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CFD Analysis of Explosions with Hydrogen-Methane-Air Mixtures in Congested Geometries

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Hydrogen is an enabler for de-carbonising the energy system in Europe by 2050. In the UK, several projects are investigating the feasibility of gradually blending hydrogen into the natural gas pipelines with the aim to reach 100% hydrogen in the gas network. However, the safe use of hydrogen as a fuel presents different challenges than conventional hydrocarbon-based fuels Advanced consequence models are powerful tools that can be used to support the design process and estimate the consequences of potential accidents. This paper analyses the predictive capabilities of two combustion models for explosion for hydrogen, methane and hydrogen-methane blends. The analysis involves the default combustion model in the commercial version (FLACS-CFD *v21.2*), and a new combustion model implemented in an in-house development version where the model for premixed turbulent combustion incorporates Markstein number effects (FLACS-CFD *v21.2 IH*). Experiments performed by Shell in unconfined pipe-racks, some of which were part of the EU funded project NaturalHy, are considered. The simulation results from both versions of FLACS-CFD are within a factor of 2 of the overpressures observed in the experiments. However, FLACS-CFD *v21.2 IH* appears to give an improved representation of the overpressure trend with variations in the hydrogen equivalence ratio observed in the experiments.

1. Introduction

The use of hydrogen as an energy carrier increases world-wide. Several research and innovation initiatives have been undertaken to promote the use of hydrogen as a decarbonisation option. In the UK, the Hy4Heat and the H21 projects are examining the feasibility of gradually blending hydrogen into the natural gas pipelines, with the aim to reach 100% hydrogen in the gas network. However, the safety-related properties of hydrogen are fundamentally different from those of the conventional hydrocarbon-based fuels. Therefore, significant efforts are directed towards developing methodologies and technologies for ensuring safe production, transport, storage and use of hydrogen in industry and society.

Advanced consequence models are powerful tools that can be used to support the design process and estimate the consequences of potential accidents. The CFD tool FLACS-CFD (Gexcon AS, 2021) has been continuously validated for fuel-air explosions involving hydrocarbons since the tool was first developed more than 40 years ago. Over the last two decades, efforts have been made to develop and validate the submodule FLACS-Hydrogen for hydrogen-air mixtures, including the PhD work of Middha (2010) and the EU funded project HySEA (Lucas et al., 2021). However, apart from the study presented in Middha et al. (2011), there has been less focus on simulating explosions involving hydrogen blended with other fuels.

The predictive capabilities of two combustion models for representing explosion overpressures for hydrogen, methane and hydrogen-methane blends are presented in this paper. The analysis involves the default combustion model in the commercial version of FLACS-CFD (*v21.2*), and a new combustion model implemented in an in-house development version where the model for premixed turbulent combustion incorporates Markstein number effects (*v21.2 IH*). Experiments performed by Shell in unconfined pipe-racks, some of which were done as part of the EU funded project NaturalHy, are considered here to document the performance of the two models.

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2. FLACS-Hydrogen

FLACS-Hydrogen is a module of the CFD tool FLACS-CFD (Gexcon AS, 2021) for hydrogen safety applications that was first developed in connection with the Network of Excellence (NoE) HySafe, funded by the European Commission. The model has since been developed through several R&D projects at Gexcon and is continually validated for hydrogen applications. This paper compares two versions of FLACS-Hydrogen: FLACS-CFD *v21.2* (released in 2021) and FLACS-CFD *v21.2 IH* (an in-house version).

