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Author: Ruipengyu Li Weeratunge Malalasekera Salah Ibrahim Bo Liu

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On the Mechanism of Pressure Rise in Vented Explosions: A Numerical Study

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

^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*

^c*Department of Mechanical Engineering, University of Sheffield, Sheffield, S1 4ET, UK*

Abstract

Accidental gas explosions are a significant concern in process industries. In an explosion event, the promotion of flame acceleration due to turbulence generated from obstacles is responsible for many severe damages. This paper discusses the numerical evaluation and the mechanism of pressure rise in vented explosions in the presence of obstructions using computational fluid dynamics (CFD). The large eddy simulation (LES) technique is employed with a dynamic flame surface density (DFSD) in the combustion model to account for the filtered chemical source term. The experimental test case considered for the validation of simulations is a small-scale explosion chamber with removable baffle plates and obstacles. It is found that the maximum overpressure increases with the baffle plates moved downstream from the ignition source or when additional baffles are placed in sequence. Large separation between baffles and the central obstacle results in lower overpressure due to the relaminarisation of the flame front. The trend of explosion overpressure is related to the competition between the strength of venting and expansion in the explosion chamber. Extensive interactions between the flame and the obstruction-generated turbulence are found to wrinkle the flame front and increase the burning rate. Satisfactory agreements have been obtained between LES and the experimental data. This confirms the capability of the developed model in predicting essential safety-related parameters in vented explosions. Results reveal the potential of using LES in the selection of design aspects for loss prevention, such as the area of vents and distance between congested regions in chemical processing plants.

Keywords: Pressure rise, Vented explosions, Obstacles, Dynamic model, LES

*Corresponding author

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

1. Introduction

Accidental release of flammable gas or vapour into a cloud may produce a combustible fuel-air mixture. In such a situation a deflagration wave can be triggered if a suitable ignition source is present. It may subsequently lead to high overpressure in the presence of confinements and obstructions. Gaseous explosion hazards often lead to the destruction of buildings, off-shore plants and process industries. The damage caused by the initial overpressure is generally more severe than the ensuing fires. Figure 1 briefly illustrates the mechanism of pressure build-up in partially-confined vented explosions with the presence of obstacles.

Figure 1: Illustration of the mechanism driving pressure rise in a vented explosion with obstructions. Positive effect (+). Negative effect (-). The strength of gas expansion and venting determines the overpressure build-up. Obstacle-generated turbulence promotes the combustion rate.

Explosions in process industries are often highly complex, and predicting the produced overpressure for safety guidance could be a challenging task. In the final report of the Buncefield incidence (Powell, 2008), for example, the investigation board estimated that 700 to 1000 mbar of overpressure would have been generated in the Northgate and Fuji car parks of the site, based on the degree of damage to the adjacent buildings. However, overpressure calculation using available simple models largely underestimated the case, giving only up to about 50 mbar in a similar

environment. This indicates the uncertainties in the overpressure predictions and the complex mechanism involved in the explosion at the Buncefield scenario.

Parameters such as maximum explosion overpressure and its time of incidence are important for design engineers and safety managers. Hence, there is a growing need for prediction and risk assessment tools for the safe design of many industrial structures and processes. However, the timing and magnitude of overpressure in explosions depend on various conditions including the type of the fuel (Alharbi et al., 2014), the stoichiometry (Alharbi et al., 2014), ignition location (Rocourt et al., 2014) and the configuration of obstruction (Ibrahim et al., 2009; Na et al., 2017), etc. Thus, accurate prediction and assessment of explosion is a challenging task.

There have been several early attempts to use simple correlations and formulas for predictions of explosion pressures in compartments (Bjerketvedt et al., 1997). However, the typical weakness with such formulas is that they do not take into account turbulence generation and flame acceleration, therefore, the results can be an order of magnitude different from experiments (Bjerketvedt et al., 1997). Numerically solving a simplified series of governing equations is another approach to obtain pressure history in simple vessels (Chippett, 1984). Very recently, a computational platform has been proposed to account for various vent sizes and container shapes in vented explosions (Ugarte et al., 2016). The main advantage of such numerical calculations is the much cheaper computational cost compared to 3-D numerical simulations and they also account for simple flame shapes and geometries. However, as a typical explosion in process industries often involves obstacles such as complex pipes racks or congested plants, such zero-dimensional models are generally unable to consider the effects of obstacle-generated turbulence and flame stretch.

Applying computational fluid dynamics (CFD) in process and plant safety is a relatively new research field. Thanks to the improvements in computational technology and resources, CFD is becoming a more attractive and reliable tool as an alternative to experiments in process industries. Reynolds-averaged Navier-Stokes

(RANS) methods have been applied in studying explosions for safety-related structures (Birkby et al., 2000; Catlin et al., 1995; Popat et al., 1996). While RANS-based method remains as the major numerical tool in explosion-related studies, the accuracy is generally not sufficient and a certain degree of tuning of model parameters is usually required. Although it is computationally more expensive, the large eddy simulation (LES) technique is emerging to be applicable to simulate unsteady flows in practical industrial devices. Explosions in vessels with obstacles are highly unsteady and often involve complicated flow patterns such as shear layers and recirculation zones, and LES is expected to provide more promising predictions compared to RANS. There have been a few studies of explosion-related scenarios where simulations have been performed using LES (Chen et al., 2017; Di Sarli et al., 2009; Ibrahim et al., 2009; Wen et al., 2012).

The central matter of using LES in safety-related studies is the inclusion of sub-models for the closure of the filtered chemical source term. The issue is that the flame thickness is generally smaller than the LES grid size, meaning combustion needs to be modelled completely. One solution is to introduce a spatial filter larger than the mesh size to resolve the filtered flame on LES (Boger et al., 1998). It generally involves solving a transport equation for the filtered reaction progress variable with the source term modelled using the flame surface density (FSD) approach. The original Boger et al. (1998) algebraic FSD model has been refined subsequently to include the control of filtered flame thickness and reproduction of laminar propagation speed when turbulence effects diminish (Boger and Veynante, 2000). A dynamic procedure (Wang et al., 2012) was also proposed recently in which the subgrid-scale (SGS) part of the flame wrinkling is evaluated dynamically. The dynamic flame surface density (DFSD) model was first proposed in simulating a growing turbulent flame kernel and it is further adapted for present explosion study. It is advantageous because the model coefficient is self-adjusted depending on the wrinkling of the resolved flame. This is considered beneficial in safety-related simulations as an explosion is highly dynamic and the flame can transit from initially laminar to fully

turbulent in the presence of obstacles. Furthermore, since explosions can occur in both small and large scales, the DFSD model is expected to perform better compared with the more common algebraic models where the model parameter may require tuning from case to case.

