This item was submitted to [Loughborough's Research Repository](#) by the author.
Items in Figshare are protected by copyright, with all rights reserved, unless otherwise indicated.

Numerical study of vented hydrogen explosions in a small scale obstructed chamber

PLEASE CITE THE PUBLISHED VERSION

<https://doi.org/10.1016/j.ijhydene.2018.07.078>

PUBLISHER

Elsevier © Hydrogen Energy Publications

VERSION

AM (Accepted Manuscript)

PUBLISHER STATEMENT

This paper was accepted for publication in the journal International Journal of Hydrogen Energy and the definitive published version is available at <https://doi.org/10.1016/j.ijhydene.2018.07.078>

LICENCE

CC BY-NC-ND 4.0

REPOSITORY RECORD

Li, Ruipengyu, Weeratunge Malalasekera, and Salah Ibrahim. 2018. "Numerical Study of Vented Hydrogen Explosions in a Small Scale Obstructed Chamber". Loughborough University.
<https://hdl.handle.net/2134/34073>.

Numerical study of vented hydrogen explosions in a small scale obstructed chamber

Ruipengyu Li^{a,*}, Weeratunge Malalasekera^a, Salah Ibrahim^b

^a*Wolfson School of Mechanical, Electrical and Manufacturing Engineering, Loughborough University, Loughborough, LE11 3TU, UK*

^b*Department of Aeronautical and Automotive Engineering, Loughborough University, Loughborough, LE11 3TU, UK*

Abstract

There is a growing need to understand and estimate the explosion hazards associated with hydrogen storage and utilisation. This paper presents a comprehensive numerical study on the explosion characteristics of a lean hydrogen-air mixture in a small-scale obstructed vented chamber. The large eddy simulation (LES) technique is employed to study the highly unsteady turbulence-driven explosion when the flame propagates past successive obstructions. A dynamic flame surface density (DFSD) model is applied to the filtered chemical source term in the LES to account for the progressive wrinkling of the deflagrating flame. The driving mechanism of pressure rise and the underlying physics of flame-obstacle interactions are illustrated using the detailed LES results. The paper considers 11 individual flow experimental configurations of various obstacle number, size and location. They are further classified into six groups to investigate the influence of the level of blockage and the separation distance between adjacent obstructions. Critical safety-related parameters including the maximum overpressure and its incidence time are analysed. A comparison with propane is also made to highlight the substantial overpressure and flame acceleration of hydrogen deflagrations. Satisfactory agreements have been obtained between the LES and the experimental data, and this confirms the capability of the developed computational models in capturing essential explosion features and information for the study of vented hydrogen explosions.

Keywords: Hydrogen explosions, Flame-obstacle interaction, Dynamic LES model, Overpressure, Flame wrinkling

*Corresponding author

Email address: r.li3@lboro.ac.uk (Ruipengyu Li)

1. Introduction

Hydrogen (H_2) as an alternative fuel and an energy carrier has many benefits due to its high heat value, renewable capability and the exclusion of harmful emissions [1]. The utilisation of hydrogen lies in hydrogen fuel cell electric vehicles [2, 3], hydrogen-fuelled internal combustion engines [4] and heating in buildings and industry [5]. However, some of its properties require additional engineering controls and considerations to ensure the safe use [6, 7]. As hydrogen is much lighter than air and rapidly dissipates when released, a leak often leads to fast mixing with surrounding air. Also, it has a wide range of flammability limits and relatively low ignition energy, making burning and accidental explosion of hydrogen-air mixtures more likely. The situation may be less severe in an open space since H_2 rises quickly into the atmosphere, but it can be a dangerous gas in confined or partially-confined regions involved in its production, storage, transport and end-user application [8].

Explosion hazards and safety issues while working with hydrogen has been a significant concern in its related storage, buildings and processing plants [7–10]. Compared with other common fuels such as methane (CH_4) and propane (C_3H_8), hydrogen explosions are potentially more dangerous due to its high combustion speed and excessively generated overpressure. The possibility of hydrogen leaks and subsequent explosions in situations such as tunnels and refuelling stations [7, 11] necessitates an improved understanding of the features and behaviours of hydrogen explosions. Yanez et al. [12] reported the production, discharge, accumulation and explosion of hydrogen during the Fukushima-Daiichi accident (March 11th 2011) and highlighted the devastating consequence even with the amount of H_2 involved.

Methods for protecting structures from internal explosions including venting and suppression require the knowledge of the explosion characteristics [13, 14]. It is known that the generated overpressure significantly contributes to the destruction of an explosion event. The overpressure is dependent on various conditions such as the fuel/air equivalence ratio and ignition location. Furthermore, the surrounding obstacle-generated turbulence can significantly enhance the explosion overpressure.

30 Thus an appropriate estimation of hydrogen explosion hazards has to consider the
31 effect of obstacles and turbulence. There has been a significant amount of experi-
32 mental work regarding the explosion features of H_2 . Besides medium or large scale
33 explosion tests [15], a few lab-scale experimental studies [16–19] have been conducted
34 in order to gain insights into the factors that influence the hydrogen-explosion be-
35 haviours such as vent area [18], vent burst pressure [16] and the position of ignition
36 sources [17, 18].

37 Computational fluid dynamics (CFD) is evolving as an efficient and reliable alter-
38 native to experiments and has been used in safety-related research in buildings and
39 off-shore processing plants [20–23]. There has also been literature related to hydro-
40 gen dispersion [7, 24–26], high-speed propagating hydrogen flames [27], impinging
41 hydrogen jet flame [28] and hydrogen explosions [8, 29, 30]. The abundant results
42 obtained from CFD simulations such as the overpressure and the detailed flow field
43 are particularly useful in assisting the assessment and the design of equipment, build-
44 ings and other structures. For example, Hansen et al. [13] have recently extracted
45 and estimated the explosion loads (actual forces) on the equipment with different
46 geometrical shapes from CFD simulations in large-scale scenarios using the com-
47 mercial software FLACS. Furthermore, performing a large number of well-validated
48 simulations can provide a database for various operating conditions including the
49 gas concentration, object geometries, vent area size, etc., and such statistically anal-
50 ysed data can help to propose new correlations as a fast and efficient tool for engi-
51 neers to estimate overpressure in gas explosions [31]. It is hoped that CFD results
52 will potentially help to give guidance to the engineers and safety consultants, e.g.
53 determining the optimal separation distance between adjacent buildings in a con-
54 gested area and the design strength of facilities. Despite the beneficial information
55 provided for hazards and risk analysis of hydrogen technologies, applying CFD mod-
56 els should be with cautiousness regarding their limitations and accuracy in certain
57 cases. Vyazmina and Jallais [29] pointed out that an explosion model validated for
58 large-scale enclosures may not be well-adapted for small-scale chambers ($< 1\text{ m}^3$).

Eventually, new CFD models for safety issues should go through a series of rigorous steps of validation and evaluation before being available to the end users, and this is also the idea of the model evaluation protocol for CFD assessment of hydrogen safety issues [32], recently proposed in the hydrogen community.

Although considered cost-effective in exploring explosion hazards and designing safer structures, the accuracy of the CFD method still relies on the modelling approaches for turbulence and combustion [29, 33]. For large-scale industrial applications, the use of Reynolds-averaged Navier-Stokes (RANS) [11, 29, 30, 32–35] has been dominant due to the computational efficiency and moderate accuracy. Within the academic research on gas explosions, the large eddy simulation (LES) based models are becoming more popular [36–42]. Gubba et al. [40] and Di Sarli et al. [41] have demonstrated that LES can be used to study and understand the sophisticated features of vented explosions in the presence of obstacles. Also, Molkov et al. [39] applied and validated an LES combustion model for hydrogen/air deflagration in a large-scale (78.5 m long) obstructed tunnel. The significant advantages of LES such as the ability to sufficiently account for the primary features of turbulent flows, as well as resolving the highly unsteady flame propagation may compensate the extra computational cost compared with RANS. For example, Di Sarli et al. [41] obtained an improved prediction of overpressure and flame speed using LES compared to the RANS simulation performed previously by Patel et al. [43] in the same explosion chamber.

Since modelling techniques for turbulent premixed flames are used for most gas explosions, an essential factor to consider when using LES is the sub-grid scale (SGS) combustion model as no portion of the filtered chemical source term can be resolved on an LES grid [44]. Another complexity lies in if the SGS model can adequately account for the effects of obstructions that are generally present in hydrogen production and processing facilities. The wrinkling and distortion of the deflagrating flame front significantly increase as it interacts with surrounding obstacles and the explosion can start from initially laminar and progress to be fully turbulent. Among

the available SGS models in the literature, the flame surface density (FSD) based models have been applied in a wide range of test cases of premixed combustion [45, 46]. FSD based approaches in LES often include solving a transport equation for the reaction progress variable with the filtered source term commonly closed by using algebraic formulations [47, 48] or solving an additional transport equation [49]. The algebraic FSD approaches have been used in several explosion-related studies [34, 36, 40, 41] due to its simplicity and robustness. However, as the model parameter is typically fixed in the simulation by the user, it may fail to predict the explosion features with a wide range of obstacle configurations and operating conditions.

