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Numerical Modeling of Premixed Combustion of Hydrogen and Steam Mixtures in Large Scale Experiments with Buoyancy Effects

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ABSTRACT

In the context of severe accident scenarios in a nuclear power plant, hydrogen management is an important component to ensure the reliability and proper functioning of critical systems. If the concentration of hydrogen reaches flammability limits, explosions in the containment can damage crucial safety systems and even compromise the integrity of the walls. CFD codes can serve as a numerical tool for the evaluation of the risks associated with hydrogen combustion during severe accidents. The objective of the present work consists of assessing the effects of a new correlation for the flame speed in order to further develop and validate the in-house code when dealing with hydrogen combustion. Furthermore, it has been observed that the new correlation predicts large values of the flame speed near the wall. In order to make the model as general as possible and to implement no user-defined parameters to cut off the wall distance, a wall-bounded version of the new combustion model is introduced, by means of a blending function similar to the one used in the $k-\omega-$SST turbulence model. Different combustion models are validated for slow deflagrations in a closed containment, namely the Thermalhydraulics Hydrogen Aerosol and Iodine (THAI) facility. Effects of flame propagation and buoyancy forces are investigated. Numerical results are presented and analyzed in terms of flame front development and pressure rise. Overall, the new combustion model results in a more robust approach that also provides good predictions in terms of flame evolution and pressure rise.

1 INTRODUCTION

During a severe accident in a nuclear power plant, hydrogen management is an important component to ensure the reliability and proper functioning of critical systems. If the concentration of hydrogen reaches flammability limits, combustion or explosion of hydrogen-air-steam mixtures in the containment can damage crucial safety systems and can even compromise the integrity of the walls. Computer Fluid Dynamics (CFD) codes are being used as a more accurate alternative to Lumped Parameter (LP), as they provide three-dimensional information with detailed temporal transients. Thus, numerous studies have been carried out to model hydrogen combustion with CFD codes, many of them also using the THAI facility as the benchmark case. Previous inhouse studies [1] have shown the potential of the Turbulent Flame-speed Closure (TFC) model for resolving the flow dynamics in THAI, even when using Reynolds Averaged Navier Stokes (RANS) for turbulence modeling. The same combustion model, along with the Eddy Dissipation Concept (EDC), were implemented in [2], obtaining similar results. The TFC model was tested with RANS and Large Eddy Simulation (LES) for the THAI vessel in [3] obtaining similar results in terms of the pressure rise. Alternative models have also been tested, like the one proposed in [4] where the flame development has been split into wrinkling due to the turbulence generated by the flame itself, wrinkling due to the fractal, wrinkling enhancement due to the leading point mechanism, and wrinkling generated due to the turbulence in the flow. For a comparison with LP codes, the reader can look at the work introduced in [5], where the results of different runs of THAI with LP codes are presented. Overall, the calculated temperature was higher than the experimental findings.

2 EXPERIMENT DESCRIPTION

The Thermalhydraulics Hydrogen Aerosol and Iodine (THAI) facility (described in [6]) is a containment with a main vessel of 9.2 m of height and 3.2 m of inner diameter made out of stainless steel, having a total volume of 60 m^3. The main cylindrical part has double walls with an inner wall of 22 mm thickness, a gap of 16.5 mm filled with thermal oil to control the wall heating and cooling, and an outer wall of 6 mm. All the containment is surrounded in its entirety with a 120 mm Rockwool thermal insulation. The instrumentation is mainly composed of an advanced flame front detection of 43 fast thermocouples installed at different radial and axial locations (to measure the flame arrival time as the appearance of the first temperature steep change) and a pressure measurement system comprised of four strain-gauge transducers (although as it is a slow deflagration case, there is not a considerable pressure difference between them, taking the results of the upper one for comparison with numerical results).