The ultimate purpose of this research is to develop LES sub-models and tools for realistic explosion scenarios where the scales can range from several meters to hundreds of meters. It is thus essential to ensure that LES can capture all phases of an explosion event and the starting point is to study a small-scale experiment of vented explosion (Alharbi et al., 2014). The first objective of this paper is to investigate the mechanism of pressure rise and flame acceleration in vented explosions with obstacles using LES. The second is to assess the capability of LES and the DFSD model in capturing the unsteady explosion behaviours and predicting essential safety-related parameters. Calculations of a wide range of obstacle arrangement in the explosion chamber are performed to explore aspects such as the effects of location and number of obstacles as well as the level of blockage. The present work aims to provide detailed information of a typical vented deflagration including overpressure history, flame speed, flame/turbulence interaction and venting effectiveness, which can be further used in the design and assessment of buildings and process plants. The computational setup presented in this paper may also be extended to large-scale and more complex cases of the vented explosion that typically occur in the processing industries. In addition, it may be further applied to calibrate existing or provide new engineering correlations and models in the industry to better understand and predict turbulence-driven explosions.

2. Experimental test case

The experimental test case from the Sydney combustion group (Alharbi et al., 2014) is used here for model validation and analysis. The schematic diagram of the laboratory-scale explosion rig is shown in Figure 2a.

The $50 \times 50 \times 250$ mm chamber is square in cross-section and has a volume

Figure 2: Specifications of the explosion chamber used in the experiment (Alharbi et al., 2014) (Dimensions are in mm).

of 0.625 L. It can accommodate three baffle plates positioned at 20 mm, 50 mm and 80 mm from the base to create varying degree of blockage (obstruction). Each baffle plate, a schematic of which is also shown in Figure 2b, consists of five 4-mm wide strips each with a 5-mm wide space spreading them throughout the chamber, creating a blockage ratio of 0.4. Downstream of the baffle plates, a further solid obstruction with a square cross-section may be placed with its bottom surface kept at 96 mm from the base. Two solid obstacles can be used, a small one with a cross-section of 12×12 mm or a large one with a 25×25 mm cross-section. The blockage ratios of the two square obstructions are 0.24 and 0.5, respectively. This chamber is of specific interest due to its smaller volume and its capability to hold a deflagrating flame, resulting from the strong turbulent environment generated by solid obstacles at different downstream locations from the closed bottom end.

The present study focuses on the liquefied petroleum gas (LPG). It constitutes 95% C_3H_8 , 4% C_4H_{10} , 1% C_5 and other hydrocarbons by volume. Thus, LPG has been approximated by its dominant component (propane) in the LES simulations. In the experiments, the stoichiometric fuel-air mixture is injected and allowed to rest. Hence, the initial turbulence level is considered low. Subsequently, the quiescent mixture is ignited by focusing an infrared output from a Nd:YAG laser 2 mm above the base and this marks the start of each experiment, or time zero. Venting at atmospheric pressure is maintained at the top of the chamber throughout the explosion process. Pressure is measured using two Keller type PR21-SR piezoelectric pressure transducers at 25 kHz, located in the base plate as well as in the wall of the chamber just upstream of the exit plane.

For the present investigation, eight configurations with different number and position of baffle plates are studied. In order to facilitate the discussion in the remainder of this paper, detailed analysis of pressure trends and flame behaviours are only given for five configurations. These are clustered into two families as shown in Figure 3 and Figure 4. Each configuration has an associated code representing the number and position of obstructions. For example, configuration BB0S indicates

Figure 3: Configuration 00BS, 0BBS, and BBBS in family 1 (not to scale). Baffles are progressively increased and kept furthest from ignition end.

Figure 4: Configuration B00S, BB0S, and BBBS in family 2 (not to scale). Baffles are progressively increased from the ignition end.

baffles at the first two locations near the ignition end and a small solid square obstacle. Family 1 intends to investigate the effects of increasing the number of baffle plates starting from one baffle furthest from the ignition point (configuration 00BS, 0BBS and BBBS), while family 2 is to study the impact of increasing baffle plates starting from one plate closest to the ignition point (configuration B00S, BB0S and BBBS).

3. Numerical setup

This section provides the basic setup for the simulations performed in this paper. It focuses on the DFSD model and an effective way of providing the profile of the initial flame kernel. The full governing equations and other numerical details for simulations in this paper can be found elsewhere (Kirkpatrick et al., 2003) and only a brief description is given here.

3.1. The dynamic flame surface density model

The structure of a premixed flame and the thermochemical state of the gas mixtures are commonly represented by a single progress variable c . It may be defined by the normalised fuel mass fraction, temperature, etc. so that $c = 1$ in the fully burned gas and $c = 0$ in the fresh unburned gas, under the assumption of single-step chemistry and unity Lewis number (Bray et al., 1985). In LES, the filtered transport equation for $\tilde{c}$ is (Boger et al., 1998)

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

The filtered reaction rate term, $\tilde{\omega}_c$, may be modelled as (Boger et al., 1998)

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

by introducing the subgrid-scale flame surface density Σ . The flame surface density is generally determined from an additional transport equation (Hawkes and Cant,

2000) or modelled using algebraic expressions (Boger et al., 1998; Boger and Veynante, 2000). In this work, the Boger et al. (Boger et al., 1998; Boger and Veynante, 2000) parabolic algebraic expression is retained as

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

where Δ is the filter width and Ξ_{Δ} is the subgrid-scale flame wrinkling factor. Note that Δ should be larger than the mesh size Δ_x (typically $\Delta \geq 5\Delta_x$) so that the filtered progress variable gradients can be well resolved on an LES grid (Boger et al., 1998; Mercier et al., 2015). $\Delta = 6\Delta_x$ is used in present study. The $\tilde{c}$ -equation adopted for the present study is (Boger and Veynante, 2000; Wang et al., 2012):

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

where the modified diffusion term is included to control the filtered flame thickness and to reproduce the correct laminar propagation speed in the absence of subgrid-scale turbulence effect (Boger and Veynante, 2000; Ma et al., 2013; Mercier et al., 2015).

The SGS flame wrinkling factor Ξ_{Δ} measures the ratio between total and resolved flame surfaces locally and the Wang et al. dynamic model (Wang et al., 2012) is used for the present investigation:

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

where the inner cut-off scale δ_c (Gülder and Smallwood, 1995; Knikker et al., 2002) is prescribed by the user and should be of the order of the laminar flame thickness, δ_L^0 . In present work, $\delta_c = 4\delta_L^0$ is used (Veynante and Moureau, 2015). The model parameter β is determined dynamically by comparing the test-filtered and resolved

flame fronts (Wang et al., 2012; Veynante and Moureau, 2015):

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

where $\widehat{\Delta}$ is the width of the test filter. Here, the test-filtering ($\widehat{\cdot}$ operator) and the spatial-averaging ($\langle \cdot \rangle$ operator) procedures are carried out using a Gaussian filter (Boger et al., 1998; Wang et al., 2012). The test-filter and averaging-filter widths are set as $\widehat{\Delta} = 1.1\Delta$ and $\Delta_m = 1.5\widehat{\Delta}$, respectively (Veynante and Moureau, 2015). The unstrained laminar burning velocity and flame thickness are set as $S_L^0 = 39.0$ cm/s (Metghalchi and Keck, 1980) and $\delta_L^0 = 0.37$ mm (Wang et al., 2012), respectively, for the stoichiometric propane/air mixture.