2.1 Turbulence model

In line with the porosity/distributed resistance (PDR) concept, the standard *k-ε* turbulence model (Launder and Spalding, 1974) is modified to include the volume porosity, β_V, and the area porosity, β_j, of the control volume, resulting in the following transport equations for turbulent kinetic energy, *k*, and its rate of dissipation, *ε*

$$\frac{\partial}{\partial t}(\beta_v \rho k) + \frac{\partial}{\partial x_i}(\beta_j \rho u_i k) = \beta_v P_k - \beta_v \rho \varepsilon + \frac{\partial}{\partial x_i}\left[\beta_j \frac{\mu_{eff}}{\sigma_k}\frac{\partial k}{\partial x_i}\right] \text{ and} \quad (1)$$

$$\frac{\partial}{\partial t}(\beta_v \rho \varepsilon) + \frac{\partial}{\partial x_i}(\beta_j \rho u_i \varepsilon) = \beta_v P_\varepsilon - \beta_v C_{2\varepsilon} \rho \frac{\varepsilon^2}{k} + \frac{\partial}{\partial x_i}\left[\beta_j \frac{\mu_{eff}}{\sigma_\varepsilon}\frac{\partial \varepsilon}{\partial x_i}\right]. \quad (2)$$

Here ρ is the density, μ_{eff} is the effective dynamic viscosity, u_i, is the velocity in the ith direction, P_k and P_ε are the production of turbulence kinetic energy and of the dissipation rate of turbulence kinetic energy, respectively; $C_{2\varepsilon}$, σ_k and σ_ε are model constants.

2.2 Combustion model

The conservation equation for the fuel mass fraction, Y_F, is expressed as

$$\frac{\partial}{\partial t}(\beta_v \rho Y_F) + \frac{\partial}{\partial x_j}(\beta_j \rho u_j Y_F) = \frac{\partial}{\partial x_j}\left(\beta_j \rho D \frac{\partial Y_F}{\partial x_j}\right) + R_F, \quad (3)$$

where the diffusion coefficient, D, and the chemical reaction source term, R_F, are given by

$$D = C_{\beta D}\, s\Delta \text{ and } R_F = C_{\beta R_F}\frac{S}{\Delta}\rho\, min\left(1 - \frac{Y_F}{Y_{F0}}, 9\frac{Y_F}{Y_{F0}}\right). \quad (4)$$

Here, $C_{\beta D}$ and $C_{\beta RF}$ are model constants, S is the burning velocity, Δ is the control volume length in the direction of flame propagation and Y_{F0} is the initial fuel mass fraction.

The laminar burning velocity at atmospheric pressure, S_{L0}, is tabulated for different equivalent ratios. FLACS-CFD *v21.2* applies a correction to the hydrogen laminar burning velocity based on the Lewis number. Figure 1a shows the laminar burning velocity for different equivalence ratios used in FLACS-CFD *v21.2 IH* (S_L), before the correction, the laminar burning velocity used in FLACS-CFD *v21.2* with the Lewis correction ($S_{L,Le}$) and the laminar burning velocity presented by Taylor (1991). For mixtures of more than one gas component, the combustion properties are calculated as a weighted average of all the selected components, considering the volume fraction and the relative consumption of oxygen. Figure 1b shows the laminar burning velocity as a function of the hydrogen concentration for hydrogen-methane blends with an equivalence ratio of 1.1. The figure compares the laminar burning velocity used in FLACS-CFD *v21.2 IH,* before the correction (S_L), and the laminar burning velocity used in FLACS-CFD *v21.2* with the Lewis correction ($S_{L,Le}$) with the laminar burning velocity calculated using CHEMKIN presented by Ennetta (2017).

To model the regime of cellular flame propagation, both FLACS-CFD *v21.2* and FLACS-CFD *v21.2 IH* use the quasi-laminar burning velocity concept. In FLACS-CFD *v21.2*, the quasi-laminar burning velocity, S_{QL}, is modelled as

$$S_{QL} = S_L\left(1 + C_{QL} {r_F}^a\right), \quad (5)$$

where C_{QL} is a mixture-dependent model constant, r_F is the flame radius and a is a model constant. In FLACS-CFD *v21.2 IH*, the burning velocity in the quasi-laminar regime is described by

$$S_{QL} = S_L C^*_{QL}\left(\frac{r_F}{r_{F,cr}}\right)^{a^*}, \quad (6)$$

where $r_{F,cr}$ denotes the critical radius of the appearance of a cellular flame, and the model constants C^*_{QL} and a^* are both concentration- and mixture dependent.

