Large Eddy Simulation of Syngas and Biogas Explosions Accounting for High Temperature and Pressure Effects

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Extended Abstracts

Environmental concerns and dwindling fossil fuel resources are placing ever growing demand for sustainable and pollution-free future energy sources. Hydrogen and hydrogen blended fuels generated from renewable sources such as syngas and biogas are promising potential candidates as future energy carriers. Synthesis gas (or Syngas) is a gas mixture containing carbon monoxide (CO) and hydrogen (H_2). Syngas can also contain carbon dioxide (CO_2) and other components such as water (H_2O). Biogas mainly comprises of methane (CH_4) and carbon dioxide (CO_2), produced by the anaerobic digestion of organic material by mesophilic bacterias. The composition of these gases depends on the type of process used to refine them. Several promising technologies are being developed for sustaining an economically viable production demands of biogas and syngas [1].

The future wide spread use of these blended fuels requires the knowledge of explosion parameters to help ensure their safe handling. Effect of fuel composition, maximum overpressures, maximum rate of pressure rise and burning velocity are the most important parameters for the assessment of process hazards and the safe design of handling equipment. However, there is limited knowledge of these parameters in the literature.

In the present study, numerical simulations have been conducted to aid our understanding of the combustion behaviour of syngas in elevated temperature and pressure conditions using an in-house version of the open source Computational Fluid Dynamics (CFD) code OpenFOAM. Combustion is treated with the Coherent flame model (CFM), which assumes that combustion takes place in the so-called flamelet regime in the relatively thin layers that separate regions of unburned and fully burned gases. The flame front locally propagates as unstretched laminar flame speed and under turbulence gets stretched and strained. This flame stretching due to turbulence increases flame surface which results in an increase of the burning velocity. Therefore the CFM combustion modeling simplifies the turbulent combustion problem by separating the combustion modeling from the analysis of the turbulent flow field. The unstretched laminar flame speed and laminar flame thickness are

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important parameters for this model. CFM was originally developed in the context of Reynolds Averaged Navier Stokes (RANS) approach with different source-term formulations [2-4]. It was recently extended to Large Eddy Simulations (LES) by [5] based on filtering the reaction progress variable and modelling the reaction rate through solving a balanced transport equation for the sub-grid flame surface density. A transport equation for subgrid flame surface density is better suited for non uniform grids and the also accounts for non-equilibrium effects within the source terms. This modified and extended CFM for LES has been previously implemented into the code by the authors and tested for simulating flame wall interaction [12].

The unstretched laminar flame speed (S_l) correlation for mixture of H_2/CO/CO_2/CH_4 in air is adopted from the work of [6]. This correlation was recommended to be valid for Syngas as base fuel with the blend of CO_2 in the range of (0 – 40%) and CH_4 in the range of (0 – 50%) at equivalence ratios (ϕ = 0.7 - 1.5) at 295 K and equivalence ratios (ϕ = 0.8 - 1.2) at 300 – 450 K for 1 atm pressure. The S_L correlation is presented as a function of initial mixture temperature, equivalence ratio and volume concentration of the constituent gases, respectively. Fundamentally laminar flame speeds for a reacting mixture are functions of unburnt reactants temperature and pressure (strong function of temperature and weak function of pressure). To account for the temperature and pressure effects in the situation of explosion, the S_l correlation is further modified to include the high pressure effects using power law expression following [7]. The recent experimental results of [8-10] were taken into account to data fit the temperature and baric indexes in the power law expression.

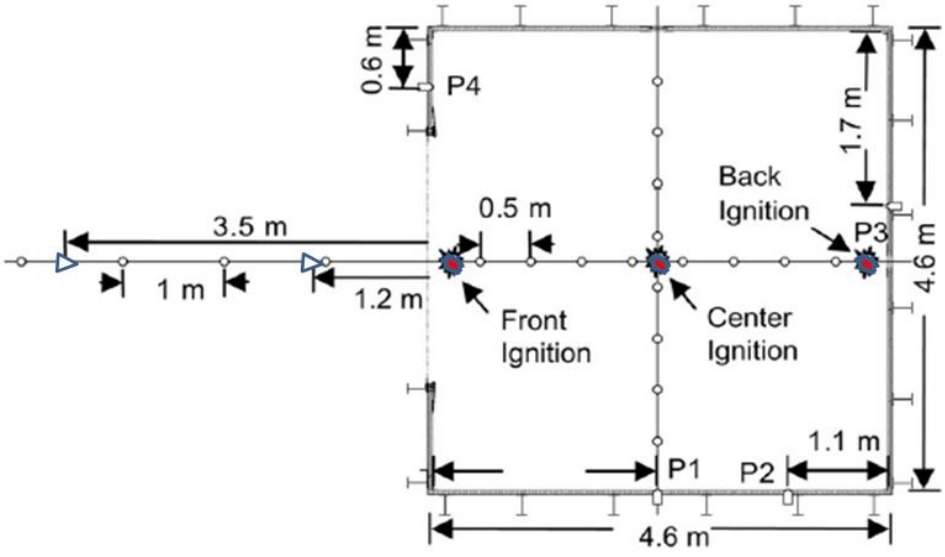

Figure 1. Configuration of the vented explosion test chamber showing pressure transducers (rectangles), thermocouples (circles) and blast-wave transducers (triangles) [11].

