SIMULATION OF HYDROGEN DISTRIBUTION IN THE CONTAINMENT DURING A SEVERE ACCIDENT WITH FAST HYDROGEN-STEAM RELEASE

D. Papini, M. Andreani, B. Ničeno, and H.-M. Prasser
Laboratory for Thermal-Hydraulics, Paul Scherrer Institut (PSI)
5232 Villigen PSI, Switzerland
davide.papini@psi.ch

P. Steiner and J.-U. Klügel
Kernkraftwerk Gösgen-Däniken AG
4658 Däniken, Switzerland
psteiner@kkg.ch

ABSTRACT

Three-dimensional simulations are required for a reliable analysis of the risk of hydrogen stratification, accumulation and combustion during a severe accident in light water reactors. This paper reports on a plant application of the GOTHIC containment code to simulate the hydrogen distribution in case of fast release of hydrogen-steam mixture from hot-leg creep rupture during a postulated total Station Black-Out (SBO). The utilization of GOTHIC shows advantages compared to Lumped Parameter (LP) codes, which predict only averaged conditions for each compartment of the containment, and to Computational Fluid Dynamics (CFD) codes, mainly in terms of lower calculation costs thanks to the adoption of a relatively coarse mesh. The prevailing mixing processes of the hydrogen are described with reference to a base scenario that maximizes the hydrogen convective flows assuming an irreversible opening of the dampers on top of the steam generator towers. The mitigation strategy relies solidly on the dilution resulting from the large free volume of the containment and the high value of the design pressure. Sensitivity analyses investigate the importance of the steam generator dampers and the influence of the liquid sump on bottom of the break volume. The closure of the dampers in the steam generator towers after the initial lift results in higher hydrogen concentration in the compartmented inner space and less mixing in the containment dome. The effect of steam condensation on the surface of the sump is negligible in terms of hydrogen risk. The flammability of the mixture is finally assessed using the Shapiro diagram. Flammable states are obtained during the transient but the Adiabatic Isochoric Complete Combustion (AICC) pressure limit results in (static) pressure peaks below the containment design pressure.

KEYWORDS
Severe accident, plant application, GOTHIC code, flammability analysis, AICC pressure

1. INTRODUCTION

In the framework of the EU stress tests the operating NPPs (Nuclear Power Plants) have been asked to prove their SAMG (Severe Accident Management Guideline) strategies with respect to the risk of combustion load and containment failure. A large amount of hydrogen produced in the event of a severe accident may be released to the containment, usually together with steam. When mixing with the air of the containment, pockets of flammable mixture can build up and lead to slow deflagration, fast turbulent deflagration (with flame acceleration) or deflagration-to-detonation transition. A detailed assessment of the combustion risk and the design of the respective mitigation measures (e.g., the Passive Autocatalytic Recombiners – PARs [1]) require accurate three-dimensional simulations to compute the local distribution of the gas species. LP codes, usually used in the simulation of severe accidents, have inherent limitations concerning the conservation of momentum and turbulent mixing, therefore they are not suited to predict local/regional hydrogen concentration as well as stratification and mixing phenomena in presence of flow structures such as jets or plumes.

On the one hand, a significant confidence has been reached in CFD-based methods for hydrogen risk assessment in reactor containments [2]. Three-dimensional CFD analyses might be necessary to simulate the combustion of the mixture and assess the dynamic pressure loads in the containment, which depend primarily on the turbulence generated at the flame front [3]. On the other hand, the GOTHIC containment code offers a practical approach to the different time and spatial scales involved during a severe accident. The coarse-mesh approach typical of GOTHIC is gaining nowadays interest, on the account, e.g., of the results of the recent OECD/NEA-PSI CFD benchmark [4], which highlighted the fair accuracy of GOTHIC coarse-mesh models. The prediction of the erosion of a stratified helium-rich layer in a single vessel (of the PANDA facility in Switzerland) was validated for GOTHIC using a rather small number of cells compared to standard CFD codes (~8 k cells compared to ~2 M cells), which turned out in drastically reduced calculation times against a similar prediction accuracy. Extensive validation exercises of GOTHIC have been conducted in the last decade based on experiments among others in the large PANDA multi-compartment facility, using air, steam and helium (simulant of hydrogen) mostly under idealized conditions [5] but also in test sequences scaled from generic containment calculations [6].

This paper presents a full scale plant application of the GOTHIC code aimed at hydrogen risk assessment. Predictions of local hydrogen concentrations in PWR containments using GOTHIC were already performed by Grgić et al. [7] but considering a multi-volume, mostly lumped-parameter model, with internal subdivision only for the largest compartment (i.e., the containment dome). A detailed three-dimensional representation of the containment with GOTHIC has been afforded recently by Jiménez et al. [8] with similar scope as our analyses. The present work addresses specifically the impact of the ceiling dampers in the steam generator towers as well as the influence of the liquid sump on the hydrogen risk. The analysis is fully characterized with a preliminary assessment of the ignition potential using the Shapiro diagram (following the roadmap presented in the State-of-the-Art report of the OECD/NEA [9]). Assuming a slow deflagration regime, the integrity of the containment is finally investigated calculating the AICC (Adiabatic Isochoric Complete Combustion) pressure with the gas species concentrations and containment ambient conditions computed by the GOTHIC simulation.

2. GOTHIC MODEL

The thermal-hydraulic program GOTHIC [10] is based on a two-phase, multi-fluid formulation, and solves the conservation of mass, energy and momentum for three fields: a multi-component gas mixture, a continuous liquid, and droplets. A full treatment of the momentum transport terms is considered, with inclusion of turbulent shear and turbulent mass and energy diffusion. GOTHIC has the necessary capabilities for simulating the 3D (three-dimensional) distribution of hydrogen from the time point of release to the time point of possible combustion. These capabilities include fundamental models for transport phenomena (turbulent and molecular diffusion, natural convection, multiple gases and steam condensation), capability to handle complex geometry, operation of engineering devices (valves, doors, hatches, PARs, etc.), possibility of easy transfer of proper initial and boundary conditions from severe accident codes and, compared to CFD codes, the aforementioned capability to obtain accurate results with relatively coarse mesh [4].

The analyzed containment is a spherical steel containment (large dry PWR containment, Konvoi type) bounded by a concrete shell with annular gap of air. The GOTHIC model represents only the inner spherical containment (filled with air), which is highly compartmentalized. The main feature of this type of containment is an internal cylindrical concrete structure (named cylindrical shielding wall or missile protection cylinder), which envelopes the primary system components and related compartments (component room). The steam generator ceiling dampers (flaps opening on top of the steam generator towers based on pressure difference) represent the main hydraulic connection between the component room and the large open space above the upper deck (the dome or operating room). Table I characterizes volumes and surfaces of the investigated reactor containment.