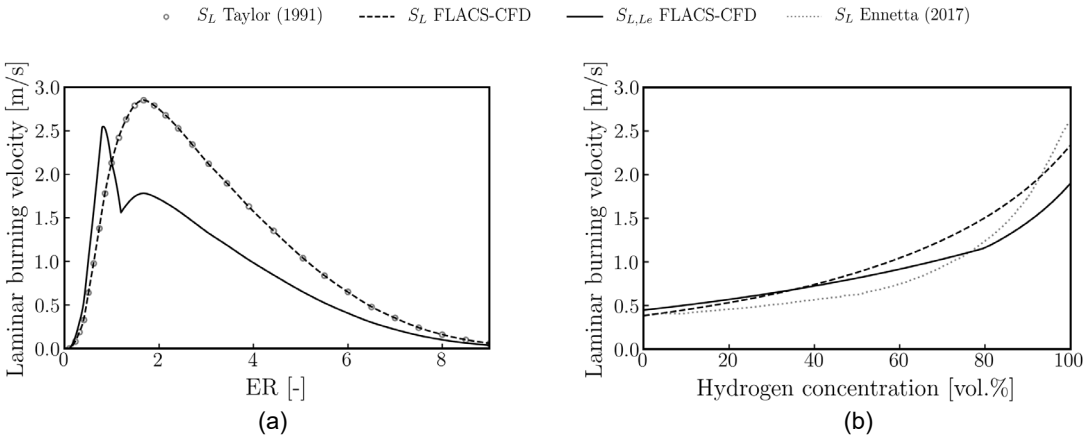

Figure 1: Laminar burning velocity vs. equivalence ratio for 100% hydrogen mixtures (a). Laminar burning velocity vs. hydrogen concentration for hydrogen-methane blends (b).

For the high intensity turbulent regime, the turbulent burning velocity correlation proposed by Bray (1990) is used in FLACS-CFD *v21.2*. The turbulent burning velocity, s_T, is expressed in terms of the effective root-mean-square turbulence velocity, u_{0k}, and the Karlovitz stretch factor, K, following Bradley et al. (2013)

$$\frac{s_T}{u'_k} = \alpha\, K^{-\beta}, \qquad K = 0.25\left(\frac{u'}{s_L}\right)^2\left(\frac{u' l_C}{\upsilon}\right)^{-0.5}, \tag{7}$$

with constant α and β empirical parameters. Here v is the kinematic viscosity and l_C is the combustion length scale. l_C is proportional to the distance from the point of ignition to the flame front in many scenarios. For confined geometries, this growth is bounded by a parameter that is proportional to the distance between the enclosing walls.

FLACS-CFD *v21.2 IH* computes α and β as a function of the strain rate Markstein number, Ma_{sr}, which depends on the mixture and the equivalence ratio. The expressions used for positive Ma_{sr} are

$$\alpha = C_\alpha 0.023(30 - Ma_{sr}) \text{ and } \beta = 0.0103(30 - Ma_{sr}), \tag{8}$$

where C_α is a model constant. For negative Ma_{sr} the expressions become

$$\alpha = C_\alpha 0.085(7 - Ma_{sr}) \text{ and } \beta = -0.0075(30 + Ma_{sr}). \tag{9}$$

The low intensity turbulent burning velocity correlation for both versions is (Arntzen, 1998)

$$s_T = 0.96 u'^{0.912} s_L^{0.284} \frac{l_C^{0.196}}{\upsilon} + s_L. \tag{10}$$

3. Experiments and model setup

(a) (b)

Figure 2: Experimental configuration (a) and geometry model in FLACS-CFD (b) for the 9-gate congestion type.

