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# Report on results of ATTICA- DORT/TORT calculations

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**Summary**

This document describes first results of calculations with the coupled code system TORT-TD/ATTICA3D for an assumed accident scenario with water ingress. The calculations have been carried out for a reference plant design oriented at the Chinese HTR-PM [1]. In order to be able to perform the neutron dynamics calculations, appropriate nuclear cross section data had to be prepared for the TORT-TD code that take into account the presence of water. This has been done by means of the code system ZIRKUS of IKE [1] in which the NEA spectral code MICROX2 is embedded [3]. Initial and boundary conditions for the accident scenario with water ingress have been defined taking into account previous published literature [4][5]. The consequences of the water ingress are mainly analysed with respect to two major effects: The initial fast power increase due to the addition of moderator and a long term heat-up phase with corrosion due to the decay heat of the reactor. The results of the TORT-TD/ATTICA3D calculations are presented. Concerning the initial power increase the results are compared with those of TINTE calculations available from literature. Here a good agreement was obtained. Concerning the long-term effect of corrosion over up to 80 hours, only a moderate attack of the fuel elements was found. The maximum burn-off of the fuel sphere graphite matrix material is only 2.7%.

Approval

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# 1 Introduction

The aim of this task is to establish a state-of-the-art analysis chain for the safety relevant analysis of water ingress events into a High Temperature Gas-cooled Reactor (HTGR). The computational analysis of water ingress to the reactor core of an HTGR has not been improved in the last decades because the prevailing HTGR designs did not use steam generators for power conversion. Recent developments, however, aim again at producing steam for generation of electricity or supply of process heat.

IKE is further developing the three-dimensional thermal hydraulic code ATTICA-3D (Advanced Thermal hydraulic Tool for In-vessel and Core Analyses), see [9]. ATTICA-3D is designed to model heat and mass transport in HTRs with pebble or block fuel elements. It allows the calculation of concentrations for an arbitrary number of gas components, taking into account convection and diffusion as well as sources/sinks from chemical reactions.

A basic model of carbon chemistry (reactions with oxygen and steam) was implemented in ATTICA3D. Also the interface to neutronics was enhanced to transfer an additional parameter, the hydrogen density in either steam or hydrogen. The coupling with the transient neutron transport code TORT-TD (developed by GRS); see [7] [8], was implemented in the framework of a nationally sponsored project (German Federal Ministry of Economics and Technology Förderkennzeichen/support code1501382), see [9].

Within this task the ATTICA-3D/TORT-TD code combination shall be used for calculation of water ingress scenarios with particular emphasis on:

- Reactivity effects (heterogeneous temperature model of the fuel element is implemented for spheres, work for block type fuel elements is ongoing)
- carbon chemistry
- estimation of the source term for combustion in the containment/reactor building (formation of combustible gases in the vessel)

In D22.23 there is detailed description of the models used in both ATTICA3D and TORT-TD. This deliverable is available to ARCHER partners on the online platform.

The present report describes first results of calculations with the coupled code system TORT-TD/ATTICA3D for an assumed accident scenario with water ingress carried out for a reference plant design oriented at the Chinese HTR-PM [1]. The preparation of nuclear cross section data that take into account the presence of water by means of the code system ZIRKUS is described in Chapter 2. Initial and boundary conditions for the accident scenario with water ingress are given in Chapter 3. Chapter 4 presents results of the TORT-TD/ATTICA3D calculations. The consequences of the water ingress are analysed with respect to the initial fast power increase due to the addition of moderator and a long term heat-up phase with corrosion due to the decay heat of the reactor.

# 2 Generation of cross sections for water ingress

To be able to simulate a water ingress both neutronically and thermal hydraulically, it is necessary to have the appropriate cross sections (XS) available. Otherwise no feedback can come from the introduction of additional moderator. To generate these XS for the reference system selected: the Chinese HTR-PM [1], the 2-d steady-state and long-term transient HTR simulation system ZIRKUS [2] is used. With ZIRKUS, we have the possibility to produce XS for the equilibrium core, with respect to a number of variation parameters. Due to the lack of possibility to simulate transients that demand real modelling of reactor kinetics (including of neutron precursor equations), the XS generated with ZIRKUS are afterwards extracted from the output files and transferred in a format that our transient time-dependent neutron code TORT-TD can work with, i.e. the NEMTAB format.

For XS generation with ZIRKUS, a geometry is used that comprises 399 material zones, 144 burn up zones for the core region, and 24 spectral zones (zones with different temperatures). Note that the core region (from zone 1 to 144) is sub-divided in eight so called flow channels. This is necessary to account for the constant reload and discharge of pebble fuel elements during operation and also to account for the fact that like in an hour glass, the pebbles in the most inner channel have a shorter residence time in the core compared to the pebbles in the most outer channel. The difference in residence time of a pebble can be found in the differing number of zones in each channel. While the innermost channel has 16 axial subdivisions, the most outer channel has 24 axial subdivisions. When one fuel reload step is executed, the number densities of the upper zone, e.g. zone 1 is passed to zone 2 at the end of a burn-up step. The same applies to all other zones. One can now see that after 16 reload steps the innermost fuel pebbles will be discharged or recycled, while the pebbles in the outermost channel still have to undergo 8 more reload steps until reaching the discharge tube. This is how ZIRKUS accounts for the different flow velocities of each channel. The fact, that the outermost channel takes about 1.5 times longer than the innermost channel was determined by experiments.

13 neutron groups are used for the computation and the generation of XS, and it is this elevated number of neutron groups that allows for omitting the buckling dependency for neutronics which otherwise, with a smaller number of groups, should have been taken into account.

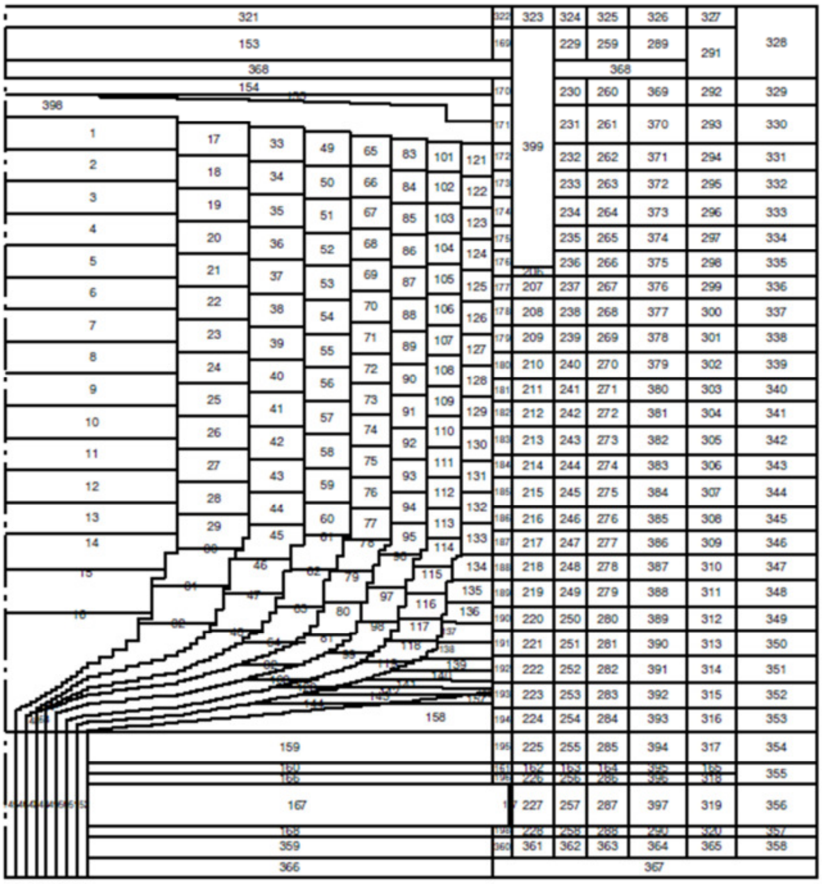


Figure 1 : Geometry of the HTR-PM in the ZIRKUS HTR simulation system

For a TORT-TD calculation, the spatial meshes are condensed with respect to a simplified geometry for a transient calculation. This reduces computational time. For the TORT-TD geometry only 232 material zones are used. However the number of burn-up zones and also, since burn-up and spectral zones are roughly the the same, are increased to 154. Note, that in the TORT-TD geometry the flow channels introduced above are dissolved. The reason for this lies within the fact, that for a transient incident or accident, the recycling of the fuel is assumed to be turned off. This goes hand in hand with the safety regulations that would prohibit business-as-usual operation during an incident or accident.
For the transient calculation the initial number of 13 neutron groups will be condensed to only 7 neutron groups using a condensation routine within the ZIRKUS code. The condensed XS were also tested in the condensed ZIRKUS geometry for consistency. For the control rod zone (zone 399 in ZIRKUS, zone 192 in TORT-TD) the XS were manipulated manually in order to have spatially resolved control rods instead of the 2-d grey curtain assumption made in ZIRKUS. Here, a MCNP [6] calculation for the control rod was done, and the $\sigma_a$ and $\sigma_{tot}$ had to be modified such that MCNP and TORT-TD had the same increase in reactivity for the equilibrium and totally withdrawn position of the control rods (about 0.4% reactivity increase per spatially resolved control rod, 1.2 % reactivity increase when the whole control rod bank is fully withdrawn).


