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# Hydrogen Analyses in the EPR

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## ABSTRACT

In severe accidents with core melting large amounts of hydrogen may be released into the containment. The EPR provides a combustible gas control system to prevent hydrogen combustion modes with the potential to challenge the containment integrity due to excessive pressure and temperature loads. This paper outlines the approach for the verification of the effectiveness and efficiency of this system.

Specifically, the justification is a multi-step approach. It involves the deployment of integral codes, lumped parameter containment codes and CFD codes and the use of the sigma criterion, which provides the link to the broad experimental data base for flame acceleration (FA) and deflagration to detonation transition (DDT). The procedure is illustrated with an example.

The performed analyses show that hydrogen combustion at any time does not lead to pressure or temperature loads that threaten the containment integrity of the EPR.

## 1 INTRODUCTION

In a severe accident with core melting large amounts of hydrogen may be produced due to the oxidation of zirconium, most of it from the fuel claddings, by steam at high temperatures and later on from the molten core concrete interaction (MCCI). The hydrogen is released into the containment and can form combustible gas mixtures. For large amounts or high local concentrations of hydrogen an ignition could lead to combustion modes potentially threatening the containment integrity by excessive pressure or temperature loads. Three fundamentally different types of containment loads could originate from a combustion.

1. A slow hydrogen combustion produces a slow pressure increase with no dynamic effects, however the absolute value could exceed the maximum pressure for which the containment was designed. The pressure increase by a combustion is enveloped by the so-called adiabatic isochoric complete combustion pressure $p_{AICC}$. This is a theoretical and conservative value which would result if the energy equivalent to the complete burning of all hydrogen present in the containment would be released into the containment atmosphere without any heat transfer to structures or walls. It depends only on the available masses of hydrogen and oxygen. If the value of $p_{AICC}$ is below the design pressure of the containment then any slow combustion cannot threaten the containment due to pressure loads.
2. A fast deflagration with flame velocities of several hundred meters per second and even worse a detonation, where the flame velocity reaches sound velocity, would produce strong pressure or shock waves. These waves are a highly dynamic pressure load, where the local pressure peaks on the containment structure or across inner walls can possibly exceed the $p_{AICC}$. Fortunately a direct initiation of detonation in the containment is not possible, because too much energy would be necessary. So, the only possibility is that the slow combustion, which follows an ignition, is accelerated, until the flame velocity is sufficient for generating large dynamic pressure loads. This process is promoted by high hydrogen concentrations, turbulence generating obstacles and a confinement of the flame. These phenomena and processes are described exhaustively in [1]. In case of flame acceleration (FA) it is important that also the dynamic loads are tolerable by the contain-

ment and the frequencies of dynamic pressure load are not near the Eigen frequency of the reactor building to exclude damages induced by resonance phenomena.

3. Finally, a long-lasting, localized slow burning is conceivable, e.g. by the burning of the hydrogen generated by MCCI in the reactor pit after the failure of the reactor pressure vessel. This would mean that for a long time hot gases could be transported to a relatively small area of the containment shell provided appropriate flow conditions. This part of the containment shell could be overheated, although the average containment surface temperature is still uncritical. Local analyses of the containment surface temperature for long lasting burnings have to be performed to exclude that possible threat.

The European Pressurized Water Reactor (EPR) is equipped with a combustible gas control system (CGCS) to prevent such excessive loads. It consists of components enabling a global mixing of the containment atmosphere, and passive autocatalytic recombiners (PARs). The mixing quickly reduces high concentration gradients by the enabling of global convection loops in the containment. The PARs remove hydrogen from the atmosphere by catalytic, flameless oxidation and reduce the hydrogen concentration in the long term below the flammability limit. This paper describes the approach for the verification of the capability of the CGCS to prevent the above mentioned threats to the containment.

## 2 PROCESS FOR JUSTIFICATION OF THE CGCS

### 2.1 General Remarks

#### 2.1.1 Best Estimate Assumptions and Hydrogen Release

The justification of the effectiveness and efficiency of the CGCS is based on a careful selection of accident scenarios which are analysed. For safety analyses often so-called conservative assumptions are used to envelope uncertainties in the sequence of the accident events or in the involved physical processes. However, totally unphysical assumptions should be avoided, especially for severe accident analysis where as far as possible best-estimate analyses are performed.