Hydrogen-air (Shirvill et al., 2019a) and hydrogen-methane-air blends (Shirvill et al., 2019b) were ignited in a 3 m x 3 m x 2 m rig with metal bars serving as obstacles at the Health and Safety Laboratory. Table 1 summarises the experimental setup. For the hydrogen-methane blends, an equivalence ratio (ER) of 1.1 was used. For the hydrogen tests, both lean and rich mixtures were tested. The congestion consisted of vertical and horizontal

pipes of about 26 mm diameter. In the lower part of the rig, 1 m long pipes were located vertically. For the 4-gate congestion type, four series of pipes were located around the ignition location. The 7-gate type consisted of seven series of pipes and the 9-gate type consisted of nine series of pipes. In the upper part, four layers of pipes were located horizontally for the 4-gate congestion type and seven layers for the 7-gate and 9-gate congestion types. Figure 2b shows the geometry used in the simulations. A core grid size of 12.5 cm was used, i.e. there were 16 cells across the minimum cloud size.

Table 1: Experimental configurations

Test	Hydrogen [vol.%]	Methane [vol.%]	ER [-]	Congestion type
Hydrogen06	100	0	0.969	4-gate
Hydrogen07	100	0	0.967	4-gate
Hydrogen08	100	0	1.226	4-gate
Hydrogen10	100	0	1.711	4-gate
Hydrogen11	100	0	0.800	4-gate
Hydrogen15	100	0	1.253	4-gate
Hydrogen16	100	0	1.167	7-gate
NatHy02	0	100	1.06	9-gate
NatHy04	25	75	1.09	9-gate
NatHy03	50	50	1.06	9-gate
NatHy05	75	25	1.08	9-gate
NatHy01	100	0	1.28	9-gate

4. Results

Figure 3a compares the maximum pressure observed in the experiments with the predicted maximum pressure by FLACS-CFD *v21.2* and FLACS-CFD *v21.2 IH* for different equivalence ratios. The highest maximum overpressure in the experiments occurs for the mixture with ER=1.253 and the lowest maximum overpressure is observed for the lean mixture with an equivalence ratio of 0.8. FLACS-CFD *v21.2 IH* predicts the maximum overpressure at an ER of 1.25, as observed in the experiments. This trend is in line with the higher laminar burning velocity for ER=1.25 than for the other ER tested (see Figure 1a). However, FLACS-CFD *v21.2* predicts the highest overpressure at an ER of about 0.97. The laminar burning velocity in FLACS-CFD *v21.2* is higher at ER=0.97 than at ER=1.25 due to the Lewis number correction. The predicted overpressure for lean hydrogen mixtures is lower with FLACS-CFD *v21.2 IH* than with FLACS-CFD *v21.2*. For the richest mixtures (ER=1.8), neither FLACS-CFD version captures the significant reduction in overpressure compared to the near-stoichiometric mixtures. At ER=1.8 the maximum simulated overpressure is about 1.5 higher than the observed overpressure. The maximum overpressures predicted by both FLACS-CFD versions are within a factor 2 of the measured values.