3.2. Flame kernel initialisation

Ignition is a complex phenomenon and LES can only resolve a flame of the size typically larger than the filter width Δ , therefore the very early stage of flame kernel formation is not considered for the present study. Simulation is initiated by imposing a flame kernel of burned gases at the position of the ignition source. The initial profile of filtered progress variable $\tilde{c}$ across the flame front is given by filtering the steady solution of one-dimensional propagating laminar flame under the LES filter scale Δ .

The procedure practically includes 1-D calculation of laminar flame with detailed chemistry, filtering the flame profile according to the LES filter size and impose a filtered burned flame kernel on the LES grid. First, a one-dimensional calculation of stoichiometric propane/air mixture is performed using a detailed chemical reaction mechanism, GRI 3.0 (Smith et al., 1999) in a specialised software, FlameMaster (Pitsch, 1998). Note that the resulting flame profile is thinner than the mesh size of LES. Hence, a one-dimensional Gaussian filter (Fiorina et al., 2010) is employed to obtain the filtered progress variable $\tilde{c}$ under specified LES filter size Δ . Finally, a semi-spherical flame kernel is imposed at the ignition point of the chamber and the

initial radius of the burned gases is set to 3 mm for all flow cases.

3.3. Solution details

LES computation has been carried out using the structured in-house code PUFFIN (Kirkpatrick et al., 2003). The DFSD model described above has been successfully implemented and tested in PUFFIN. Simulations are performed using an initially stagnant propane/air mixture of equivalence ratio 1.0.

The computational domain of the explosion chamber has dimensions of $50 \times 50 \times 250$ mm. It is adequately extended to 325 mm in x , y and 500 mm in the z direction. A non-reflecting boundary condition (Kirkpatrick et al., 2003) is applied on the boundaries of the extended domain, in order to minimise the effect of reflected pressure waves on the pressure field inside the chamber.

The chamber domain constitutes $85 \times 85 \times 423$ cells in the x , y and z directions, respectively. The cells within the chamber are distributed uniformly, giving a grid size of $\Delta_x \approx 0.59$ mm. The mesh size is chosen to ensure that the filtered flame thickness is smaller than the gaps between the strips of the baffle plates. Outside the explosion chamber, the grid is expanded toward the far-field boundaries to save computational time. Adiabatic and no-slip boundary conditions are employed on the chamber bottom and side walls with the 1/7th power law wall function of Werner and Wengle (Werner and Wengle, 1993) used to calculate the shear stress at the solid wall. Subgrid-scale turbulence is modelled using the dynamic Smagorinsky eddy viscosity model (Germano et al., 1991).

Conservation equations for scalars use second-order central difference scheme for diffusion terms. SHARP (Leonard, 1987) is used for advection terms of the scalar equations to avoid problems associated with oscillations in the solution. Crank-Nicolson scheme is used for the time integration of scalar equations. Further details of the numerical scheme are given in (Kirkpatrick, 2002).

Three numerical grids have been studied in order to examine the solution dependence on the mesh resolution. However, only the results of the fine grid are presented in this paper. The quality of LES for present grid resolution is charac-

terised according to Pope's criterion (Pope, 2004). It is ensured that at least 80% of the total turbulent kinetic energy is resolved in the majority of the flame region, considering the fully turbulent phase of the explosion in configuration BBBS. All the LES simulations are performed on an HP Z420 workstation with an Intel Xeon 3.5 GHz processor. Under the current grid resolution, a run for the case BBBS (the most turbulent and time-consuming) requires 408 CPU hours until the leading edge of the flame exits the explosion chamber.

4. Results and discussions

The results of stagnant, stoichiometric propane/air explosion deflagrating flames in a range of configurations are presented and discussed in this section. The first aim is to demonstrate the mechanism of pressure rise in vented explosions. The focus is on the advantage and potential of using LES in providing adequate information in order to aid safe design in relevant process industries, e.g. computation of gas expansion and venting rates can help optimise the design of vents in industrial buildings to minimise major destruction caused by high overpressure. The second aim is to assess the ability of LES and the implemented DFSD model in capturing key characteristics of explosion dynamics and predicting the essential safety-related parameters such as the peak overpressure in the chamber. A particular interest is to analyse the underlying physics associated with flame-solids interactions and illustrate the effects of number and location of obstructions in selected configurations.

4.1. Qualitative study of flame propagation

This section aims to illustrate the typical flame behaviours occurring in vented explosions with repeated obstructions. Figure 5 displays a sequence of high-speed images of laser-induced fluorescence from OH (LIF-OH) from the experiment and calculated resolved FSD contours from LES in the configuration BBBS. Note that the LIF-OH images only mark the reaction zone qualitatively, and large values of resolved FSD indicates the numerical reaction zone calculated from LES. Due to some difficulties in the experiments, two imaging tiers were used to capture the

Figure 5: Time sequence of flame propagation in configuration BBBS. Top: LIF-OH images (false coloured) (Al-Harbi, 2013). Bottom: LES images (coloured by the resolved part of the FSD). Physical times after ignition are indicated at the top of each image. Time instant when the position of flame leading edge from LES matches the corresponding LIF-OH image (t_0).

maximum viewable height but not the whole explosion chamber (Alharbi et al., 2014). Note that the right-hand side of the LIF-OH images appear blank because the laser sheet is blocked in the corresponding region (Al-Harbi, 2013). These high-speed images are compared with the contours of resolved FSD from LES to demonstrate the flame shape and to validate the global degree of contortion in the flame at various stages. As there is a slight time variation in flame position for each experimental run, the starting time t_0 of the first flame image from LES is chosen so that the furthest flame leading edge matches that of the high-speed image. The time intervals between successive LES images are kept same as in the high-speed images.

After the initialisation of the ignition, a flame kernel is formed and grows hemispherically. Evidently, from Figure 5, the leading edge of the flame hits the first baffle plate and starts protruding through the narrow vents. As a result, the flame separates into finger-like shapes. However, at this early stage, the flame is not much wrinkled because the turbulence level is low behind the first baffle. Between the first and the second baffle plates, the four finger-shape flame humps merge and are also seen to propagate laterally towards the walls of the chamber. Note that the flame forms four fingers again when hitting the second baffle plate. It is then subjected to noticeable stretch due to higher local turbulence. After jetting out of the third baffle, the flame becomes significantly stretched and wrinkled. It encounters the central square obstacle at a very high speed and subsequently wraps around it. The highly wrinkled flame front propagates past the last obstruction and gets reconnected quickly in the recirculation zone. After that, the flame propagates toward the chamber exit.

Note that the ‘geometrical’ effect of obstacles with a sharp-edged cross-section in the direction of flame propagation can be identified from the flame images. It can be seen from the successive LES images that there are small packets of unburned mixture trapped in the burned gases on the faces of some obstructions (e.g. strips of the baffle plates), left by the distorted flame front wrapping around them. For instance, the last images of both LES and experiments clearly show the trapped fresh

gases in the recirculation zone downstream of the square obstacle. As a matter of fact, the trapped fresh mixture is typically present in the upstream and downstream regions of the baffle bars and the square obstacle and they will be consumed subsequently and contribute to the internal pressure rise of the chamber at later stages of the explosion. Comparison between the LIF-OH images at 12 ms and 12.8 ms and also between their corresponding LES images confirms that the trapped mixture in the area upstream of the central obstacle has been burned. The numerical and experimental images demonstrate the capability of reproducing flame structure, propagation rates and the entrapment of the unburned gases at various stages of the explosion using LES.