An example related to hydrogen risk is the release process of hydrogen from the in-vessel oxidation of zirconium. If nothing is known about the process, it is conservative to assume the oxidation of 100 % of Zr and an instantaneous release of the complete generated hydrogen. But with up-to-date knowledge it is clearly totally unphysical to assume an instantaneous hydrogen release. The hydrogen is mainly generated by oxidation of Zr. The steam has to diffuse through the formed surface layer of ZrO to reach the elemental Zr, the reaction product $H_2$ has to diffuse the opposite way. Hence, the hydrogen generation process is time-consuming and not instantaneous, see e.g. [2]

For best-estimate analyses it is hence necessary to simulate the in-vessel processes, to get the time histories of mass and energy release of gases into the containment. The results are used as input and boundary conditions for the subsequent analysis process.

#### 2.1.2 Accident Scenario Categories

For the design of the EPR and the safety analyses concerning severe accidents two categories of accident scenarios are defined:

1. Representative scenarios are used for the design of the severe accident safety systems. The systems have to be able to cope with the conditions and loads resulting from these scenarios. An example would be a break in the reactor cooling system (RCS), large enough to initiate a severe accident.
2. Bounding scenarios have even more aggravating conditions, to show the robustness of the systems and to demonstrate that no "cliff-edge"-effect exists, i.e. that no sudden complete system failure - which could then lead to a significant higher hydrogen risk - occurs if the design conditions would be exceeded. An example for a bounding scenario would be a recovery of the safety injection systems, which have to fail for a severe accident to occur, and injection of water on the already melting core. That would lead to very high hydrogen generation rates, and hence also release rates, in the order of a few kg/s.

Accidents of both categories are analyzed to reach comprehensive results.

### 2.1.3 Used Computer Codes

The justification process is a staged approach and consists of several successive steps and employs different computer codes. The used codes cover the spectrum from the integral code MAAP, the lumped-parameter containment code COCOSYS and the computational fluid dynamics (CFD) codes GASFLOW and COM3D. The codes are used complementarily, using their specific advantages and avoiding the specific drawbacks of the codes. This approach is in accordance with the findings of the OECD International Standard Problem 47, where for containment problems the application of both - lumped-parameter and CFD codes - was found necessary for meaningful and comprehensive analyses [3]. A brief description of the codes and the application for which they are used here are given in the following.

MAAP is an integral code, developed by Fauske & Ass. capable of modelling the processes within the reactor coolant system (RCS) and the pressure vessel [4]. As typical for this type of code, it is running relatively fast, allowing the simulation of a large number of scenarios. Although the containment is also modelled by MAAP, programs exist, which are better suited for the simulation of processes in the containment atmosphere. Therefore MAAP is primarily used for screening analysis to find the most severe scenarios to be analyzed more thoroughly and for simulating the in-vessel processes of these scenarios. The detailed time histories of mass and energy release rates into the containment are used as input for other codes. MAAP is thought to deliver conservative values of hydrogen release rates, as compared with e.g. MELCOR, another widely used integral code, see [5].

COCOSYS is a dedicated lumped-parameter code for containment analyses, developed by the Gesellschaft für Reaktorsicherheit (GRS) in Germany [6]. It utilizes as far as possible mechanistic models for describing the physics and chemistry. The containment model developed for the EPR consists of 30 zones and the components of the CGCS, mixing system and PARs, are modelled in detail. COCOSYS is used for determining global thermal-hydraulics, short and long term - up to several days - development of pressure and temperature in the containment, the compliance with global goals, e.g. the hydrogen reduction below flammability limit in less than 12 hours, and the determination of the maximum $p_{AICC}$ in the scenario. Besides geometrical and structural data the code needs as input the mass and energy release rates into the containment throughout the accident, until vessel failure from an integral or in-vessel code, such as MAAP, after vessel failure during the MCCI phase with dedicated codes, such as the code COSACO, developed by AREVA NP [7]. Such an analysis delivers the hydrogen history in the containment and can be used to determine scenarios and periods of time where a detailed investigation with CFD codes is beneficial. This analytical step between integral and CFD code is necessary, because detailed CFD calculations are far more time-consuming, by up to two orders of magnitude, than COCOSYS calculations.