The modeling capabilities of GOTHIC are based on orthogonal coordinates only (Cartesian numerical grid). The developed input deck is sketched in Figure 1. The selected approach is a compromise between a fully 3D representation of the entire geometry and a schematization into convenient multiple subdivided volumes. Several subdivided control volumes are defined, in orthogonal coordinates, and then suitably connected to reproduce the 3D layout of the compartments in the containment. The GOTHIC model consists more precisely of two large 3D subdivided volumes with full 3D geometry (Vol.1s, representing the upper section with dome, and Vol.17s, representing the lower inner compartment with the break point), 15 3D prism volumes with real height and equivalent cross-sectional area, modeling the large containment room within the cylindrical shielding wall, and 23 lumped volumes, simulating the remaining volume of the containment (staircase room and annular space below the upper deck floor).

The total number of cells is ~37000. Within the control volumes with Cartesian grid of the GOTHIC model, the actual geometry with curved surfaces, concrete walls and primary system components is approximated through the implementation of "blockages", which are obstacles fully or partially obstructing cell volume occupied by fluid. ~16000 cells are fully blocked with null volume porosity. Figure 2 shows some example of the full 3D geometry reproduced in the lower containment and the upper zone with the dome. The break is located in the lower part of a steam generator room, below the lower deck floor (Figure 2-(a)). The mesh size in the break volume follows the criterion of cell size in the vicinity of the injection similar to the injection size (a validation of this criterion is given in [6]). The typical dimension of the cells is of the order of the hot leg diameter (~0.8-1 m), with a coarsening in the upper containment volume (~1.6-2 m in Vol.1s, see Figure 2-(b)). Some mesh sensitivity studies were performed in the break volume to determine a proper modeling of the impulse of the jet. Numerical difficulties were unfortunately encountered using a finer mesh (cell size less than break size), which did not permit indeed to solve the expansion of the high-velocity jet due to continuous code crashing. On the other hand, a coarser mesh was inappropriate to render the real geometry adopting blockages.

A total of 171 thermal conductors (heat structures) were implemented to model the heat capacity of the solid structures and the heat transfer between fluid and these structures. The default heat transfer options are considered, including convective heat transfer, condensation at the wall and radiation between steam and wall. Molecular and turbulent diffusion (the k-ε turbulence model is used) are considered and a second order accuracy in the spatial discretization of the advection terms is adopted, as recommended for gas transport phenomena [6]. The version of the code used in the present study is GOTHIC 8.1 [10].

Table I. Main geometrical data of the GOTHIC containment model (large dry PWR containment).

Total volume of the sphere [m^3]	73622	Steel surface [m^2]	6007
Total free volume [m^3]	55102	Inner steel shell in dome [m^2]	4672
Subdivided free volume [m^3]	49313	Number of cells	~37000
Concrete surface [m^2]	9755	Number of thermal conductors	171

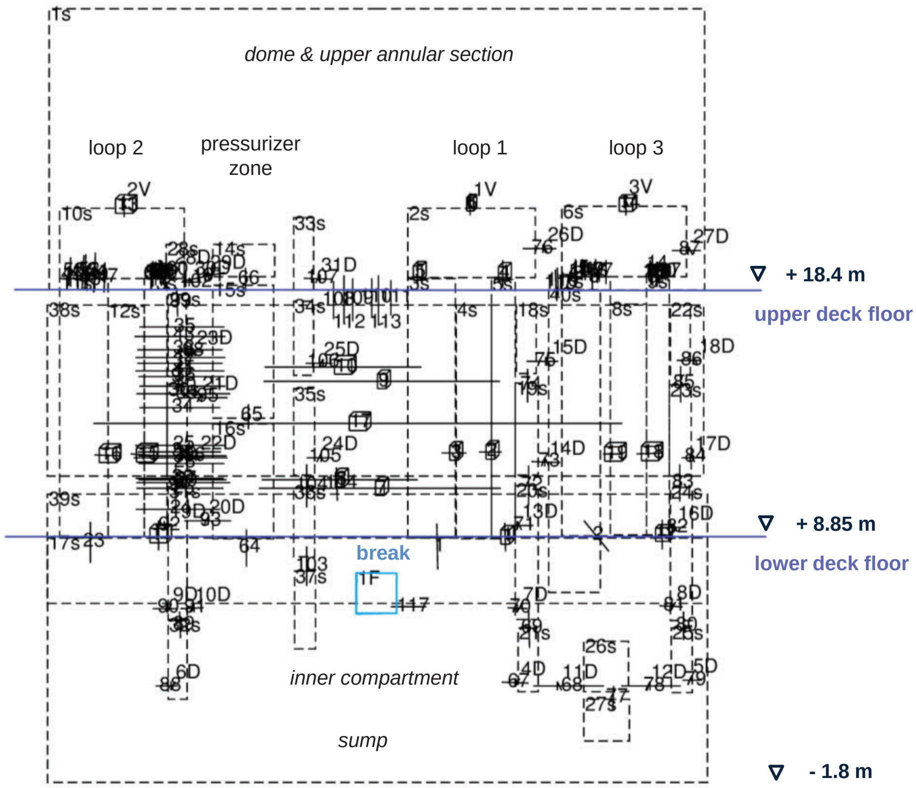

Figure 1. GOTHIC nodalization diagram of the containment.

