), right side: 3-dimensional model of PBMR

Table 1: Main parameters used for the TORT-TD/ATTICA3D model of the PBMR-400

| Description                            | Unit | Value |
|----------------------------------------|------|-------|
| Thermal power                          | MW   | 400   |
| Inlet temperature                      | °C   | 500   |
| Outlet temperature                     | °C   | ~ 900 |
| Gas mass flow rate                     | kg/s | 192.7 |
| System pressure                        | bar  | 90    |
| Control rod insertion from top of core | m    | 1.5   |

To ensure proper configuration of the respective inputs both codes were applied to the purely neutronics (exercise 1) and purely thermal hydraulics task (exercise 2); subsequently, the results were compared to results of the benchmark participants. In addition, exercise 3 comprises a steady-state calculation but with the coupled code TORT-TD/ATTICA3D. The results agree well within the scatter band of the participants' results, as reported in [4].

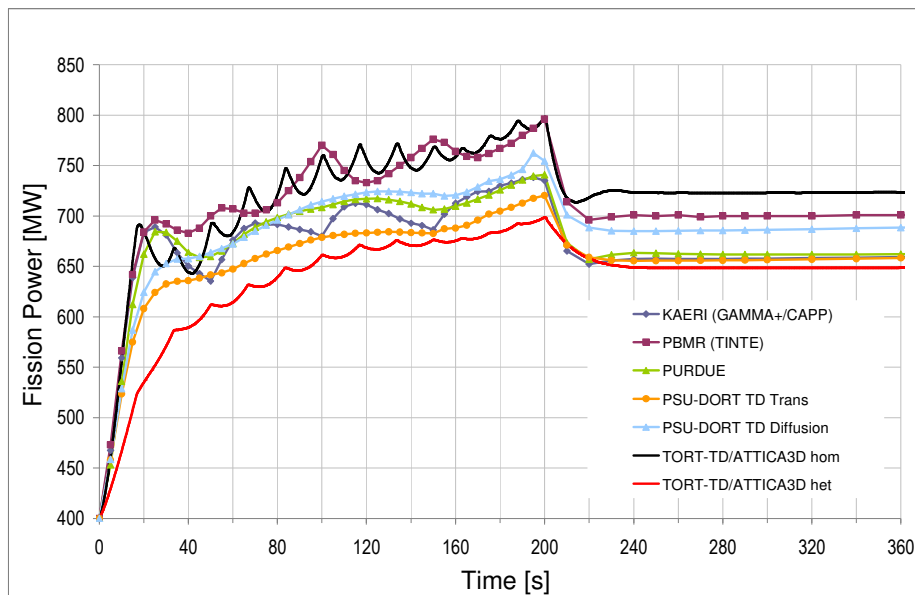
From the steady-state solution obtained with the coupled code TORT-TD/ATTICA3D the transient exercises were the next tasks. For demonstration of the time-dependent capabilities of our coupled code exercise 5a and 5b, the total control rod withdrawal (TCRW) and the total control rod ejection (TCRE), were selected.

#### 4.1 Total control rod withdrawal

In exercise 5a of the PBMR-400 benchmark, the control rods are withdrawn over a period of 200 seconds with a speed of 1 cm/s from the steady-state position, i.e. 1.5 metres from the top of the pebble bed ( $z = 9.5$  m). The final position of control rods is 50 cm above the upper end of the pebble bed ( $z = 11.5$  m). At the start of the transient all but the above mentioned input parameters remain the same. The reactor is at full power with the corresponding xenon distribution.