Because FA depends on local gas composition and turbulence generation, calculations with a fine spatial resolution are necessary. Therefore, CFD codes are also used:

GASFLOW is a CFD code, specifically developed by the Research Center Karlsruhe (FZK, Germany) and the Los Alamos National Laboratory (LANL, US) for the analysis of hydrogen distribution in nuclear reactor buildings. It is also able to calculate slow deflagrations without dynamic pressure loads, the effect of hydrogen recombiners, i.e. the reduction of hydrogen and the effect of the hot exhaust gases of each PAR, and has a model for containment spray systems [8].

COM3D is a CFD code dedicated to the calculation of fast hydrogen deflagrations. It is also developed by FZK. The code is able to calculate flame acceleration up to sound velocity but neglects heat transfer to structures. Hence, it can be used to determine pressure loads due to a fast combustion and to assess if a DDT could occur, i.e. if the flame velocity could reach sound velocity [9].

## 2.2 Steps of Justification

In this section the different steps of the justification process are described in consecutive order. The complete analysis procedure, including all six steps, is not necessary for each accident scenario.

### 2.2.1 Screening Analysis

As a first and basic step, about 100 scenarios are analysed with MAAP. From this data base, about 10-15 scenarios are picked for further analysis. The criterion for selection is the severity with respect to hydrogen risk. Important parameters for the hydrogen risk are e.g.:

- A higher released hydrogen mass increases the maximum amount of energy that could be released by a combustion
- A higher hydrogen release rate increases the concentration gradient, promoting flame acceleration
- The number of release locations influences the inhomogeneity: the less release locations, the higher the resulting concentration gradient
- A lower steam content of the atmosphere during hydrogen release means a lower flammability limit and also a higher risk for flame acceleration.

Roughly half of the scenarios selected for further analysis are representative, the rest boundary scenarios.

### 2.2.2 Global Results

All of the selected 10 - 15 scenarios are analyzed with COCOSYS. This results, as mentioned above, in more global findings, long-term pressure and temperature development, hydrogen depletion by the PARs, compliance with global goals and values for the maximum $p_{AICC}$ for the scenarios. The spatial resolution of a lumped-parameter code is limited by its nodalization, because the atmosphere within a zone is by definition homogenously mixed. Nevertheless it is possible to recognize scenarios, where the inhomogeneity of hydrogen distribution in the containment is large, because the COCOSYS model is specifically developed for severe accident containment analyses. These scenarios, and especially the periods of time, where this inhomogeneity is largest, are then selected for the further analysis with CFD codes. This is necessary because the local concentration gradients have to be assessed for estimation of the risk for flame acceleration.

### 2.2.3 Local Gas and Temperature Distributions

For the scenarios chosen for further analysis, i.e. the scenarios. with the highest hydrogen risk, see above, CFD analyses are performed with GASFLOW. The results of the calculation are the local gas and temperature distribution. So it is possible to assess, if large concentration gradients exist, which are not visible in the COCOSYS calculations, because they are "smeared out" by the lumped-parameter principle.

Furthermore, the local temperature distribution of the containment shell can be investigated. With GASFLOW also slow deflagrations can be calculated and the influence of the heat release by the combustion simulated.

Additionally, the influence of the activation of the containment spray system can be investigated with GASFLOW. This is important because the spray reduces the steam content of the atmosphere, hence increasing the hydrogen concentration and lowering the flammability limit. But spraying has also very beneficial aspects: Besides the obvious pressure reduction atmospheric mixing is promoted, thereby reducing potentially harmful concentration gradients. To investigate the interaction between these two phenomena locally, lumped-parameter calculations may not be sufficient and CFD calculations are helpful to gain insights, not only for an accidental activation of spraying but also for severe accident management guidelines.

### 2.2.4 Distribution of Risk of Flame Acceleration

It was experimentally found that a necessary condition for flame acceleration is a violation of the so-called sigma criterion, see [1] for an exhaustive overview. The sigma index is the ratio of the volume of a gas mixture after combustion to the volume before combustion, divided by an empirically derived value. The sigma criterion is violated if the sigma index exceeds 1. This criterion provides a link from calculations to the broad database of hydrogen combustion experiments. However, most of the experiments were performed in tube-like geometries without venting, i.e. the flame is confined and cannot expand into three dimensions, like in the dome of the reactor building. Hence the sigma criterion is very conservative and its violation is necessary but not sufficient for the occurrence of FA.

GASFLOW is able to calculate the sigma index locally for each computational cell. For scenarios or time periods, where the value is everywhere below 1, no FA is possible and hence no further, detailed investigation of pressure loads necessary.