In this paper, the characteristics and vital safety-related parameters of vented hydrogen explosions in a small scale chamber with obstructions have been studied using a dynamic flame surface density (DFSD) combustion model. Based on the renowned Boger et al. [47] algebraic model, the DFSD model evaluates the model coefficient on-the-fly, according to the information of the resolved flame front. Wang et al. [50] first proposed the model for simulating a growing turbulent flame kernel, while our study aims to apply and assess it in a more complex environment including flame-obstacle interactions and laminar to turbulent transition. Compared with some of the earlier numerical explosion studies such as [29], the main contribution made in this study is the insight into the pressure generation mechanism, specifically in small-scale (< 1 litre) turbulence-driven vented hydrogen explosions with multiple obstructions, as well as an assessment of the recently developed LES-DFSD approach using a series of test configurations. The objectives of this paper are twofold: (i) to study and understand the essential features of the vented hydrogen deflagrations and the influences of obstructions (e.g. number, position and size of obstacles) using LES; (ii) to evaluate the capability of the developed DFSD model in predicting the overpressure and flame acceleration in considered configurations and compared them with recent experimental data. The results presented in the paper intend to demonstrate the benefits and potential of LES as a computational tool for a range of types and scales of hydrogen explosions.

117 2. Experimental setup

118 The recent experiments from the University of Sydney [51] are used to validate
119 the developed computational model and to study the explosion characteristics of
120 hydrogen. The explosion chamber is shown schematically in Figure 1. It has a
121 square cross-section with a side of 50 *mm*, and the length is 250 *mm*, giving a
122 volume of 0.625 litres and an aspect ratio of 5:1. The chamber can accommodate
123 three removable baffle plates (also referred to as grids or obstacles in the rest of
124 the paper) with a schematic shown in Figure 1b. Each baffle consists of five 4-mm
125 wide and 3-mm thick strips evenly separated by six 5-mm gaps, producing an area
126 blockage ratio (ABR) of 40% in the flow direction. A single baffle also creates a
127 volume blockage ratio (VBR), i.e. the ratio of blocked volume to the total volume of
128 the chamber, of 0.48%. These may be located at any of the three locations: 19 mm
129 (B1), 49 mm (B2) and 79 mm (B3) from the base. A further solid obstruction with
130 a square cross-section can be placed such that its lower surface is 96 mm away from
131 the base plate. Two solid obstacles may be used, a small one with a cross-section of
132 12×12 mm or a large one with a size of 25×25 mm. They create ABRs of 24% and
133 50% (VBRs of 1.152% and 5%), respectively.

134 While the focus of this paper is on hydrogen, the experiment also uses two
135 other fuels, namely liquid petroleum gas (LPG) and compressed natural gas. In the
136 experiment, the fuel-air mixture enters the atmospheric pressure chamber through a
137 non-return valve, and it is allowed to rest before each ignition event. The stagnant
138 fuel-air mixture is then ignited by focusing the infrared output from an Nd: YAG
139 laser 2 mm above the base, and this sets the time zero for each experimental run.
140 The hinged flap at the chamber exit rises 1 second before ignition to allow venting
141 throughout the explosion. Pressure is recorded at 25 kHz using two Keller type
142 PR21-SR piezo-electric pressure transducers located in the base plate as well as in
143 the wall of the chamber. High-speed imaging of laser-induced fluorescence from OH
144 (LIF-OH) with a repetition rate of 5 kHz is also performed providing an excellent
145 representation of the evolution of the reaction zones.

Figure 1: Specifications of the explosion chamber used in the experiment [51] (not to scale, dimensions are in mm).

Table 1: Grouped configurations to study the influence of obstructions

Group	Description	Configuration
1	Baffles are progressively increased and kept furthest from ignition end	00BS, 0BBS, BBBS
2	Baffles are progressively increased from ignition end	B00S, BB0S, BBBS
3	Two baffles are positioned at different stations of the chamber	BB0S, B0BS, BBBS
4	One baffle is positioned at a different station of the chamber	B00S, 0B0S, 00BS
5	Central obstacle size increases with all three baffle plates present	BBB0, BBBS, BBBL
6	Small or large central obstacle without any baffle plates	000S, 000L

146 A total number of 11 configurations (see supplementary material for a list of
 147 schematics) has been investigated numerically for the present study. A code is used
 148 to identify each configuration to specify the obstruction locations and size of the
 149 solid obstacle. For example, 0B0S stands for the case where one baffle plate is at
 150 B2, and the small central obstacle (S) is placed downstream of the ignition point,
 151 and BBBL represents the configuration where three baffle plates B1, B2 and B3, as
 152 well as the large central obstacle (L), are positioned in the same order away from
 153 the chamber bottom.

154 Table 1 displays the configurations classified into six groups to facilitate the
 155 analysis of the impact of obstructions. Groups 1-4 aim to investigate the influence
 156 of the turbulence-generating baffle plates, while groups 5 and 6 intend to examine
 157 the impact made by changing the size of the central obstacle. This classification
 158 of flow configurations is made to represent various means of blockage including the
 159 number and location of the baffles as well as the size of the solid central obstacle.

160 3. Numerical setup

161 3.1. The combustion model

162 The premixed deflagration flame is governed by equations for conservation of
 163 mass, momentum and energy. A transport equation for a reaction progress variable
 164 c is also included, representing the chemical state of the fuel-air mixture. It is defined
 165 such that $c = 0$ where the mixture is unburned and $c = 1$ where it is fully burned.
 166 The general form of the Favre-filtered transport equation for $\tilde{c}$ is

$$\frac{\partial \tilde{\rho} \tilde{c}}{\partial t} + \frac{\partial}{\partial x_i} (\tilde{\rho} \tilde{u}_i \tilde{c}) = - \frac{\partial}{\partial x_i} (\tilde{\rho} \tilde{u}_i \tilde{c} - \tilde{\rho} \tilde{u}_i \tilde{c}) + \overline{\frac{\partial}{\partial x_i} \left(\rho D \frac{\partial \tilde{c}}{\partial x_i} \right)} + \bar{\omega}_c \quad (1)$$

167 where the filtered source term, $\bar{\omega}_c$, can be closed using the concept of the flame
 168 surface density as

$$\bar{\omega}_c = \rho_u S_L^0 \Sigma \quad (2)$$

169 where ρ_u is the density of the fresh gases, and S_L^0 is the unstrained laminar burning
 170 velocity. Σ is the sub-grid scale flame surface density, which is expressed using the
 171 algebraic formulation [45]:

$$\Sigma = 4\sqrt{\frac{6}{\pi}}\Xi_{\Delta}\frac{\tilde{c}(1-\tilde{c})}{\Delta} \quad (3)$$

172 where Δ is the combustion filter width and Ξ_{Δ} is the sub-grid scale flame wrinkling
 173 factor. Thus, the $\tilde{c}$ -equation adopted for the present study is [45, 50]

$$\frac{\partial \bar{\rho} \tilde{c}}{\partial t} + \frac{\partial}{\partial x_i} (\bar{\rho} \tilde{u}_i \tilde{c}) = \frac{\partial}{\partial x_i} \left(\frac{\rho_u \Xi_{\Delta} S_L^0 \Delta}{16\sqrt{6/\pi}} \frac{\partial \tilde{c}}{\partial x_i} \right) + 4\rho_u S_L^0 \sqrt{\frac{6}{\pi}} \Xi_{\Delta} \frac{\tilde{c}(1-\tilde{c})}{\Delta} \quad (4)$$

174 where the modified diffusion term, the third term in Eq. (4), is included to control
 175 the filtered flame thickness and to reproduce the correct laminar propagation speed
 176 in the absence of sub-grid scale turbulence effect [45]. Note that Δ should be larger
 177 than the mesh size Δ_x (typically $\Delta \geq 5\Delta_x$) so that the filtered progress variable
 178 gradients can be well resolved on an LES grid [50]. In the present study, $\Delta = 6\Delta_x$
 179 is used.