4.2. Explosion characteristics: family 1

Family 1 consists of configurations 00BS, 0BBS and BBBS with progressively increasing number of baffle plates from one to three and positioned furthest from the ignition bottom as displayed in Figure 3. Figure 6 presents the histories of overpressure at the base of the chamber from LES and experiments for the configurations in family 1. Some data processing of raw experimental pressure signals was conducted to facilitate the comparison against the numerical results. First, pressure signals are aligned based on the peak overpressure for each realisation and are then grouped in a statistical envelope, in order to perform averaging and to visualise the variation in overpressure magnitudes for all the signals. Next, the mean pressure trace is plotted within the envelope to view the pressure trend and mean peak overpressure from experiments. Lastly, as there is a slight shift in time due to the variability in the ignition for each run, the variation in the time to reach the peak (referred to as “time-to-peak”) is indicated in Figure 6. Experimental mean pressure trace is placed according to the averaged times taken to reach the peak. Predicted LES pressure is also plotted to compare with the experimental data.

It can be seen from Figure 6 that LES with the DFSD model is able to correctly predict the trend and magnitude of overpressure compared with experiments. The calculated time instant for the peak overpressure also matches the experiments

Figure 6: Comparison of predicted and measured pressure-time traces of family 1. Mean experimental pressure signal (dashed line). Statistical envelope (grey background). The range of time taken to the first peak overpressure in the experiment (“Time to peak”).

well. Furthermore, the predicted maximum overpressure is in good agreement with experiments. This is encouraging because the peak pressure is one of the most important parameters used in the safe design of buildings and equipment. It can be observed that the trend of overpressure rise is similar for all the three configurations in family 1. It is apparent that following ignition, the pressure grows in a fluctuating manner but remains relatively low (less than 10 mbar) in the initial period of the explosion. Then, it increases sharply up to the peak pressure and the process is almost monotonic. Thereafter, the overpressure begins to drop, and it oscillates towards the atmospheric pressure due to acoustics. It should be noted that considering the computational time and practical importance, calculated magnitudes of subsequent weak pressure peaks are not validated in the present study. Figure 6 also shows the impact of number of baffle plates and their positions with respect to distance from the ignition bottom. Evidently from both LES and experiments, increasing the number of baffles gives rise to increased turbulence, faster flames and shortens the time to reach the peak pressure. Generally, the maximum overpressure also increases when extra baffle plates are added from 00BS to BBBS. From experiments, the magnitude of the peak pressure increases by about 52% when an additional baffle is added upstream of the third one, i.e. from 00BS to 0BBS, which is also excellently reproduced by LES. Interestingly, although configuration BBBS gives the highest overpressure level as expected, the relative growth is considered

small when the first baffle is added in configuration 0BBS. Changing from 0BBS to BBBS, LES predicts an increase in peak pressure by around 18% while it is only by 1.4% in the experiments. It may reveal that the effect of the first baffle is not as significant as predicted numerically. One possible interpretation is that the DFSD model tends to overestimate the level of flame wrinkling in this case, while the influence of turbulence on the flame is practically not that strong when the flame passes the first baffle. It also explains the slight advance in the calculated time-to-peak for configuration BBBS compared with experiments. Nevertheless, LES is able to mimic the pressure rise and fluctuation in the early stage of the explosion. It is also satisfactory in predicting the peak overpressure, its time of incidence as well as pressure gradient in all three configurations.

Figure 7: Propagation speed of the flame's leading edge from LES and experiments of family 1. Positions of three baffle plates (B1, B2, B3) and the central square obstacle (Sq.Ob.).

Flame acceleration is responsible for fast burning and subsequent rise in internal pressure in an explosion enclosure. It is known that the flow around the obstacles results in an increase of flame surface and it can lead to flame acceleration. In addition to the 'geometrical' factor, turbulence and eddies may also wrinkle the flame front at the same time. Figure 7 displays the speed of flame leading point from LES and experimental measurements. Locations of the midpoints of the three baffle plates (B1, B2, B3) and the central square obstacle (Sq.Ob.) are also annotated in the figure. Experimentally, flame displacements are derived from the measured LIF-OH flame images. The speed of the flame leading point is then computed knowing that high-speed imaging system has a repetition rate of 5 kHz. Numerically, it is

calculated from the flame position identified by $\tilde{c} = 0.5$.

In general, the flame speed calculated from LES is in good agreement with experimental measurements. To understand the phenomenon and mechanism of flame acceleration, configuration BBBS is taken here for the illustration. Throughout the explosion event, the flame front speed increases significantly from ~ 5 m/s close to the bottom end of the chamber to ~ 140 m/s near the top exit. Initially, the flame is laminar and expands hemispherically before touching the side walls. Consequently, the flame front moves relatively slowly within the chamber until turbulence develops. The leading-edge speed in the early stage is mainly determined by two factors: 1). the laminar burning velocity of the fuel/air mixture, and 2). thermal expansion caused by the density difference between the unburned and burned gases. A slight increase in flame speed can be observed as the flame propagates through the first baffle, B1. Flame acceleration across B1 seems to be a more of a weak ‘geometrical’ impact on the flame surface, compared to the effect of flame stretch due to turbulence. Flame speed remains relatively low (less than 20 m/s) between B1 and B2 and starts to rise again when the flame moves through B2. Interestingly, a noticeable decrease in flame speed can be observed right after the second baffle from both LES and experiments. Around B3, flame starts to accelerate remarkably due to the high turbulence level. A sudden drop in speed is then predicted by LES after wrapping around the central obstacle and a similar trend is also present in the experimental measurements. This is likely to be caused by the unavoidable lateral movement when interacting with the eddies and wake around the central obstacle. Thereafter, flame speed increases in a quasi-steady manner towards the chamber exit, as predicted by LES. However, comparison with experiments is not applicable in the region close to the open end. Notice that in spite of the high congestion of obstructions, the flame front tends to decelerate after propagating through each baffle plate mainly due to the lateral movement and interference from vortices and eddies.

Figure 7 also reveals the effects baffle plates in this series of configurations.

Comparing configuration 0BBS and BBBS with the case of the single baffle, 00BS, it is noticeable that increasing the obstruction frequency leads to greater flame propagation speed in the blow-down region after the last obstruction. The kinks in the speed profiles are because of the temporary slowdown of the flame front right before it encounters an obstacle. Globally, LES reproduces the essential dynamic behaviours of the explosion such as flame acceleration and deceleration in all three configurations very well. Slight deviations from the experimental measurements can be noticed when the flame is downstream of the square obstacle in the blow-down region. This may be partially due to the limited time resolution of high-speed images considering the high turbulence and flame front speeds within the region.