2.2.5 Calculation of Deflagration

Because the sigma criterion is conservative, it can be violated in a number of scenarios. Therefore a detailed investigation is necessary with COM3d. This code is specially suited for the calculation of fast deflagrations of hydrogen and flame acceleration.

The time for ignition and start of the COM3d calculation is chosen from GASFLOW calculations. For the selection usually a trade-off between maximum local sigma value and mass of hydrogen present in the containment is necessary. The reason is that the highest sigma values occur near the break during the maximum of the hydrogen release rate, but at that time only part of the hydrogen is already released into the containment and could be burned. At later times, the hydrogen mass is higher, but the sigma values are lower because the atmospheric mixing has already reduced the high local concentrations. So the exact time of ignition is the result of engineering judgment to find the worst conditions. This means that possibly more than one COM3d calculation is performed for an accident scenario.

The ignition location is usually easier to choose, because for a break in the primary circuit the location with the highest sigma indices are most likely found above the break and the hydrogen rises to the dome through the SG tower closest to the break. A flame would obviously follow the same path, consuming the hydrogen. In the SG tower the flame is rather confined and many turbulence generating structures are present. This combination provides the most pronounced conditions for promoting flame acceleration. In other words: if no critical FA is reached there, it is reached nowhere in the containment. When the flame leaves the SG tower and enters the dome, it can expand freely in all directions and will hence decelerate.

The COM3d calculations deliver the flame velocity and pressure distribution and the time histories of pressures and pressure differences across inner structures. The gas temperatures and hence the pressure buildup are overestimated by COM3d, because it is an adiabatic code and neglects heat transfer to the wall, both radiation of the hot gas and convective heat transfer. For short combustion calculations of a few seconds, typical for fast deflagrations, these effects are negligible.

2.2.6 Assessment of Building Response

If the COM3d calculations show that a combustion is fast enough to cause large, dynamic pressure spikes two parameters have to be examined. Firstly, the absolute values of the spikes and pressure differences across inner structures are important. It is important, that these values are not higher than the load-bearing capacity of containment shell and inner walls. Secondly, it has to be checked that the frequency of the pressure spikes is not near the building frequency, so that no resonance can occur. It was found that for no scenario a detailed performance of this last step was necessary.

## 2.3 Example

In this section a few examples for an analysis of a small break loss of coolant accident (SBLOCA) are presented, to get an impression, what the results look like. The purpose is not an exhaustive analysis, but to highlight a few important points to illustrate the verification procedure presented in section 2.2. The example is restricted to the phase until vessel failure and on the risk of pressure loads due to a fast deflagration. A complete analysis cannot be presented, simply because it would go much beyond the limits of the paper.

The scenario was calculated with MAAP, resulting in the time histories of mass and energy release. For the beginning of the hydrogen release the release rates are shows in Figure 1. The peak release rate is about 0.7 kg/s. The largest inhomogeneities will probably occur at or shortly after the peak release rate. The red vertical line in the figure indicates the time for which some distributions calculated with GASFLOW and the ignition time for a combustion calculation with COM3d are presented later in this section.

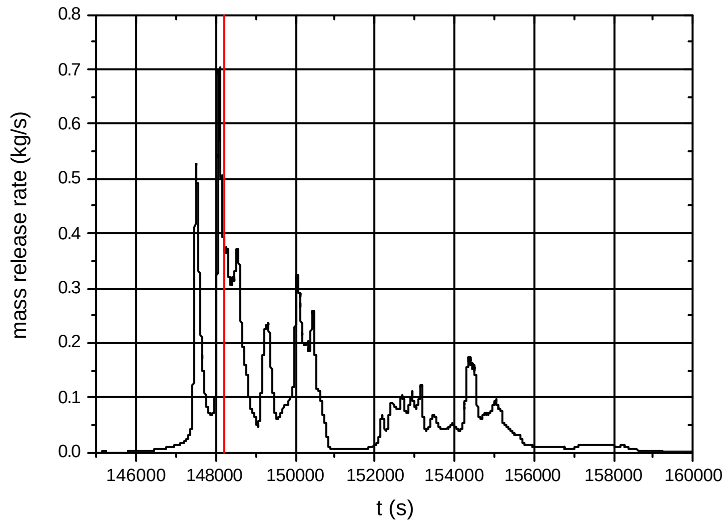


Figure 1 Start of hydrogen release, showing the peak release rate as a result of the MAAP calculation

