Simulation of ENACCEF Experiments on Hydrogen Combustion with the CONTAIN Code

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ABSTRACT

Experiments on hydrogen combustion, which were performed in the ENACCEF experimental facility, were simulated with the computer code CONTAIN. The ENACCEF facility consists of a vertical cylindrical tube connected to a cylindrical dome. In the experiments, a negative hydrogen concentration gradient was established along the tube before ignition in the tube bottom. Input models for the CONTAIN code were developed. The simulation results of flame propagation are compared to experimental data.

1 INTRODUCTION

During a severe accident in a nuclear power plant, hydrogen combustion may be generated during degradation of the reactor core. Subsequent accumulation of the hydrogen in the reactor containment may lead to hydrogen combustion, which could eventually threaten the containment integrity due to ensuing mechanical and thermal loads. This possibility has been confirmed during actual accidents in real nuclear power plants.

To investigate the phenomena of hydrogen combustion, experiments are being performed in various experimental facilities. One of these is the ENACCEF facility, located at the Institut de Combustion, Aerothermique, Reactivité et Environnement (ICARE) within the Centre National de la Recherche Scientifique (CNRS) in Orléans (France). Experiments on the ENACCEF facility were performed jointly by CNRS and IRSN (Institut de Radioprotection et de Sûreté Nucléaire, France).

Conditions in an actual nuclear power plant containment during a hypothetical hydrogen combustion should be predicted by using adequate physical models, implemented in computer codes. The codes are validated by simulating experiments and comparing experimental and simulation results. Basically, two different approaches are being used: lumped-parameter codes and Computational Fluid Dynamics (CFD) codes. Although CFD codes solve the basic equations of fluid mechanics and heat transfer (with additional constitutive equations) on the local instantaneous scale, their application to actual containments remains impractical due to long computation times. Therefore, in spite of the simplifications that lumped-parameter codes use in their description (as the space is subdivided into large control volumes - cells, in which conditions are modelled as homogeneous, and which are connected by flow paths), they are still more practical to use for actual containments (provided their results are sufficiently realistic). This is the rationale for their validation through simulation of experiments, where CFD codes could be used just as well. Although the use of lumped-parameter codes for simulation of some experiments on hydrogen combustion may seem
questionable (due to the inherent limitations of some in-built physical models), these
simulations may still provide valuable information about the code capabilities.

In the present work, the simulation of tests ENACCEF 765 and 736 with the lumped-
parameter code CONTAIN is described. In both tests, a negative hydrogen concentration
gradient was established along a vertical tube before ignition. Simulations were performed
within the participation of the Jozef Stefan Institute in the OECD International Standard
Problem No. 49 (ISP-49) on hydrogen deflagration, which took place in 2009 and 2010. The
simulated results of flame propagation are presented and compared to experimental data.

2 ENACCEF EXPERIMENTS

2.1 ENACCEF Experimental Facility

The ENACCEF facility is basically a vertical cylindrical “acceleration” tube, followed
by a cylindrical dome (Figure 1). The tube and the dome have the same axis. The internal
height of the tube is 3.2 m, and the internal diameter is 0.154 m, whereas the internal height of
the dome is 1.7 m and the internal diameter is 0.738 m. In a limited central part of the tube,
obstacles are placed at regular intervals in the form of horizontal rings with their outer
diameter equal to the tube internal diameter. A detailed description of the ENACCEF facility
is provided in the ISP-49 specification and report [1,2].
2.2 ENACCEF Tests 765 and 736

Two tests, referred to as 765 and 736, were simulated. In both tests, a negative hydrogen concentration gradient was established along the acceleration tube before ignition (Figure 3). The initial pressure was 1 bar. The air-hydrogen mixture was ignited at the bottom of the tube, and the upward flame propagation was observed.

![Initial H2 Concentration](image)

Figure 3. Initial hydrogen concentration along acceleration tube.