180 The SGS wrinkling factor Ξ_{Δ} measures the ratio between total and resolved
 181 flame surfaces locally, and it accounts for the sub-grid scale flame surface lost by the
 182 filtering process [50]. A fractal-like expression for Ξ_{Δ} , originally proposed by Wang
 183 et al. [50], is adapted for the present investigation:

$$\Xi_{\Delta} = \left(\frac{\Delta}{\delta_c} \right)^{\beta} \quad (5)$$

184 where the inner cut-off scale, δ_c , is lost in the filtering process and it requires to be
 185 prescribed by the user. Note that δ_c should be of the order of the laminar flame
 186 thermal thickness, δ_L^0 [52], and $\delta_c = 4\delta_L^0$ is used in this work. The model parameter β
 187 is determined dynamically by comparing the test-filtered and resolved flame fronts:

$$\beta \approx \frac{\ln \left(\langle |\widehat{\nabla \tilde{c}}| \rangle / \langle |\nabla \widehat{\tilde{c}}| \rangle \right)}{\ln \left(\sqrt{1 + (\widehat{\Delta}/\Delta)^2} \right)} \quad (6)$$

188 with $\hat{\Delta}$ being the width of the test filter. The test-filtering ($\hat{\cdot}$ operator) and the
 189 spatial-averaging ($\langle \dots \rangle$ operator) procedures in Eq. (6) are carried out using an
 190 implemented Gaussian filter [53]. The test-filter and averaging-filter widths are set
 191 as $\hat{\Delta} = 1.1\Delta$ and $\Delta_m = 3.0\hat{\Delta}$, respectively. Note that $\hat{\Delta}$ should be larger than the
 192 filtered flame thickness (typically, $\hat{\Delta} \geq \Delta$) [52], and the size of Δ_m has been found
 193 to have a minimal effect on the results presented in this paper. The laminar burning
 194 velocity and thermal flame thickness are set as $S_L^0 = 125$ cm/s [54] and $\delta_L^0 = 0.12$ mm
 195 [55], respectively, for the lean hydrogen-air mixture of equivalence ratio $\Phi = 0.7$. In
 196 the simulation of the deflagration, Eqs. (5) and (6) are used to automatically adjust
 197 the degree of SGS flame wrinkling Ξ_Δ based on the instantaneous resolved flame
 198 characteristics.

199 *3.2. Computational details*

200 The LES computation of the vented hydrogen deflagration has been carried out
 201 using the in-house code PUFFIN [56]. The code solves the compressible form of
 202 mass, momentum and scalar equations, discretised using a finite volume formulation
 203 on a Cartesian grid. The Gaussian spatial filtering and the DFSD model using
 204 Eqs. (4) to (6) have been implemented in the code to account for the potential
 205 progressive flame wrinkling in the deflagration.

206 The domain of the explosion chamber has dimensions of $50 \times 50 \times 250$ mm, and
 207 the size of the whole computational domain is $325 \times 325 \times 500$ mm. A non-reflecting
 208 boundary condition [46] is applied to the boundaries of the far field, to minimise the
 209 effect of reflected pressure waves on the internal pressure field of the chamber. The
 210 chamber domain constitutes $85 \times 85 \times 423$ cells in the x , y and z directions, respec-
 211 tively. They are distributed uniformly in the chamber giving a grid size of $\Delta_x \approx 0.59$
 212 mm. The mesh size is chosen to ensure that the filtered flame thickness ($\approx \Delta$) is
 213 smaller than the gaps between the strips of the baffle plates. The grid is expanded
 214 from the chamber toward the far-field boundaries to save the computational time.
 215 Adiabatic and no-slip boundary conditions are employed on the solid walls of the
 216 chamber, and the 1/7th power law wall function of Werner and Wengle [57] is used

217 to calculate the shear stress at the solid wall. Subgrid-scale turbulence is modelled
218 using the dynamic Smagorinsky eddy viscosity model [58].

219 Conservation equations for scalars use second-order central difference scheme for
220 diffusion terms. SHARP [59] is used for advection terms of the scalar equations
221 to avoid problems associated with oscillations in the solution. Time integration of
222 scalar equations uses the Crank-Nicolson scheme. Further details of the numerical
223 scheme are given elsewhere [see 56] and are thus not presented here. The initial
224 velocity field is quiescent, with a random perturbation to generate initial turbulence.
225 Flame is initialised using a burned flame kernel pre-filtered at the filter width Δ . It
226 is superimposed at the ignition point of the domain to initiate each simulation. The
227 kernel is hemispherical and has a radius of 3 mm for all the simulations. Two other
228 computational grids ($\Delta_x \approx 1 \text{ mm}$ and $\Delta_x \approx 0.75 \text{ mm}$ within the chamber) have
229 been investigated to examine the solution dependence on the mesh resolution, and
230 the variation in the maximum overpressure is found to be small ($< 4\%$) between the
231 intermediate and fine (used in this paper) grids. The quality of LES for the present
232 grid resolution ($\Delta_x \approx 0.59 \text{ mm}$ within the chamber) is characterised according to
233 Popes criterion [60]. At least 80% of the total turbulent kinetic energy is resolved
234 in the majority of the flame region, considering the fully turbulent phase of the
235 explosion in the configuration BBBS. All the LES simulations are performed on an
236 HP Z840 workstation with an Intel Xeon 3.5 GHz processor. Under the current
237 mesh resolution, a run for the case BBBS requires 312 CPU hours until the leading
238 edge of the flame exits the explosion chamber.

239 4. Results and discussion

240 Numerical simulations of vented hydrogen explosions have been performed for 11
241 individual configurations grouped in Table 1. Section 4.1 presents a global study of
242 the deflagration emphasising the underlying physics of the flame-obstacle interaction
243 and the mechanism of pressure build-up within the explosion chamber. Some crit-
244 ical safety-related parameters including the maximum overpressure and the flame

propagation speeds obtained from the LES are compared against the experimental results in section 4.2. The focus is to analyse the effects of obstructions such as the number and the location of the baffle plates and the size of the central obstacle. The ability of the developed computational setup in capturing the essential explosion characteristics is also assessed. Finally, the results between hydrogen and propane are discussed in section 4.3 to highlight the differences regarding their explosion characteristics.

4.1. A phenomenological study

The physical phenomena and the typical flame behaviours behind the hydrogen-air deflagration are discussed in this section using the configuration B0BS as an example. Figure 2 shows the shape of the typical hydrogen-air explosion flame extracted experimentally and numerically for configuration B0BS. The reaction zone is marked using a sequence of high-speed images of LIF-OH in the experiment [51], which is indicated using the contour of $\tilde{c}$ numerically from LES. Evidently from Figure 2, LES can reproduce both the flame structure and the global propagation speed. It can be noticed that the flame shape continuously changes during the explosion. Initially, the flame is laminar and expands hemispherically before impinging on the first baffle plate. It penetrates the grid and separates into four fingers primarily resulting from the ‘geometric’ stretch caused by the strips of the baffle plate. Then, they quickly merged with each other due to the lateral spread of the flame. Meanwhile, the surface area of the flame tends to decrease before reaching the next grid. The flame then jets through the gaps of B3 and immediately strikes the square obstacle. It can be seen that the flame front is very much corrugated when interacting with the obstacle. After passing the last obstruction (square obstacle), the flame is significantly wrinkled ($t = 4.4$ ms of the LIF-OH images) and propagates towards the chamber outlet. The blockage introduced by the central obstruction also leaves a small amount of unburned mixture behind it when wrapped by the flame front. It is then consumed when the leading flame point is further downstream, as indicated by both high-speed and LES images. It can be noticed that the flame spreads faster

Figure 2: Comparison of deflagration flame propagation between simulations and experiments for configuration B0BS. Top: LIF-OH high-speed images from the experiments [61]. Bottom: LES flame images contoured by $\tilde{c}$. t_0 is set to match the position of the flame leading point with the high-speed image. Time intervals between successive LES images are kept the same as the experiment.

274 in the upper part of the combustion chamber due to the increased flame distortion
275 caused by the interaction with the upstream obstacles.

276 Figure 3a shows the calculated overpressure distribution along the axial direction
277 on the mid-plane of the chamber for the configuration B0BS. The pressure has been
278 found to be nearly uniform on the xy -plane (i.e. cross-section) of the chamber.
279 During the explosion process, the magnitude of the internal pressure rises as well as
280 its spatial range of influence, which is approximately the region of the burned gases.
281 Note that the wall pressure (downstream of the central obstacle) measured in the
282 experiments is consistently lower than the base and it may suggest that a pressure
283 gradient exists within the chamber [61]. It is further confirmed by LES with a
284 negative pressure gradient vertically along the chamber, which drives the explosion
285 gases out across the outlet. A significant pressure drop to atmospheric level due to
286 venting can be found near the exit of the combustion chamber. Furthermore, both
287 the numerical (not shown here) and the experimental results [61] confirm that the
288 two pressure probes on the chamber base and the wall downstream of the central
289 obstacle have given similar pressure patterns in all the test cases. Therefore, the
290 analysis and discussion of the rest of this paper will focus on the pressure at the
291 bottom of the vessel.