Three cases are selected to validate the combustion model implemented from the Hydrogen Deflagration set of experiments: HD-15, HD-22, and HD-24. The corresponding hydrogen and steam concentrations, as well as initial conditions, are summarized in Table 1. They consist of an ascending flame of a uniform mixture of hydrogen, air, and steam, which is ignited at the bottom of the vessel (at 0.5 m) and rises initially due to buoyancy, as the initial conditions assume low values of turbulence (after injecting and recirculating the mixture, the fans are disconnected between 10 and 15 minutes before igniting). Turbulent initial levels prior to ignition were not measured, so the values used for the CFD calculations are taken from previous studies in the literature [1], having $k = 1.5 \times 10^{-4}\,\mathrm{m}^2/\mathrm{s}^2$ and $\varepsilon = 4.8 \times 10^{-5}\,\mathrm{m}^2/\mathrm{s}^3$ for the three selected cases.

Table 1: Experimental initial conditions for the three selected cases.

Run	p (bar)	T (K)	x_{H_2} (%)	x_{H_2O} (%)
HD-15	1.504	366.0	9.9	0.0
HD-22	1.487	365.0	9.8	25.0
HD-24	1.472	363.5	9.9	48.0

3 COMBUSTION MODELS AND NUMERICAL SETUP

The solver used for this work is constructed over `XiFoam`, which is a solver in OpenFOAM developed for premixed combustion [7] that uses the regress variable $\widetilde{b}$ to determine the state of combustion. Thus, the progress of combustion is determined by the following transport equation:

$$\frac{\partial}{\partial t}\left(\overline{\rho}\widetilde{b}\right) + \frac{\partial}{\partial x_i}\left(\overline{\rho}\widetilde{u}_i\widetilde{b}\right) - \frac{\partial}{\partial x_i}\left(\overline{\rho}\left[D_l + D_t\right]\frac{\partial \widetilde{b}}{\partial x_i}\right) = -\overline{\rho}_u S_L \Xi \left|\frac{\partial \widetilde{b}}{\partial x_i}\right| , \tag{1}$$

where D_l is the laminar mass diffusivity, D_t is the turbulent mass diffusivity, ρ_u is the unburnt density, S_L is the laminar flame speed, and Ξ is the flame wrinkling factor. Combustion models are used to determine the D_t and Ξ variables. Three different models are implemented in this work, namely:

- **Turbulent Flame-speed Closure (TFC):** to be consistent with previous work carried out in Fluent [1], the TFC model [8] has also been implemented in OpenFOAM. The turbulent diffusivity is given by:

  $$D_t^{\text{TFC}} = D_t^{\text{TFC-Fluent}} = D_t^{\infty} = \frac{C_\mu}{\text{Sc}_t/\text{Le}}\frac{k^2}{\varepsilon} , \tag{2}$$

  where $C_\mu = 0.09$, Sc_t is the turbulent Schmidt number, Le is the Lewis number, k is the turbulent kinetic energy and ε is the turbulent dissipation. The wrinkling factor of the TFC combustion model can be expressed as:

  $$\Xi^{\text{TFC}} = \frac{Au'}{S_L}\text{Da}^{1/4} = \frac{Au'}{S_L}\left(\frac{l_t}{u'\tau_c}\right)^{1/4} , \tag{3}$$

  where the root mean square of the velocity fluctuations is expressed as $u' = \sqrt{2k/3}$, the integral length scale is given as $l_t = 0.2014k^{3/2}/\varepsilon$ [9] and the chemical timescale is $\tau_c = \kappa_u/S_L^2$ (where κ_u is the unburnt thermal diffusivity). With respect to [1], effects of preferential diffusion and quenching due to stretching effects are not included for brevity. Future efforts will focus on the inclusion of such effects.

- **Goulier Turbulent Flame-speed Closure (GTFC):** a recently obtained experimental correlation for the turbulent flame speed in lean hydrogen mixtures [10] was used to construct a combustion model called GTFC [11]. The turbulent diffusivity is given by:

  $$D_t^{\text{GTFC}} = D_t^{\infty}\left[1 - e^{-t/\tau_L}\right] = \frac{C_\mu}{\text{Sc}_t/\text{Le}}\frac{k^2}{\varepsilon}\left[1 - e^{-t/\tau_L}\right] , \tag{4}$$

  where t is the time measured from ignition and the timescale τ_L is given by:

  $$\tau_L = \frac{D_t^{\infty}}{u'^2} = \frac{1}{u'^2}\frac{C_\mu}{\text{Sc}_t/\text{Le}}\frac{k^2}{\varepsilon} . \tag{5}$$

  The flame wrinkling factor is obtained as:

  $$\Xi^{\text{GTFC}} = 1.613\left(\frac{R_f}{l_T}\right)^{0.333}\left(\frac{u'}{S_L}\right)^{0.526}(\text{Le})^{-0.140} \tag{6}$$

  where R_f is the flame radius, which is taken as the distance Y_f between the ignition and the highest location at which $\widetilde{b} = 0.5$, similarly to the THAI experimental runs.