Figure 2 : TORT-TD geometry for the HTR-PM

The variation parameters that are used for the XS generation are:

- Fuel temperature
- Moderator temperature
- Xenon density
- Hydrogen content

The range of parameters that are possible are presented in Table 1. Some constellations within these variations are physically irrelevant, e.g. moderator temperatures lower than the fuel temperatures, but they are nevertheless provided since it would demand modifications of the XS generation with ZIRKUS treatment of the latter.

Table 1 : Range of XS with supporting points

| Variation parameter | Unit | Number of supporting points | Supporting points |
|---|---|---|---|
| Fuel temperature | K | 10 | 300, 500, 700, 900, 1100, 1300, 1500, 1700, 1900, 2100 |
| Moderator temperature | K | 7 | 300, 600, 900, 1200, 1500, 1800, 2100 |
| Buckling | - | 0 | - |
| Xenon density | $(barn^* cm)^{-1}$ | 3 | 0.0, 2.0E-11, 8.0E-10 |
| Water content | kg | 3 | 0, 200, 800 |

What might seem strange is the "water content" in kg ranging from 0 to 800 kg; since in the text above, the variation parameter is introduced as the hydrogen density. The reason for this is that ZIRKUS adds a certain $H_2O$-density homogeneously to each of the core zones. Corrosion processes are not implemented, so the steam will not react with the hot graphite to produce hydrogen and either CO or $CO_2$.
In ATTICA3D however these corrosive processes are implemented. Since there would be two moderating media, namely hydrogen and steam, this would also demand for a further variation parameter. To circumvent this fact, only the hydrogen density is transferred from ATTICA3D to TORT-TD. The fraction of hydrogen contained in steam, i.e. about 2/18, the relative atomic weight of hydrogen in $H_2O$, is calculated for each core zone and added to the hydrogen content of the respective zone. Proceeding like that one obtains the increase of moderation, with a little detour over the hydrogen density, but for the benefit of saving of an additional variation parameter that would further increase computational time. In the water ingress scenario and results chapter, the reader will find that the power increase and the following increase in fuel and moderator temperature will feed-back neutronically and will shut the reactor down before the onset of a significant hydrogen production. This justifies the use of the ZIRKUS method to account for steam content within the core.
With the average temperature distribution from ZIRKUS which is coupled to the 2-d thermal hydraulic code THERMIX/KONVEK, see [2][1], the spectral groups are a weighted. The detailed comparison of the codes THERMIX and ATTICA3D applied for HTR-PM problem geometry can be found in [11].
For demonstration purposes the solid temperature at two different radial positions (deviations of radii due to application of different discretisation methods) is depicted in Figure 3.

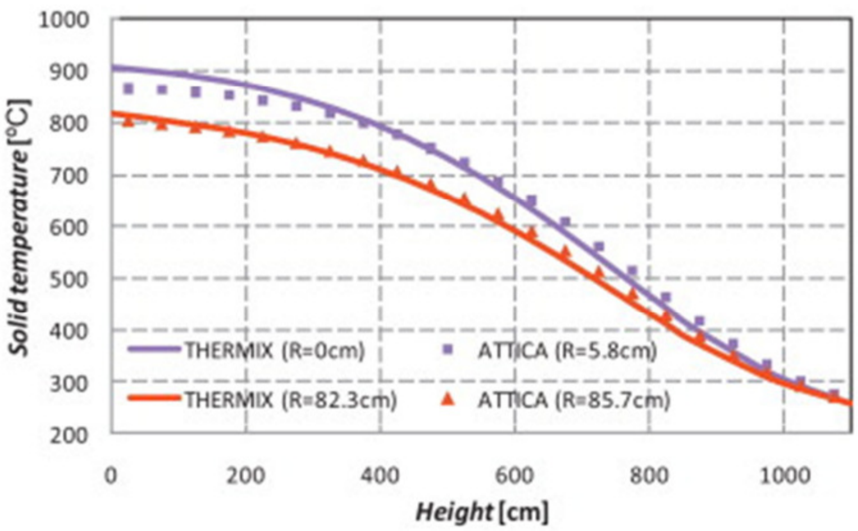



Figure 3 : Axial solid temperature distribution comparison for the HTR-PM at different radial positions, from [11]

The increase of reactivity for the HTR-PM in nominal operational conditions with 0, 200 and 800 kg in the core is displayed in

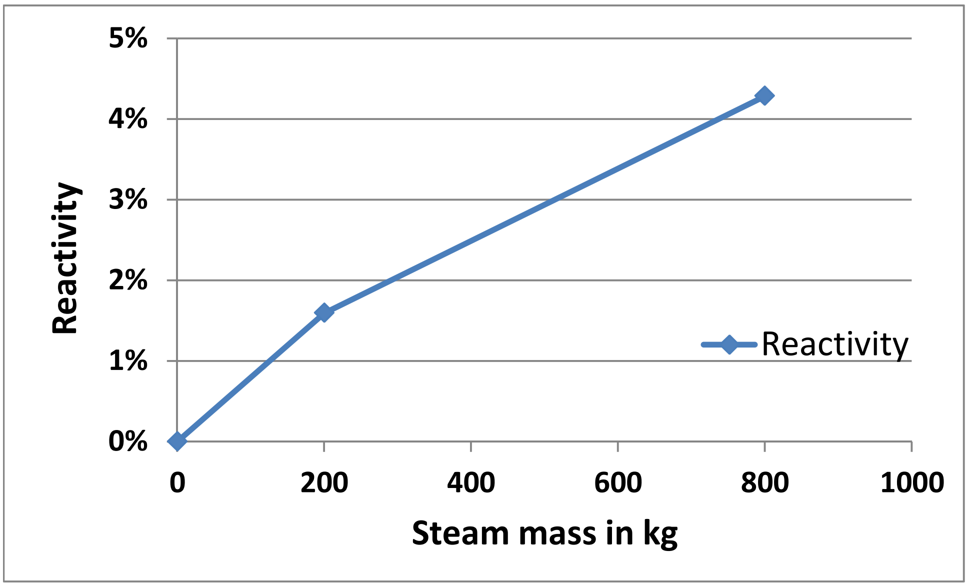



Figure 4 : Reactivity increase with steam content in the core

# 3 Accident scenarios for the water ingress

For the reference plant – the HTR-PM - the scenario to be calculated is a common 2F break of a single steam generator tube. Since ATTICA3D does only simulate processes inside the reactor pressure vessel, important parameters and boundary conditions of the accident for the beginning have to be taken from other analysis in literature. Here references [4] and [10] prove to be helpful. In these publications the water ingress is also analysed and source terms for water are determined with the help of whole primary circuit (and also secondary circuit) simulations. The design basis accident will be taken as starting point. This scenario considers a double-end break of one steam generator tube that is detected and, subsequently, the steam generator will be isolated with the two steam generator isolation valves and drained with the steam generator emergency draining system allowing approximately 600 kg to enter the primary circuit, see [4].

## 3.1 Design basis accident

As design basis accident (DBA) a 2 F break of one of the steam generator tubes is assumed. Since the pressure on the secondary side is much higher (139 bar) than the pressure in the primary circuit (70 bar), water/steam will pour into the primary circuit. As a consequence, the total pressure will immediately rise in the primary circuit. Analysis of Zheng et al in [4] determined the pressure rise to be 4 bar due to ingress of steam and water. Corrosion of graphite in a steam atmosphere will produce corrosion products like CO, $CO_2$ and $H_2$. These additional gas components will gradually lead to a further increase in pressure, but in the range of several hours. After the set point of the pressure relief valve is reached (79 bar), the valve will open reducing the primary pressure slightly below the operational pressure.

### 3.1.1 Assumptions and sequence of events for the DBA

The sequence of events is taken from the water ingress analysis described in [4]. Some additional assumptions had to be made, e.g. the amount of steam that reaches the core.