292 Figure 3b shows the overpressure history computed by LES and the correspond-
293 ing gas expansion and venting strength in the explosion chamber, with the purpose
294 of describing the trend of pressure development during the hydrogen explosion. It is
295 known that the pressure rise in the semi-confined enclosure is a consequence of the
296 competition between the two events: (i) gas expansion caused by combustion tends
297 to promote the pressure build-up; (ii) discharge of the explosion gases through vent-
298 ing tends to release the internal pressure. The volumetric flow rates of gas expansion,
299 $\dot{V}_{expa}$ and venting, $\dot{V}_{vent}$ can be readily computed using the LES velocity field. $\dot{V}_{expa}$
300 can be represented by the rate of volume change of the fresh unburned gases with the
301 burned gases. In LES, this may be evaluated from $\dot{V}_{expa} = \frac{\partial}{\partial t} V_b \left(1 - \frac{\rho_b}{\rho_u} \right)$, where ρ_u
302 and ρ_b are the densities of unburned and burned mixtures, respectively. The volume

303 occupied by the burned gases, V_b , can be evaluated by integrating $\bar{c}$ over the entire
 304 computational domain Ω : $V_b = \int_{\Omega} \bar{c} dV$ [50]. The venting rate $\dot{V}_{vent}$ is computed as
 305 the volume flow rate across the chamber exit plane: $\dot{V}_{vent} = \int_{A_{exit}} \vec{u} \cdot \vec{n} dA$, where
 306 $\vec{u}$ and $\vec{n}$ are the velocity and its normal direction, respectively. It is clear that
 307 $\dot{V}_{expa} > \dot{V}_{vent}$ will lead to a rise in the internal overpressure, while the opposite will
 308 result in a pressure drop.

Figure 3: Distribution of pressure along the chamber and the mechanism driving the pressure rise: configuration B0BS.

309 Shown in Figure 3b is the evolution of $\dot{V}_{expa}$ and $\dot{V}_{vent}$ with time during the
 310 explosion event. The overpressure is also shown to compare with the venting and
 311 expansion profiles. As it can be seen from Figure 3b, $\dot{V}_{expa}$ is only slightly greater
 312 than $\dot{V}_{vent}$ in the early stages of the explosion, so the chamber pressure slowly in-
 313 creases. The absence of B2 in configuration B0BS gives a relatively large separation
 314 distance between the two baffles. It leads to a slower rise in the combustion rate due
 315 to a long residence time so that the venting strength takes over the expansion at t
 316 ≈ 3.15 ms, and consequently, LES predicts a slower pressure rise close to B3. The
 317 intense flame-obstacle interaction after passing B3 leads to a sharp rise in the gas
 318 expansion. It also promotes the venting as the fast explosion flame pushes more un-

319 burned gases exhausted from the chamber. However, there is a time delay for $\dot{V}_{vent}$
 320 to respond and catch up with $\dot{V}_{expa}$ and the pressure thus rises considerably after
 321 passing through B3. The numerical difference between them eventually contributes
 322 to a pressure peak, denoted as ‘Max’ in Figure 3b. After that, $\dot{V}_{expa}$ decreases as
 323 the leading edge of the flame leaves the chamber. Combustion is only sustained by
 324 burning the small amount of trapped mixture in the recirculation areas behind the
 325 obstacles and at the corners of the chamber. Meanwhile, venting is continued by ex-
 326 hausting some of the burned gases. Accordingly, the overpressure starts to decrease
 327 a while after the venting rate exceeds the combustion rate. Note that the both $\dot{V}_{expa}$
 328 and $\dot{V}_{vent}$ will fall alternately to zero, and the pressure will oscillate towards the
 329 atmospheric level due to acoustics.

Figure 4: Numerical snapshots of the flame front represented by the iso-line of $\tilde{c} = 0.5$ with vorticity contours for configuration B0BS. Time instants correspond to $t = 0.1, 2.2, 3.1, 3.8$ and 4.1 ms (from left to right).

330 Figure 4 shows the flow dynamics and flame-flow interactions in the hydrogen
 331 explosion for the configuration B0BS extracted from LES. The recirculation zones

332 and the turbulence level may be seen from the vorticity contour, and the flame
 333 front is defined using the iso-line of $\tilde{c}$. As demonstrated earlier, the presence of
 334 obstacles may promote the combustion rate and significantly increase the explosion
 335 overpressure. The obstacles can induce vortices and turbulence of various length
 336 scales and strength. For instance, at $t = 2.2$ ms, weak recirculation regions behind
 337 the downstream obstacles can be observed even if the flame front is only interacting
 338 with the first grid. The turbulence intensity in the wake area of B3 and Sq.Ob.
 339 gradually becomes stronger with the rapid approach of the flame front. Intense
 340 flame-turbulence interactions make the flame surface wrinkle. As can be seen from
 341 $t = 3.8$ ms in Figure 4, this not only speed up the flame but also creates more
 342 turbulence. Note that even in the downstream area of the last obstruction, the
 343 fast explosion is sustained by the continuous interactions between the propagating
 344 flame front and the generated turbulence in this region. As hydrogen explosions are
 345 usually rapid and highly unsteady, LES proves itself as a valuable tool in visualising
 346 the entire explosion process and in helping to understand its underlying physics.

347 *4.2. Overpressure and flame speed*

348 Figure 5 compares the maximum overpressure and its time of incidence between
 349 LES and the experiments for all the configurations (grouped in Table 1) studied
 350 in this paper. It is clear that the magnitude and timing of the peak pressure are
 351 strongly related to the configuration of the explosion chamber. Maximum pressure
 352 can increase by up to 400% by changing from configuration 000S to BBBL. In
 353 this case, the VBR changes from 1.15% (000S) to 6.44% (BBBL), and the peak
 354 overpressure increases from less than 200 mbar (000S) to ~ 1000 mbar (BBBL). It
 355 is important to realise that a real explosion in hydrogen process plants is likely to
 356 occur in much larger scales. Thus, the generated maximum overpressure may be
 357 much higher in larger-scale scenarios. As can be seen from groups 1 and 2, the more
 358 congested the obstacles, the higher the overpressure peak it can reach. The position
 359 of the baffle plates also plays a vital role in determining the maximum pressure, e.g.
 360 groups 3 and 4. Generally, the peak pressure decreases when the grids are closer

361 to the ignition source, or considerable separation distance is present between two
 362 successive obstacles. Results of groups 5 and 6 reveal that the size or the blockage
 363 level of the central square obstacle significantly affects the pressure magnitude.

Figure 5: Comparison of the peak overpressure and its incidence time between the experiments and LES for all studied configurations: (a) group 1, (b) group 2, (c) group 3, (d) group 4, (e) group 5, and (f) group 6. Experimental mean values and variations (hollow symbols with error bars of time to peak and maximum overpressure).

364 Overall, LES gives satisfactory results compared with experiments regarding
 365 both the timing and magnitude of the maximum overpressure, and this implies that
 366 the applied DFSD model successfully accounts for the flame wrinkling in a range
 367 of flow configurations with various turbulence level. The numerical calculations
 368 give excellent predictions for cases such as 0BBS, BBBS and BBBL regarding the
 369 overpressure magnitude, while a small degree of over-estimation can be seen on the
 370 configuration BB0S, 0B0S and BBB0. The most substantial discrepancy (absolute
 371 error) lies in the case 00BS where it is under-predicted by ~ 250 mbar. Calculated
 372 time taken to reach the peak pressure, $t_{p,LES}$, is generally within or close to the
 373 range of the experimental measurement for all the test cases. Experimentally, the

374 mean time taken to reach the peak overpressure varies approximately from 4 ms to 7
 375 ms depending on the configuration. In general, one may expect that the higher the
 376 pressure peak, the shorter the time of occurrence. While it is true when the number
 377 of grids increases, i.e. groups 1 and 2, there are some exceptions where the rela-
 378 tionship between the two is more complicated. For example, in group 3 (Figure 5c),
 379 the maximum pressure of BB0S is only half of 0BBS, but its time of incidence is
 380 apparently shorter than the latter. As it can be seen, LES also shows a correct pre-
 381 diction behaviour consistent with the experimental results. Note that the variation
 382 in the timing and magnitude of the peak overpressure does exist in the experimen-
 383 tal measurements, e.g. a comparatively wide range of $t_{p,exp}$ for configuration 000S.
 384 Considering that LES results are from single realisation, factors including the initial
 385 turbulence level, numerical schemes and thermochemical properties of the fuel can
 386 affect the results to an extent. However, a complete parametric study to investigate
 387 all modelling options is beyond the scope of this paper. Thus, with the current mod-
 388 elling setup, the discrepancies shown in Figure 5 are thought to be acceptable. In
 389 general, all trends seen in experiments for crucial parameters such as peak pressure
 390 and time to peak are predicted reasonably well. Sections 4.2.1 and 4.2.2 will further
 391 discuss the influence of location, number and size of the obstruction, as well as the
 392 LES prediction.

393 *4.2.1. Effect of obstacle number and location*

394 This section focuses on the impact of the number and location of obstacles on the
 395 hydrogen-air explosion characteristics within the chamber. Note that the configura-
 396 tions in groups 1-4 (see Table 1) are equipped with a small central obstacle down-
 397 stream of the baffles, representing various arrangements of turbulence-generating
 398 grids. Considering the conciseness of the paper and that the pressure trends are
 399 similar to an extent between configurations, results of overpressure and flame speed
 400 for groups 1 and 3 are not included in the main text but can be found in the sup-
 401plementary material.