3 MODELLING OF HYDROGEN COMBUSTION IN CONTAIN CODE

The lumped-parameter CONTAIN code [3] was developed at Sandia National Laboratories (USA) under the sponsorship of the US Nuclear Regulatory Commission for analyzing containment phenomena under design-basis and severe accident conditions. CONTAIN also allows the simulation of hydrogen combustion. Three different combustion models may be used:

— a deflagration model,
— a diffusion flame burning model, and
— a bulk spontaneous recombination model.

In the present work, the deflagration model was used. The cell gas volume for deflagration burning is assumed to be well mixed with no accounting for variation of concentrations such as may be present ahead of and behind the flame front. CONTAIN is limited to modelling only low-velocity combustion: it does not model accelerated flames and detonation. Under circumstances where flame acceleration occurs, CONTAIN’s prediction of the loads, to which the containment will be subjected, may be non-conservative.

The deflagration model initiates a deflagration when threshold conditions are satisfied: the effective combustible mole fraction and the oxygen mole fraction must be higher than threshold values, whereas the mole fraction of the diluent must be lower than the threshold value. Threshold values are either internal values in the code or prescribed by the user.

The burn in a cell continues for a time (“burn time”) that is either prescribed by the user, or calculated by dividing a characteristic burn length by the flame velocity. The characteristic burn length is equal to the characteristic cell length, which is either calculated as the cube root of the cell volume or prescribed by the user. The flame velocity is either internally calculated or specified by the user. The CONTAIN model treats each deflagration
as a discrete event, and the burn time of that event is fixed once the deflagration is calculated to occur. The burn rate is determined by estimating the number of moles of combustibles and oxygen available to burn over the remainder of the burn time. The number of moles available to participate in the burn is determined from the number of moles present at a given time during the burn and by the mole fraction of combustibles or oxygen that must remain at the end of the burn. The burning rate is then set assuming a steady depletion rate of the most limiting constituent over the remaining burning time.

The burn can propagate to adjacent cells if:
- a connecting gas flow path is present,
- either the gas flow is into the adjacent cell or the flame velocity exceeds the absolute value of the gas flow velocity,
- the combustible gas, oxygen and water vapour concentrations in the adjacent cell allow propagation.

A time delay factor (between 0 and 1) delays the propagation of a burn to an adjoining cell by a fraction of the total burn time in the cell from which the burn propagates. Because CONTAIN is a lumped-parameter code, burned and unburned gases are mixed uniformly at each time step in the cell where the burn takes place. These gases flow into adjacent cells. If the time delay is too large, mixtures in adjacent cells may be rendered non-flammable because of the nonphysical introduction of burned gases and the burn may not propagate. If the time delay is too small, the total burn time may be too short and the peak containment pressure and temperature may be over-predicted.

4 MODELLING OF ENACCEF EXPERIMENT

Input models of the ENACCEF facility to simulate both tests with the CONTAIN code were developed. The flow and heat transfer parameters in the input models for the CONTAIN code were prescribed so that the flame propagates (at least) to the end of the tube. Two different simulation methods were used:
- “default” simulations, where the value of the flame propagation velocity in each cell was prescribed as two different values (corresponding to the regions below and above the first obstacle), and flame propagation to the end of the tube was achieved by a combination of flow-loss coefficients and time delay factors, and reducing the dome volume;
- “corrected” simulations, where the flame propagation to the end of the tube was achieved by prescribing independently the flame velocity in each cell and varying it adequately along the acceleration tube.

4.1 Geometric Parameters

The acceleration tube was subdivided into 20 cells which extend over the tube cross-section (Figure 2). In the region with obstacles, the region between two successive obstacles was modelled as one cell.

The dome was modelled in two different ways. For the default simulations, the dome was modelled as a single cell with a cross-section equal to the actual cross-section, and a height of 0.1670 m. This was necessary to achieve flame propagation over the entire acceleration tube with the prescribed values of other parameters. For the corrected simulations, the dome was modelled with the actual volume subdivided into 10 equal cells, which extend over the entire dome cross-section (as shown in Figure 2).
4.2 Flow Modelling

For the default simulations, the flow-loss coefficients were set to 0.3 for flow paths between all cells within the tube. These values (and other prescribed combustion parameters – see below) were adjusted for the flame to reach the end of the tube in the simulation of test 765 in approximately 0.1 s, as was observed in the experiment. For the corrected simulations, the flow-loss coefficients were set to 1.0 for flow paths between all cells within the tube as well as within the dome.