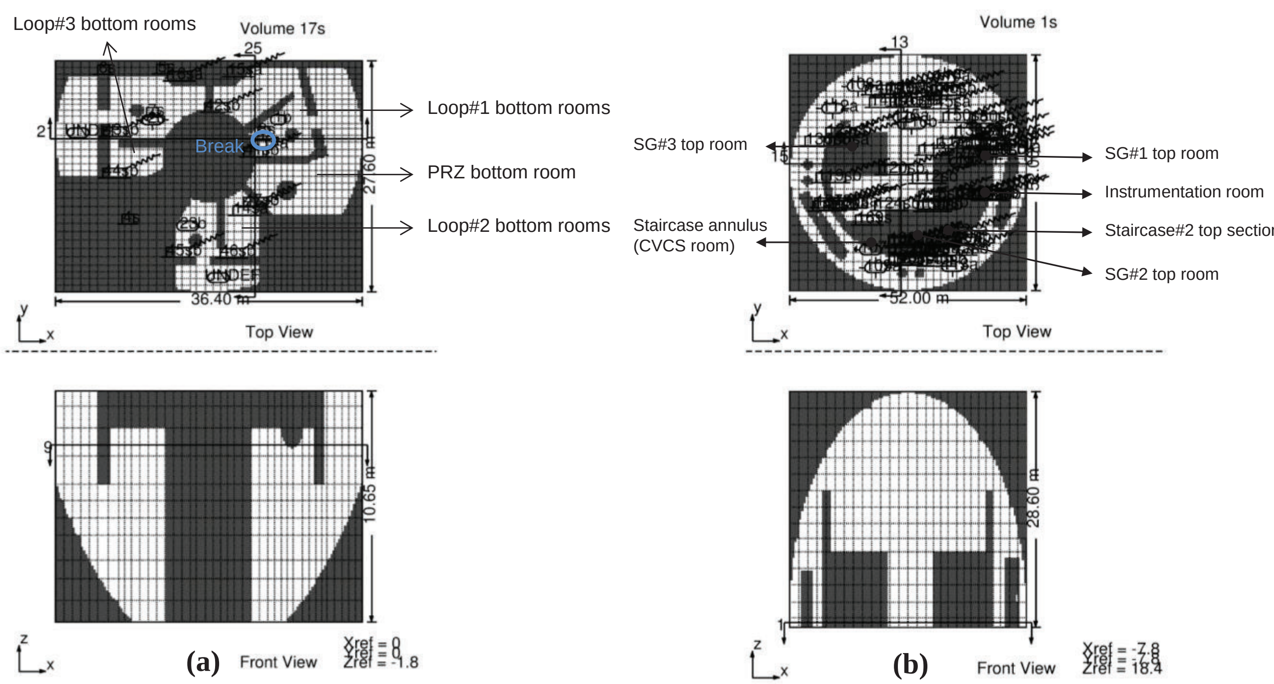

Figure 2. Nodalization detail for lower containment volume (Vol. 17s) (a) and upper containment volume (Vol. 1s) (b).

3. INVESTIGATED SCENARIO

The considered accident is a total SBO with high temperature creep rupture in the hot leg, identified as the most severe postulated event with respect to the hydrogen risk. The source term comes from a MELCOR calculation, by assuming, however, in the GOTHIC simulation conservatively twice the amount of the hydrogen obtained from MELCOR (only in-vessel generation of hydrogen is accounted, no reflood of the primary system occurs before the break). A total of ~310 kg of hydrogen are considered (inclusive of the 100% safety margin) and are defined to be released through a fast release. Fast-release scenario means that all the gases contained in the primary system are injected in few seconds to the containment. In BDBA (Beyond Design Basis Accident) the hydrogen gets injected with high steam content, while no liquid is assumed to be present in the primary system (or, equivalently, the liquid immediately evaporates at containment conditions).

The thermodynamic conditions of the primary system (upstream the break) and the containment (downstream the break) at the time of creep rupture, as derived from MELCOR, are summarized in Table II. They represent the initial conditions for the GOTHIC model. The initial temperature of the containment (83.5°C) is assumed uniform for all the compartments. The initial steam content in the atmosphere is 45% (molar concentration) and comes from previous releases of the pressurizer relief valves. The large initial pressure difference between the primary circuit (167 bar) and the containment (1.3 bar) leads to choked flow, which produces an underexpanded, sonic, high-velocity jet into the break compartment. The composition of the steam-hydrogen mixture at the release is based on the ideal gas law applied in the primary system conditions, obtaining a boundary composition of 40% hydrogen and 60% steam. The dynamics of the break flow was defined using a separate, simple model considering the critical flow limitation in GOTHIC. The hydrogen-steam mixture release takes place in 3 s. More details on the definition of the boundary conditions are discussed in [11].

It is just mentioned that the release conditions investigated in this study are not fully covered by the validation of the GOTHIC code, which has not been extended to the high temperature and high speed of a sonic jet (a validation case of GOTHIC during a fast release, but lower velocity, in a two-compartment geometry is discussed in [12]). Nevertheless, the simulation of the fast hydrogen release with the GOTHIC code and a coarse 3D nodalization (respecting the recommendations discussed in Section 2) can be expected to provide reliable information on the hydrogen distribution in containment.

Table II. Break upstream and downstream conditions from MELCOR calculations of the postulated SBO scenario with creep rupture in hot leg.

	Pressure [kPa]	Temperature [K]	Volume [m^3]
Primary system	16705	1531 *	300.9
Containment	128	356.6	55102

*Temperature calculated in the hot leg, leading to creep failure.

4. RESULTS AND DISCUSSION

The simulations with GOTHIC addressed the prevailing processes for hydrogen distribution and mixing as well as the effect of the dampers of the steam generator towers. The steam generator ceiling dampers represent the main convective path between component room and operating room. The opening of the lateral doors gives an alternative path. In absence of PARs and sprayers the hydrogen mixing is based on the gas dilution in the large volume of the operating room. The running time for 1000 s of transient was about 2 days parallelizing the computation on 12 nodes of the high performance cluster available at PSI.

4.1. Base case with irreversible opening of steam generator dampers

The base case assumes that the dampers stay open once lifted by the initial pressure difference. The liquid sump (hence corresponding condensation/evaporation phenomena) is initially neglected due to numerical difficulties [11]. Figure 3 illustrates the distribution of hydrogen and respective flow field through a suitable vertical cut of the containment in the zone of the break. The origin of the break is just below the lower deck on the side of the steam generator close to the pressurizer (right-hand-side from reactor pressure vessel structure) and is indicated in the sketches with a white circle.

The released hydrogen-steam mixture forms a sonic jet that flows in the lower containment, rises immediately through the steam generator towers and impinges on the dome spherical shell (Figure 3-(a)). The doors connecting the compartmented inner volumes to the outer room are opened by the pressure difference caused by the jet (the opening of the doors is always irreversible). The main phenomenon that can be observed within the first 10 s of transient is the convective mixing of hydrogen induced by the jet and related vortices as a result of the jet deflection at the wall (Figure 3-(b)). The vortex-induced mixing takes advantage of the large free volume in the dome region and is effective in about one minute in stabilizing the maximum hydrogen concentration in the upper part of the dome to 10%. A buoyancy-driven flow is established in all the containment leading to the formation of a stratified cloud of hydrogen in the upper dome (10% concentration). This stratified cloud is clearly visible at 300 s (Figure 3-(c)).