402 Figure 6 presents the pressure and flame speed evolutions for group 2 configura-

Figure 6: Comparison between LES and experiments for group 2. *Top:* Overpressure traces. Mean experimental signal (----). The variation in $t_{p,exp}$ (—|—). *Bottom:* Flame propagation speed. Locations of the baffle plates (B1, B2 and B3) and the central square obstacle (Sq.Ob.).

403 tions. It is worth noticing here that the mean overpressure for each case presented
 404 in this paper is averaged from 50 individual experimental realisations, and an illus-
 405 tration of the averaging process is provided in the supplementary material. As the
 406 pressure trends in each experiment are very similar [61], the averaging procedure
 407 is performed after shifting all the pressure traces in time to match the maximum
 408 overpressure of each one. The range of the overpressure magnitude and the time
 409 taken to reach the peak pressure ($t_{p,exp}$) are also shown in the processed data (e.g.
 410 Figure 6) to facilitate the comparison with the numerical results. For flame speed
 411 profiles, the flame front position is numerically tracked by $\tilde{c} = 0.5$ furthest from the
 412 ignition end, while it is determined from the LIF-OH images experimentally.

413 Figure 6 shows that in group 2, the maximum pressure almost doubles when an
 414 additional grid is placed in the order starting closet to the ignition end. Compar-
 415 ison between the overpressure history and the corresponding flame speed indicates

that considerable flame propagation speed commonly accompanies high overpressure. Therefore, additionally placed grids contribute to the higher flame speed in the region downstream of the central obstruction. Since the introduction of more obstructions (i.e. groups 1 and 2) in the path of the flame propagation increases the overall turbulence level generated within the chamber, the more intensive flame-obstacle interactions give rise to the higher overpressure peak. Interestingly, both LES and experiments (Figure 5b) indicate that adding another grid to the case 0BBS (i.e. changing from 0BBS to BBBS) does not significantly increase the overpressure peak, and this may reflect the weak effect of having the lower grid compared to the other two.

Another observation made from Figure 6 is that the hydrogen flame substantially accelerates after passing successive obstacles, resulting from the local blockage and the high reactivity of hydrogen. The velocity reaches ~ 160 m/s for the case BBBS just downstream of the square obstacle, and the flame can accelerate up to about 300 m/s close to the exit as predicted by LES. The kinks in the speed profiles due to the temporary slowdown of the flame front right before it encounters an obstacle are also correctly reproduced numerically, indicating that the developed model successfully captures the essential dynamics of the flame propagation. Slight deviations in flame speeds from the experimental measurements can be noticed when the flame is downstream of the square obstacle in the blow-down area. It may be partially due to the limited time resolution of high-speed images considering the high turbulence and flame front speeds within the region.

Note that the exact mechanism of flame acceleration due to obstacles and confinement is complex. It may involve several types of flow instabilities such as the well-known Rayleigh-Taylor (RT) instability [62]. Furthermore, self-acceleration resulted from the intrinsic wrinkling of expanding laminar flame [62] may be present in the early development and quasi-laminar stage of the explosion. To the authors' knowledge, well-developed models are currently not available for these instabilities of the laminar flame [34]. However, for all the test cases considered here, the effect

445 of obstacle-generated turbulence is expected to be so dominant that the sub-grid
 446 contribution of the flame surface growth due to these instabilities may be neglected.

Figure 7: Comparison between LES and experiments for group 4. *Top:* overpressure traces. Mean experimental signal (----). The variation in $t_{p,exp}$ (|—|). *Bottom:* flame propagation speed. Locations of the baffle plates (B1, B2 and B3) and the central square obstacle (Sq.Ob.).

447 Recalling that Figure 5c demonstrates the effect of alternating the position of
 448 two baffle plates for group 3 configurations. Note that these cases have the same
 449 blockage ratio (i.e. VBR), and only the location of the grids varies. It clearly shows
 450 that higher overpressure is generated when the two baffles are closer to the central
 451 obstruction. Figure 7 provides a further illustration of the influence of the obstacle
 452 position using the group 4 configurations. It shows that the location of a single grid
 453 inside the chamber increases the pressure to different degrees. For the configuration
 454 B00S, due to the closeness of the lower baffle plate to the ignition source and the
 455 small thickness of the grid (3 mm), the flame front is only slightly stretched by
 456 B1 and then relaminarises as it passes. It is identified in Figure 7 by a noticeable
 457 bump in the pressure trace at ~ 4 ms from both LES and experiments. It is also

458 interesting to see that adding B1 to case 000S does not alter the peak overpressure
459 very much (see Figure 5) even though the blockage ratio increases.

460 Based on Figures 6 and 7, LES has satisfactory performance in reproducing the
461 overpressure trends, and even details such as small turning points in the pressure
462 curves due to sudden changes in the burning rate are correctly captured. It reflects
463 the main advantage of the DFSD model as the model coefficient accounting for
464 the SGS flame wrinkling adjusts automatically in the simulation. It is particularly
465 useful in the present test cases since the level of the flame front wrinkling can vary
466 significantly for various configurations of obstacles.

467 As mentioned earlier, there appears to be an apparent underestimation (~ 250
468 mbar less than the mean experimental value) in peak pressure for the configura-
469 tion 00BS (Figure 5d) compared with the other cases. A closer look at its pressure
470 trace in Figure 7 reveals that the early-stage overpressure matches well with the
471 experiment despite the under-prediction when approaching the peak. Further in-
472 vestigation shows that the computed flame wrinkling factor for the case 00BS (see
473 supplementary material) in the turbulent phase of the deflagration is of the similar
474 magnitude as that of 0B0S in group 4. However, considering that the experimental
475 peak pressure of the case 00BS is almost twice as large as that of 0B0S, the numer-
476 ically under-predicted pressure peak may result from the underestimation of Ξ_{Δ} in
477 the later stage of the explosion.

478 Figure 8 illustrates the effect of the single grid on the flame front structure just
479 before contacting the square obstacle. For both cases of 000S and B00S, the flame
480 front essentially travels to the square obstacle in a quasi-laminar manner. Although
481 the greater vertical flow velocity of the latter indicates that the flame does propagate
482 faster, it also promotes the venting from the top of the chamber. The efficient venting
483 may also explain the lack of pressure generation by adding the first grid after the
484 flame passes B1, resulting from the relatively long distance away from the next
485 downstream obstruction. Accordingly, LES predicts a maximum overpressure of $\sim$
486 200 mbar for both 000S and B00S despite that the experimental values are slightly

487 lower (see Figure 5).

Figure 8: Effect of the single grid as illustrated by the flame front structure (iso-lines of $\tilde{c} = 0.2$ and $\tilde{c} = 0.8$) before reaching the square obstacle for configuration 000S, B00S and 0B0S (from left to right). Contours of negative axial velocity indicate recirculation regions in the flow.

488 A closer look at Figure 8 reveals that the flame structure substantially changes
 489 when moving the grid from the lower (B1) to the middle position (B2). Since the
 490 axial velocity (~ 40 m/s .vs. ~ 10 m/s) at the baffle openings increases in time, the
 491 Reynolds number of the fresh gases based on the scale of the grid is higher. Fur-
 492 thermore, the formation of a few disconnected flame islands behind the baffle strips
 493 confirms the presence of stronger recirculation zone when flame-baffle interactions
 494 occur. It explains the more wrinkled and corrugated flame front for case 0B0S. The
 495 significant growth of the flame surface area before reaching the central obstacle also
 496 enhances their subsequent interactions, and the sub-grid wrinkling will be higher
 497 (see supplementary material). Consequently, the computed maximum overpressure
 498 of the case 0B0S is more than twice of that in the case B00S (~ 400 mbar .vs. ~ 200
 499 mbar), as also proved by the experiments. Therefore, it may be concluded that
 500 the distance between the grid and the ignition source serves as a controller and the
 501 generated overpressure is higher as the grid moves further downstream.

4.2.2. Influence of the obstacle size

It is recalled from Table 1 that group 5 consists of configuration BBB0, BBBS and BBBL in which central obstacle starts from none to large, while group 6 constitutes configuration 000S and 000L where no baffles are present. As confirmed from the peak overpressure calculations and experiments (Figure 5e), increasing the size of the central obstruction enhances the peak pressure. On the other hand, when the central obstacle is the only obstruction in the chamber, the maximum overpressure is nearly doubled by using a large one according to Figure 5f. In this case, the ABR almost doubled by changing from 000S to 000L, and the VBR of the latter (5%) is about 4 times of the former ($\sim 1.2\%$). The computed pressure signals of group 5 are presented in Figure 9, while that of group 6 are included in the supplementary material.

Figure 9: Comparison of overpressure signals between LES and experiments for group 5 cases. Mean experimental signal (----). The variation in $t_{p,exp}$ (—|—).