- **Goulier Turbulent Flame-speed Closure wall-bounded (GTFC-wb):** preliminary simulations have shown that the GTFC combustion model predicts unrealistically large values of Ξ close to the wall, since the effects of the walls were not considered in the experimental campaign [10]. To address that, a wall-bounded model is created, where the wrinkling factor is a combination of TFC and GTFC, having:

$$\Xi^{\text{GTFC-wb}} = \Xi^{\text{GTFC}} + \mathcal{BF}\left(\Xi^{\text{TFC}} - \Xi^{\text{GTFC}}\right) , \tag{7}$$

where the blending function goes from $\mathcal{BF} = 1$ at the wall (leading to the TFC model) to $\mathcal{BF} = 0$ far from it (transitioning to the GTFC model). The blending function is defined similarly to the $k - \omega-$SST turbulence model:

$$\mathcal{BF} = \tanh\left(\left[\max\left(\frac{k^{3/2}}{\varepsilon y}, \frac{500\nu C_\mu k}{y^2\varepsilon}\right)\right]^4\right) . \tag{8}$$

The turbulent diffusivity of the GTFC-wb is that of the GTFC (see Equation 4).

Specific meshing strategies, such as simplifying the curved walls with straight ones, have been followed to obtain a grid with high-quality levels. Even if asymmetries have been found experimentally, as they are caused by stochastic processes like turbulence or hydrodynamic instabilities rather than by fixed obstacles (like the ignition system or injection pipe) [6], an axisymmetric grid has been used for simplicity. A mesh sensitivity study has been carried out, choosing as the final mesh one with 71614 cells and local refinement in correspondence to the walls and in the ignition region. The turbulence model used is the $k - \varepsilon$ with buoyancy source terms. The governing equations are solved with a pressure-based segregated PIMPLE algorithm with variable time step based on the maximum Courant number. The laminar flame speed has been obtained using the Bentaib correlation and a pressure correction term [1]. The temporal discretization has been performed with an `Euler` scheme whereas the convective terms use a `limitedLinear` scheme, which is based on the Sweby limiter for central differences.

4 RESULTS

Two figures are presented for each one of the three cases. On the left one, the vertical flame position Y_f in time t is shown, taking Y_f as the distance between ignition and the highest flame front location $\widetilde{b} = 0.5$, following the experimental approach. On the right, the pressure p evolution in time t is presented. Experimentally, a pressure probe located at the top of the facility was used. Numerically, the pressure value is more or less constant throughout the domain, taking the value from the axial location in the same location as the experimental probe. Numerical results obtained with Fluent in previous work [1] are included for comparison.

4.1 HD-15 case: 10% hydrogen, 0% steam

The first case is the mixture without steam. It can be seen in the left graph of Figure 1 what was previously mentioned: GTFC produces very large velocities that make the flame quickly expand. TFC and TFC-Fluent match at the end of the flame development but not at the beginning. Most probably, this can be caused by the different terms of the Fluent implementation. The GTFC-wb predictions lie between GTFC and TFC, tending at the beginning to GTFC (no wall-flame interaction yet) and to the trend of the TFC after half the vessel (once the flame fully reaches the wall). The pressure development from the OpenFOAM models overestimate the pressure peak, having a similar discussion as with the flame location: GTFC quickly burns the mixture, the GTFC-wb goes next, and then the TFC model. The comparison with

Fluent for the TFC shows again differences in the results, being likely related to the solver approach that Fluent uses (like implicit time marching or density-based solution algorithm). It is worth noting here that a density based approach in OpenFOAM is not available in the current implemetation. Hence, such effects will be the focus of future work. Nevertheless, the blending function adopted in the GTFC-wb appears to be a good strategy in terms of improving the current implementation of GTFC.