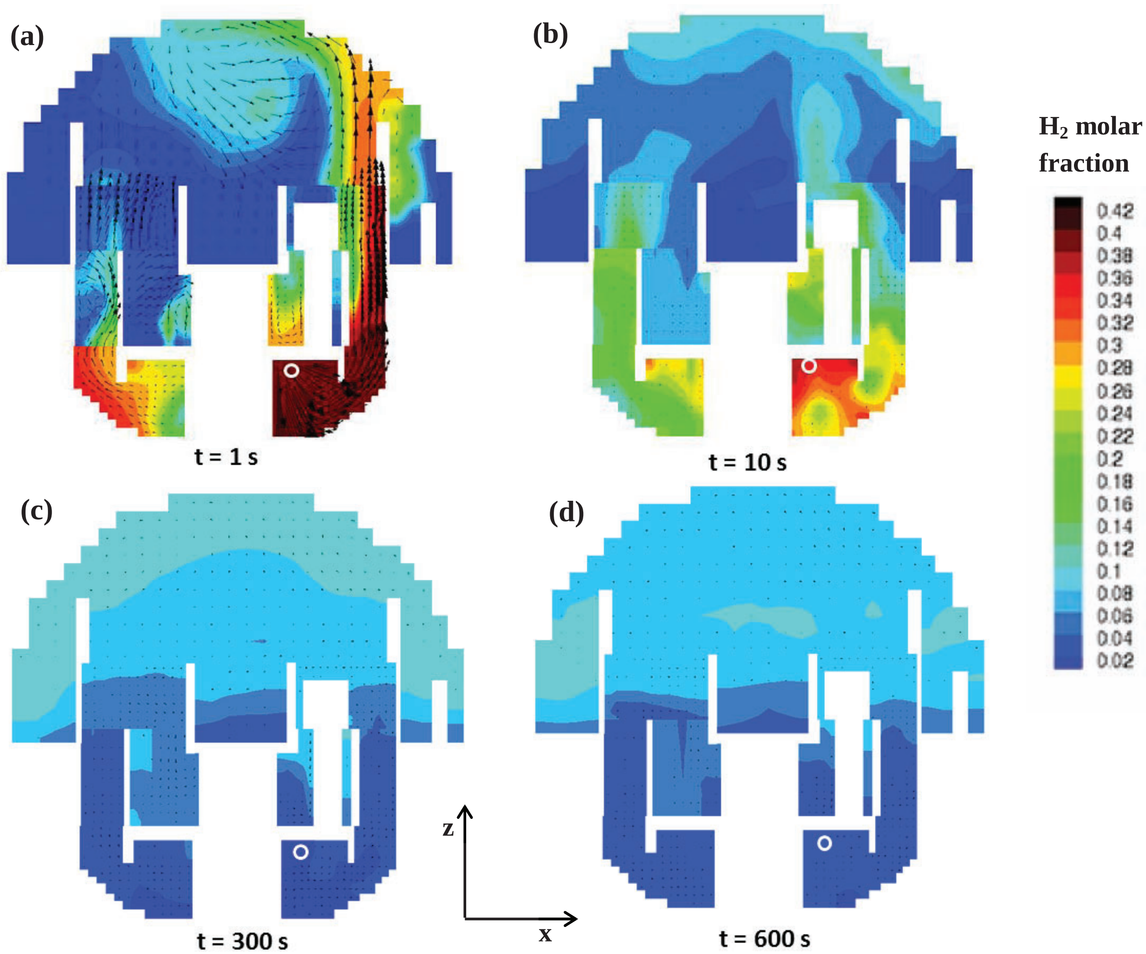

Figure 3. Contour maps of hydrogen concentration: base case transient sequence.

On a more extended time-scale another physical process seems relevant (here visible after 600 s, see Figure 3-(d)). The steam condensation on the steel structure of the dome locally increases the gas density and induces a downward-directed flow that mitigates the stratified region. This behaviour is consistent with the simulations from Royl et al. [13] using the GASFLOW code. They defined this mixing process as condensation-sedimentation effect. Condensation-sedimentation takes place thanks to the wet atmosphere established in the dome and acts as a key mechanism for the homogenization of the stratified hydrogen cloud. In our case, the condensation-induced mixing reduces the hydrogen concentration in the dome from 10% to 8%.

Additional information can be obtained from 3D visualization of the results. Figure 4-(a) shows 3D cut of the containment excluding the large upper volume. Strong heterogeneous regional conditions are evident in the compartment room for the early seconds of the transient. Less affected by the initial jet are the steam generator opposite to the break and the pressurizer area. Stratification in dome resulting from buoyant flow is clear from Figure 4-(b).

The isenthalpic expansion of the hydrogen-steam jet leads to a fast pressure peak in the containment within the first second of the transient. The choked (under-expanded) jet coming from full primary system pressure causes a series of high-frequency pressure shocks in the cells near the release point. Pressure and temperature transients are discussed with some details in [11]. In response to the hydrogen fast release, the containment pressure increases from 1.3 bar to 2.2 bar.

Evaluation of the flammability of the mixture and the potential of auto ignition (the successive steps being flame acceleration and deflagration-to-detonation transition) in each compartment of the containment can be performed by using the Shapiro diagram [9]. A minimum concentration of air of about 30% is required to ignite the mixture. Steam presence is beneficial to dilute the mixture but at least 60% steam is necessary to exclude any combustion risk. Concentrations of gas species in containment are reported in Figure 5. Based on the considerations above, the combustion risk can be excluded only in the first instants in the lower containment, as the air is depleted by the initial hydrogen-steam jet. The jet itself is not flammable only at the early stage, before widening and mixing with the dome atmosphere. Critical gas concentrations are reached in the dome (Figure 5-(a)) and in the steam generator room. It is interesting to discuss the behavior of the lower compartment (Figure 5-(b)). When the air is restored after the initial jet flow, enough hydrogen is still entrapped in the lower compartment such to establish a flammable mixture.

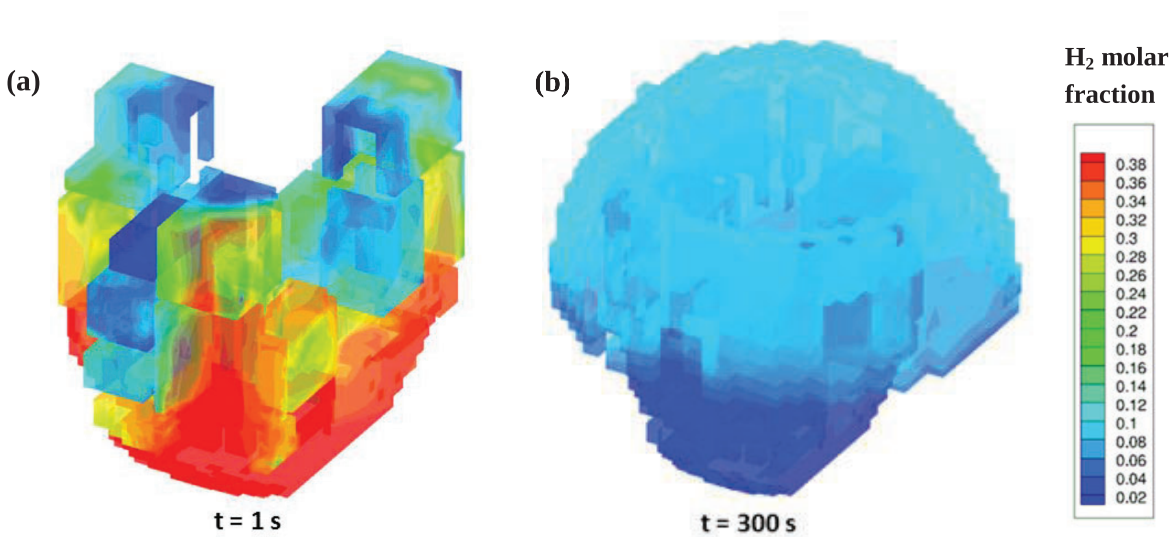

Figure 4. 3D visualization of hydrogen distribution: (a) initial jet; (b) stratified cloud.

