Simulation of Hydrogen Combustion Experiment THAI HD-22 with ASTEC Code

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ABSTRACT

The experiment on hydrogen combustion THAI HD-22, performed in a large cylindrical vessel, was simulated with the lumped-parameter severe accident code ASTEC. Simulated pressure, temperature and flame propagation are compared to experimental results. The simulated flow pattern in the vessel is also analysed.

1 INTRODUCTION

During a severe accident in a light water reactor nuclear power plant, substantial quantities of hydrogen may be generated by Zircaloy oxidation during the degradation of the reactor core. If the hydrogen concentration in the plant containment is within flammability limits, hydrogen combustion may occur, threatening the containment integrity. For this reason, both experimental and theoretical research of hydrogen combustion is being carried out.

Many experiments on hydrogen combustion in containment were performed in the THAI experimental facility, located at Becker Technologies in Eschborn (Germany). The THAI facility is a large vertical cylindrical vessel. The experiment THAI HD-22 dealt with hydrogen deflagration in a steam-air atmosphere [1]. A homogeneous air-steam-hydrogen mixture was ignited at the vessel bottom, and the upward and radial flame propagation were observed.

Within the field of nuclear safety, the main purpose of theoretical simulations of experiments on hydrogen combustion is to develop and validate computer codes that could be used for safety analyses of actual nuclear power plants. At present, the simulations may be divided in two groups:
— simulations with Computational Fluid Dynamics (CFD) codes that solve the transport equations of fluid mechanics using local instantaneous description, and use additional constitutive equations to describe combustion,
— simulations with lumped-parameter codes that describe the considered space as a network of control volumes, in which conditions are modelled as homogeneous, and simulate the combustion within the control volumes using algebraic models.

Although CFD codes solve the basic equations of fluid mechanics on the local instantaneous scale, the long computation times make them impractical for simulations of
combustion in actual plants. For this reason, simulations with lumped-parameter codes are useful, in spite of the relatively simple treatment of the complex phenomenon of combustion.

The experiment THAI HD-22 has already been simulated using various computer codes within the OECD International Standard Problem No.49 (ISP-49), which took place in 2009 and 2010 [2]. Although the experiment was quite successfully simulated by some participants, the differences between calculated results shows that additional simulations might still be useful.

In the present paper, the simulation of the THAI HD-22 experiment with the lumped-parameter severe accident code ASTEC is presented. Calculated pressure, temperature and flame propagations are compared to experimental results to assess the code. In addition, the simulated flow pattern in the vessel, caused by the combustion process, is analysed.

2 EXPERIMENT THAI HD-22

2.1 THAI Experimental Facility

The THAI experimental facility is located at Becker Technologies GmbH in Eschborn (Germany). It is basically a single-volume cylindrical vessel, with a volume of 60 m$^3$, an internal height of 9.2 m, and an internal diameter of the main part of 3.2 m (Figure 1). The vessel is insulated on the outside. The temperature of the walls is not controlled.

Figure 1. Schematic of THAI experimental facility (simplified figure based on [2])

Figure 2. Nodalisation of THAI experimental facility for ASTEC code (16-cells model)
2.2 Initial Conditions and Execution of the Experiment

In the present paper, only the rudimentary facts of the experiment, necessary for the understanding of the simulation, are provided. A detailed description may be found in the experiment report [2].

The following initial conditions were established before the ignition of the combustible air-steam-hydrogen mixture:

- pressure: 1.5 bar,
- atmosphere temperature: 92 °C,
- steam volumetric concentration: 25%,
- hydrogen volumetric concentration: 10%.

The mixture was ignited in the vessel lower plenum, 0.5 m above the floor (Figure 1). The pressure and temperature during combustion were measured. The upward and radial flame propagation were inferred from temperature measurements. Local hydrogen concentration was measured prior and after hydrogen combustion.