Predictions were conducted for the vented explosion tests of [8], which were performed in a test chamber of 4.6 × 3.0 × 4.6 (m^3) with a square vent of either 5.4 m^2 or 2.7 m^2 area located on one of the vertical walls. Four chamber pressure transducers were mounted to the chamber, one at the centre of the wall opposite the vent, one on the wall containing the vent, and two on a wall perpendicular to the vent (one on-axis with the centre of the chamber, one off-axis) as

shown in Figure 1. An hybrid hex-tet computational mesh was generated for the 64 m^3 using the 'snappyHexMesh' utility in OpenFOAM. The mesh distribution in the computation domain is shown in Figure 2. The volume enclosing the chamber is 30.0 × 15.0 × 35 m was also meshed to capture the venting of burned gas, the external explosions and to reduce the effect of boundary conditions on the numerical results. A cell size of 3 cm was used in the region inside the chamber and in the area immediately outside the chamber to resolve the external explosion. The total cells in computational mesh are approximately is 5 M.

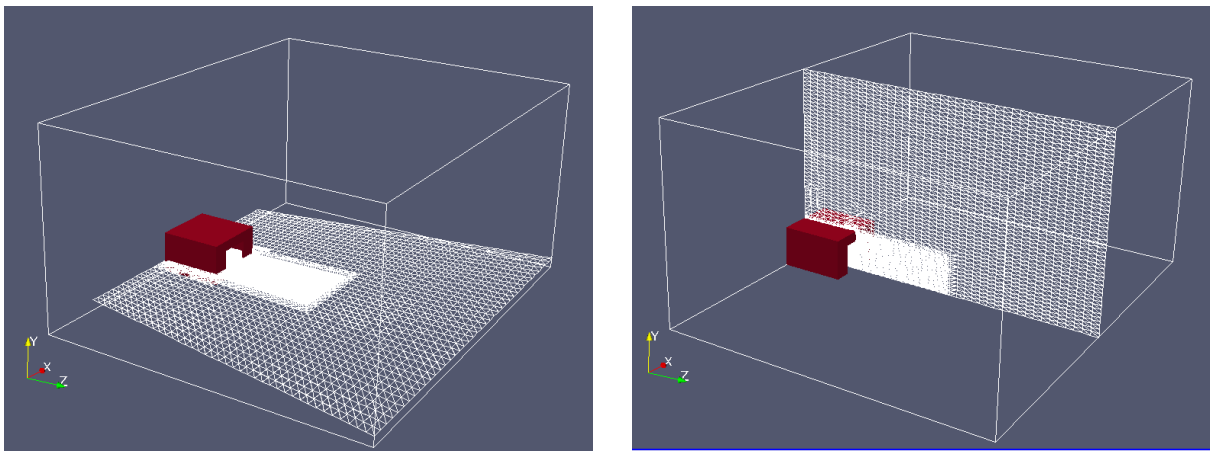

Figure 2. Computation domain and the mesh distribution in the vertical and horizontal directions.

The boundary conditions applied to the geometry were non-slip, adiabatic walls for the chamber walls and ground, and partial reflective 'wave- transmissive' pressure boundary conditions were used for the open boundaries to minimize pressure oscillation within the domain.

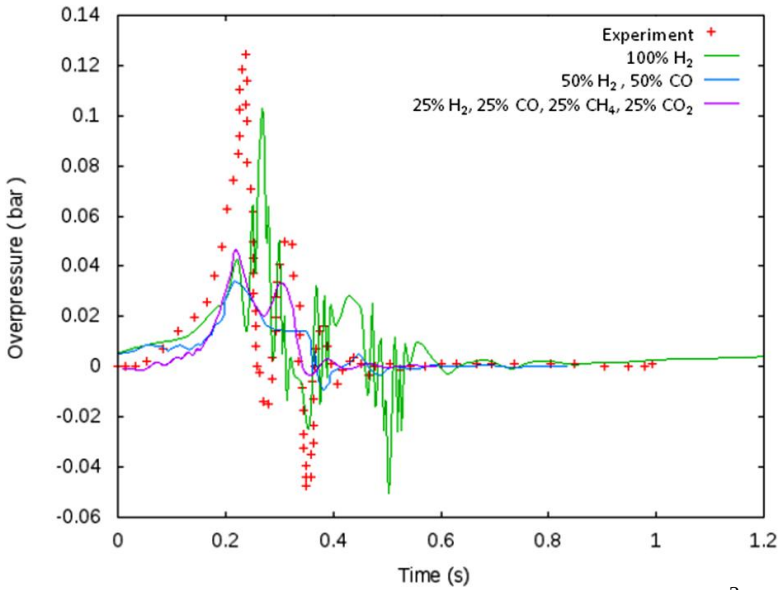

Figure 3. Pressure trace curves for the different fuel for the vent of 5.4 m^2 with ignition at the center of the chamber.

An open vent was used in the simulations with premixed fuel mixture initialized in the chamber volume. The random velocity field of the turbulence root mean square velocity u'= 0.5 m/s was initialized in the entire domain to match the experimental conditions. Three mixture compositions are considered, i.e. 18% hydrogen – which is approximately 0.53 equivalence ratio; 50% H_2 and 50% CO_2 at equivalence ratio 0.98 and 25% H_2, 25% CO, 25% CH_4, 25% CO_2 at equivalence ratio 1.1. These mixture compositions were chosen because of their similar laminar flame speeds.

In Figure 3, comparison is made between predicted and measured overpressures for the pure hydrogen explosion tests with the 5.4 m^2 vent inside the chamber, while the predicted overpressures for the two fuel compositions are also shown. It is seen that the peak over pressure increases with the increase of the mixture reactivity, i.e. the laminar flame speed values at high temperature and pressure. Hydrogen is the most reactive among the three and exhibits the highest overpressure. The addition of CO_2 and CO dilutes the fuel-air mixtures and decreases the burning rates of the blended fuels.

The laminar flame speed correlation considered in the present study is hence able to predict the laminar flame speed at high pressures with reasonable accuracy. The results have demonstrated the potential of the present numerical solver for simulating premixed turbulent flames of syngas and biogas under elevated temperature and pressure conditions.

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