Experimental and Numerical Study of Flame Propagation with Hydrogen Gradient in a Vertical Facility: ENACCEF

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In case of hypothetic severe accident in a Pressurized Water Reactor (PWR), the interaction of the melted core with the cooling water can generate large amounts of hydrogen. Hydrogen can also be generated by oxidation of metals present in the corium recovery pool or in the basemat during the molten corium-concrete interaction phase. Then hydrogen is dispersed into the containment by convection loops arising essentially from condensation of steam released via the Reactor Cooling System (RCS) break or during corium-concrete interaction. The distribution of hydrogen can be more or less homogeneous, depending on mixing in the containment atmosphere. If considerable hydrogen stratification exists, then local concentration of hydrogen may become substantial, and may exceed the lower flammability limit. In case of ignition, the subsequent overpressure may adversely affect the containment building, internal walls and equipments integrities.

The evaluation of such scenarios needs CFD codes. However, a thorough validation process is necessary before using such codes with a high level of confidence. The original vertical facility ENACCEF, which represents a scale down of a PWR Steam Generator casemate, has been built to fulfill this objective.

The present work aims to validate the commercial code FLACS on ENACCEF flame acceleration tests characterized by a hydrogen gradient. Positive and negative gradients are considered and experimental data are compared to 3D calculations.

**Keywords**: hydrogen, hazard, combustion, gradient, CFD, FLACS.

1. Introduction

In case of hypothetic severe accident in a Pressurized Water Reactor (PWR), hydrogen would be produced during reactor core degradation and released to the reactor building, which could subsequently raise a combustion hazard. A local ignition of the combustible mixture would give birth initially to a slow flame, but depending on the composition of the reactive mixture and on the geometrical configuration of the containment (size, obstacles, etc.), it can accelerate strongly. For some conditions the accelerated flame can transit to detonation or be quenched after a certain distance. Even if no detonation transition occurs, the flame acceleration is responsible for the generation of high pressure loads that could damage the reactor’s building which is the last barrier to radioactive products release.
Different tools and methodologies are available to assess this risk, including semi-empirical criteria and lumped parameter codes, but CFD analysis is necessary for situations where the premixed flame can potentially accelerate in complex and densely obstructed geometries. The problem is then to build a predictive multidimensional model, in order to calculate the pressure load on the containment walls and equipments due to the different existing combustion regimes (slow and fast deflagrations, detonations) in sub-stoichiometric non-uniform hydrogen-air mixtures.

This article presents a specific validation of FLACS code based on three tests performed on ENACCEF facility. The first one deals with flame propagation in uniform gas mixture of 13% hydrogen and 87% air. The two other tests concern flame propagation in stratified initial mixture (test1: negative hydrogen gradient from 13 to 10.5 % and test2: positive hydrogen gradient from 10.5 to 13 %). After a brief description of ENACCEF, the experimental results are given, followed by the numerical results which are compared to the experiments.

1. ENACCEF EXPERIMENT

ENACCEF is a vertical facility of 5 m high and can be equipped with repeated obstacles in the bottom part. It is divided in 2 parts:

- the acceleration tube (3.2 m long and 154 mm i.d.), is equipped at its bottom-end with 2 tungsten electrodes as a low energy ignition device. At a distance of 1.9 m from the ignition point, 3 rectangular quartz windows (40 mm x 300 mm optical path) are mounted flush with the inner surface, 2 of them are opposed to each other the third one being perpendicular to the others (see figure 1, right). These windows allow the recording of the flame front during its propagation along the tube using either a shadowgraph or a tomography system. The tube is also equipped with 11 small quartz windows (optical diameter: 8 mm, thickness: 3 mm) distributed along it,

- the dome (1.7 m long, 738 i.d.) is connected to the upper part of the acceleration tube via a flange. This part of the facility is also equipped with 3 silica windows (optical path: 170 mm, thickness: 40 mm), perpendicular to each other 2 by 2 (see figure 1, left). Through these windows, the arrival of the flame can be recorded via a Schlieren or a tomography system.
Several obstacles can be inserted in the acceleration tube. Two different shapes have been used, annular obstacles of different blockage ratios (from 0.33 up to 0.63) and hexagonal mesh grids (with holes of 10 mm diameter spaced by 15 mm) for which the blockage ratio was equal to 0.6 (see Figure 3).