Comparison between groups 5 and 6 (Figure 5e and f) reveals that with the presence of the three baffle plates, the maximum pressure is generally higher than the configurations with only the central obstruction. It shows the effectiveness of the baffles plates in creating turbulence and the contribution of continuous flame-turbulence interaction to the internal pressure of the explosion chamber. The high turbulence intensity in the shear layer of the sharp-edged baffle strips leads to the substantially wrinkled flame front when reaching the central obstruction. Figure 5 also shows that the maximum pressure increases by $\sim 30\%$ when adding a small

522 obstacle to the case BBB0. A further rise of $\sim 20\%$ is seen when the large one replaces
523 it. It is worth mentioning that the overpressure generated by the configuration
524 BBBL is the highest among all the cases and it can reach nearly 1 bar, and LES
525 successfully captures the details on its pressure trace such as the sudden decrease in
526 the overpressure at about 4 ms (Figure 9).

527 It is worth mentioning that both ABR and VBR are critical explosion-related
528 parameters [63]. However, as has been demonstrated in section 4.2.1, the explosion
529 overpressure is also influenced by the arrangement of obstacles in a multi-obstruction
530 environment. Hence, LES is potentially a useful tool in complex obstructed process
531 areas where simple correlations using parameters such as the blockage ratio are not
532 sufficient.

533 Figure 10 shows the later stages of the explosion extracted from LES for config-
534 uration BBB0, BBBS and BBBL at various time instants. It can be seen that the
535 deflagrating flame behaves differently based on the size of the obstacle at the central
536 position. Without the central obstruction (i.e. configuration BBB0), the fingers-like
537 flame fronts induced by B3 merge and it propagates towards the outlet. When an
538 obstacle is placed, the flame tends to wrap around it and get further distorted. Note
539 that the size of the obstacle plays a vital role in the flame behaviour. The passage
540 between the side of the obstacle and the wall of the combustion chamber becomes
541 narrower when the size is larger, causing the flame to be ejected from there at high
542 speed. Furthermore, the large obstacle introduces a more extensive turbulent wake
543 behind it where the flame is significantly wrinkled, and some unburned hydrogen-air
544 mixture is trapped when passing it, as shown at $t = 3.9$ ms from Figure 10.

545 Figure 10d displays the flame location where the overpressure peaks ($t \approx t_{p,LES}$)
546 for each configuration in the simulation. It can be seen that when the maximum
547 pressure is reached, the flame is at a position closer to the outlet if the degree of
548 obstruction is increased, and this may be due to the higher propagation speed of the
549 flame front. For the case BBBL, the peak pressure is reached when the leading edge
550 of the flame nearly at the exit of the chamber. Experimental findings [61] confirms

Figure 10: Flame snapshots (contoured by $\tilde{c}$) of group 5 configurations (BBB0, BBBS and BBBL) showing the effect of the size of the central obstacle. (a) $t = 3.6$ ms; (b) $t = 3.7$ ms; (c) $t = 3.9$ ms; (d) $t \approx t_{p,LES}$.

that the flame location where the maximum overpressure is reached depends on the obstacle arrangement, and it may be more downstream when the overall turbulent intensity of the chamber is higher.

4.3. Comparison with propane

Hydrogen and propane are expected to be largely different regarding the consequences of the explosions hazards. This section provides a comparative study between the lean hydrogen/air ($\Phi=0.7$) and stoichiometric propane/air ($\Phi=1.0$) explosions using the same numerical and experimental setup. Note that LPG used in the experiment constitutes 95% C_3H_8 , 4% C_4H_{10} , 1% C_5 and other hydrocarbons by volume. It is thus approximated by its dominant component (propane) in the LES simulation. The laminar burning velocity and the thermal flame thickness entering the DFSD model for C_3H_8 are set to $S_L^0=39.0$ cm/s and $\delta_L^0=0.37$ mm [50], respectively.

Figure 11: Comparison of overpressure signals and flame propagation speed between LES and experiments for configuration BB0S. *Left:* hydrogen, $\Phi=0.7$. *Right:* propane, $\Phi=1.0$. Mean experimental signal (----). The variation in $t_{p,exp}$ (|—|).

Figure 11 presents the overpressure and flame speed of configuration BB0S using the two fuel/air mixtures, showing the distinct explosion behaviours. It is apparent that even for stoichiometric propane/air mixture, the generated maximum overpressure is almost an order-of-magnitude lower (~ 500 mbar .vs. ~ 60 mbar) than the lean hydrogen/air explosion. Also, the time taken to reach the peak is more than twice as slow as the hydrogen case, and the rate of pressure rise is considerably lower. As it can be seen from the speed-up locations in Figure 11, deflagrating hydrogen flame not only propagates faster but also responds more to the obstructions. The higher sensitivity to the obstacles for hydrogen leads to a magnified effect of flame-obstacle interactions compared with propane. While this section only includes one obstacle arrangement, the conclusions to the comparison between the two fuels drawn here are generally valid for other cases [61].

Note that the LES-DFSD approach excellently reproduces the experimental pressure trends, and it also captures the slightly different dynamics of the pressure traces for the same configuration between the two fuels. For example, it can be noticed from both LES and experiments in Figure 11 that there is a tiny pressure peak before the maxima at around 4 ms for hydrogen, while it is not present for propane. In contrast, a small peak can be found at about 10 ms for propane in the experiment, and it is also predicted numerically.

5. Conclusions

In this paper, large eddy simulations have been performed to investigate the vented hydrogen explosion in a small-scale obstructed chamber. A dynamic flame surface density model is applied to account for the progressive wrinkling of the flame front. The considered laboratory-scale explosion chamber has removable baffle plates and sharp-edge obstacles of different sizes, and a total of 11 flow configurations have been studied extensively. The highlight of the present work lies in the assessment of the recently developed LES-DFSD framework in modelling small-scale turbulent hydrogen explosions, as well as the insight into the mechanism driving the hydrogen

592 explosion process.

593 Comparison between lean hydrogen-air ($\Phi=0.7$) and stoichiometric propane-air
594 ($\Phi=1.0$) mixtures confirms that the magnitude of the peak pressure is an order higher
595 for the configuration BB0S using hydrogen. Furthermore, the deflagrating flame of
596 hydrogen is found to be more sensitive to the effect of obstacles compared with
597 propane. Based on the numerical and the experimental studies discussed earlier,
598 the following conclusions can be made on the influence of obstruction:

- 599 • The hydrogen flame is laminar at the beginning, but the degree of flame stretch
600 and wrinkling increases as the flame front propagates past repeated baffles and
601 obstacles. Thus, the explosion may involve different phases covering from quasi-
602 laminar to fully turbulent.
- 603 • Considerable flame propagation speed over successive obstructions generally links
604 with strong overpressure.
- 605 • The peak overpressure grows with an increase in volume blockage ratio and with
606 decreasing distance between successive obstructions. Maximum overpressure can
607 be as low as ~ 200 mbar when only the small obstacle is present (i.e. configuration
608 000S). It may reach approximately 1 bar with the highest degree of obstruction
609 (i.e. configuration BBBL).
- 610 • The overpressure is not only affected by the obstacle ABR and overall VBR, and
611 the number of obstacles and their locations relative to the ignition source also
612 influence the pressure build-up.
- 613 • Large separation between consecutive obstacles can lead to flame relaminarisation
614 and flame deceleration, and the pressure may rise slowly or even decrease.
- 615 • The effect of the first grid on the peak pressure and flame velocity is small. Greater
616 axial flow speeds (or the Reynolds number) and stronger recirculation zones at
617 the baffle plate contribute to the higher level of flame-baffle interaction when the
618 grid is moving downstream.

619 • Size of the central obstacle affects both the peak overpressure and the location of
 620 the flame front when it is reached.

621 Comparison between the numerical and the experimental pressure histories and
 622 flame front speeds shows satisfactory agreement considering the variation and un-
 623 certainties in the experiments. It has been demonstrated that LES is capable of re-
 624 producing the critical features and dynamics of the hydrogen explosion process. The
 625 calculated overpressure corresponds well with the experimental data in both mag-
 626 nitude and trend over a range of obstacle arrangements. Encouragingly, LES also
 627 captures some details on the pressure-time curve such as sudden pressure rise and
 628 drop in the magnitude due to immediate changes in the burning rate. It is believed
 629 to be the capability of the LES-DFSD approach as the level of flame-turbulence in-
 630 teraction is appropriately accounted for at different stages of the explosion and also
 631 for configurations of various degree of obstructions. Satisfactory results obtained
 632 from LES encourages the application of the current models to study larger-scale hy-
 633 drogen explosions with complex obstructions that are typically encountered in the
 634 actual hydrogen storage and processing areas.