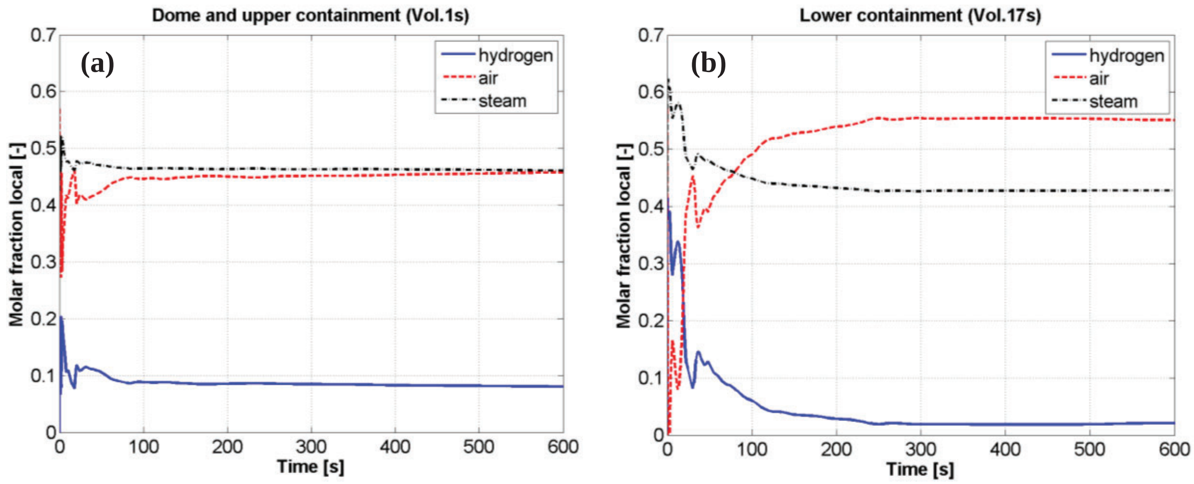

Figure 5. Gas species concentration: (a) upper containment volume; (b) break volume.

4.2. Sensitivity cases

4.2.1. Steam generator dampers closing

A first sensitivity case is studied by constraining the main convection path from the compartment room to the dome. This is obtained by allowing the steam generator dampers to reclose once the pressure difference across them vanishes. Therefore, after the first seconds (3-5 s) no large connections from the compartment area to the upper volume are directly available and the hydrogen can flow upwards just through the lateral doors leading to small staircase room and, from there, to the annulus section. It is mentioned that the real "best-estimate" scenario for the power plant is somewhere in between the two simulated cases, with a section of dampers staying open and a section reclosing, but it is not deemed of interest for the discussions in the paper.

The resulting hydrogen distribution is shown in Figure 6. Most of the hydrogen still reaches the dome in the first seconds, with the initial jet rising along the towers and impinging on the dome shell. Due to the confinement from the dampers closure, a marked separation is evident between compartment room and dome later in the transient. High hydrogen concentrations are trapped in the steam generator zone (30% hydrogen still visible after 30 s, Figure 6-(b)). The clearing of the lower containment is much slower. On the other hand, lower hydrogen concentrations are found in the dome, with average value stabilizing to 7-8%. The hydrogen mixing in the large free volume is also less effective. No evidence of condensation-sedimentation process is visible. Overall, the containment response with respect to the hydrogen risk is worsened, with more critical accumulations in the steam generator compartments (Figure 6-(c) and (d)).

4.2.2. Sump effect

The base case of this study was repeated by including the liquid sump on the bottom of the inner compartment (break volume), which increased the computation costs to solve the droplets flow induced by the interaction of the high velocity jet with the liquid field and consequent entrainment and de-entrainment phenomena.

The global behavior of the 3D hydrogen distribution is not noticeably affected by the sump. A striking effect is the occurrence of an increased concentration on the sump, as suggested by the analysis of Grgić et al. [7] too. These high hydrogen levels are evident after 60 s of simulation (Figure 7) and are plausibly caused by steam condensation on the liquid interface.