For all the experiments reported here, the acceleration tube was equipped with 9 annular obstacles, the first one being 0.638m from the ignition point and the distance between the obstacles was fixed to 0.154 m. The used obstacles correspond to a blockage ratio BR of 0.63;

\[ BR = 1 - \left( \frac{d}{D} \right)^2 \quad (1) \]
where D (D=0.154m) is the acceleration tube diameter and d (d=0.093) represents the inner diameter of the annular obstacle. The thickness of such obstacles is about 2 mm.

1.1. Instrumentation

ENACCEF facility is highly instrumented to follow the flame propagation: 16 UV-sensitive photomultiplier tubes (HAMAMATSU, 1P28) are mounted across silica windows (optical diameter: 8 mm, thickness: 3 mm) in order to detect the flame as it propagates (5 photomultiplier tubes are located along the dome and 11 along the acceleration tube).

Several high speed pressure transducers, (7 from CHIMIE METAL and 1 PCB) are mounted flush with the inner surface of the tube in order to monitor the pressure variation in the tube as the flame propagates and the pressure build-up is monitored via a PCB pressure transducer mounted at the ceiling of the dome.

Moreover, gas samplings are used to measure the gas composition along the facility. 6 gas sampling are located along the acceleration tube and 1 on the dome. Figure 4 shows the sensors location along the facility height.
1.2. Gas Injection system

The combustible mixtures were constituted of hydrogen distributed by Air Liquide (purity larger than 99.95%) and laboratory dry compressed air. Before each run, the whole facility was vacuumed down below 1 Pa. Then, the mixture is introduced in ENACCEF via flow meter controllers (MKS1179A) at the desired composition up to a final pressure of 100 kPa. All the experiments were performed at ambient temperature. The injection system is shown in figure 5.

![Injection system](image)

Figure 5: Injection system in the lower part of the facility

1.3. Ignition system

The ignition point is located at 138 mm from the bottom of the facility. Ignition system is composed of two electrodes. The energy delivered is estimated to 100 mJ.

2. EXPERIMENTAL PROCEDURE

All the experiments reported here are performed at ambient temperature (T=23°C) and atmospheric pressure. Three tests are considered:

**Test1: Uniform mixture test**

In order to produce a homogenous mixture, the facility is vacuumed down to 1 Pa before the premixed gas filling. The premixed gas composition (13%H2 + 87% air) is injected in the bottom and the top of the facility up to 10^5 Pa.
After ignition, the spatial flame velocity is derived from the flame luminosity recorded by photomultipliers (Figure 6). Several shots were carried out in order to obtain an average flame speed profile in the vessel and to assess the repeatability of the flame behaviour as it is illustrated on Figure 7.

From figure 7, one can see that the flame accelerates strongly in the obstacles field and reaches a maximum flame velocity of 535 m.s\(^{-1}\) before it drops to a velocity of about 400 m.s\(^{-1}\). This mixture is characterized by an expansion factor of 4.21. In this case, the ratio between the maximum speed and sound speed in the burned gas is higher than 0.5 and is in the choked regime.

**Test 2: Negative hydrogen gradient test**

In order to produce the H\(_2\) gradient in the lower tube, the facility is filled with a premixed gas composed by 10.5\% H\(_2\) and 89.5\% air up to 99725 Pa. Then, pure hydrogen is injected during 2 minutes in the bottom of the facility with rate of 0.5 l/min up to 1 bar. About 5 min later, gas sampling is done and the mixture is ignited. The 6 gas samplings are analyzed using a GC apparatus (Carboplot P7 column + TCD) with a relative uncertainty lower than 3\% in mass. The test is repeated 7 times and hydrogen gradient average is calculated (see figures 6 and 7)
As shown in Figure xx, flame velocity reaches 600 m/s which corresponds to choked regime as for test1.

**Test3: Positive hydrogen gradient test**

In order to produce the positive H$_2$ gradient in the lower tube, the facility is filled with a premixed gas composed by 13%H$_2$ and 87% air up to 89,325 Pa. Then, air-hydrogen mixture is injected during 9 minutes in the bottom of the facility with rate of 7.2l/min as follow:

- During the first 180 seconds, the injected mixture is composed by 13% H$_2$ and 87% air,
- From 181 to 300 seconds, the injected mixture is composed by 12% H$_2$ and 88% air,
- From 301 to 420 seconds, the injected mixture is composed by 11% H$_2$ and 89% air,
- From 421 to 541 seconds, the injected mixture is composed by 10.5% H$_2$ and 89.5% air,

At the end of this phase, gas sampling is done and the mixture is ignited. The gas samplings are analysed with a relative uncertainty lower than 3% in mass. The test is repeated 7 times. This injection procedure allows having hydrogen gradient as shown in the following figures 8 and 9.
Figure XX shows that for test 3, the flame speed remains lower than tests 1 and 2 and the speed depends on the gradient when a positive hydrogen gradient is established.