635 **Nomenclature**

636	β	Model coefficient in the DFSD model
637	Δ	LES combustion filter width
638	δ_c	Inner cut-off scale
639	δ_L^0	Laminar (thermal) flame thickness
640	Δ_m	Filter width of volume averaging
641	Δ_x	LES grid size
642	$\dot{\omega}_c$	Reaction rate in terms of c
643	$\dot{V}_{expa}$	Volumetric flow rate due to expansion
644	$\dot{V}_{vent}$	Volumetric flow rate due to venting
645	$\langle \dots \rangle$	Volume averaging operation
646	$\vec{n}$	Vector of normal direction
647	$\vec{u}$	Velocity vector

648	Ω	Volume of computational domain
649	$\overline{\phi}$	LES filtered quantity of ϕ (unweighted)
650	Φ	Equivalence ratio
651	ρ	Density
652	ρ_b	Burned gas density
653	ρ_u	Unburned gas density
654	Σ	Flame surface density
655	$\hat{\cdot}$	Test-filtering operation
656	$\hat{\Delta}$	Test-filter width
657	$\tilde{\phi}$	LES filtered quantity of ϕ (mass weighted)
658	Ξ_{Δ}	Sub-grid flame wrinkling factor
659	A	Area
660	A_{exit}	Area of chamber exit plane
661	c	Reaction progress variable
662	D	Molecular diffusion coefficient
663	S_L^0	Laminar burning velocity
664	t	Time
665	$t_{p,exp}$	Time to reach peak pressure from experiments
666	$t_{p,LES}$	Time to reach peak pressure from LES
667	u_i	Velocity component
668	V	Volume
669	V_b	Volume occupied by burned gas
670	x_i	Direction in Cartesian coordinate
671	ABR	Area blockage ratio
672	B1	Baffle plate no. 1
673	B2	Baffle plate no. 2
674	B3	Baffle plate no. 3
675	CFD	Computational fluid dynamics
676	DFSD	Dynamic flame surface density

677	FSD	Flame surface density
678	L	Large central obstacle
679	LES	Large eddy simulation
680	LIF-OH	Laser-induced fluorescence of OH
681	LPG	Liquid petroleum gas
682	RANS	Reynolds-averaged Navier-Stokes
683	S, Sq.Obs	Small central obstacle
684	SGS	Sub-grid scale
685	VBR	Volume blockage ratio

686 **Acknowledgement**

687 The authors would like to thank Dr Bo Liu from the University of Sheffield
688 for his valuable suggestions on the modelling conducted in this paper. The original
689 experimental data provided by Professor Assaad Masri from the University of Sydney
690 are gratefully appreciated.

691 **Reference**

- 692 [1] G. Marbán, T. Valdés-Solís, Towards the hydrogen economy?, *International*
693 *Journal of Hydrogen Energy* 32 (2007) 1625–1637.
- 694 [2] A. Veziroglu, R. MacArio, Fuel cell vehicles: State of the art with economic and
695 environmental concerns, *International Journal of Hydrogen Energy* 36 (2011)
696 25–43.
- 697 [3] T. E. Lipman, M. Elke, J. Lidicker, Hydrogen fuel cell electric vehicle per-
698 formance and user-response assessment: Results of an extended driver study,
699 *International Journal of Hydrogen Energy* 43 (2018) 12442–12454.
- 700 [4] C. M. White, R. R. Steeper, A. E. Lutz, The hydrogen-fueled internal combus-
701 tion engine: a technical review, *International Journal of Hydrogen Energy* 31
702 (2006) 1292–1305.
- 703 [5] P. E. Dodds, I. Staffell, A. D. Hawkes, F. Li, P. Grünewald, W. McDowall,
704 P. Ekins, Hydrogen and fuel cell technologies for heating: A review, *Interna-*
705 *tional Journal of Hydrogen Energy* 40 (2015) 2065–2083.
- 706 [6] Y. Lee, J. Kim, J. Kim, E. J. Kim, Y. G. Kim, I. Moon, Development of a web-
707 based 3D virtual reality program for hydrogen station, *International Journal*
708 *of Hydrogen Energy* 35 (2010) 2112–2118.

- [7] E. Kim, J. Park, J. H. Cho, I. Moon, Simulation of hydrogen leak and explosion for the safety design of hydrogen fueling station in Korea, *International Journal of Hydrogen Energy* 38 (2013) 1737–1743.
- [8] B. Angers, A. Hourri, P. Benard, E. Demaël, S. Ruban, S. Jallais, Modeling of hydrogen explosion on a pressure swing adsorption facility, *International Journal of Hydrogen Energy* 39 (2014) 6210–6221.
- [9] S. Kikukawa, H. Mitsuhashi, A. Miyake, Risk assessment for liquid hydrogen fueling stations, *International Journal of Hydrogen Energy* 34 (2009) 1135–1141.
- [10] Y. F. Khalil, Science-based framework for ensuring safe use of hydrogen as an energy carrier and an emission-free transportation fuel, *Process Safety and Environmental Protection* 117 (2018) 326–340.
- [11] A. G. Venetsanos, D. Baraldi, P. Adams, P. S. Heggem, H. Wilkening, CFD modelling of hydrogen release, dispersion and combustion for automotive scenarios, *Journal of Loss Prevention in the Process Industries* 21 (2008) 162–184.
- [12] J. Yanez, M. Kuznetsov, A. Souto-Iglesias, An analysis of the hydrogen explosion in the Fukushima-Daiichi accident, *International Journal of Hydrogen Energy* 40 (2015) 8261–8280.
- [13] O. R. Hansen, M. T. Kjellander, J. A. Pappas, Explosion loading on equipment from CFD simulations, *Journal of Loss Prevention in the Process Industries* 44 (2016) 601–613.
- [14] O. J. Ugarte, V. Akkerman, A. S. Rangwala, A computational platform for gas explosion venting, *Process Safety and Environmental Protection* 99 (2016) 167–174.
- [15] C. R. Bauwens, J. Chaffee, S. B. Dorofeev, Vented explosion overpressures from combustion of hydrogen and hydrocarbon mixtures, *International Journal of Hydrogen Energy* 36 (2011) 2329–2336.
- [16] J. Guo, Q. Li, D. Chen, K. Hu, K. Shao, C. Guo, C. Wang, Effect of burst pressure on vented hydrogen-air explosion in a cylindrical vessel, *International Journal of Hydrogen Energy* 40 (2015) 6478–6486.
- [17] J. Guo, X. Sun, S. Rui, Y. Cao, K. Hu, C. Wang, Effect of ignition position on vented hydrogen-air explosions, *International Journal of Hydrogen Energy* 40 (2015) 15780–15788.
- [18] X. Rocourt, I. Sochet, B. Pellegrinelli, Small-scale flame acceleration and application of medium and large-scale flame speed correlations, *International Journal of Hydrogen Energy* 42 (2017) 1327–1336.
- [19] X. Lv, L. Zheng, Y. Zhang, M. Yu, Y. Su, Combined effects of obstacle position and equivalence ratio on overpressure of premixed hydrogenair explosion, *International Journal of Hydrogen Energy* 41 (2016) 17740–17749.

- [20] N. R. Popat, C. A. Catlin, B. J. Arntzen, R. P. Lindstedt, B. H. Hjertager, T. Solberg, O. Saeter, A. C. Van Den Berg, Investigations to improve and assess the accuracy of computational fluid dynamic based explosion models, *Journal of Hazardous Materials* 45 (1996) 1–25.
- [21] B. J. Arntzen, Modelling of turbulence and combustion for simulation of gas explosions in complex geometries, Ph.D. thesis, Norwegian University of Science and Technology, 1998. URL: <http://ntnu.diva-portal.org/smash/record.jsf?pid=diva2:122240{%}%5Cnhttp://ntnu.diva-portal.org/smash/get/diva2:122240/FULLTEXT01>. doi:10.1016/j.jlp.2005.06.012.
- [22] L. Sun, H. Yan, S. Liu, Y. Bai, Load characteristics in process modules of offshore platforms under jet fire: The numerical study, *Journal of Loss Prevention in the Process Industries* 47 (2017) 29–40.
- [23] K. B. Mishra, The influence of Volume Blockage Ratio on IOCL Jaipur explosion, *Journal of Loss Prevention in the Process Industries* (2018) —.
- [24] P. Middha, O. R. Hansen, I. E. Storvik, Validation of CFD-model for hydrogen dispersion, *Journal of Loss Prevention in the Process Industries* 22 (2009) 1034–1038.
- [25] K. Matsuura, H. Kanayama, H. Tsukikawa, M. Inoue, Numerical simulation of leaking hydrogen dispersion behavior in a partially open space, *International Journal of Hydrogen Energy* 33 (2008) 240–247.
- [26] T. Beard, M. Bragin, W. Malalasekera, S. S. Ibrahim, Numerical Simulation of Hydrogen Discharge in a Partially Enclosed Space, *Energy Procedia* 66 (2015) 153–156.
- [27] M. A. Abdel-Raheem, S. S. Ibrahim, W. Malalasekera, A. R. Masri, Large Eddy simulation of hydrogen-air premixed flames in a small scale combustion chamber, *International Journal of Hydrogen Energy* 40 (2015) 3098–3109.
- [28] K. K. J. Ranga Dinesh, X. Jiang, J. A. Van Oijen, Numerical simulation of hydrogen impinging jet flame using flamelet generated manifold reduction, *International Journal of Hydrogen Energy* 37 (2012) 4502–4515.
- [29] E. Vyazmina, S. Jallais, Validation and recommendations for FLACS CFD and engineering approaches to model hydrogen vented explosions: Effects of concentration, obstruction vent area and ignition position, *International Journal of Hydrogen Energy* 41 (2016) 15101–15109.
- [30] A. Marangon, M. Schiavetti, M. Carcassi, P. Pittiglio, P. Bragatto, A. Castellano, Turbulent hydrogen deflagration induced by obstacles in real confined environment, *International Journal of Hydrogen Energy* 34 (2009) 4669–4674.
- [31] J. Li, F. Hernandez, H. Hao, Q. Fang, H. Xiang, Z. Li, X. Zhang, L. Chen, Vented Methane-air Explosion Overpressure Calculation-A simplified approach based on CFD, *Process Safety and Environmental Protection* 109 (2017) 489–508.