The release rates into the containment are used as input for the COCOSYS calculation. The COCOSYS results give the history of hydrogen in the containment and an impression of the homogeneity of the distribution, hence indicating periods where flame acceleration could be possible. The history of the hydrogen in the containment from start of hydrogen release until failure of the reactor pressure vessel is shown in Figure 2. Nearly 1000 kg of $H_2$ are released, but due to depletion by the PARs the maximum mass of hydrogen in the containment atmosphere is clearly below 500 kg. At vessel failure only less than 200 kg $H_2$ are present in the atmosphere. The discrepancy between the curves of released and present mass at the time t < 148000 s is only an artefact, because the time resolution of the COCOSYS output values was not chosen fine enough for this overview plot.

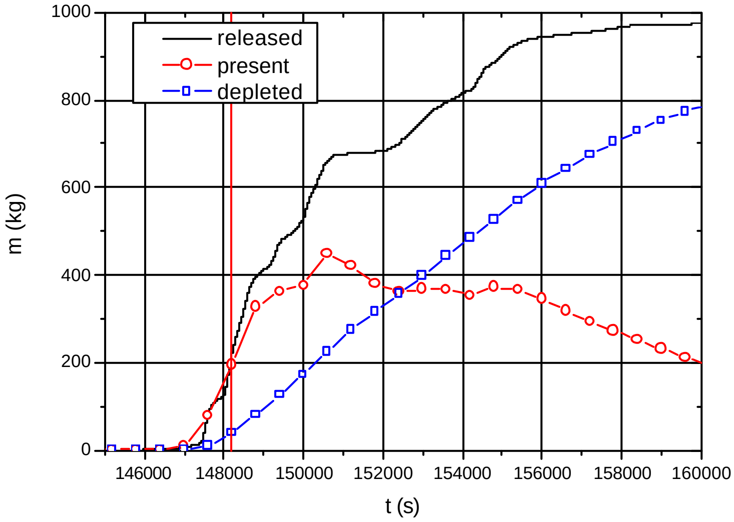


Figure 2 Time histories of hydrogen mass released into the containment, present in the containment and depleted by PARs as a result of the COCOSYS calculation

In Figure 3 the hydrogen concentration in the COCOSYS zones representing the dome and the top of the steam generator tower on the side of the break in the RCS and on the opposite side, covering roughly 1/3 of each SG tower volume, is shown. The dome is by far the largest zone and its concentration is very similar to the average concentration of the whole containment, which is therefore not explicitly presented here. Obviously a large concentration gradient is present in the containment during the first two release peaks, i.e. for $t < 149000$ s. The hydrogen concentration reaches levels of nearly 9 vol.% in the top of the SG tower of the break side. This strong inhomogeneity exists only for a very limited time, after about 151000 s the concentration is very similar to the values in the dome and stays below 6 vol.%. Note that at 148100 s the hydrogen concentration in the dome would still be below the flammability limit, if the hydrogen would be homogenously distributed, as assumed by lumped-parameter codes.

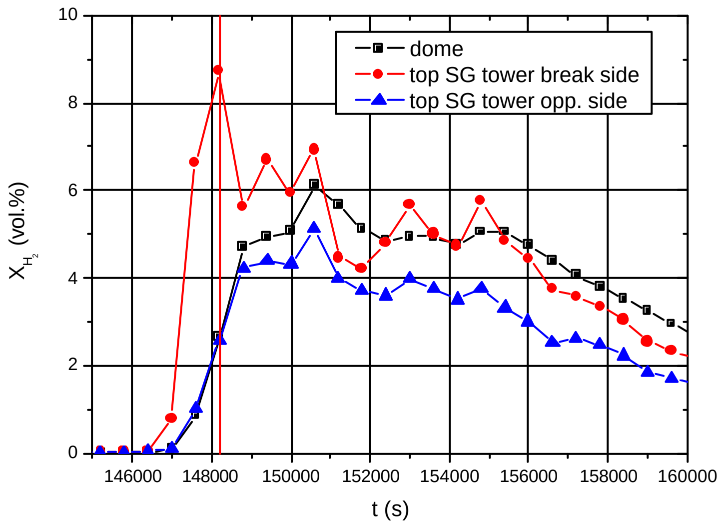


Figure 3 Time history of the hydrogen concentration in the COCOSYS zones dome, top of SG tower of the break side and the opposite side.