0 seconds :

- Reactor runs at 105 % of the operational power level (262.5 MWth), also on 105 % of the helium mass flow (100.5 kg/s)
- Steam generator tube ruptures
- Steam/water pours into the primary circuit

10 seconds:

- Humidity sensors detect excess humidity
    - Actuation of blower shutdown
    - Blower runs out with decreasing power
    - Isolation of the steam generator via the steam generator isolation valves
    - Steam generator emergency draining system will dump the water left in steam generator
- Control rods insertion starts (takes 50 seconds)

after 40 seconds:

- Blower flaps close to completely stop the mass flow through the steam generator
- Onset of loss of forced cooling accident including corrosion of the graphite structure in presence of steam

The pressure in the primary circuit is taken from the TINTE analysis by Zheng et al in [4] and is depicted in Figure 5

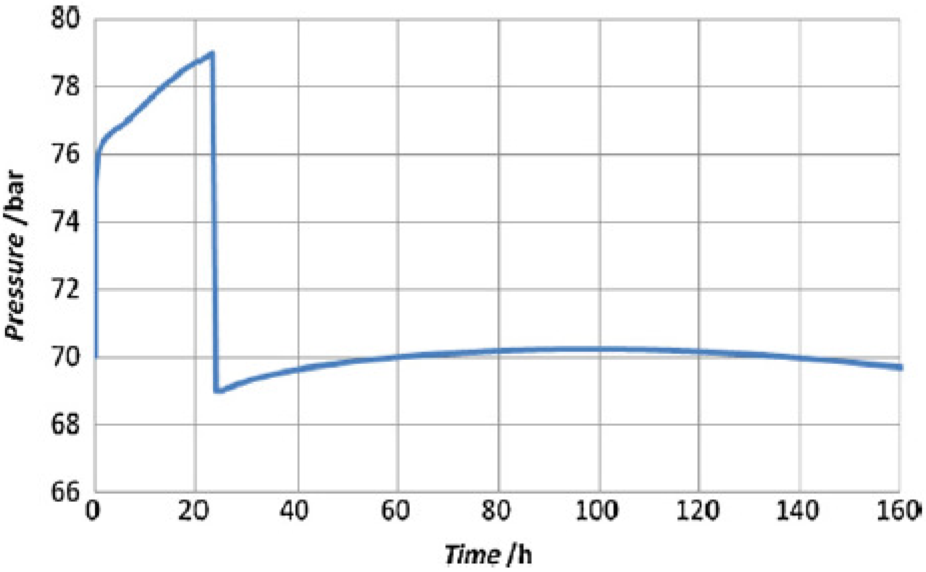



Figure 5 : Primary pressure during the design basis accident and the anticipated transient without scram (ATWS), from Zheng et. al [4]

Additional assumptions:

- The steam needs about 3 seconds from the steam generator to the reactor pressure vessel, so the steam flow in ATTICA3D will be started after 3 seconds of the transient.
- The steam mass flow increases parabolically from 0 to 5.44 kg/s within 7 seconds, and decreases linearly after the blower stops (like the helium mass flow), see Figure 6.

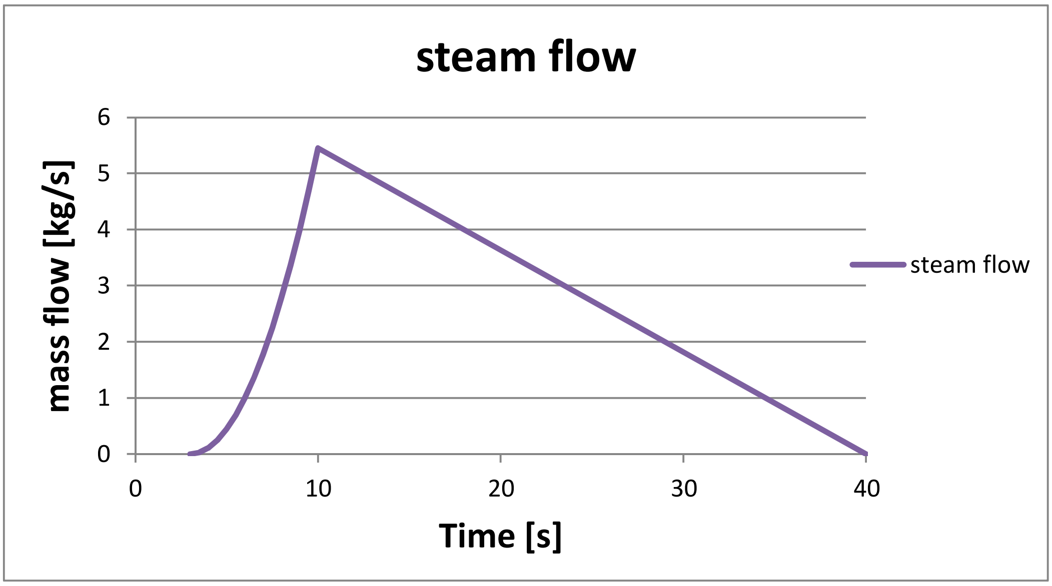



Figure 6 : Steam flow rate over time for the design basis accident

- The relative steam concentration at the outlet is increased to 0.0545 within 10 seconds. This steam concentration will be « sucked in » from the outside and is assumed to decrease linearly over 500,000 seconds in order to account for reduction of steam partial pressure. (This assumption will only hold as long as there is no total steam consumption balance implemented in ATTICA3D, i.e. the amount of steam that is available for chemical reaction will decrease with increasing time. If the 600 kg that entered the primary circuit due to a break of a single steam generator tube is consumed the steam partial pressure on the in- and outlet should be reduced to zero.)

Conditions at t = 0 seconds, i.e. initial conditions for the water ingress are presented in Figure 7

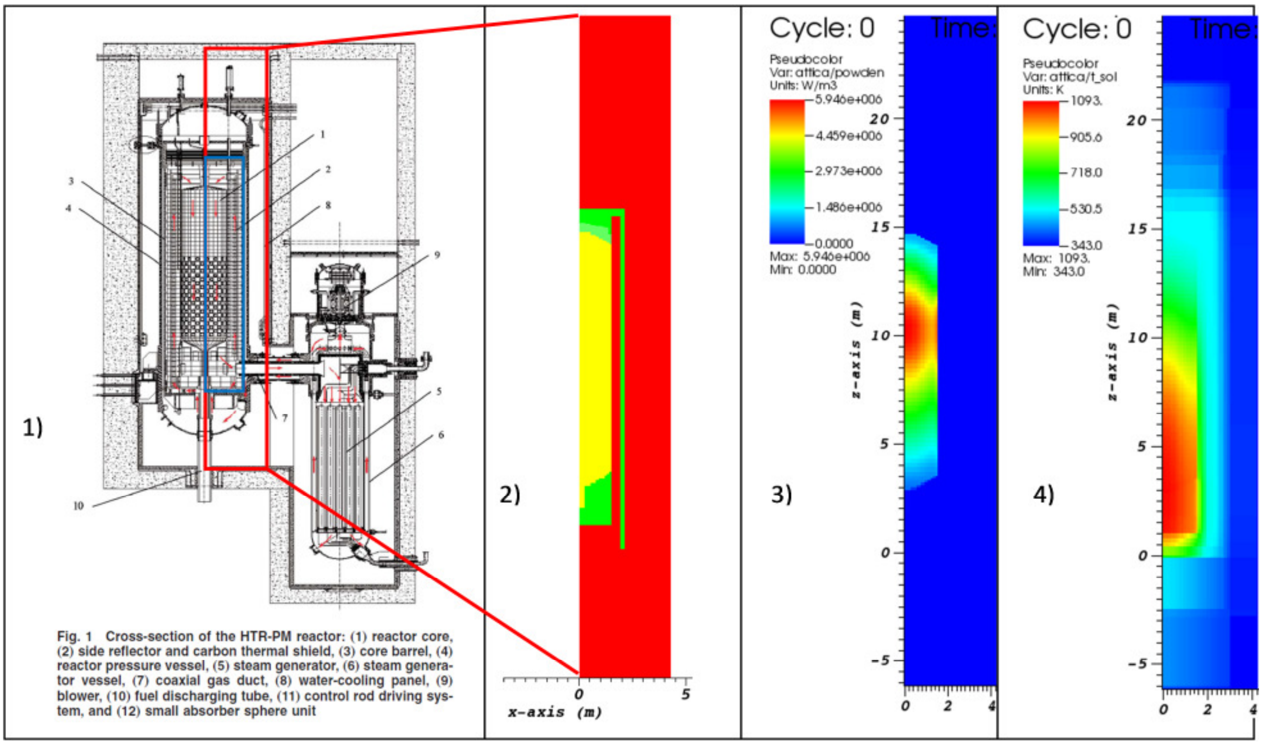



Figure 7 : 1) Geometry of the HTR-PM with the computational domains of TORT-TD in blue and ATTICA3D in red frame, 2) flow path of helium with core (yellow), 3) power distribution 4) solid temperature distribution

# 4 Results for the water ingress (design basis accident)

The consequences of the water ingress are two-fold. There is a quick power increase in the range of seconds due to the addition of moderator and a long term heat-up phase with corrosion due to the decay heat of the reactor.