4.3. Explosion characteristics: family 2

Family 2 consists of configuration B00S, BB0S and BBBS where baffles increase from 1 to 3 from the ignition end. The explosion characteristics of configurations in this family and comparison with family 1 are discussed in this section.

Figure 8: Comparison of predicted and measured pressure-time traces of family 2. Mean experimental pressure signal (dashed line). Statistical envelope (grey background). The range of time taken to the first peak overpressure in the experiment (“Time to peak”).

Figure 8 and Figure 9 present the pressure history and flame front speed, respectively for this family. Within the family, peak pressure increases with respect to the number of baffles and its incidence time also advances. This is expected as additional baffles increase the turbulence level and the interaction with the flame front, enhancing the burning rate as a result. Compared to family 1, configuration B00S and BB0S have lower peak pressures than their counterparts 00BS and 0BBS where

the same number of baffles are applied. It can be observed that for the cases of a single baffle plate and a square obstacle, moving the baffle from B3 to B1 leads to $\sim 50\%$ reduction in peak overpressure. This is reflected from both experiments and LES although the peak pressure is somewhat overestimated in LES for case B00S. It reveals the influence of the baffle position with respect to the square obstacle and ignition end. Figure 9 proves that for case B00S, the relatively large distance

Figure 9: Propagation speed of the flame's leading edge from LES and experiments of family 2. Positions of three baffle plates (B1, B2, B3) and the central square obstacle (Sq.Ob.).

between the baffle and square obstacle allows the flame to relaminarise before it reaches the central obstacle. This results in a noticeable small increase in the pressure history after the flame passes the first baffle. Encouragingly, LES is able to reproduce the first pressure peak for this case though there is a slight time difference against the experiments. Similarly, for configuration BB0S, the separation between the second baffle and the obstacle allows the flame to relaminarise. Therefore, it can be concluded that the distance between the baffle plate and the ignition source controls the pressure level and the global flame propagation. It is worth mentioning that relaminarisation can occur in a deflagration if the distance between adjacent obstructions is sufficiently large. Another interesting observation is that for case BB0S only, there is a noticeable small pressure peak when it is dropping at around 10 ms. The weak peak has been found to occur when the flame is located between the central obstacle and the chamber exit, which is also reproduced by LES. From the numerical perspective, the instantaneous increase in overpressure can be reflected by the sudden rise in the flame wrinkling factor or global burning rate within

the chamber. As mentioned before, there could be trapped unconsumed fresh gases upstream and downstream the obstructions after propagating past them and they may be a large source of turbulence depending on the configuration. Therefore, the subsequent consumption of a relatively large amount of trapped unburned mixture may contribute to the weak overpressure rise after the main pressure peak in configuration BB0S. However, further experimental and numerical investigations of flow and flame structures around this weak peak are needed for a complete explanation.

Figure 10 and Figure 11 show the comparison of the simulation results of the main pressure peak with the experimental data. In terms of time, the calculated values are almost all within the range of experimental errors. The largest deviation occurs in the case BBBS where it is $\sim 11\%$ ahead of the experimental average. For the pressure magnitude, the predictions of configuration 00BS, B0BS and 0BBS are most consistent with the experiments and the relative error is less than 7%. The trend of maximum pressure with configurations is also correctly calculated by LES. Notable discrepancies are found in case B00S and 0B0S where they are overestimated by ~ 20 mbar. It is noted that slight over-prediction in peak pressure is also present in several other configurations (e.g. 000S and BB0S). This may be partly due to the neglect of the chamber heat loss as a result of the adiabatic boundary condition on the walls of the chamber. However, as the flame/wall interactions and heat transfer in a highly unsteady explosion event are not well understood, the present treatment is thought to be effective.

Comparing Figure 10 with Figure 11, it can be seen that the time to peak and the magnitude of the pressure peak are not always negatively correlated. For instance, the maximum pressure of case 0BBS is almost twice that of BB0S, but the incidence time for the latter is more than 2 ms faster, as indicated by both LES and the experiment. This may be explained by the difference in the flame front location where the main pressure peak is reached. The study of obstacle arrangement within the chamber (Figure 11) also shows that the optimal case for producing internal pressure is the BBBS configuration which has three baffles and a square obstacle.

Figure 10: Summary of the time taken to reach the main pressure peak from experiments and LES for 8 configurations.

Figure 11: Summary of the magnitude of the main pressure peak at the base of the chamber from experiments and LES for 8 configurations.

In this case, the flame stretches to a high level as it passes the three successive baffles, which is a result of high level of turbulence caused by the baffle plates. The resulting increase in burning rate leads to acceleration of flame propagation. Therefore, a large amount of pressure builds up over the obstacles thus a very high peak pressure occurs.

Calculations and analysis of a range of configurations using LES have been proved to be successful in predicting the maximum overpressure and exploring aspects such as the effects of location and number of obstacles as well as the level of blockage. It may be concluded that in an explosion, the impact of the number and location of obstacles on the timing of the pressure peak is very complex and simple correlations may not be applicable. The promising results and details from LES in the small-scale explosion chamber suggest the possibility of extending the study to large-scale industrial buildings with complex obstacles.

4.4. Gas expansion and venting in the explosion chamber

This section aims to explicate the mechanisms associated with the accumulation and release of the chamber internal pressure. The goal is to illustrate the link between the overpressure history and the flame propagation for explosions in a vented enclosure using LES. Configuration BBBS is used here as a demonstration and the analysis can also be extended to all other cases. Figure 12 presents the spatial distribution of the internal overpressure at five instants from the LES. As pressure is found to be nearly homogeneous in the cross-section of the explosion chamber, only the axial profiles are given. It can be seen from Figure 12 that the pressure remains nearly uniform in the region of obstacles while there is a negative gradient from the most downstream obstruction towards the chamber exit (250 mm). As expected, the maximum internal pressure is located near the closed end of the chamber where ignition takes place. Hence, the overpressure monitored on the chamber base is considered for the analysis and discussion in the rest of the section.

The increase and decrease of overpressure within the explosion chamber can be directly explained by the competition between the two phenomena: expansion of the

Figure 12: Spatial distribution of overpressure along the axial direction from the ignition end and between the first two baffle strips for configuration BBBS. Pressure profiles are extracted from the LES and the physical times are indicated.

gases and venting at the chamber exit. The rate of gas expansion can be represented by the rate of volume change of the fresh unburned gases with the burned gases. In LES, this may be calculated from

$$\dot{V}_{expansion} = \frac{\partial}{\partial t} V_b \left(1 - \frac{\rho_b}{\rho_u} \right) \quad (7)$$

where ρ_u and ρ_b are the densities of unburned and burned mixtures, respectively. The volume occupied by the burned gases, V_b , can be evaluated by integrating $\bar{c}$ over the entire computational domain Ω : $V_b = \int_{\Omega} \bar{c} dV$ (Wang et al., 2012). The venting rate is computed as the volume flow rate across the chamber exit:

$$\dot{V}_{vent} = \int_{A_{exit}} \vec{u} \cdot \vec{n} dA \quad (8)$$

where $\vec{u}$ and $\vec{n}$ are the velocity and its normal direction, respectively.