The GASFLOW analysis shows that the risk for flame acceleration is highest at the time of the maximum hydrogen release rate, i.e. at 148100 s, and lower at all earlier and later times. Especially it shows that the risk for flame acceleration is higher than at the time when the hydrogen mass present in the containment is near its maximum, at about 150000 - 151000 s. In Figure 4 a cut through the containment, specifically through the SG tower on the break side is shown. Obviously local hydrogen concentrations reach values much higher than the values of the COCOSYS results, up to 15 vol.% in the SG tower and 10 vol.% in the dome. The latter is much above the flammability limit and combustion in the dome hence possible. This shows that CFD calculations give a much more detailed view of the situation and that lumped-parameter calculations cannot be regarded a-priori as conservative.

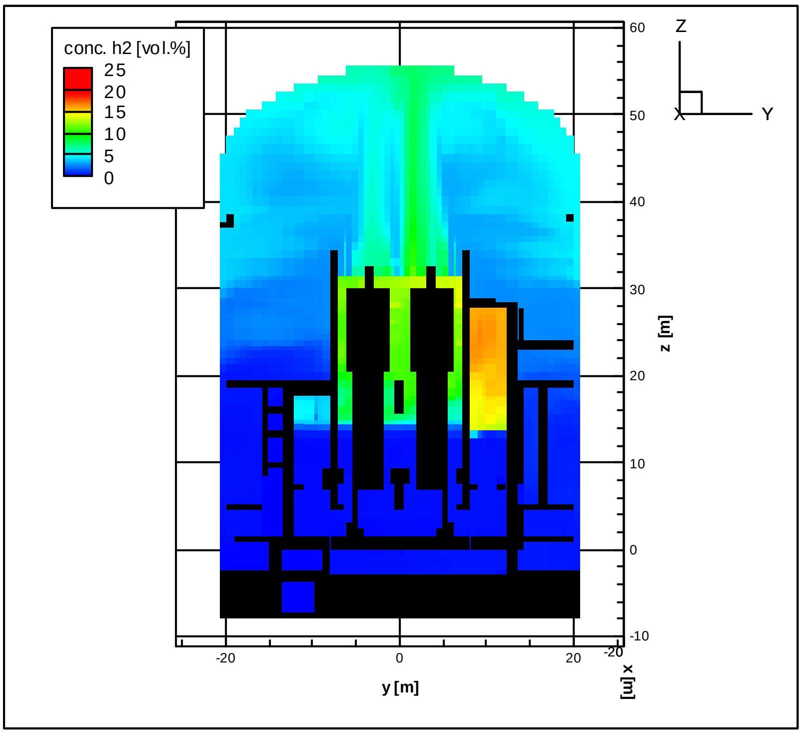


Figure 4 GASFLOW result: cut through the SG tower on the break side showing the hydrogen distribution at 148100 s

In Figure 5 the spatial distribution of the sigma criterion is shown, the location of the cut and the time are the same as in Figure 4. The sigma index is about 1 at the top of the SG tower and greater than 1 in the top of pump room above the break, located in the picture on the right side of the SG tower, coloured in orange. Therefore FA cannot be ruled out and a COM3d calculation is performed.