- [32] D. Baraldi, D. Melideo, A. Kotchourko, K. Ren, J. Yanez, O. Jedicke, S. G. Giannissi, I. C. Tolas, A. G. Venetsanos, J. Keenan, D. Makarov, V. Molkov, S. Slater, F. Verbecke, A. Duclos, Development of a model evaluation protocol for CFD analysis of hydrogen safety issues the SUSANA project, *International Journal of Hydrogen Energy* 42 (2017) 7633–7643.
- [33] D. Baraldi, A. Kotchourko, A. Lelyakin, J. Yanez, A. Gavrikov, A. Efimenko, F. Verbecke, D. Makarov, V. Molkov, A. Teodorczyk, An inter-comparison exercise on CFD model capabilities to simulate hydrogen deflagrations with pressure relief vents, *International Journal of Hydrogen Energy* 35 (2010) 12381–12390.
- [34] R. S. Cant, W. N. Dawes, A. M. Savill, Advanced CFD and Modeling of Accidental Explosions, *Annual Review of Fluid Mechanics* 36 (2004) 97–119.
- [35] H. Hisken, G. A. Enstad, P. Middha, K. Van Wingerden, Investigation of concentration effects on the flame acceleration in vented channels, *Journal of Loss Prevention in the Process Industries* 36 (2014) 447–459.
- [36] J. Williamson, J. McGill, A. Trouve, Large Eddy Simulation Modeling of Turbulent Deflagrations, in: *Fire Safety Science - Proceedings of the Eighth International Symposium, 2005*, pp. 1375–1386. URL: http://iafss.org/publications/fss/8/1375/view/fss_{_}8-1375.pdf. doi:10.3801/IAFSS.FSS.8-1375.
- [37] V. Molkov, D. Makarov, J. Puttock, The nature and large eddy simulation of coherent deflagrations in a vented enclosure-atmosphere system, *Journal of Loss Prevention in the Process Industries* 19 (2006) 121–129.
- [38] D. Makarov, V. Molkov, Y. Gostintsev, Comparison Between Rng and Fractal Combustion Models for Les of Unconfined Explosions, *Combustion Science and Technology* 179 (2007) 401–416.
- [39] V. Molkov, F. Verbecke, D. Makarov, LES of Hydrogen-Air Deflagrations in a 78.5-m Tunnel, *Combustion Science and Technology* 180 (2008) 796–808.
- [40] S. R. Gubba, S. S. Ibrahim, W. Malalasekera, A. R. Masri, LES Modeling of Premixed Deflagrating Flames in a Small-Scale Vented Explosion Chamber with a Series of Solid Obstructions, *Combustion Science and Technology* 180 (2008) 1936–1955.
- [41] V. Di Sarli, A. Di Benedetto, G. Russo, Using Large Eddy Simulation for understanding vented gas explosions in the presence of obstacles, *Journal of Hazardous Materials* 169 (2009) 435–442.
- [42] R. Li, W. Malalasekera, S. Ibrahim, B. Liu, On the mechanism of pressure rise in vented explosions : A numerical study, *Process Safety and Environmental Protection* 117 (2018) 551–564.
- [43] S. Patel, S. Jarvis, S. Ibrahim, G. Hargrave, An experimental and numerical investigation of premixed flame deflagration in a semiconfined explosion chamber, *Proceedings of the Combustion Institute* 29 (2002) 1849–1854.

- [44] H. Pitsch, Large-Eddy Simulation of Turbulent Combustion, *Annual Review of Fluid Mechanics* 38 (2005) 453–482.
- [45] M. Boger, D. Veynante, Large eddy simulations of a turbulent premixed v-shape flame, in: C. Dopazo (Ed.), *Eighth European Turbulence Conference, Eighth European Turbulence Conference, Barcelona, Spain, 2000*, pp. 448–452. doi:10.1016/0142-727X(90)90030-F.
- [46] M. P. Kirkpatrick, S. W. Armfield, A. R. Masri, S. S. Ibrahim, Large Eddy Simulation of a Propagating Turbulent Premixed Flame, *Flow, Turbulence and Combustion* 70 (2003) 1–19.
- [47] M. Boger, D. Veynante, H. Boughanem, A. Trouvé, Direct numerical simulation analysis of flame surface density concept for large eddy simulation of turbulent premixed combustion, *Symposium (International) on Combustion* 27 (1998) 917–925.
- [48] T. Ma, O. T. Stein, N. Chakraborty, A. M. Kempf, A posteriori testing of algebraic flame surface density models for LES, *Combustion Theory and Modelling* 17 (2013) 431–482.
- [49] E. R. Hawkes, R. S. Cant, A flame surface density approach to large-eddy simulation of premixed turbulent combustion, *Proceedings of the Combustion Institute* 28 (2000) 51–58.
- [50] G. Wang, M. Boileau, D. Veynante, K. Truffin, Large eddy simulation of a growing turbulent premixed flame kernel using a dynamic flame surface density model, *Combustion and Flame* 159 (2012) 2742–2754.
- [51] A. Alharbi, A. R. Masri, S. S. Ibrahim, Turbulent premixed flames of CNG, LPG, and H₂ propagating past repeated obstacles, *Experimental Thermal and Fluid Science* 56 (2014) 2–8.
- [52] D. Veynante, V. Moureau, Analysis of dynamic models for large eddy simulations of turbulent premixed combustion, *Combustion and Flame* 162 (2015) 4622–4642.
- [53] G. Wang, M. Boileau, D. Veynante, Implementation of a dynamic thickened flame model for large eddy simulations of turbulent premixed combustion, *Combustion and Flame* 158 (2011) 2199–2213.
- [54] K. T. Aung, M. I. Hassan, G. M. Faeth, Flame stretch interactions of laminar premixed hydrogen/air flames at normal temperature and pressure, *Combustion and Flame* 109 (1997) 1–24.
- [55] O. Vermorel, P. Quillatre, T. Poinso, LES of explosions in venting chamber: A test case for premixed turbulent combustion models, *Combustion and Flame* 183 (2017) 207–223.
- [56] M. P. Kirkpatrick, A large eddy simulation code for industrial and environmental flows, Ph.D. thesis, The University of Sydney, 2002.

- 868 [57] H. Werner, H. Wengle, Large-Eddy Simulation of Turbulent Flow Over and
869 Around a Cube in a Plate Channel, in: F. Durst, R. Friedrich, B. E. Launder,
870 F. W. Schmidt, U. Schumann, J. H. Whitelaw (Eds.), *Turbulent Shear Flows*
871 8, Springer Berlin Heidelberg, Berlin, Heidelberg, 1993, pp. 155–168.
- 872 [58] M. Germano, U. Piomelli, P. Moin, W. H. Cabot, A dynamic subgrid-scale eddy
873 viscosity model, *Physics of Fluids A: Fluid Dynamics* 3 (1991) 1760–1765.
- 874 [59] B. P. Leonard, A stable and accurate convective modelling procedure based
875 on quadratic upstream interpolation, *Computer methods in applied mechanics*
876 and engineering 19 (1979) 59–98.
- 877 [60] S. B. Pope, Ten questions concerning the large-eddy simulation of turbulent
878 flows, *New Journal of Physics* 6 (2004).
- 879 [61] A. Alharbi, *Turbulent Premixed Flames Propagating Past Repeated Obsta-*
880 *cles*, Ph.D. thesis, University of Sydney, 2013. URL: [http://hdl.handle.net/](http://hdl.handle.net/2123/9765)
881 [2123/9765](http://hdl.handle.net/2123/9765).
- 882 [62] S. B. Dorofeev, Flame acceleration and explosion safety applications, *Proceed-*
883 *ings of the Combustion Institute* 33 (2011) 2161–2175.
- 884 [63] D. Bjerketvedt, J. R. Bakke, K. van Wingerden, Gas explosion handbook,
885 *Journal of Hazardous Materials* 52 (1997) 1–150.