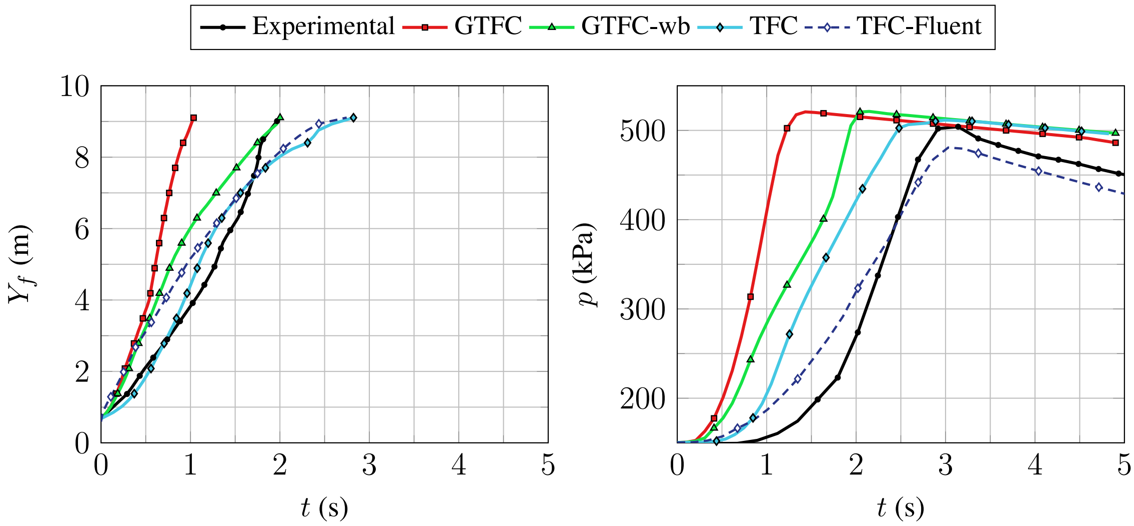


Figure 1: Flame front location (left) and pressure (right) evolution in time for the HD15 case.

4.2 HD-22 case: 10% hydrogen, 25% steam

The results for the case with low steam concentration are similar to those of the case without steam (see Figure 2): TFC and TFC-Fluent match at the later stages, GTFC burns really fast and GTFC-wb is between GTFC and TFC. However, in this case, it can be seen how the GTFC-wb captures the change in trend that occurs between 350 kPa and 400 kPa and predicts a faster flame front development towards the end of the vessel than the TFC (having a closer slope to the experimental values).

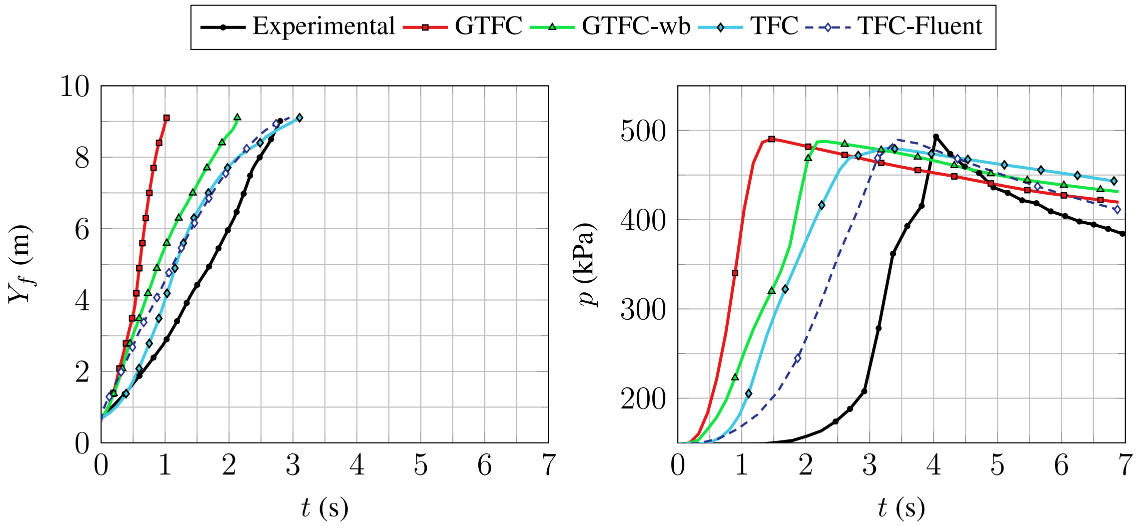


Figure 2: Flame front location (left) and pressure (right) evolution in time for the HD22 case.