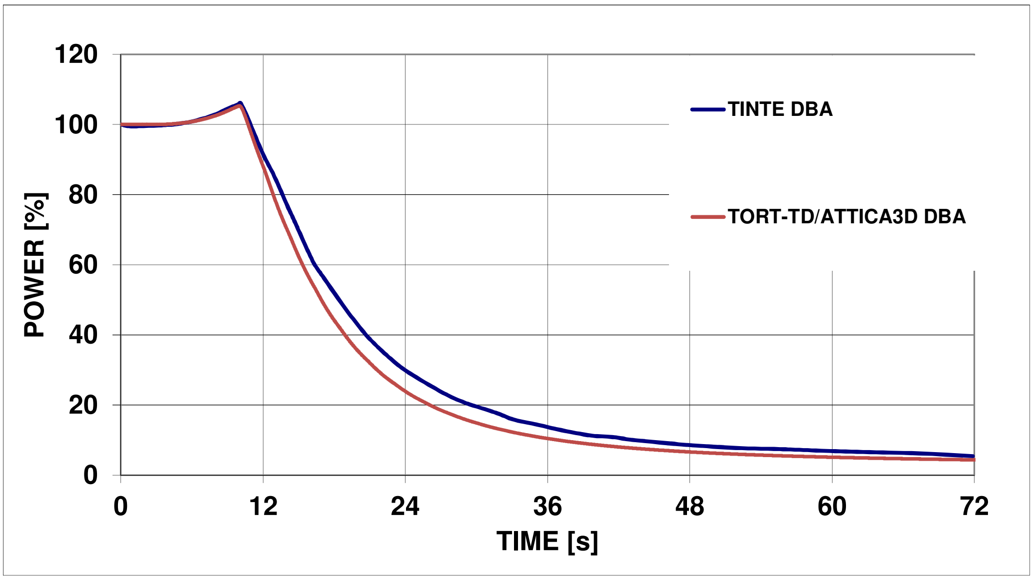



Figure 8 : Power increase after steam reaches the core, TINTE result taken from [4]

After the steam is detected by the humidity sensors, the blower is turned off and the rods are inserted over 55 seconds ending the power increase for the design basis accident. The decay heat distribution of 105% of nominal conditions is taken from the ZIRKUS analysis. The short power increase in the range of seconds will not change decay heat distribution significantly, and therefore will be taken as decay heat source for the long-term corrosion effects.
The long-time behaviour is characterised best by a pressurised loss of forced cooling case. In the beginning of the transient, the steam enters. However with the temperature distribution of nominal operation, even though at a higher level, the upper part of the reactor where the cold gas (250℃) enters is far below temperatures where corrosion takes place. Only at the outlet, where the solid temperatures reach (780℃) there is a slight corrosion attack. But the major part of corrosion due to steam in the core will take place in the course of hours. The reason is that the core first needs to heat up with the decay heat, so that temperatures with significant corrosion rates are reached.
As mentioned above, the flow pattern in the water ingress design basis accident resembles the pressurised loss of forced cooling accident. After the blower stops, the bottom core and reflector are the hottest parts. The gas still under pressure heats up in the bottom and flows up in the central core. When the gas reaches cold top reflector (250℃ in the beginning of the transient), it transfers its heat to the top reflector. The cooler gas flows downwards next to the side reflector in the outer part of the core.

In Figure 9 the flow patterns in steady state conditions and also after 11,800 seconds are shown. Here, the above described effect is visible.

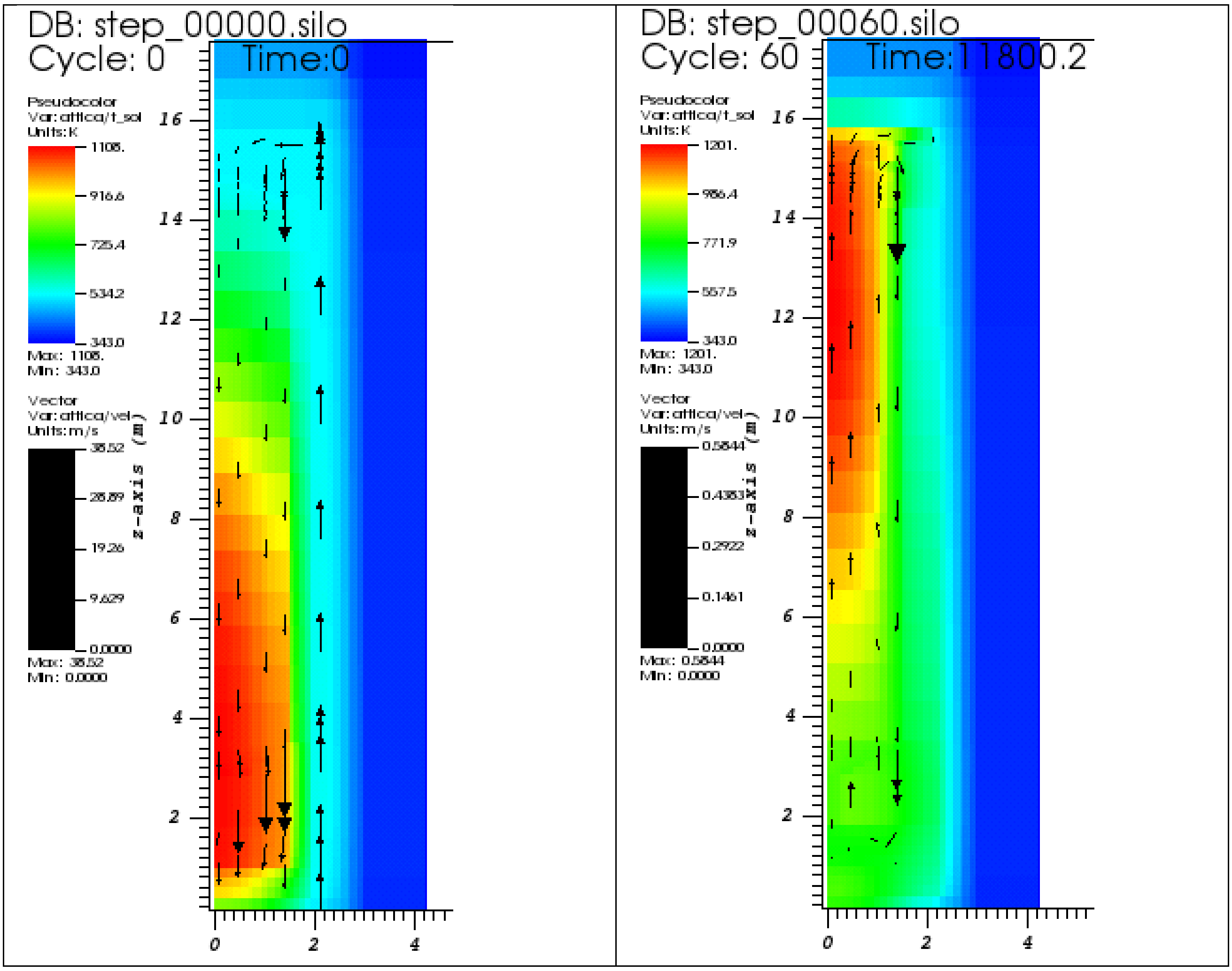
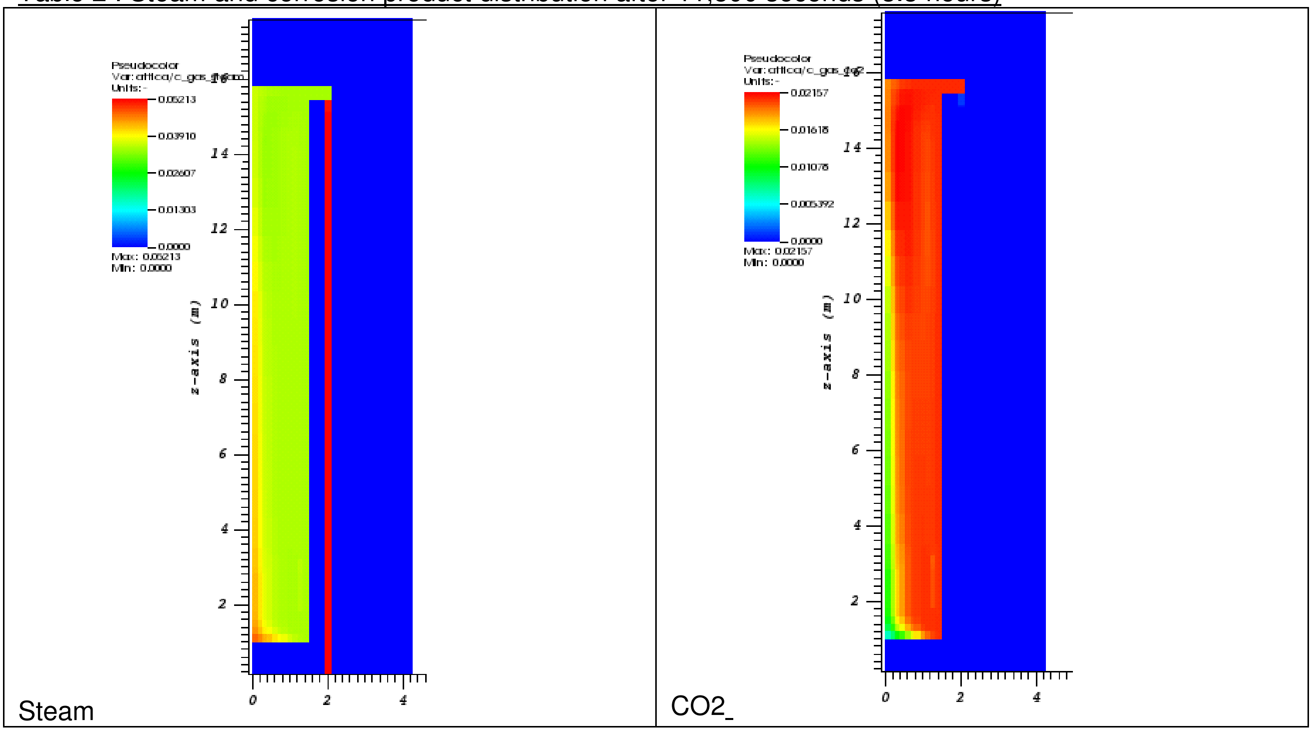
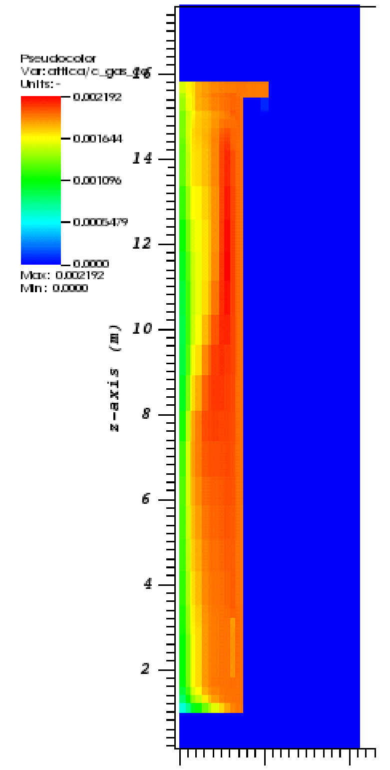