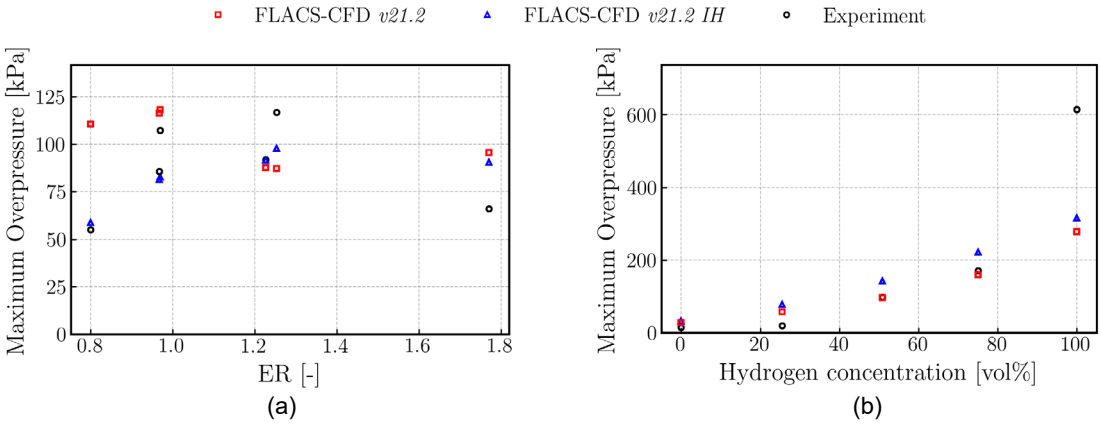

Figure 3: Maximum overpressure for 100% hydrogen tests for different equivalence ratios (a) and maximum overpressure for different hydrogen concentration for hydrogen-methane blends (b).

Figures 4a and 4b show the maximum overpressure with distance from ignition for tests Hydrogen06 and Hydrogen11, respectively. The maximum observed overpressure for the 4-gates geometry at sensors located perpendicular to the rig face occurred at 1.4 m from the ignition location except for test Hydrogen11. The simulated overpressure was also highest at 1.4 m for Hydrogen11. The flame speed increases when the flame front propagates between the obstacles. The flame propagates faster in simulations than in experiments.

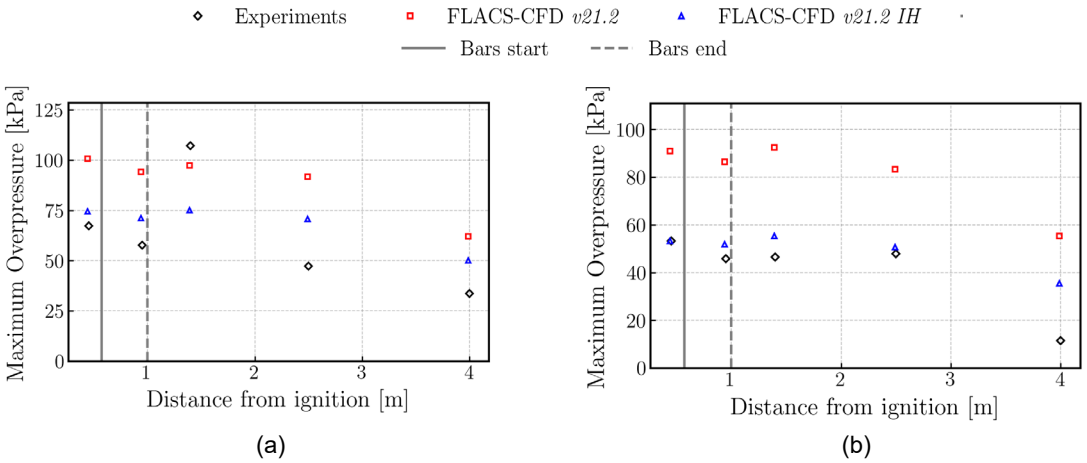

Figure 4: Maximum overpressure with distance from ignition for tests Hydrogen06 (a) and Hydrogen11 (b).