4.3 HD-24 case: 10% hydrogen, 48% steam

For the case with the highest steam concentration (see Figure 3), GTFC-wb and TFC-Fluent give similar results for the flame front development, being between the GTFC and TFC values. However, for both the flame front development and pressure evolution, all the models return similar results that are closer between them than the results for the previous two cases.

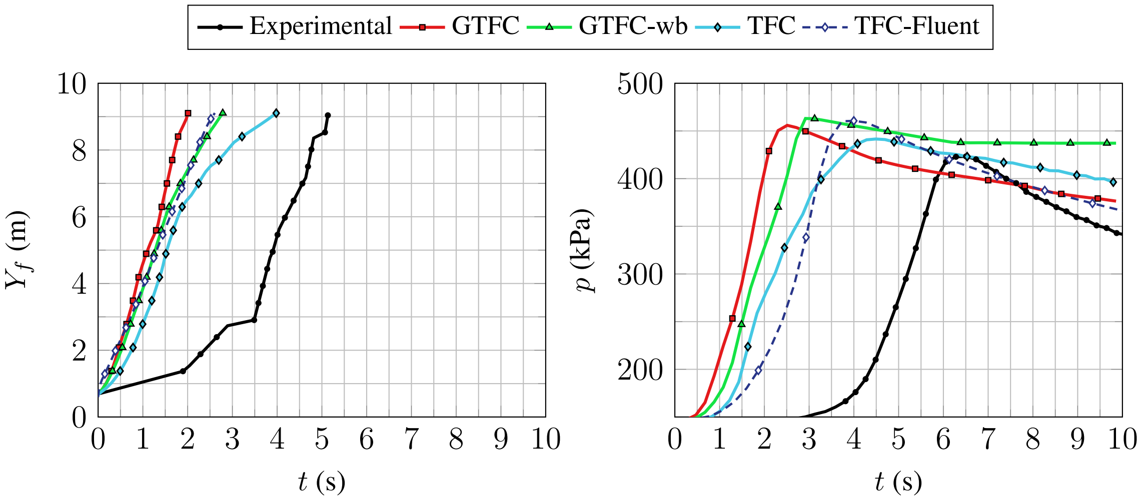


Figure 3: Flame front location (left) and pressure (right) evolution in time for the HD24 case.

4.4 DISCUSSION

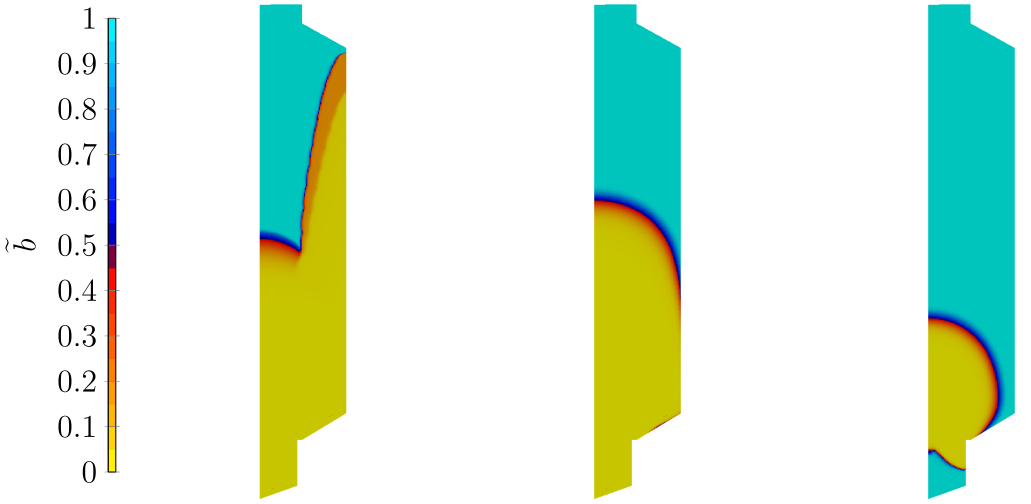
To further support the previous results, pressure metrics are compared, as summarized in Table 2. Three metrics are shown: the maximum peak pressure, the maximum pressure rise p', and the mean pressure rise (averaging only those values larger than 0.1 MPa/s before the peak pressure is reached). Each metric has the relative error with respect to the experimental value, keeping the sign in order to show both the overpredicting and underpredicting scenarios.