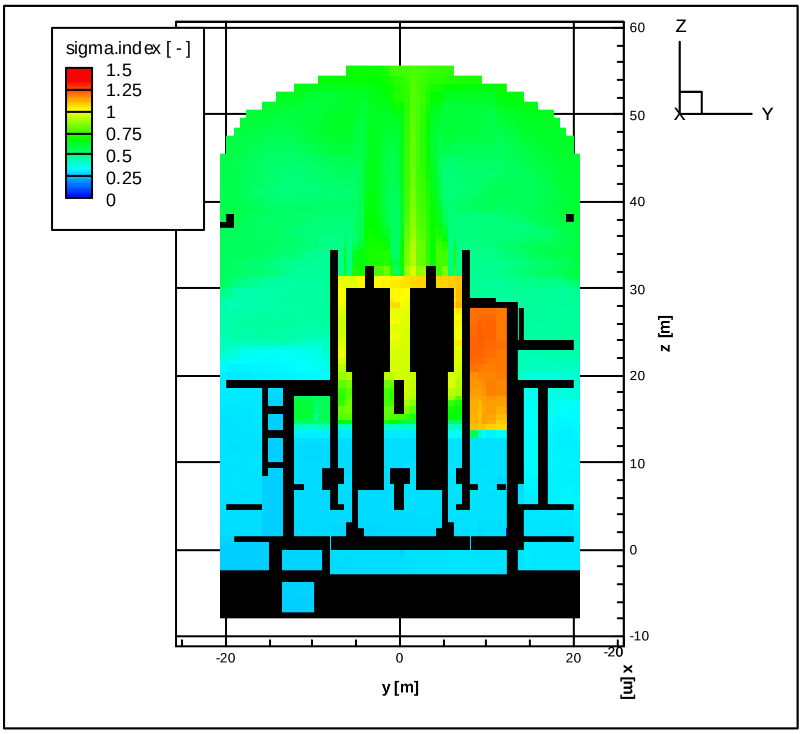


Figure 5 GASFLOW result: cut through the SG tower on the break side showing the distribution of the sigma index at 148100 s

The location of the ignition is above the break in the RCS, as described in section 2.2.5, the ignition time is 148100 s. In Figure 6 and Figure 7 the flame velocity distribution at about 1.3 s and 2.5 s after the ignition are shown. The location of the cuts is similar to the GASFLOW plots. After 3 s the combustion process is over. The figures show the expected behaviour of the flame velocity: it is relatively high when it leaves the SG tower into the dome and subsequently decelerates. The flame speed reaches several hundred meters per second, which is nevertheless much below sound velocity for the given gas composition and temperature in the containment The maximum pressure differences caused by the combustion are about 50 mbar and no dynamic effects are observable. Hence no further analyses regarding the risk of fast deflagration would be necessary for this scenario.