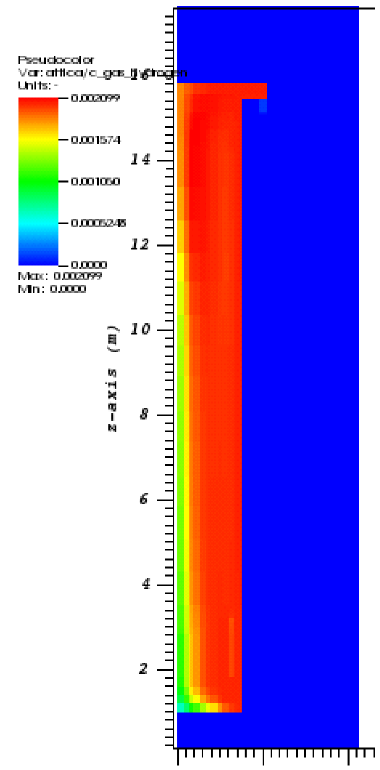

Figure 9 : Temperature distribution and velocities at t = 0seconds (left) and after 11,800 seconds (right)

Table 2 : Steam and corrosion product distribution after 11,800 seconds (3.3 hours)





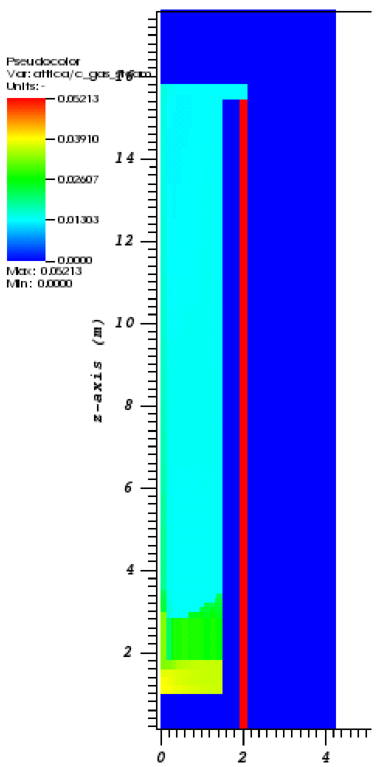

CO



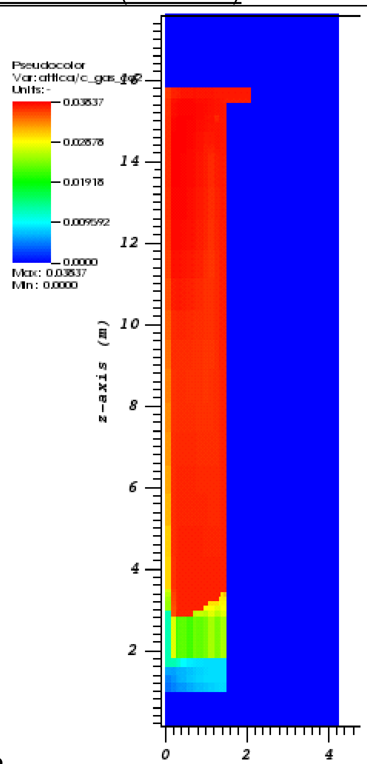

Hydrogen

In Table 2 above, the distribution of corrosion gases is presented. Here, it is to be noted, that the $CO_2$ is about five times as high as the corresponding CO concentration.

Table 3 : Steam and corrosion gas distribution after 108,000 seconds (30 hours)