Table 2: Pressure metrics, grouped in three blocks: HD15, HD22, and HD24

Model	$p_{\max}$ (kPa)	$\epsilon_{p_{\max}}$ (%)	$(dp/dt)_{\max}$ (kPa/s)	$\epsilon_{(dp/dt)_{\max}}$ (%)	$(dp/dt)_{\text{mean}}$ (kPa/s)	$\epsilon_{(dp/dt)_{\text{mean}}}$ (%)
GTFC	520.96	1.08	560.26	55.60	350.24	49.07
GTFC-wb	521.87	1.25	445.71	23.79	215.22	−8.39
TFC-Fluent	481.91	−6.49	195.06	−45.83	154.66	−34.17
TFC	511.69	−0.72	280.55	−22.08	197.89	−15.77
GTFC	490.66	−7.25	498.48	5.64	328.43	21.35
GTFC-wb	489.05	−7.55	371.67	−21.24	198.06	−26.82
TFC-Fluent	489.58	−7.45	193.32	−59.03	167.85	−37.98
TFC	480.00	−9.26	238.88	−49.38	167.76	−38.01
GTFC	455.96	6.81	253.06	24.57	181.11	28.53
GTFC-wb	463.84	8.65	208.80	2.78	158.72	12.64
TFC-Fluent	460.99	7.99	230.90	13.66	165.00	17.10
TFC	441.70	3.47	179.32	−11.73	138.08	−2.01

It can be seen that the predictive capabilities of the GTFC-wb combustion model are consistently better than those of the GTFC with a few exceptions. When compared with the TFC, the GTFC-wb also shows better results, as it retains the information from the new correlation developed for lean hydrogen mixtures on which the GTFC is constructed. Even if there are some differences between TFC and TFC-Fluent, the results with Fluent have been included in order to have a comparison of the order of magnitude of the relative errors.

Finally, and to show how the wall-bound works, three regress variable $\widetilde{b}$ fields are presented in Figure 4 for the HD15 case. The original formulation of the GTFC has a fast flame developments in the proximity of the wall. The wall-bounded model restricts the flame development at the wall but still presents a faster flame development than the TFC. Similar results are obtained for the other cases and are not shown here for brevity.



(a) GTFC
$Y_f = 8.31$ m, $t = 1.0$ s.

(b) GTFC-wb
$Y_f = 5.59$ m, $t = 1.0$ s.

(c) TFC
$Y_f = 3.39$ m, $t = 1.0$ s.

Figure 4: Flame front development (regress variable field $\widetilde{b}$) for different models (HD15 case).

5 CONCLUSIONS

In this work, a new combustion model based on an experimental correlation for lean mixtures of hydrogen, relevant for nuclear safety management, is investigated in the context of the THAI test facility. It has been observed that the new correlation predicts large values of the flame speed near the wall, since wall effects were not considered in the experimental campaign. In order to overcome such limitation, a wall-bounded version of the new combustion model is introduced, by means of a blending function similar to the one used in the $k-\omega-$SST turbulence model. This new implementation shows good agreement with the experiments, performing accurately with three runs of the THAI vessel that had different mixture compositions. The $k-\varepsilon$ turbulence model with buoyancy source terms is adopted. One of the main future developments is to implement the buoyancy source terms in a $k-\omega-$based turbulence model, as it should give better results for internal flows, such as the one considered here. The performance of the wall-bounding should also be evaluated with other facilities to ensure that the behavior is robust and general. Nevertheless, the results obtained for this vessel already show an improvement with respect to previous models and they show the promising predictive capabilities of the wall-bounded combustion model.

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