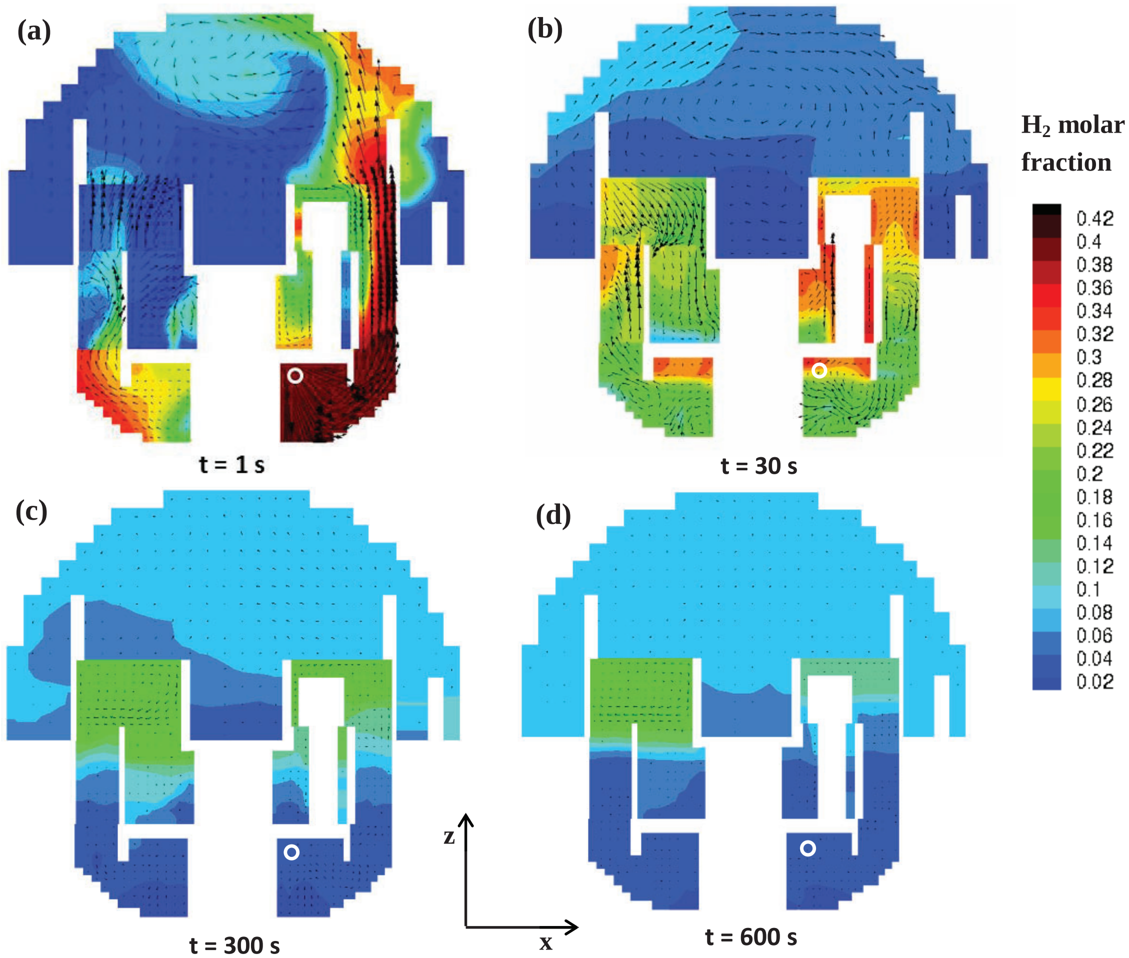

Figure 6. Contour maps of hydrogen concentration: steam generator dampers closing case.

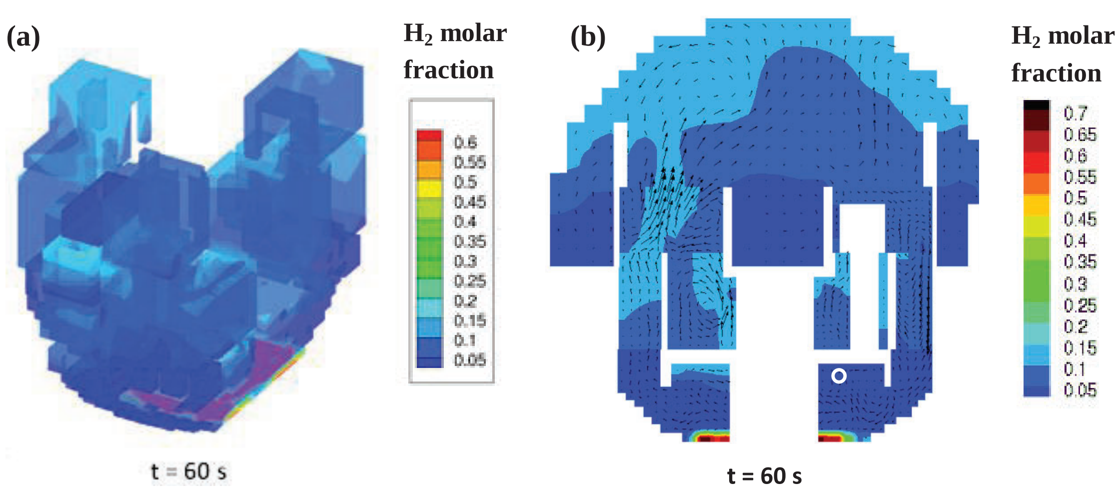

Figure 7. High local hydrogen concentration computed in the sump zone: (a) 3D view; (b) 2D contour map.

Nonetheless, it must be recognized that not enough spatial resolution is available in the model to accurately resolve interface phenomena. Further investigations are still required on these "potentially dangerous" regional accumulations. Instead, the "potentially beneficial" effect from sump evaporation when in contact with the hot jet is not such to give actual improvements to the hydrogen risk.

The results of the performed sensitivity studies are summarized in Figure 8 by comparing the local prediction of hydrogen concentration in dome (Figure 8-(a)) and in the steam generator compartment above the break release (Figure 8-(b)). While the sump effect does not alter the global stratification of hydrogen in containment, the operation of the steam generator dampers shows bigger influence. The steam generator towers are characterized by strong hydrogen accumulation if the convective flow to the dome is blocked.

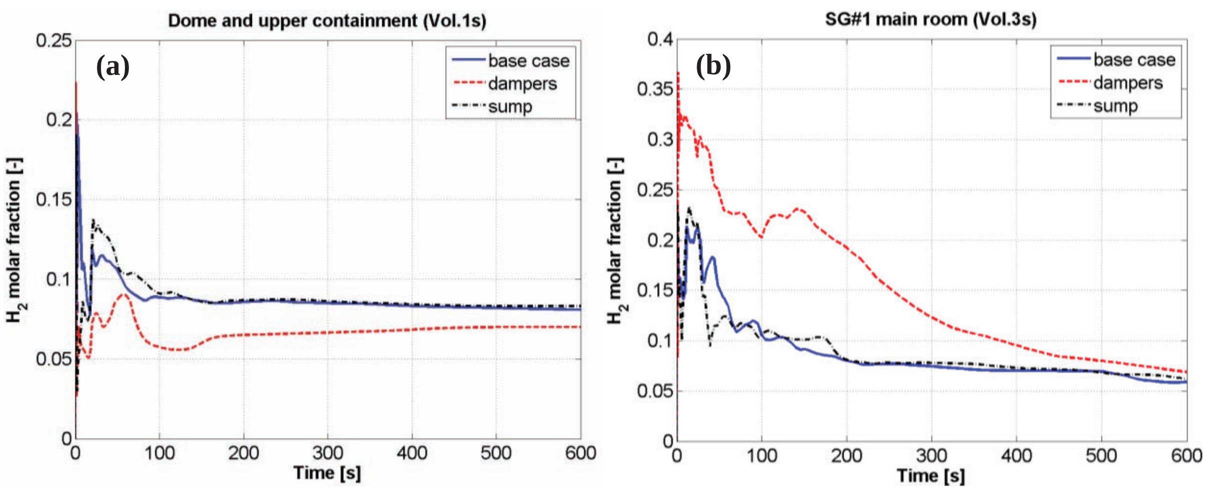

Figure 8. Comparison of hydrogen concentration in selected cells (top location) in upper containment volume (a) and steam generator compartment (b).