Steam




CO2

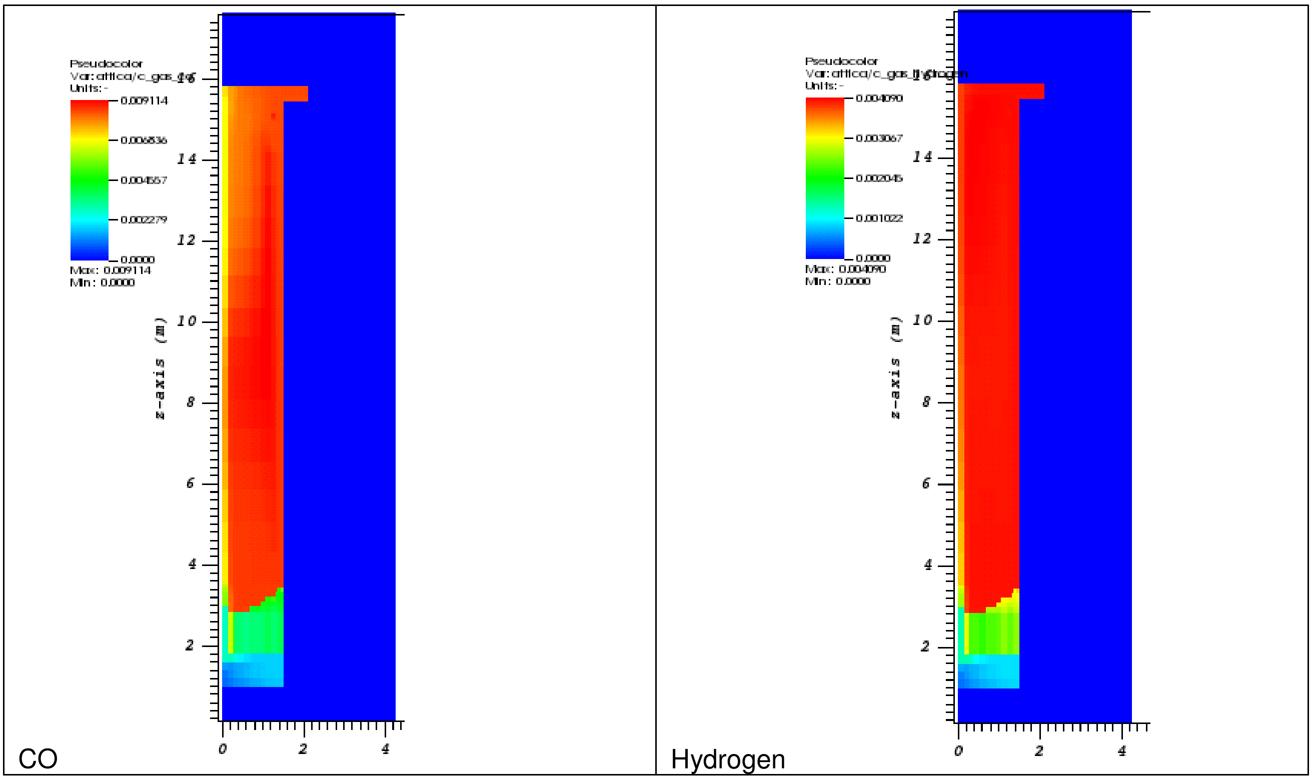
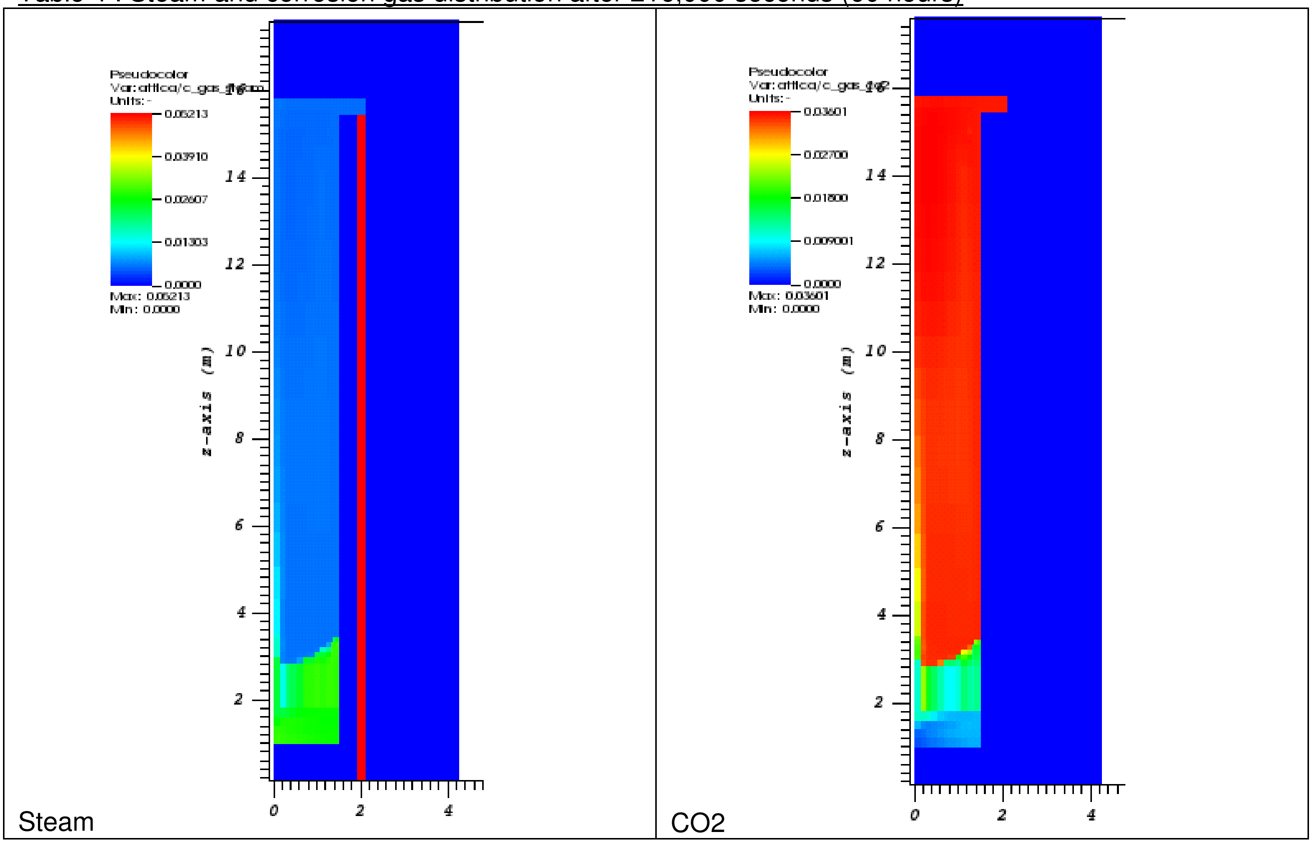



Table 4 : Steam and corrosion gas distribution after 216,000 seconds (60 hours)