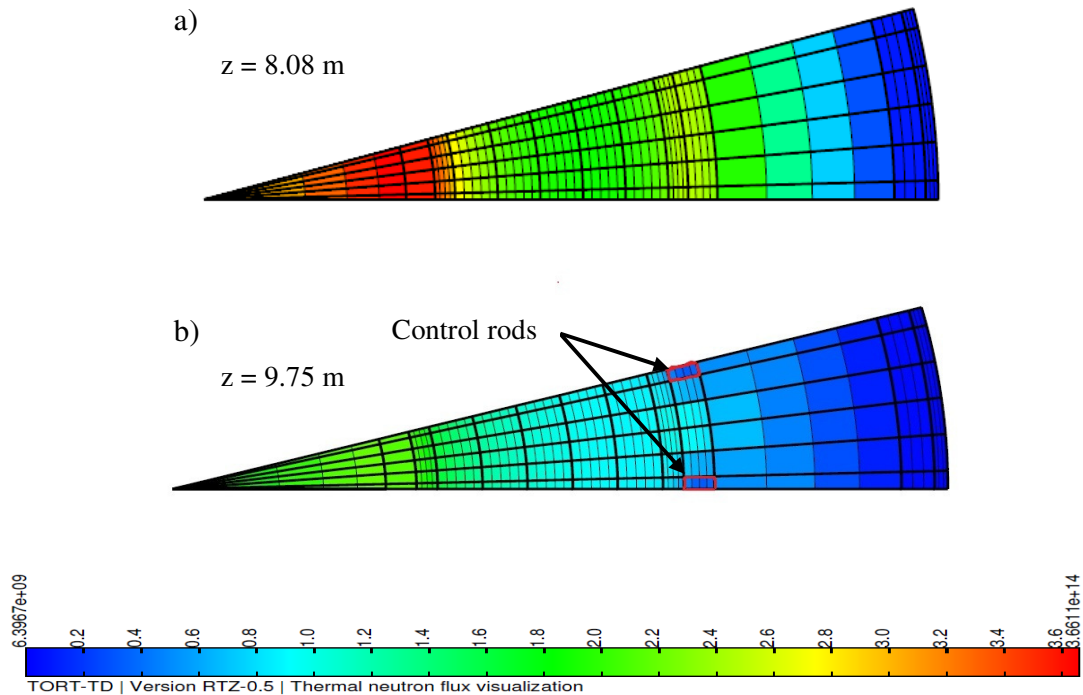
In the benchmark description [7], a model for the fuel temperature is proposed. This model subdivides the fuel element into five shells and appoints the maximum fuel temperature to the innermost shell containing both graphite and fuel particles. However, the proposed fuel temperature model was NOT used; instead, the fuel was modelled homogeneously and, additionally, our own HTM was applied.

According to the benchmark specification, the response of the whole system (e.g. possible increase of the inlet temperature) is not taken into account. The TCRW is modelled using the provided homogenised ‘grey curtain’ cross sections reducing the problem to a 2-dimensional one. Additionally, the TCRW was calculated where control rods were spatially resolved, see Figure 5 where the neutronics mesh grid is depicted. For clarification, the control rod positions are outlined in red. To achieve the same rod worth for spatially resolved control rods as in the homogenised case, several steady-state calculations with different insertion depths of the rods were simulated and the absorption and total cross sections for the rods were adjusted such that same reactivity insertion was obtained.



**Figure 4: Power evolution during TCRW for homogeneous fuel modelling (black) and heterogeneous fuel modelling (red) in comparison to other benchmark participants**

In Figure 4, the increase of power following a TCRW is shown. TORT-TD/ATTICA3D lies well within the other benchmark participants' results. The final power level which is reached after approximately 240 seconds is slightly higher for the homogeneous case and slightly lower for the HTM.



**Figure 5: Thermal neutron flux distribution a) at flux maximum, b) with spatially resolved control rod positions (outlined in red)**

Figure 5 displays the thermal neutron flux in the maximum position at  $z = 8.08$  metres, and at  $z = 9.75$  metres where rods are shown including the neutronics discretisation. Between the rods the flux increases (b).

## 4.2 Total control rod ejection

In exercise 5b of the PBMR-400 benchmark, all control rods are ejected within 0.1 sec from the reflector while all other input parameters remain unchanged. Here, the fast Doppler feedback of the HTM on the power distribution is investigated. The results of the participants display large differences in the power evolution.