4.3. Flammability analysis

A preliminary evaluation of the flammability of the gas mixture was made for each compartment of the containment by application of the traditional Shapiro diagram (original data at 25°C and 1 bar; large variability is not expected though for pressure and temperature effects, see [9][15]). Figure 9 plots a "trajectory cloud" along the entire base case transient. The points of the cloud are provided with a color pattern based on a suitably defined "flammability index", which represents the distance from a linear interpolation of the limit curve [11]. The flammability based on the Shapiro diagram reads 0 in the inert zone and increases linearly to 1 in the flammable zone, as the followings (*x* denote gas molar fractions):

$$\begin{gathered} Flam = \min(a,b)\cdot c \\ a = \max(1-|0.6-x_A|/0.35,0); \quad b = \max(1-|0.4-x_{H2}|/0.35,0); \quad c = \max((0.6-x_{St})/0.6,0) \end{gathered} \tag{1}$$

The blue points in the inert region with high hydrogen concentration represent the initial jet, which is sufficiently diluted by the high volume fraction of steam. Both the diffusion and deflection of the jet in the dome as well as the buoyant flow of hydrogen in all compartment room lead to flammable states. The more flammable conditions (green points) characterize the transient response. Stabilized conditions in dome and steam generator upper room stay slightly beyond the flammability limit (pale blue zone). Figure 10 shows the results of the dampers sensitivity case. Flammable conditions are still reached in the dome, whereas states with higher flammability (the red spot) characterize the steam generator compartments.

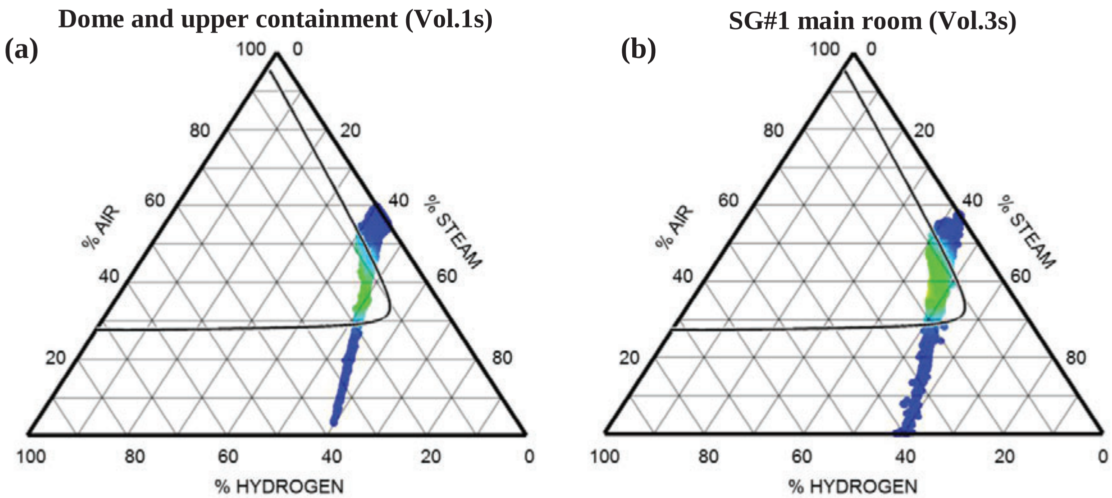

Figure 9. Trajectory clouds on the Shapiro diagram (1000 s transient): base case.

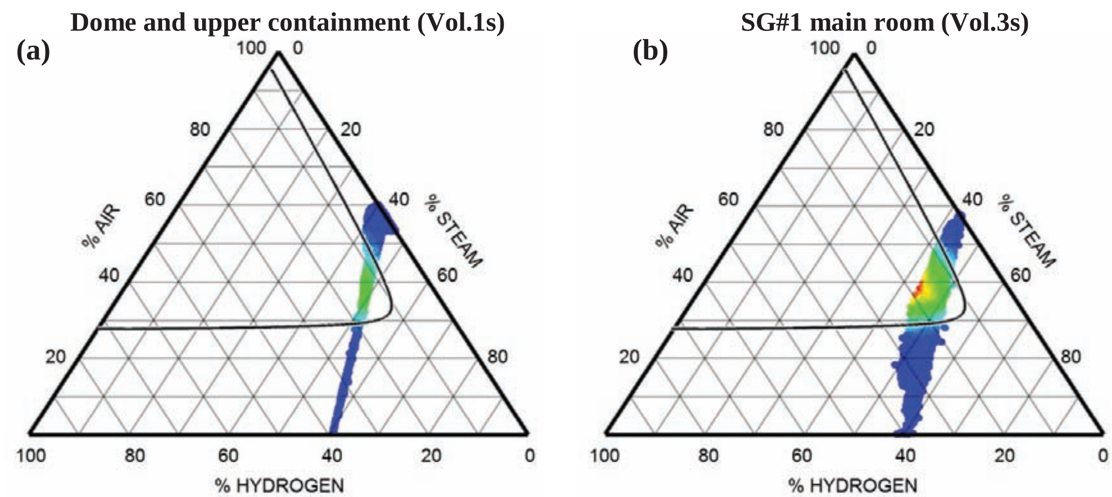

Figure 10. Trajectory clouds on the Shapiro diagram (1000 s transient): sensitivity with dampers closing.

4.4. Pressure peak analysis in case of deflagration

The static load associated with a slow deflagration regime is limited by thermodynamics. An assessment of the containment integrity is given by calculating the corresponding pressure peak according to the so-called AICC (Adiabatic Isochoric Complete Combustion) method [14].

All the chemical energy available in the gas mixture is assumed to be converted into temperature and pressure, under the conservative assumptions that all the hydrogen in the containment is instantaneously burnt and the heat losses to the structures/environment are neglected. The AICC methodology assesses the most conservative case, if one accepts that just static loads to the wall are considered. Dynamic pressure loads are not limited by the AICC value because the local pressure at the wall is due to very rapid, non-equilibrium combustion where turbulence at the flame front plays a relevant role [3]. Therefore, the actual pressure peak endangering for short time intervals the containment integrity might be strongly underestimated (short time peaks usually exceed static pressure by a factor of 2-2.5 [14]).

The fundamentals of the AICC methodology are presented in Appendix A. Figure 11 shows the AICC results for the base case sequence discussed in this paper. The AICC formula takes as input the masses of the gas species (hydrogen, air and steam) and the containment ambient conditions before the combustion. The conditions pertaining to the dome, where the build-up of hydrogen stratification has been computed, are considered. Post-deflagration temperature is found to be below 700°C, while the AICC pressure value does not exceed 4 bar. The AICC value is lower than the design pressure of the containment (5.89 bar). Even though the resulting dynamic pressure would be higher than the design pressure, it should be realized that the oscillation frequency of such dynamic loads may be much higher than the natural frequency of containment wall. Therefore, the danger from short-time dynamic peaks can be neglected.