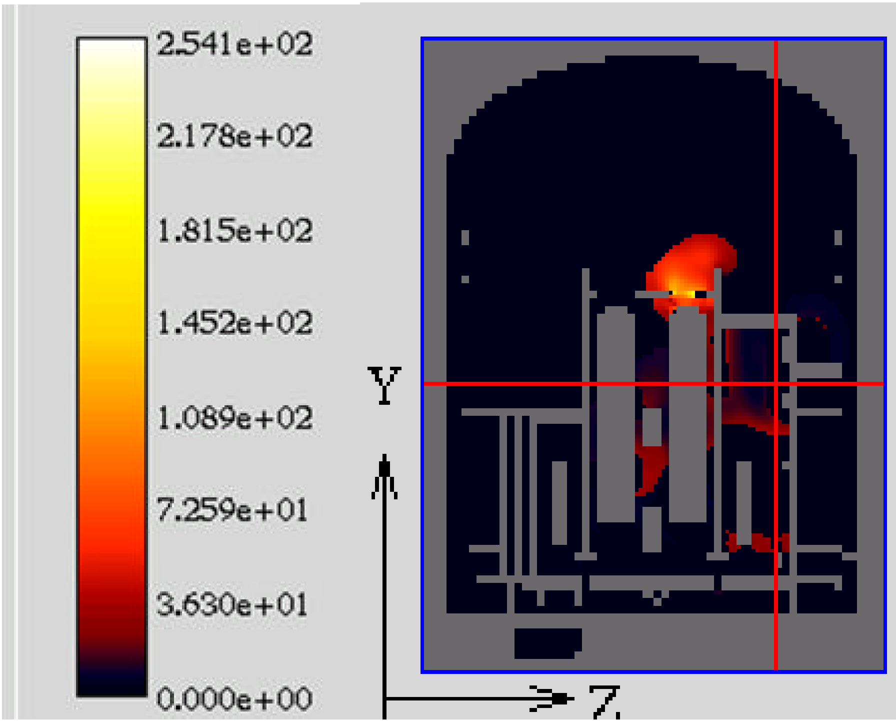


Figure 6 COM3d result: flame velocity in m/s about 1.3 s after ignition

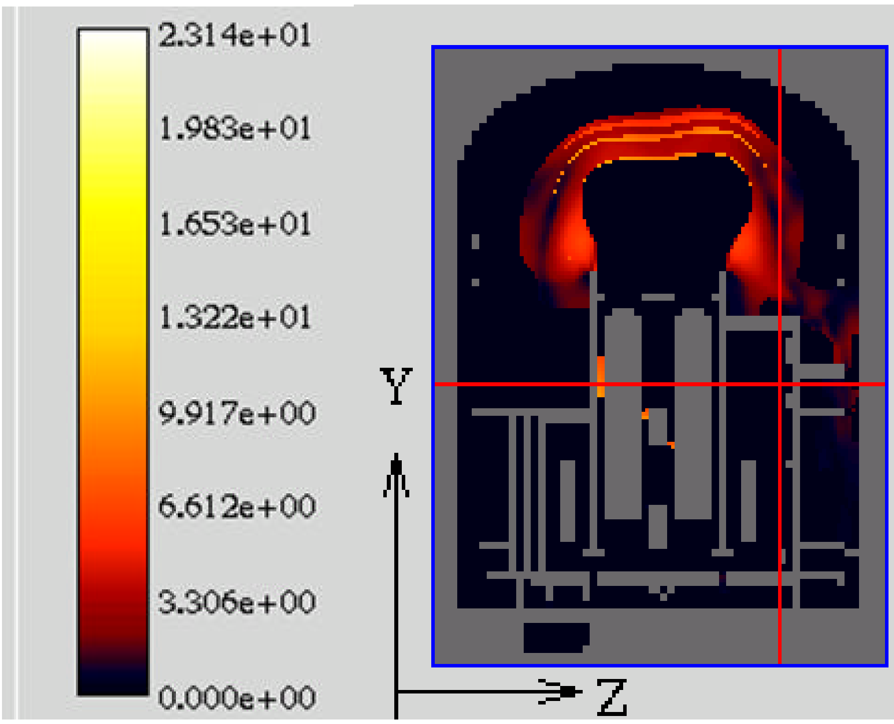


Figure 7 COM3d result: flame speed in m/s about 2.5 s after ignition

## 3 SUMMARY AND CONCLUSION

In this paper the procedure for the verification of the CGCS of the EPR was presented. The purpose of this system is to prevent excessive temperature or pressure loads due to the combustion of hydrogen, which is generated in a severe accident.

The justification is a staged approach and makes complementary use of integral, lumped-parameter containment and CFD codes, thereby utilizing the specific advantages and minimizing the effect of the specific drawbacks of the code classes.

The integral code MAAP is used for calculating in-vessel phenomena and the release rates into the containment. A large number, about 100, accident scenarios are calculated for a screening analysis to find the scenarios with the highest hydrogen risk. The 10 - 15 most challenging scenarios are then analyzed further.

COCOSYS is a lumped-parameter code for containment analyses. All of the selected scenarios are calculated with COCOSYS. This results in long term behaviour of containment pressure and temperature, the compliance of global goals, like hydrogen depletion and $p_{AICC}$-values, and the time history of the hydrogen mass and concentration in the containment, obviously limited in spatial resolution by the nodalization. From these analyses the scenarios and periods of time are chosen, where the hydrogen risk is highest, especially with respect to flame acceleration and dynamic pressure loads, but also to the temperature loads of potential slow deflagration.

Again, the most severe scenarios and periods are chosen for further analyses with the CFD code GASFLOW. The results of GASFLOW are the local gas and temperature distributions for atmosphere and structures, especially containment shell. Additional analysis of special aspects, like temperature loads due to slow combustion and influence on local hydrogen concentration by an activation of the spraying system, are also performed with the code.

GASFLOW delivers also the distribution of the sigma index, which is a link between simulation and experimental data. The sigma criterion is conservative: its violation, i.e. if the sigma index exceeds 1, is necessary but not sufficient for the occurrence of flame acceleration. Hence, more detailed investigations of the combustion process are performed with the dedicated CFD code COM3D if the sigma criterion is violated.

For these analyses the most severe time(s) and location is chosen for ignition. The results of the COM3d calculation show the distribution of flame velocity and pressure and the time histories of pressure differences. If large dynamic pressure loads are found, an analysis of the structural response of the building could be necessary. This was not necessary for any of the calculations for the EPR.

This analysis procedure is suited for investigating the temperature and pressure loads which could result from the hydrogen combustion in a severe accident. By applying integral, lumped-parameter and CFD codes comprehensive and meaningful analyses are possible within a reasonable timeframe. With this verification procedure it could be shown that the CGCS of the EPR is suitable for preventing excessive loads onto the containment by the combustion of hydrogen.

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