Figure 13 displays the rates of expansion and venting and their relation to the

Figure 13: Pressure rise and oscillations of configuration BBBS illustrated by expansion and venting of gases. Top: Overpressure time trace from LES. Bottom: Expansion and venting rates evaluated from LES. Time instants of flame reaching the three baffle plates (B1, B2, B3), the central square obstacle (Sq.Ob.) and chamber outlet ('Out'). Time of the first peak overpressure ('Peak').

evolution of overpressure in the explosion for case BBBS. Times of flame moving through the midpoints of all the obstructions are also identified as B1, B2, B3, and Sq.Ob. The figure also indicates the time taken to reach the peak overpressure and the time when the flame exits the chamber. When $\dot{V}_{expansion} > \dot{V}_{vent}$, pressure builds up inside the chamber. In contrast, $\dot{V}_{expansion} < \dot{V}_{vent}$ will lead to a decrease in overpressure.

Clearly, from Figure 13, the overpressure history is closely related to the competition between gas expansion and venting. Before the flame reaches the second baffle, pressure increases gradually in a fluctuating way. A similar pattern can also be observed from the experimental pressure signals in other configurations, e.g.

from Figure 8. The fluctuation is represented by the alternative evolution of both expansion and venting rates. When the flame is at the upstream position of B2, the explosion chamber is efficiently vented, given that the expansion and venting rates grow at very close values and the pressure remains relatively low. At this early stage of the explosion, the expanded volume created by the burned gas from the combustion process can be properly exhausted through the venting from the chamber outlet. Overpressure begins to rise sharply between B2 and B3 where the flame starts to transit from quasi-laminar to fully turbulent. This is reflected by the significant growth in the expansion rate at almost the same time. Meanwhile, rapid burning also pushes more unburned mixture towards the chamber exit, inducing a corresponding enhancement in explosion venting. However, a lag between the two phenomena means that the flow is not sufficiently expelled from the chamber and it gives rise to the pressure rise. Maximum overpressure is reached when the venting rate takes over the expansion rate. It takes place between the square obstacle and the chamber open end as it is the furthest obstruction downstream encountered by the flame. Beyond this point, overpressure drops because venting is relatively more efficient than combustion for the rest of the fresh gases within the chamber. At about 10.2 ms, the leading edge of the flame exits the chamber and the expansion rate stops rising. Combustion is only maintained for a very short period before decreasing, as a result of burning of the remaining fresh gases at the corners of the chamber and in the wake area of the obstructions. In the meantime, the venting rate is adjusted by the acoustic reflection, and consequently, pressure drops and oscillates towards the atmospheric level. As shown in Figure 13, both venting and expansion rates decrease in an alternative manner after the flame leaves the chamber, generating weak peaks observed in the pressure history from LES. The oscillations of overpressure after the first peak reproduced by LES agree with the frequency observed in experiments (not shown in this paper) (Al-Harbi, 2013). The computation of these oscillations is closely related to the size and the velocity boundary condition of the extended computational domain which resembles the external

atmosphere. However, reliable prediction of pressure oscillations due to acoustics is outside the scope of this study. The discussion here primarily aims to demonstrate the identification and quantification of venting and expansion processes related to the whole overpressure history in an explosion event.

In general, current numerical setup for LES performs excellently in capturing the details of pressure build-up and fluctuations. The evaluation of venting effectiveness from LES reveals the direct effect of chamber length and inbuilt obstructions on overpressure evolution. This analysis is of specific interest since it potentially offers a systematic and efficient way of design parameter studies such as chamber length, locations, and sizes of the vents for effective pressure relief in safety-related assessment.

4.5. *Effects of obstacle-generated turbulence*

The previous discussion has highlighted that the blockage level, relative position and number of obstructions and venting effectiveness influence the explosion overpressure and flame propagation. The objective of this section is to physically understand the effects of solid obstacles in the vented explosion using detailed flow and flame information provided by LES.

Figure 14 shows the snapshots of flame propagation in configuration BBBS at $t = 5.2, 7.5, 8.6, 9.1$ and 9.6 ms on the mid-plane of the chamber. In the figure, the flame front can be identified from the iso-line denoted by $\tilde{c} = 0.5$ and the turbulence structures may be seen in the vorticity contour field. In practice, the fresh gas being pushed away by the burned combustion products can generate vortices and turbulence ahead of the flame in the presence of an obstruction. Interactions between the propagating flame front and the surrounding turbulent eddies lead to an increase in burning rate. Evidently, from Figure 14, vortex shedding is present throughout the flame propagation and the overall vorticity level rises with respect to time. Wakes and recirculation zones can be observed spreading on the edge and back of each baffle bar and the square obstacle. At $t = 5.2$ ms when the flame is interacting with the first baffle, the expanding gases generate vortex cores in the wake of B2, B3,

Figure 14: LES snapshots of flame propagation for configuration BBBS at times 5.2, 7.5, 8.6, 9.1 and 9.6 ms following ignition, from left to right. Vorticity field and isoline of $\bar{c} = 0.5$.

and Sq.Ob. downstream even though the flame is still at B1. However, turbulence is still relatively weak compared to the later stages. At $t = 7.5$ ms, the wake area behind the second and third baffles has grown significantly, and the propagating flame front is stretched by the resulting vortices. At this instant, the most intense recirculation appears near the vertical sides of the central obstacle. Since B3 and Sq.Ob. are relatively close, a strong turbulent flow field is generated between them, as can be seen from the snapshot at $t = 8.6$ ms. Thereafter, the flame front vigorously interacts with the turbulent eddies of the region. This largely wrinkles the flame front, expand the flame surface and consequently, raise the burning rate. After $t = 9.1$ ms when it passed the square obstacle, the flame has become wrinkled and corrugated and the peak overpressure occurs subsequently. At $t = 9.6$ ms, even if there is no more obstruction downstream, turbulent structures in this region support the deflagration and the flame still accelerates until exiting the chamber. However, the level of flame/turbulence interaction may not increase any further.

Figure 15: LES snapshots of flame propagation for configuration BB0S at times 4.6, 7.2, 8.3, 9.0 and 9.7 ms following ignition, from left to right. Vorticity field and isoline of $\tilde{c} = 0.5$.

Figure 15 shows the same snapshots for configuration BB0S as a comparison. Comparison between the two configurations (BB0S and BBBS) shows that the introduction of obstructions in the path of the flame clearly increases the turbulence throughout the chamber. The level of turbulence for configuration BB0S is generally lower than BBBS in various phases of the explosion, as shown in Figure 14 and Figure 15. Besides the difference in flow pattern and flame front structure, the absence of the third baffle greatly reduces the vorticity magnitude especially in the wake of the square obstacle. Thus, the flame can relaminarise before touching the central obstacle. Consequently, the interactions between the flame and the vortices are much weaker, resulting in a significantly lower (by $\sim 50\%$) peak overpressure. After passing the square obstacle, a considerable less wrinkling and surface area of the flame can be observed, when changing the configuration from BBBS to BB0S.

The snapshots in Figure 14 and Figure 15 clearly identify that the vortex cores and turbulence interacting with the flame front greatly affect the flame behaviour.