Theses tests were numerically investigated with FLACS CFD code of which the physical and numerical models used to calculate the hydrogen combustion are presented in the following section.

2. FLACS software and models

The description of FLACS software and its abilities mainly come from three papers (Middha & Hansen, 2009a; 2009b; Middha, Hansen & Storvik, 2009) and FLAC users’ manual (Gexcon, 2010).

FLACS is a computational fluid dynamics (CFD) code that solves the compressible Navier-Stokes equations on a 3D Cartesian grid using a finite volume method; it was developed in the early 1980s to simulate gas explosions in offshore oil and gas production platforms. Hjertager (1985, 1986) and Arntzen (1998) describe the basic equations used in FLACS. FLACS uses the Reynolds Averaged Navier-Stokes (RANS) equations and a k-ε model for turbulence (Harlow & Nakayama, 1967). The numerical model uses a second-order scheme for resolving diffusive fluxes and a second order k-scheme (hybrid scheme with weighting between second order upwind and second order central difference, with delimiters for some equations) to resolve the convective fluxes. The time stepping scheme used in FLACS is a first order backward Euler scheme. The SIMPLE pressure correction algorithm is applied (Patankar, S.V., 1980), and extended to handle compressible flows with additional source terms for the compression work in the enthalpy equation. Iterations are repeated until a mass residual of less than $10^{-4}$ is obtained. FLACS uses a “distributed porosity concept” which enables the detailed representation of complex geometries using a Cartesian grid. This approach represents geometrical details as porosities (opposite of blockage) for each control volume.

FLACS contains a combustion model that assumes that the flame in an explosion can be regarded as a collection of flamelets. One-step reaction kinetics is assumed, with the laminar burning velocity being a measure of the reactivity of a given mixture. The combustion model consists of two parts: a flame model and a burning velocity model. The β-flame model gives the flame a constant flame thickness equal to 3-5 grid cells, and assures that the flame propagates into the reactant with the specified velocity. A flame folding model has also been implemented to represent flame folding around sub-grid obstacles.

The burning velocity model consists of the following three models:

- a **laminar burning velocity model**, when the flame is smooth and governed by molecular diffusion, that describes the laminar burning velocity as a function of gas mixture, concentration, temperature, pressure, oxygen concentration in air and amount of inert diluents. For each fuel, the laminar burning velocities at different equivalence ratios are tabulated;
- a model describing **quasi-laminar combustion** in the first phase of flame propagation after ignition. Due to flame instabilities, the observed burning velocity increases as the flame
propagates away from ignition (due to flame wrinkling). In the quasi-laminar regime, the
turbulent burning velocity is given by:

\[
S_{\text{QL}} = S_L + 8S_L^{0.284} \mu^{0.912} \bar{l}_T^{0.196}
\]

- \( u' \): root mean square of velocity \([\text{m.s}^{-1}]\)
- \( \bar{l}_T \): turbulent length scale \([\text{m}]\)

- a model that describes turbulent burning velocity as a function of turbulence parameters
  (intensity and length scale). The model is based on a broad range of experimental data
  (Abdel-Gayed, Bradley & Lawes, 1987; Bray, 1990). The real flame area is described
  properly and corrected for curvature at scales equal to and smaller than the reaction zone.
  The turbulent burning velocity is given by:

\[
S_T = 15S_L^{0.784} \mu^{0.412} \bar{l}_T^{0.196}
\]

Then FLACS selects burning velocity as follows:

\[
S_u = \max\{S_L, \min\{S_{\text{QL}}, S_T\}\}
\]

FLACS has been evaluated with data from hundreds of gas explosion experiments in the
laboratory and in the field (Hansen, Storvik & Van Wingerden, 1999). A strong effort has been
made in recent years by GexCon to learn more about hydrogen dispersion and explosions and
improve FLACS in that area (Hansen, Renoult, Sherman & Tieszen, 2005; Middha, Hansen
& Storvik, 2007), so simulations of small and large-scale hydrogen explosions have also been
carried out. Comparison with experimental data revealed that in general, FLACS was able to
predict very representative values of concentrations and explosion overpressures (Middha,
Hansen, Grune & Kotchourko, 2007).