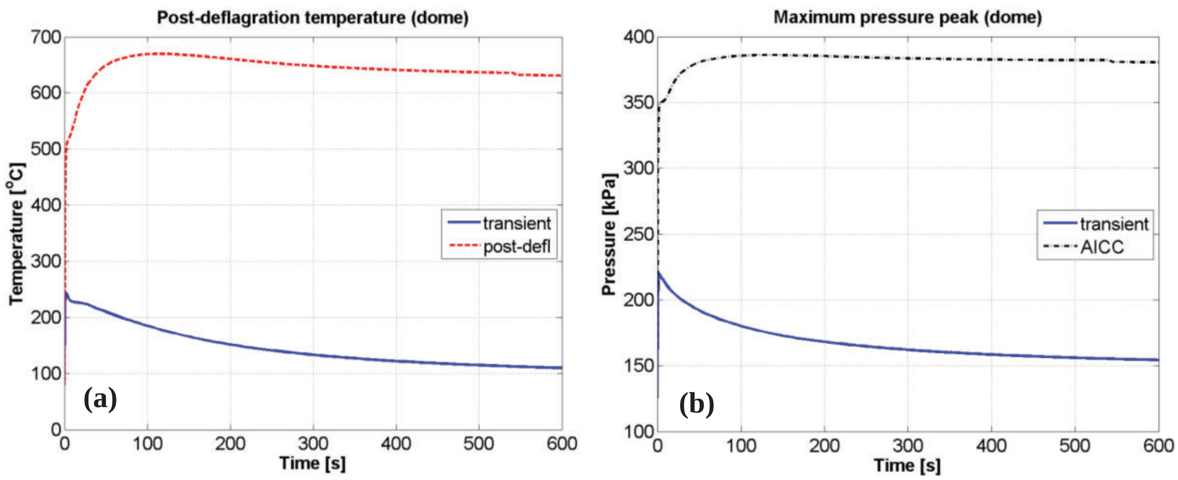

Figure 11. Computation of post-deflagration temperature (a) and AICC pressure value (b) for average conditions in containment dome (Vol.1s). Base case results.

5. CONCLUSIONS

The understanding and quantification of the hydrogen risk in containment requires reliable computer analyses, capable to solve three-dimensional flow pattern and gas distribution from the hydrogen release to the combustion characterization. Final step is the determination of thermal and mechanical loads on the containment shell. In this work, a SBO scenario with fast hydrogen-steam release from creep rupture of hot leg is identified as the most severe event for combustion hazard. An application of GOTHIC code modeling to full scale containment (large dry PWR containment) is detailed in order to demonstrate the practical applicability of GOTHIC for hydrogen risk assessment.

The conditions of the study are not fully covered by the validation of the code, which does not include high temperatures and the high velocity of the simulated choked jet. Nevertheless, reliable results are expected as the model respects the known guidelines, first of all a proper mesh size on the account of the injection size. GOTHIC is shown to be capable to predict build-up of hydrogen stratified conditions in containment dome and characterize the prevailing mixing mechanisms. A stratified cloud of hydrogen with 10% molar concentration forms in few minutes in the dome upper part. Sensitivity studies identified the importance of the opening of the steam generator room dampers in establishing an effective mixing flow with the dome. The effect from liquid sump in the break volume is minimal and can be reasonably neglected. Traditional analysis methods confirmed the reaching of flammable states which, however, do not endanger the containment integrity (statement valid without consideration of dynamic pressure loads).

Future work is foreseen on the study of specific hydrogen mitigation systems. Number and location of PARs to reduce the hydrogen risk can be studied using the developed GOTHIC model.

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APPENDIX A

The AICC methodology implemented in our study is described in this Appendix. The starting point to calculate the AICC pressure level is given by the following energy and mass balance equations [14]:

$$\left(m_{H2,i}c_{vH2,i} + m_{A,i}c_{vA,i} + m_{St,i}c_{vSt,i}\right)T_i + m_{H2,i}Q_{H2} = \left(m_{A,f}c_{vA,f} + m_{St,f}c_{vSt,f}\right)T_f \tag{2}$$

$$m_{H2,i} + m_{A,i} + m_{St,i} = m_{A,f} + m_{St,f} \tag{3}$$

where the left-hand-side corresponds to the reactants of the combustion chemical reaction (initial state denoted by subscript *i*) and the right-hand-side corresponds to the products (final state denoted by subscript *f*). The initial components of the gas mixture are hydrogen (subscript *H2*), air (subscript *A*) and steam (subscript *St*). All the hydrogen burns so that no hydrogen is present among the products. As defined for a closed thermodynamic system, the internal energy of the gas mixture is given by the product between the isochoric specific heat c_v and the temperature T. Q_{H2} represents the energy released per mass unit of burnt hydrogen (assuming that the steam produced by the combustion does not condense, Q_{H2} is given by the lower calorific heat, i.e. 120 MJ/kg).

The complete burn makes possible to calculate the mass of the components in the gas mixture after the burn. The so called Air Fuel Ratio (AFR), defined as the mass ratio of air to fuel (hydrogen) for a theoretical (stoichiometric) combustion, can be obtained from the balanced combustion reaction*. The following mass balances derive:

$$m_{A,bu} = m_{H2,i} \cdot AFR \tag{4}$$

$$m_{A,f} = m_{A,i} - m_{A,bu} \tag{5}$$

$$m_{St,f} = m_{St,i} + m_{H2,i} + m_{A,bu} \tag{6}$$

where $m_{A,bu}$ is the mass of air burnt for a stoichiometric combustion of the hydrogen in the gas mixture. Eq.(2) is solved considering the c_v of air and hydrogen from ideal gas model ($c_v = 5/2\,R$ for biatomic molecules) and the c_v of steam defined from steam tables. The gas temperature after the burn is obtained with an iterative procedure, on the account of the dependence of $c_{vSt,f}$ from the final temperature T_f.

Finally, the peak pressure that is theoretically achieved in the containment is calculated from the temperature of the gas mixture using the ideal gas law. One can either apply the ideal gas law using the free volume of the containment (or of the corresponding compartment of analysis), or alternatively [14]:

$$P_{AICC} = P_i \left(\frac{T_f}{T_i}\right)\left(\frac{n_{tot,f}}{n_{tot,i}}\right) \tag{7}$$

where n_{tot} is the total number of moles in the gas mixture. Eq.(7) is obtained from the ideal gas law by conserving the volume before and after the burn.

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* The balanced combustion reaction is $2H_2 + O_2 \rightarrow 2H_2O$. Half a mole of oxygen corresponds to a mole of hydrogen, which gives 8 kg oxygen per kg hydrogen (M_{O2} = 32 g/mol and M_{H2} = 2 g/mol). The mass fraction of oxygen in air is 23%, therefore the AFR results in 34.5 kg air per kg hydrogen burnt.