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On the mechanism of pressure rise in vented explosions: A numerical study

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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.

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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. Fig. 1 briefly illustrates the mechanism of pressure build-up in partially-confined vented explosions with the presence of obstacles.

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 700–1000 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,

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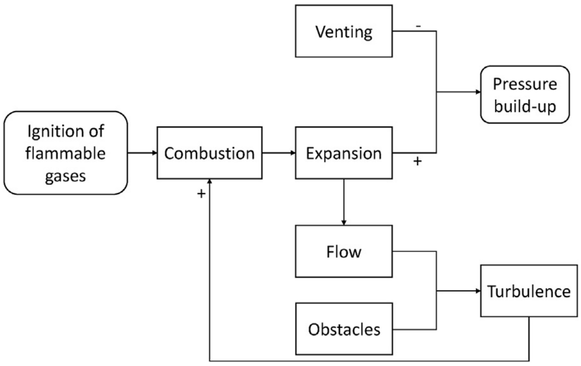

Fig. 1. Illustration of the mechanism driving pressure rise in a vented explosion with obstructions. Positive effect (+). Negative effect (−). The strength of gas expansion and venting determines the overpressure build-up. Obstacle-generated turbulence promotes the combustion rate.

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 submodels 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 Fig. 2a.

The 50 × 50 × 250 mm chamber is square in cross-section and has a volume 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 Fig. 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

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