4.3 Combustion Modelling

The only parameters that were prescribed in the burning model were the flame velocity and the time delay factor for flame propagation to adjacent cells. Other parameters were calculated by the code.

For the default simulations, the flame velocity was prescribed as 15.0 m/s in the cells below the obstacles (that is, in the first four cells), and as 30.0 m/s in the remaining cells. For the corrected simulations, the following procedure was adopted: in each cell, the flame velocity was first prescribed as 15.0 m/s. If the flame did not propagate to the next cell, then the prescribed flame velocity was gradually increased, until propagation actually occurred. Then, the procedure was repeated in the next cell. Thus, flame acceleration was introduced implicitly in the input model, although the CONTAIN code does not model it.

For the default simulations, the time delay factor for propagation to an adjacent cell was set to 0.7 in all cells. For the corrected simulation, the value was set to 0.5 in all cells (which is in fact the default value used by the code).

It should be emphasized again, that the parameters in the combustion model were adjusted to allow the flame to reach the tube end. Thus, the calculated results do not demonstrate the capability of the CONTAIN code to predict flame propagation, but merely the way the flame propagates once it is assumed that it will indeed occur.

5 RESULTS AND DISCUSSION

The flame propagation results of the default simulations are shown in Figures 4 and 5. As could be expected, the simulated flame velocity is nearly constant, as CONTAIN does not model flame acceleration, and the prescribed flame velocity did not vary much (compared to variations actually observed in experiments).

As already mentioned, for the corrected simulations, flow velocities were prescribed in each cell of the input model. Following the procedure described above, the flame velocities were prescribed for simulation of test 765 as shown in Figure 6. Thus, flame acceleration was introduced implicitly in the input model, although the CONTAIN code does not model it.

The flame propagation results of the corrected simulation of test 765 are shown in Figure 7. It may be observed that the experimental and simulation curves assume more similar shapes than on Figure 4. Due to the complexity and short duration of the experiment, the time 0 s does not necessarily correspond to the ignition. Thus, the flame propagation might have been reasonably well replicated by the simulation.

The same procedure was used to prescribe flame velocities for the corrected simulation of test 736. The values are shown in Figure 8.

The flame propagation results of the corrected simulation of test 736 are shown in Figure 9. It may be observed that the experimental and simulation curves assume very similar shapes. Again, as, due to the complexity and short duration of the experiment, the time 0 s does not necessarily correspond to the ignition, the flame propagation might have been very well replicated by the simulation.
Figure 4. Test 765 (default simulation): experimental and calculated flame position.

Figure 5. Test 736 (default simulation): experimental and calculated flame position.

Figure 6. Prescribed flame velocities in corrected simulation of test 765.
Figure 7. Test 765 (corrected simulation): experimental and calculated flame position.

Figure 8. Prescribed flame velocities in corrected simulation of test 736.
6 CONCLUSIONS

Experiments on hydrogen combustion, performed in the ENACCEF experimental facility, during which flame acceleration occurred, were simulated with the CONTAIN code. Two different methods were used. In the default simulations, modeling of flame velocity by the CONTAIN code, which does not model flame acceleration, was applied. In the corrected simulations, flame acceleration was modelled by prescribing different flame velocities in different cells in the input model along the flame propagation path. The final results show that the flame propagation may, in this way, also be quantitatively predicted by the code, assuming that the user assumes that the flame will indeed propagate to the end of the tube.

In principle, the proposed approach could be extended to safety analyses of actual plants. However, additional validations, using experiments performed on other facilities, are necessary to prove (beyond reasonable doubt) the adequacy of the method.

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REFERENCES