3 MODELLING WITH ASTEC CODE

The ASTEC code is a severe accident code, developed jointly by the Institut de Radioprotection et de Sûreté Nucléaire – IRSN (France) and the Gesellschaft für Anlagen- und Reaktorsicherheit – GRS (Germany) [3-5]. The module CPA (Containment Part of ASTEC), which deals with phenomena in the containment atmosphere, uses a lumped-parameter description: the containment is simulated as a network of control volumes (sometimes called “cells” or “zones”), which are connected by flow paths (“junctions”). The control volumes of the input model may correspond to actual containment compartments or not. Thus, to model a non-homogeneous atmosphere, large volumes may be divided into several control volumes. In each control volume, conditions are modelled as homogeneous. Thus, a “zero-dimension” description is used. The flow paths that connect control volumes are not repositories of mass or energy.

3.1 Geometric Models

Two different geometric models of the THAI vessel have been developed (Figure 2) [6]:

- a 2-cells model,
- a 16-cells model (Figure 2).

In the 2-cells model, the vessel was divided into cell 1 (Figure 2 – same cell 1 as in the 16-cells model) and cell 2 (all remaining volume). In the 16-cells model, the main cylindrical part was divided into 7 levels. Each level was further divided into 2 cells: a central cell, corresponding to the core region, with the base area equal to the cross-section of the vessel lower plenum, and another cell, which represents the remaining toroidal part. However, as ASTEC uses a lumped-parameter description, the actual shape of the cells is irrelevant.

The purpose of using the 16-cells model is to observe, apart from the pressure, also the flame propagation in the vertical direction, the non-homogeneous temperature and the flow pattern caused by the combustion process. The 2-cells model enables only the calculation of the pressure and of the average temperature in the main part of the vessel. However, the 2-cells model enables the validation of the ASTEC code for a coarser nodalisation that may have to be used for safety analyses, as the volume of a cell in the modelling of the containment of an actual nuclear power plant is usually at least of the order of several tens of m³.
The flame propagation is influenced by the modelling of the junctions. For both models, the length of each junction was prescribed as the distance between cell centres multiplied by 0.4. This value was selected, as it provided a good general agreement between experimental and theoretical results. Although a better agreement might have been obtained by fitting individual junction lengths (see section Results and Discussion), a single multiplying factor was used for consistency.

### 3.2 Modelling of Hydrogen Combustion

The FRONT model, incorporated in the ASTEC code, was applied. The model is described in detail in the corresponding manual [7]. In the input model, a number of adjustable parameters have to be prescribed. In the present work, the values used in the validation of the ASTEC code with the same experiment THAI HD-22, and provided in the description of the FRONT model, were prescribed.

The exact time of the ignition was not provided in the experimental results. From the analysis of temperature measurements in the lower plenum, the ignition time in the input model was prescribed as 1.61 s.

### 4 RESULTS AND DISCUSSION

In nuclear safety, the main threat of hydrogen combustion is the overpressure, which could cause containment failure. Thus, the calculated pressure is the first parameter that is compared to measured values when performing simulations of hydrogen combustion related to accidents in nuclear power plants. The calculated and measured pressures are shown in Figure 3. Although the maximum pressure obtained with the 2-cells model is somewhat lower than the measured value, the agreement of the timing of the pressure increase is the best. However, due to the coarseness of the 2-cells model, this agreement should not be given undue importance.

Figure 4 shows, also for the 2-cells model, the calculated temperature in the main vessel part and the measured temperatures at different elevations along the vessel axis. The general agreement is satisfactory. Thus, the results obtained with the 2-cells model show that, as to the values of calculated pressure and temperature, the ASTEC code could be used to model hydrogen combustion in an actual nuclear power plant containment with large volumes of individual cells.

For the 16-cells model, the calculated pressure is also shown in Figure 3. The agreement of the maximum value, as well as of the rate of pressure increase, is very good. However, the pressure increase in the simulation occurs much too early. To investigate the influence of the junction length on the timing of the pressure increase, an additional simulation was performed with the length of the junction connecting cell 1 (in which ignition occurs) to cell 2-1 equal to the actual distance between cell centres (which makes it longer than in the default model). As shown in Figure 3, this causes a somewhat later pressure increase. Thus, the timing of the pressure increase could be modified by varying the length of individual junctions.