3. FLACS simulation

ENACCEFF modeling
Before comparing experiments to numerical results, mesh sensitivity study has been performed
to choose the adequate mesh to be used. Coarse and fine meshes had been built and compared.
The following table summarizes their characteristics:

<table>
<thead>
<tr>
<th>Meshes</th>
<th>Number of cells</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mesh1</td>
<td>419265</td>
</tr>
<tr>
<td>Mesh2</td>
<td>1002625</td>
</tr>
</tbody>
</table>

As obstacles play an important role in turbulence production, fine grids were needed to describe
the region around obstacles. To save CPU time, the obstacles thickness had been considered to
be equal to 10 mm instead of 2mm. As shown in the following figure, this hypothesis allows having the same results as with fine mesh.

![Flame speed graph](image1)

Mesh 1 with obstacle thickness of 10 mm had been used to analyse tests 1, 2 and 3.

- **Test1 analysis**

To perform the calculation, uniform initial mixture with 13H2 and 87%air had been considered. Moreover, heat exchanges between ENACCEF and the surrounding environment had been neglected.

As shown in Figures XX and XX, experiment and numerical results are in good agreement:

- flame acceleration phase in the acceleration tube is well predicted even if the maximal value is numerically underestimated. The deceleration phase after obstacle is well predicted,
- pressure time evolution is well calculated. The first pressure peak is predicted as well as the increase of pressure during the flame propagation in the dome area. As heat losses were neglected, numerical results overestimate the pressure.

![Pressure evolution graph](image2)

Figure XX: test 1- experiment and calculation comparison of flame speed

Figure: test 1- experiment and calculation comparison of pressure time evolution

Commentaire [t4] : Ajouter obstacles sur les graphs excel des résultats
Test 2

Test 2 had been repeated experimentally seven times. For simulation and as shown in figure XX, the mean initial mixture of the several shots had been considered. As for test 2, heat exchanges between ENACCEF and the surrounding environment had been neglected.

![Figure XX: test 1- hydrogen profile](image1)

![Figure XX: test 1- experiment and calculation comparison of flame speed](image2)

As shown in Figures XX, Flacs predict quite well the flame speed shape. Indeed, the acceleration and the deceleration phases are predicted. However, maximal flame speed is underestimated. To overcome this limitation, two parameters effect had been investigated:

- the first parameter concerns the laminar flame speed correlation used in FLACS (see eq XX).
  In fact, the default correlation used in FLACS underestimates laminar flame velocity for lean air-hydrogen mixtures compared to experimental results of F. Malet [FM] as shown in FigureXX. The use of this new correlation leads to an small increase of maximal flame speed.
√ the second parameter concerns the hydrogen concentration value near the ignition location which is not measured experimentally. For this propose, the hydrogen initial profile had been modified as shown in Figure XX. The combination of new laminar flame correlation and the hydrogen profile increases consequently the maximal value of flame speed (see Figure XX)

The effect of initial hydrogen concentration had been investigated by considering the hydrogen profile presented in figure XX.

Commentaire [t6] : Ajouter obstacles sur les graphs excel des résultats

Commentaire [t7] : Ajouter obstacles sur les graphs excel des résultats
Test 3

As Test2, Test3 had been repeated experimentally seven times. For simulation and as shown in figure XX, the mean initial mixture of the several shots had been considered. As shown in Figures XX, Flacs predict quiet well the flame speed shape but the maximal flame speed still underestimated even with the new laminar flame velocity correlation.

![Figure XX: test 1- hydrogen profile](image1)

![Figure: test 1- experiment and calculation comparison of flame speed](image2)

4. Conclusions

Flame acceleration has been studied experimentally and numerically by considering initial homogenous and stratified mixtures in the vertical ENACCEF facility. Flacs CFD simulations had successfully performed for homogenous 13% H2 and in the case where the H2 gradient varies initially from 13% to 10.5 and from 10.5% to 13%. The main features of the flame propagation profile along the setup have been correctly modelled by the code even though the modelled maximum flame velocity was lower than the one obtained in the experiments. Some improvements have to be implemented in the combustion model especially the correlation of turbulent flame velocity.

References


GexCon (2010). *FLACS v9.1 user’s manual*.


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