Note that vortex structures are present in the wake of all obstructions from the early to the later stage of the explosion. This highlights the significance of capturing the vortex pattern and the flow dynamics within the chamber in all phases of the explosion.

5. Conclusion

LES simulations of a stagnant, stoichiometric propane/air mixture have been carried out to study the mechanism of pressure rise in vented explosions with various obstacle arrangement.

The considered test cases are a series of experiments conducted in a small-scale vented explosion chamber where three baffle plates and a central square obstacle can be installed. The numerical simulation work considered here uses the large eddy simulation technique. The main advantage of using a DFSD model in LES is being able to account for flame wrinkling due to obstacle-generated turbulence at the subgrid scale and dynamically calculate the burning rate for various phases of the deflagration.

Results from the numerical simulations are first validated against the experimental data. It is proved that LES with the DFSD model is capable of reproducing key flame characteristics in an explosion event. Comparison between LES and high-speed images from the experiment shows that the flame is quasi-laminar in the early stage, but the degree of wrinkling increases as the flame front propagates past successive baffles and obstacles. Present numerical setup has been proved successful in predicting essential safety-related parameters such as the timing and magnitude of the maximum overpressure and flame propagation speed at distinct stages of the explosion. In general, the LES predictions for all flow configurations are in good agreement with experimental measurements of the overpressure and flame propagation.

Another highlight of the present investigation is the study of effects of solid obstructions on the global explosion characteristics. The blockage level, number and

location of the solid obstacles, and their relative position to the ignition source have been found to have a significant impact on the magnitude of overpressure and the spatial flame structure. Numerical study of different groups of configurations reveals that the pressure rise within the chamber is linked to the position of the successive obstacles. It can be summarised that the maximum overpressure increases as the baffle plates are moved downstream from the ignition source or when additional baffles are positioned closely in the sequence. Extensive interactions with obstructions and wrinkling of the flame front have been observed and they lead to substantial flame acceleration and pressure rise. However, large separation between the baffles and the square obstacle allows for sufficient residence time for turbulence decay. This may result in laminarisation of the flame front unless disturbed by a new obstacle, causing a lower overpressure.

The overpressure history has been associated with the evolution and competition of two phenomena inside the chamber: expansion and venting. Identification and quantification of the mechanisms driving the pressure build-up using LES potentially provide a systematic and effective way of studying venting efficiency for safe design of vents in process industries.

The obstacle-generated turbulence is responsible for the large overpressure and the underlying physics are illustrated by the LES results. Generation of vortices and turbulence from the obstacles have been observed throughout the explosion. It has been identified that an explosion event may involve various stages considering the level of flame/turbulence interactions. In the early quasi-laminar stage, the flame propagation is relatively slow, and the resulting overpressure remains low. While in the later fully turbulent stage, the flame front strongly interacts with the surrounding turbulent eddies and is subsequently wrinkled, and it significantly contributes to the pressure build-up. Therefore, accurately reproducing the flow dynamics in all phases of the explosion is essential to perform reliable LES.

In conclusion, the pressure rise in a vented explosion is driven by the relationship between combustion and venting. The timing and the magnitude of the peak over-

pressure are strongly dependent on the level of flame/turbulence interaction which originates from the number and location of obstructions. LES is a useful tool for illustrating and quantifying mechanisms of pressure build-up in an obstacle-embedded environment that are generally encountered in real gas explosions. Although it still relies on the sub-models used in the simulation, it is promising in predicting essential safety-related parameters.

References

- Al-Harbi, A., 2013. Turbulent Premixed Flames Propagating Past Repeated Obstacles. Ph.D. thesis. University of Sydney. URL: <http://hdl.handle.net/2123/9765>.
- Alharbi, A., Masri, A.R., Ibrahim, S.S., 2014. Turbulent premixed flames of CNG, LPG, and H₂ propagating past repeated obstacles. *Experimental Thermal and Fluid Science* 56, 2–8. URL: <http://dx.doi.org/10.1016/j.expthermflusci.2013.11.012>, doi:10.1016/j.expthermflusci.2013.11.012.
- Birkby, P., Cant, R.S., Savill, A., 2000. The application of a laminar flamelet model to confined explosion hazards. *Flow, Turbulence and Combustion* 63, 361–377. doi:10.1023/A:1009932203310.
- Bjerketvedt, D., Bakke, J.R., van Wingerden, K., 1997. Gas explosion handbook. *Journal of Hazardous Materials* 52, 1–150. URL: <http://www.sciencedirect.com/science/article/pii/S0304389497816202>, doi:[https://doi.org/10.1016/S0304-3894\(97\)81620-2](https://doi.org/10.1016/S0304-3894(97)81620-2).
- Boger, M., Veynante, D., 2000. Large eddy simulations of a turbulent premixed v-shape flame, in: Dopazo, C. (Ed.), Eighth European Turbulence Conference, Eighth European Turbulence Conference, Barcelona, Spain. pp. 448–452. doi:10.1016/0142-727X(90)90030-F.
- Boger, M., Veynante, D., Boughanem, H., Trouvé, A., 1998. Direct numerical simulation analysis of flame surface density concept for large eddy simulation of turbulent premixed combustion. *Symposium (International) on Combustion* 27, 917–925. URL: <http://www.sciencedirect.com/science/article/pii/S008207849880489X>, doi:10.1016/S0082-0784(98)80489-X.
- Bray, K.N.C., Libby, P.A., Moss, J.B., 1985. Unified modeling approach for premixed turbulent combustion-Part I: General formulation. *Combustion and Flame* 61, 87–102. doi:10.1016/0010-2180(85)90075-6.
- Catlin, C.A., Fairweather, M., Ibraiim, S.S., 1995. Predictions of turbulent, premixed flame propagation in explosion tubes. *Combustion and Flame* 102, 115–128. doi:10.1016/0010-2180(94)00245-N.