As in the TCRW case, the proposed fuel temperature model was NOT used, but our own HTM was applied, see 4.1. Since the major source of heat is always due to fission in the kernels, homogenisation of fuel and moderator can lead to underestimation of the temperature development, especially for fast reactivity changes, and, as a consequence, can lead to an unrealistically high power evolution (up to a factor of 250-300).

By applying the HTM, the feedback is much stronger compared to a homogeneous temperature model, see Figure 6 and magnified in Figure 7. When looking at these figures, it can be seen that the proper modelling of the fuel kernel is a substantial issue and has to be treated with care. While a completely homogeneous approach might lead to a power increase in the range of a factor 300 for the homogeneous TORT-TD/ATTICA3D calculation, the heterogeneous approach has a strong feedback limiting the power values to a factor around 5.

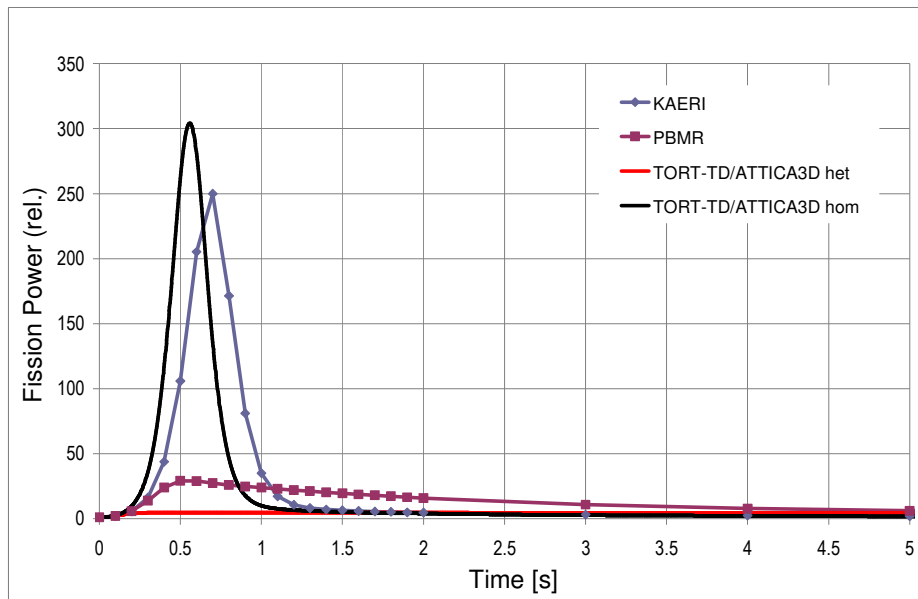


Figure 6: Comparison of relative fission power during TCRE

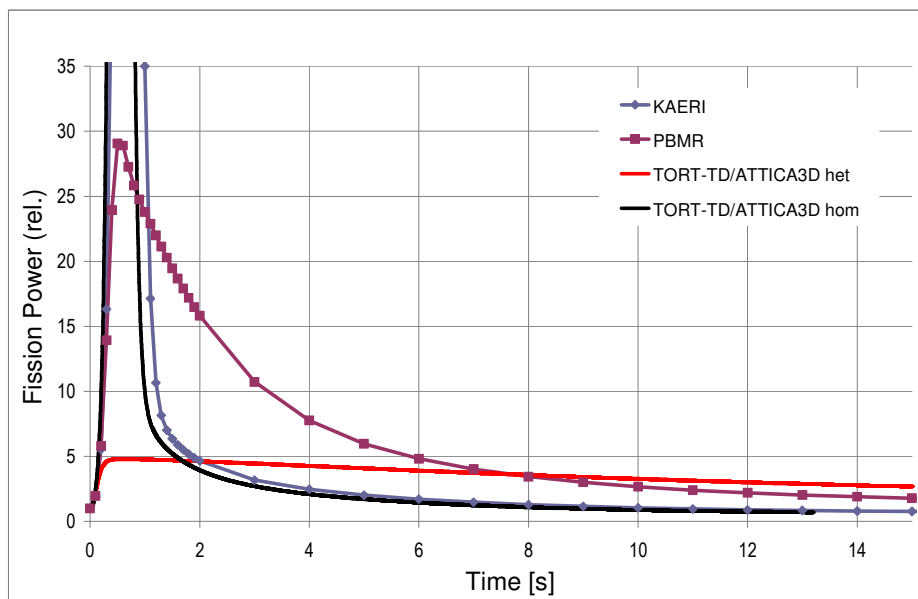


Figure 7: Comparison of relative fission power (magnified)