Figure 3b compares the maximum overpressure observed in the experiments with the predicted maximum overpressure by FLACS-CFD *v21.2* and FLACS-CFD *v21.2 IH* for different hydrogen concentrations (in hydrogen-methane blends). The maximum overpressure increases with the hydrogen concentration. The increase in maximum overpressure is more pronounced for the predictions by FLACS-CFD *v21.2 IH* than for experiments and FLACS-CFD *v21.2.* This can be explained by the differences in the burning velocity. As shown in Figure 1b, the laminar burning velocity in FLACS-CFD *v21.2 IH* is higher than the laminar burning velocity in FLACS-CFD *v21.2* and the one presented by Ennetta (2017) with 50% and 75% hydrogen. In test NatHy01, with 100% hydrogen, a deflagration-to-detonation transition was identified right after the end of the rig. The normalized pressure gradient at the exit of the rig predicted by FLACS-CFD *v21.2* and FLACS-CFD *v21.2 IH* exceeded 3 indicating that deflagration-to-detonation transition is likely to occur (Gexcon, 2021).
Figure 5 shows the maximum overpressure with distance from ignition for tests NatHy02 (5a) and NatHy03 (5b). In the NatHy02 experiment the maximum overpressure occurs when the flame reaches the end of the congested region, while in the simulations the maximum overpressure occurs inside the congested region. Both FLACS-CFD versions predict similar flame speeds before and after the congested region. In the congested region, the flame burns faster in FLACS-CFD *v21.2 IH*, resulting in higher overpressures. For test NatHy03 (50% hydrogen-50% methane), the laminar burning velocity computed by FLACS-CFD *v21.2 IH* is 1.347 m/s, while for FLACS-CFD *v21.2* is 1.093 m/s. At 0.32 m from the ignition location, the maximum overpressure predicted by FLACS-CFD *v21.2 IH* exceeds by about 1.9 times the overpressure observed in experiments. This overprediction is also observed for NatHy04 and NatHy05. The overpredictions by both versions are within a factor two of the values observed in the experiments.

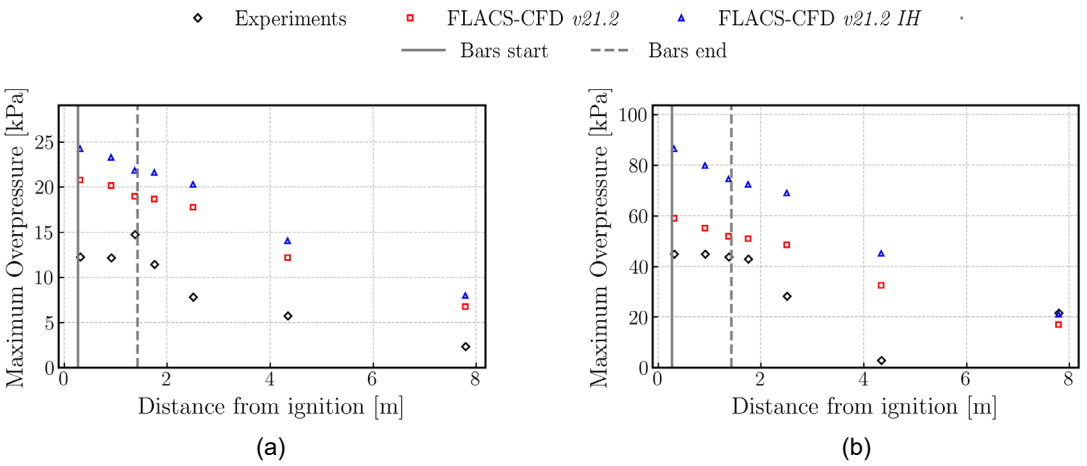

Figure 5: Maximum overpressure with distance from ignition at the line of sensors parallel to the wall for tests NatHy02 (a) and test NatHy03 (b)

5. Conclusions

Overpressure and flame speed predictions from FLACS-CFD *v21.2 IH* are compared to predictions from the released version FLACS-CFD *v21.2* for an experimental campaign involving explosions with various mixtures of hydrogen and/or methane with air. The in-house version FLACS-CFD *v21.2 IH* captures the trend of maximum overpressure with ER for pure hydrogen-air mixtures more accurately than FLACS-CFD *v21.2*. FLACS-CFD *v21.2* overpressure predictions are very conservative for ER=0.97. For methane-air and for hydrogen-methane-air blends, the maximum overpressure predictions by both versions are conservative. These comparisons do not consider the experimental uncertainty. Shirvill et al. (2019a) shows a difference of about 25% in maximum overpressure for Hydrogen06 with ER 0.969 than for Hydrogen07 with ER of 0.967. This suggests that it is not straightforward to assess the predictive capabilities of FLACS-CFD based on point-by-point comparisons. Further validation is necessary to understand the limitations of the versions for further model development.

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