- Chen, P., Guo, S., Li, Y., Zhang, Y., 2017. Experimental and LES investigation of premixed methane/air flame propagating in a tube with a thin obstacle. *Combustion Theory and Modelling* 21, 274–292. URL: <http://dx.doi.org/10.1080/13647830.2016.1218054>, doi:10.1080/13647830.2016.1218054.
- Chippett, S., 1984. Modeling of vented deflagrations. *Combustion and Flame* 55, 127–140. doi:10.1016/0010-2180(84)90022-1.
- Di Sarli, V., Di Benedetto, A., Russo, G., 2009. Using Large Eddy Simulation for understanding vented gas explosions in the presence of obstacles. *Journal of Hazardous Materials* 169, 435–442. doi:10.1016/j.jhazmat.2009.03.115.
- Fiorina, B., Vicquelin, R., Auzillon, P., Darabiha, N., Veynante, D., Fiorina, B., Vicquelin, R., Auzillon, P., Darabiha, N., Gicquel, O., 2010. A filtered tabulated chemistry model for LES of premixed combustion. *Combustion and Flame* 157, 465–475. URL: <http://dx.doi.org/10.1016/j.combustflame.2009.09.015>, doi:10.1016/j.combustflame.2009.09.015.
- Germano, M., Piomelli, U., Moin, P., Cabot, W.H., 1991. A dynamic subgrid-scale eddy viscosity model. *Physics of Fluids A: Fluid Dynamics* 3, 1760–1765. doi:10.1063/1.857955.
- Gülder, Ö.L., Smallwood, G.J., 1995. Inner cutoff scale of flame surface wrinkling in turbulent premixed flames. *Combustion and Flame* 103, 107–114. doi:10.1016/0010-2180(95)00073-F.
- Hawkes, E., Cant, R., 2000. A flame surface density approach to large-eddy simulation of premixed turbulent combustion. *Proceedings of the Combustion Institute* 28, 51–58. URL: <http://www.sciencedirect.com/science/article/pii/S0082078400801940>, doi:10.1016/S0082-0784(00)80194-0.
- Ibrahim, S.S., Gubba, S.R., Masri, A.R., Malalasekera, W., 2009. Calculations of explosion deflagrating flames using a dynamic flame surface density model. *Journal of Loss Prevention in the Process Industries* 22, 258–264. URL: <http://dx.doi.org/10.1016/j.jlp.2008.05.006>, doi:10.1016/j.jlp.2008.05.006.
- Kirkpatrick, M.P., 2002. A large eddy simulation code for industrial and environmental flows. Ph.D. thesis. The University of Sydney.
- Kirkpatrick, M.P., Armfield, S.W., Masri, A.R., Ibrahim, S.S., 2003. Large Eddy Simulation of a Propagating Turbulent Premixed Flame. *Flow, Turbulence and Combustion* 70, 1–19.
- Knikker, R., Veynante, D., Meneveau, C., 2002. A priori testing of a similarity model for large eddy simulations of turbulent premixed combustion. *Proceeding of Combustion Institute* 29, 2105–2111. doi:10.1016/S1540-7489(02)80256-5.
- Leonard, B.P., 1987. SHARP Simulation of Discontinuities in Highly Convective Steady Flow. Technical Report 100240. Institute for Computational Mechanics in Propulsion, NASA Lewis Research Center. Cleveland, OH, United States.

- Ma, T., Stein, O., Chakraborty, N., Kempf, A., 2013. A posteriori testing of algebraic flame surface density models for LES. *Combustion Theory and Modelling* 17, 431–482. URL: <http://dx.doi.org/10.1080/13647830.2013.779388>, doi:10.1080/13647830.2013.779388.
- Mercier, R., Moureau, V., Veynante, D., Fiorina, B., 2015. LES of turbulent combustion: On the consistency between flame and flow filter scales. *Proceedings of the Combustion Institute* 35, 1359–1366. URL: <http://dx.doi.org/10.1016/j.proci.2014.05.149>, doi:10.1016/j.proci.2014.05.149.
- Metghalchi, M., Keck, J., 1980. Laminar burning velocity of propane-air mixtures at high temperature and pressure. *Combustion and Flame* 38, 143–154. URL: <http://www.sciencedirect.com/science/article/pii/0010218080900462>, doi:10.1016/0010-2180(80)90046-2.
- Na, A.M., Phylaktou, H.N., Andrews, G.E., 2017. Explosion flame acceleration over obstacles : Effects of separation distance for a range of scales. *Process Safety and Environmental Protection* 107, 309–316. URL: <http://dx.doi.org/10.1016/j.psep.2017.01.019>, doi:10.1016/j.psep.2017.01.019.
- Pitsch, H., 1998. FlameMaster: A C++ computer program for 0D combustion and 1D laminar flame calculations. URL: <https://www.itv.rwth-aachen.de/index.php?id=flamemaster>.
- Popat, N.R., Catlin, C.A., Arntzen, B.J., Lindstedt, R.P., Hjertager, B.H., Solberg, T., Saeter, O., Van Den Berg, A.C., 1996. Investigations to improve and assess the accuracy of computational fluid dynamic based explosion models. *Journal of Hazardous Materials* 45, 1–25. doi:10.1016/0304-3894(95)00042-9.
- Pope, S.B., 2004. Ten questions concerning the large-eddy simulation of turbulent flows. *New Journal of Physics* 6. doi:10.1088/1367-2630/6/1/035.
- Powell, T., 2008. The Buncefield Incident 11 December 2005, The Final Report of the Major Incident Investigation Board. Technical Report. URL: <http://www.hse.gov.uk/comah/buncefield/>.
- Rocourt, X., Awamat, S., Sochet, I., Jallais, S., 2014. Vented hydrogen-air deflagration in a small enclosed volume. *International Journal of Hydrogen Energy* 39, 20462–20466. URL: <http://dx.doi.org/10.1016/j.ijhydene.2014.03.233>, doi:10.1016/j.ijhydene.2014.03.233.
- Smith, G.P., Golden, D.M., Frenklach, M., Moriarty, N.W., Eiteneer, B., Goldenberg, M., Bowman, C.T., Hanson, R.K., Song, S., Gardiner Jr, W.C., Others, 1999. GRI 3.0 Mechanism. Gas Research Institute (http://www.me.berkeley.edu/gri_mech) .
- Ugarte, O.J., Akkerman, V., Rangwala, A.S., 2016. A computational platform for gas explosion venting. *Process Safety and Environmental Protection* 99, 167–174. URL: <http://dx.doi.org/10.1016/j.psep.2015.11.001>, doi:10.1016/j.psep.2015.11.001.

- Veynante, D., Moureau, V., 2015. Analysis of dynamic models for large eddy simulations of turbulent premixed combustion. *Combustion and Flame* 162, 4622–4642. URL: <http://dx.doi.org/10.1016/j.combustflame.2015.09.020>, doi:10.1016/j.combustflame.2015.09.020.
- Wang, G., Boileau, M., Veynante, D., Truffin, K., 2012. Large eddy simulation of a growing turbulent premixed flame kernel using a dynamic flame surface density model. *Combustion and Flame* 159, 2742–2754. URL: <http://dx.doi.org/10.1016/j.combustflame.2012.02.018>, doi:10.1016/j.combustflame.2012.02.018.
- Wen, X., Yu, M., Liu, Z., Sun, W., 2012. Large eddy simulation of methane-air deflagration in an obstructed chamber using different combustion models. *Journal of Loss Prevention in the Process Industries* 25, 730–738. URL: <http://dx.doi.org/10.1016/j.jlp.2012.04.008>, doi:10.1016/j.jlp.2012.04.008.
- Werner, H., Wengle, H., 1993. Large-Eddy Simulation of Turbulent Flow Over and Around a Cube in a Plate Channel, in: Durst, F., Friedrich, R., Launder, B.E., Schmidt, F.W., Schumann, U., Whitelaw, J.H. (Eds.), *Turbulent Shear Flows* 8, Springer Berlin Heidelberg, Berlin, Heidelberg. pp. 155–168.

Highlights

- Pressure rise in the vented explosion is illustrated by gas expansion and venting.
- Vortices and turbulence generated behind the obstacles wrinkle the flame front.
- Number and position of obstacles have an effect on flame acceleration and overpressure.
- LES is able to capture key safety-related parameters such as the maximum overpressure.