In the remaining part of the paper, the analysis is restricted to results, obtained with the default 16-cells model. Namely, although a better agreement between experimental and simulation results might eventually be obtained by separately adjusting individual parameters, from the point of nuclear safety, it is much more important to assess the results, obtained with a unified modelling.
Figure 5 shows that, with the present model, the simulated flame propagation occurs much faster than in the experiment. To investigate the behaviour of the model implemented in the ASTEC code, a better fit of the flame front propagation with the experimental results was obtained by:
— dividing the proportionality coefficient, used to calculate the turbulence intensity, by 4 (instead of using the default value);
— prescribing that for each transition of the flame between cells, conditions are taken from the cell where the flame starts from to calculate the flame velocity, instead of using the conditions in the cell with the larger hydrogen concentration and the corresponding initial temperature (as was done for the default and simulation with the long 1st junction).

With these modifications, a better agreement between simulated and experimental flame propagation was obtained (Figure 5). However, the corresponding maximum pressure was much too low (Figure 3), and the pattern of the simulated pressure was different from the pattern of the measured pressure, contrary to the pressure when the simulated flame propagated much too fast. Thus, the results with the faster flame propagation were considered as more relevant for the time being. A discussion of the reasons of the observed behaviour will necessitate a thorough analysis of the model, implemented in the ASTEC code, and is beyond the scope of the present paper.

Temperatures at three representative vertical levels are shown in Figures 6, 7 and 8. In the experimental results, the highest maximum temperature always corresponds to the centre-line, whereas the other measurements correspond to the region at approximately two thirds radius distance from the vessel axis, at different orthoradial angles. In general, the temperature increase occurs much earlier in the simulation, which is similar to the discrepancy between the measured and calculated pressure (Figure 3). Also, the calculated temperature is much higher (up to 200 °C) than the measured one. Finally, the difference between the temperature in the centre-line and in the outer region after they have reached a maximum is noticeable in the simulation, whereas in the experiment the temperature has apparently become much more homogeneous over the vessel cross-section.

Figure 9 shows the simulated flow pattern at time 4.5 s. This value was selected as a characteristic time soon after the flame had propagated to the end of the vessel, and the pressure and temperatures have already reached their maximum values. The following pattern, caused by buoyancy, was established: the gas rises in the core region; in the middle and upper part of the vessel, the gas also flows in the radial direction to the outer region, whereas in the
lower part, the gas flows back from the outer region to the core region. This circulation loop is consistent with the analysis, presented in the OECD ISP-49 report. These results show that:

— atmosphere circulation, due to buoyancy, within a large vessel may be adequately simulated using a lumped-parameter description,
— the agreement between theoretical and experimental results is not merely in the pressure and temperature, which is constrained anyway by mass and energy balances, but also in terms of the flow process within the vessel.

At first sight, the discrepancies between simulation and experimental results (of all considered quantities) are sometimes too large. However, one should keep in mind the relatively simplified treatment of the complex phenomena of gas flow, heat transfer and hydrogen combustion used in lumped-parameter codes. Essentially, the simulation has qualitatively replicated the considered experiment. Quantitative discrepancies are indeed sometimes large (essentially for the temperature in the core region), but still not excessive. The overall outcome of the assessment will not be, that the agreement is “satisfactory” or “not satisfactory”, but that the simulation with the ASTEC code has replicated, with a sufficient similarity, the performed experiment.
5 CONCLUSIONS

The experiment on hydrogen combustion THAI HD-22 was simulated with the ASTEC computer code. The comparison between experimental and simulation results revealed the following:
— the pressure increase rate and maximum value were well simulated, although the simulated increase occurred earlier than in the experiment;
— the simulated flame propagated upwards much faster than in the experiment;
— the simulated temperature increased earlier than in the experiment as well, reaching higher values, and causing a less homogeneous temperature field later into the transient;
— the simulated atmosphere circulation, caused by combustion, is in accordance with the analysis of the experiment.

In terms of nuclear safety, the most important quantitative difference is between measured and calculated maximum pressure, which was less than 10% (although on the non-conservative side). Concerning the temperature, the highest quantitative differences were observed between measured and calculated values in the vessel core, which may even reach almost 50%. However, despite these large quantitative discrepancies, given the complexity of the simulated phenomena, the results support the applicability of the ASTEC code for simulations of hydrogen combustion in actual nuclear power plants.
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REFERENCES