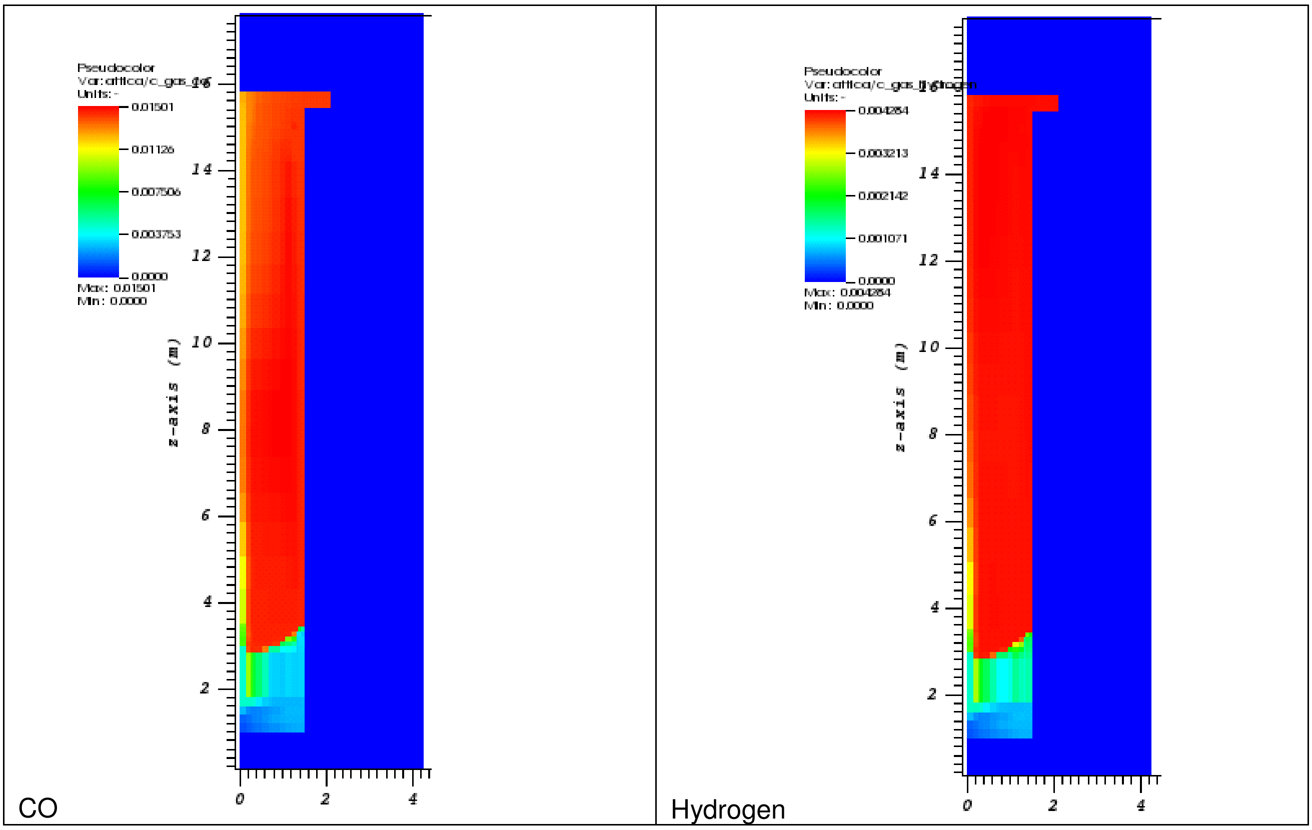
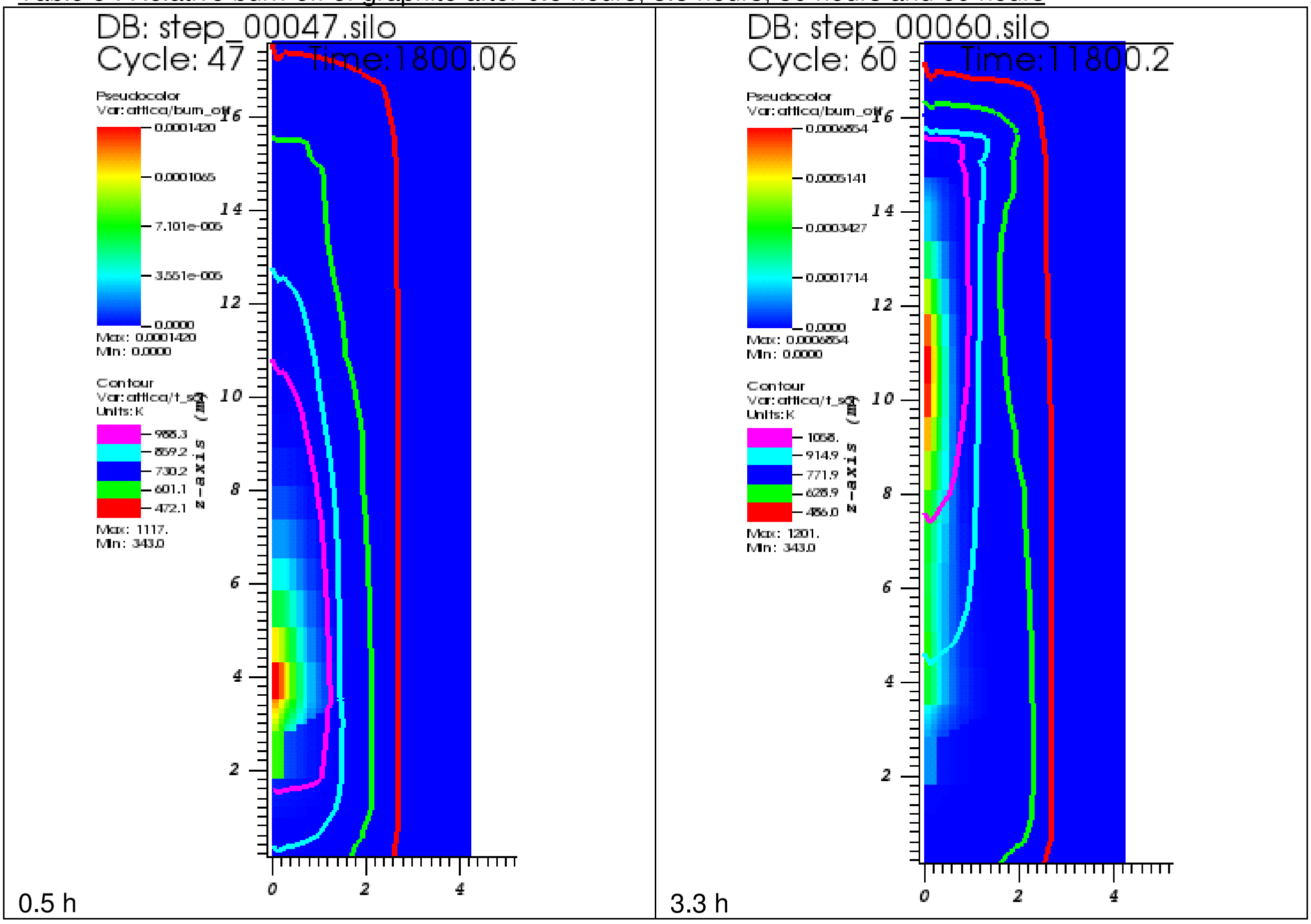
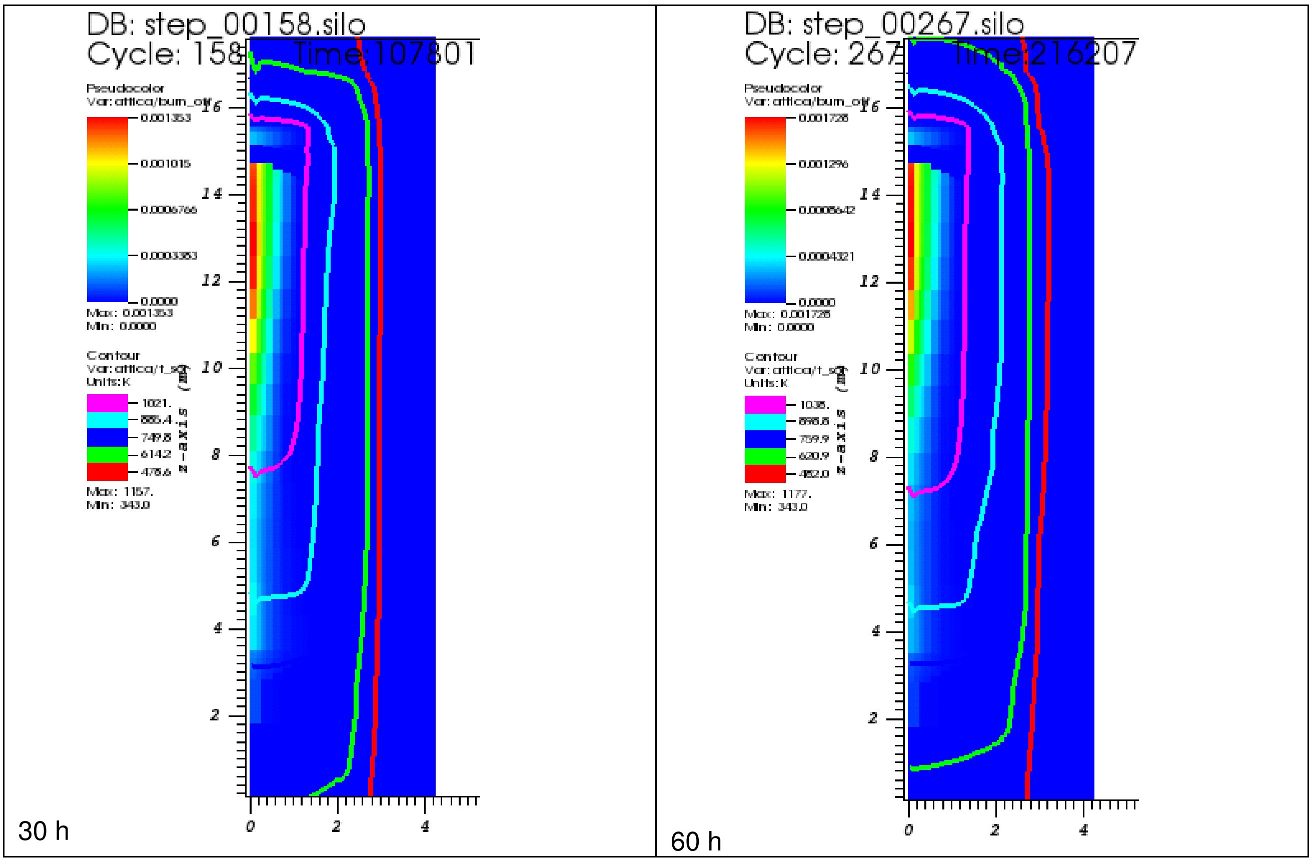



Table 5 : Relative burn-off of graphite after 0.5 hours, 3.3 hours, 30 hours and 60 hours






At the outlet, there is a concentration of steam present that corresponds to the 4 bar partial pressure out of 74 bar total pressure in the start of the transient. This steam concentration reduces linearly to 0 over 500,000 seconds. When first SPECTRA results are available, more realistic boundary conditions will be applied.
The steam flow is corresponding to the gas flow of the helium. Since the core heats up and the temperature maximum shifts from bottom to top, the first centre of corrosion can be found in the lower part. With the re-distribution of the solid temperature and the cooling down of the lower part the steam can now enter the core region and corrode fuel elements. The centre of corrosion slowly shifts upwards like the temperature maximum.
This can be seen in Figure 10 and Figure 11.