The striking differences in the power evolution are owed to the faster onset of temperature increase in the fuel, see Figure 8. In our HTM, the fuel temperatures remain lower than the other participants'. However, when taking a close look at the fuel temperature after 0.2 seconds it is obvious that there is a temperature difference of more than 100 K for the TORT-TD/ATTICA3D calculation compared to the nearest result (PBMR). This elevated temperature limits the power excursion earlier. One finding of the fast TCRE is, that with increased detail resolution of the HTM, the effects of feedback are much more pronounced.



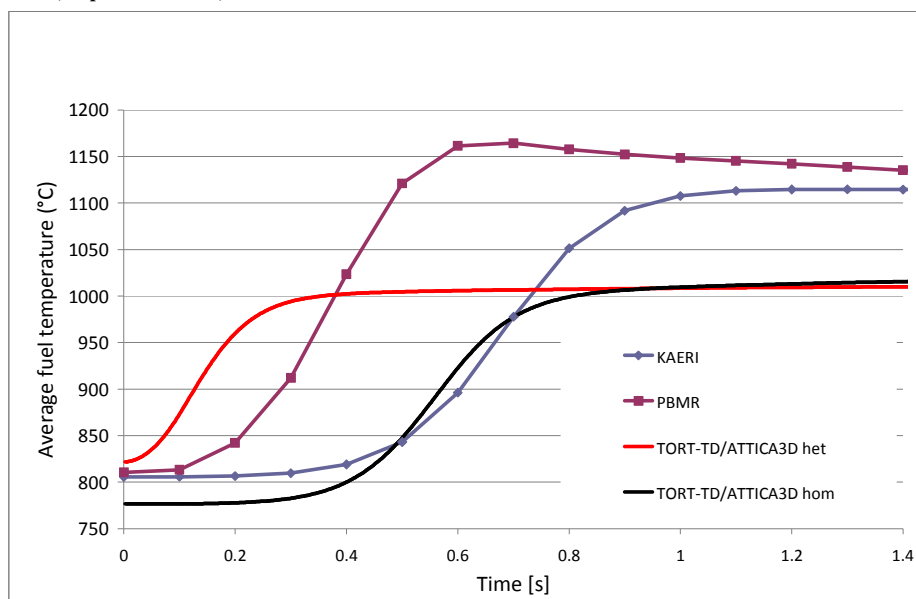


Figure 8: Fuel temperature increase in the total control rod ejection

## 5. Conclusion

The coupled code system TORT-TD/ATTICA3D was used to perform transient calculations for the PBMR-400 benchmark. Starting from the steady-state nominal conditions with xenon equilibrium, the transient exercises 5a, and 5b were calculated and compared to other participants' results. While the results showed good agreement for the TCRW case, the TCRE case needs to be checked thoroughly. For the two cases, results were produced in a 3-dimensional manner proving 3-dimensional capabilities. The HTM produces strong feedbacks on neutronics, as expected. Large deviations from other benchmark participants can be explained by different modelling, i.e. fuel is subdivided, but lumping fuel and moderator together will always introduce larger errors than would be expected by applying a time-dependent HTM.

The produced results are very promising and demonstrate that the coupled code system TORT-TD/ATTICA3D can be an important component of a future comprehensive 3-D code system for HTGR of pebble bed type.

Further improvements will be introduced to the coupled system TORT-TD/ATTICA3D. These comprise, e.g. a time-dependent HTM, and common time step search module for ATTICA3D and TORT-TD. This will considerably reduce computation times and enable calculation of e.g. long term transients like a pressurised loss of forced cooling with re-criticality.

## 6. Acknowledgements

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