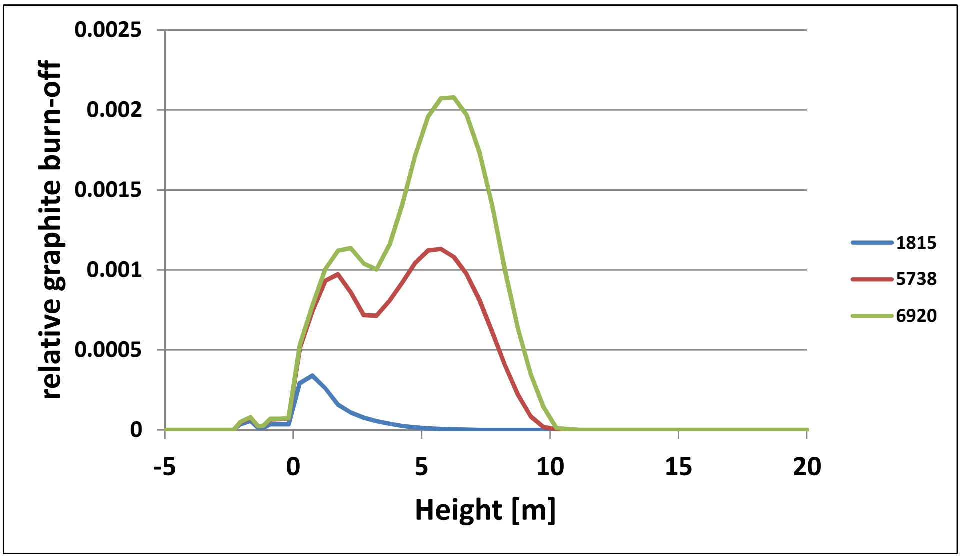



Figure 10 : Relative graphite burn-off after 1,815 seconds, 5738 seconds and 6,920 seconds in the core zone next to the centre line (at radius = 0.058 m)

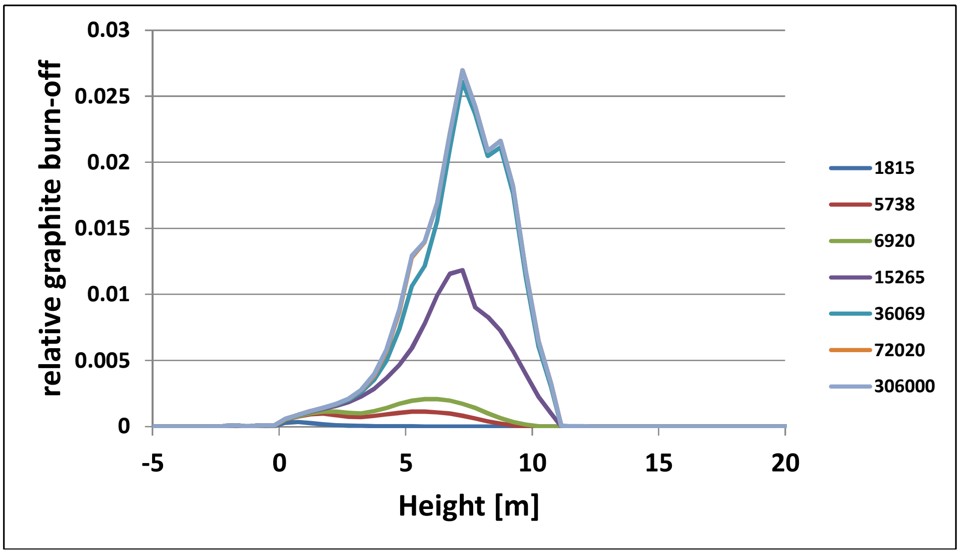



Figure 11 : Relative graphite burn-off after 1,815 seconds, 5738 seconds, 6,920 seconds, 15,265 seconds, 36,069 seconds, 72,020 seconds and 306,000 seconds in the core zone next to the centre line (at radius = 0.058 m)

## 4.1 Discussion of results

The relative graphite burn-off is a quantity that is normalised on the initial amount of graphite. When after 306,000 seconds the burn-off is 0.027, it means that only 2.7% of the graphite is corroded. Although the outer matrix graphite shell without fuel already comprises 42% of the fuel sphere volume this is not the percentage of graphite that can be lost without reaching the first particles. In a pebble bed, the gas can only flow in the porous region. The fuel pebbles are always subjected to anisotropic corrosion since the part that is perpendicular facing a flow channel will be stronger corroded than if the flow is parallel to the pebble surface. This fact can be accounted for by using a shape factor. In [4], it is stated that using a shape factor of 6 the admissible loss of graphite from the outer shell is 7%.
The results of ATTICA3D show a maximum corrosion within the core region of 2.7%. It is therefore far away from the fuel region and now coated particle will be attacked by the steam atmosphere.

The HTR-PM is designed with two helium purification systems to remove chemicals such as $H_2O$, $O_2$, CO, $CO_2$, $N_2$, $H_2$, $CH_4$ etc within the coolant; one in operation, the other one serves as back-up if the first purification system fails.
For mitigation measures of the case of water ingress in the HTR-PM there is a specially designed stand-by accident helium purification system line connected to both systems, to remove chemical impurities. This purification system has special water seperators and has a throughput of 100% of the primary circuit inventory per hour. This would further decrease the steam and hydrogen content in the reactor for long-term corrosion effects. But it is not included in the safety related systems of the HTR-PM and is assumed **not** to work to give a conservative estimate.
Therefore, the corrosion attack of the core will be less if the helium purification system with the water separators operates as designed.

# 5 Summary and outlook

In the first chapter an introduction to XS generation and the procedural steps to obtain these are described. After description of the considered cases, the scenario to be calculated was described. The earlier generated XS were then also tested and compared to results of a water ingress calculation with TINTE done by Zheng et al [4]. Here a good agreement with the TINTE results from the paper could be obtained. After presentation of the short-term results a long-term analysis including corrosion was presented. As a finding it could be shown that corrosion over up to 80 hours will lead to a moderate attack of the fuel elements. The maximum burn-off of graphite is only 2.7%. But it is only after 7% of burn-off that the first coated particles will be subject to corrosion (attack by carbon monoxide).
For further analysis, an anticipated transient without scram will be presented. Also a beyond design basis accident can be subject of further analysis

# 6 References

[1] Zh. Zuoyi,W. Zongxin, W. Dazhong, X. Yuanhui, S. Yuliang, L. Fu , D. Yujie, Current status and technical description of Chinese 2×250MWth HTR-PM demonstration plant, Nuclear Engineering and Design 239 (2009) 1212–1219.

[2] W. Bernnat, W. Feltes, Models for reactor physics calculations for HTR pebble bed modular reactors, Nuclear Engineering and Design 222 (2003) 331–347

[3] D. Mathews, An Improved Version of the Microx-2 Code, Paul Scherer Institut, PSI Bericht Nr. 97-11, (November 1997).

[4] Y. Zheng, L. Shi, Y. Wang: Water-ingress analysis for the 200 MWe pebble-bed modular high temperature gas-cooled reactor, Nuclear Engineering and Design 240 (2010), pp. 3095-3107

[5] Zh. Zuoyi,W. Zongxin, W. Dazhong, X. Yuanhui, S. Yuliang, L. Fu , D. Yujie, Current status and technical description of Chinese 2×250MWth HTR-PM demonstration plant, Nuclear Engineering and Design 239 (2009) 1212–1219.

[6] X-5 Monte Carlo Team, MCNP – A General Monte Carlo N-Particle Transport Code, Version 5, Los Alamos National Laboratory, LA-UR-03-1987, revised 10/3/05.

[7] W. A. Rhoades, D. B. Simpson, The TORT Three dimensional Discrete Ordinates Neutron/Photon Transport Code (TORT Version 3), (1991), ORNL/TM-13221.

[8] A. Seubert, K. Velkov and S. Langenbuch, The Time-Dependent 3-D Discrete Ordinates Code TORT-TD with Thermal-Hydraulic Feedback by ATHLET Models, Physor 2008, Interlaken, Switzerland, September 14-19, (2008).

[9] A. Seubert, A. Sureda, J. Bader, J. Lapins, M. Buck, E. Laurien, The 3-D time-dependent transport code TORT-TD and its coupling with the 3D thermal-hydraulic code ATTICA3D for HTGR applications, Nucl. Eng. and Design (2011), in press.

[10] D. Yujie ,Zh. Zuoyi, W. Scherer: Assessments of Water Ingress Accidents in a Modular High Temperature Gas-Cooled Reactor, Nuclear Technology 149, (2005), pp. 253-264

[11] Y. Zheng, J. Lapins, E. Laurien, L. Shi, Z. Zhang: Thermal hydraulic analysis of a pebble-bed modular high temperature gas-cooled reactor with ATTICA3D and THERMIX codes, Nuclear Engineering and Design 246 (2012), pp. 286-297.

# 7 Annexes

Annex 1 – Document approval by beneficiaries' internal QA

Annex 2 – Title 2

## 7.1 Annex 1: Document approval by beneficiaries' internal QA

Fill involved beneficiaries as appropriate (mandatory for Milestones and Deliverables, but optional for other document type)

| # | Name of beneficiary | Approved by | Function | Date |
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