

Numerical Investigation on Flame Propagation in Vented Gas Explosion

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Explosion venting technology is one of the effective and widely used methods in protection measures against accidental internal gas explosions by relieving the pressure generated within the volume. Extensive studies have been carried out to investigate factors governing to the explosion development i.e. ignition position and vent burst pressure. However, the physical and dynamic process of explosion development during the venting to ambient air is yet not well understood. The primary motivation of this research was to gain improved understanding of turbulent flame propagation in vented gas explosion, with a view to develop improved models and methods for assessing explosion risks in the process industries. Computational Fluid Dynamic (CFD) analyses using FLUENT is adopted to study the phenomenology underlying vented gas explosions. Computations were run on deflagrating turbulent flames in small-scale combustion chambers with two different volumes (0.02 m³ and 0.0065 m³), with both closed at the rear end and open at the opposite face, in order to replicate the experimental work. All cases are initialised from stagnation. Only stoichiometric concentration of propane and methane-air mixtures was considered with different ignition positions and vent static burst pressure, P_v . From the finding, end ignition gave higher reduced overpressure on both experimental and simulation results, compared to central ignition. The inclusion of vents in the enclosures provides significant reduction on the peak overpressures. However, it has been recognised on a tendency to a less effective reduction as the vent burst pressure, P_v was further increased. The competition between combustion rate and venting rate allows the explanation on both number and intensity of the overpressure peaks observed in propane-air explosion.

1. Introduction

In gas explosions, the unsteady interaction of flame propagation, geometry and turbulent flow field drives the mechanisms and phenomena determining the explosion severity at different initial/operating conditions and geometrical parameters. In the chemical, hydrocarbon and gas process industries, the explosive accidents of pressure vessel have been frequently occurring in a confined area within the vessel, pipes, channels or tunnels as they has been used as a transportation of the reactive or combustible material from one section to another section for storage purposes. In order to prevent the destructive damage to plants in industries, several techniques have been developed such as venting. The method of studying discharge technology in vessel extensively been studied extensively in experimental research (Chippett, 1984), theoretical analysis (Simpson, 1986) and numerical simulation (Bingyan et al., 2012). There are numerous influencing factors governing to the explosion development that has been studied include the type of hydrocarbon/fuel-air mixture, ignition position, and vent burst pressure (Kasmani et al., 2013).

However, the study on mechanism of combustion, physical and dynamic process of explosion is still at development stage; the experimental research is capped with site condition and test method as there is great difficulty in theory analysis. Therefore, numerical simulation is finite element software that has been one of the alternative methods of studying vessel explosion and design criteria instead of experimental and theoretical.

The numerical simulation on venting explosion process in closed vessel was built based on Computational Fluid Dynamic (CFD) analyses using FLUENT software in order to fulfil the primary motivation of this research; to gain extensive understanding of turbulent flame propagation associated with vented gas explosion, with a view to develop improved models and methods for assessing explosion risks in the process industries.

2. Numerical model

2.1 Model description

The mathematical model of the pressure field in the vented gas explosion process in closed cylindrical vessel was built based on the ANSYS Fluent CFD (2014). Venting explosion of flammable gas can satisfy three fundamental physical principles involving mass conservation, momentum, energy conservation and chemical components. The analysis of venting explosion of flammable gas in closed vessel has been performed by means of a finite-volume CFD two-dimensional (2D) model based on Navier-Stokes equations. k- ϵ model is used as the turbulence model and combustion model was described by Eddy-Dissipation model. The standard k- ϵ turbulence model was proposed by Launder and Spalding (1972). On the other hand, k- ϵ is a semi empirical model for the turbulence kinetic energy (k) and its dissipation rate (ϵ) as Eqs(1) and (2).

$$\frac{\partial}{\partial t}(\rho k) + \frac{\partial}{\partial x_i}(\rho k u_i) = \frac{\partial}{\partial x_j} \left[\left(\mu + \frac{\mu_t}{\sigma_k} \right) \frac{\partial k}{\partial x_j} \right] + G_k - \rho \epsilon \quad (1)$$

$$\frac{\partial}{\partial t}(\rho \epsilon) + \frac{\partial}{\partial x_i}(\rho \epsilon u_i) = \frac{\partial}{\partial x_j} \left[\left(\mu + \frac{\mu_t}{\sigma_\epsilon} \right) \frac{\partial \epsilon}{\partial x_j} \right] + G_\epsilon - \rho \epsilon \quad (2)$$

FLUENT provides a turbulence-chemistry interaction called Eddy dissipation model (EDM). This model was proposed by Magnussen and Hjertager (1976). The net rate of production of species, i due to reaction $R_{i,r}$, is given by the smaller i.e., limiting value of the two expressions as shown in Eqs(3) and (4):

$$R_{i,r} = v'_{i,r} M_{w,i} A \rho \frac{\epsilon}{k} \min \left(\frac{Y_R}{v'_{R,r} M_{w,R}} \right) \quad (3)$$

$$R_{i,r} = v'_{i,r} M_{w,i} A B \rho \frac{\epsilon}{k} \frac{\sum p Y_p}{\sum_j^N v''_{j,r} M_{w,j}} \quad (4)$$

2.2 Simulation conditions set-up

The size of closed cylindrical vessel for Test vessel 1 and 2 was as follows: length, L = 1 m, diameter, D = 0.162 m and L = 0.315 m and D = 0.162 m. The explosion vent was positioned at the end of the vessel (refer to Figure 1 and 2) for both test vessels but the ignition position was different for Test vessel 1 and 2. It was positioned at the end (rear) and centre of vessel for Test vessel 1 and only end ignition was considered for Test vessel 2. The vessel was filled with premixed fuel-air of stoichiometric ratio; methane and propane. The initial pressure and temperature was at normal condition which is 1 atm and 300 K. Explosion process was ignited by patching a temperature of 2,000 K as spark energy. Schematic plan of computation zones as shown in Figure 1 and 2.

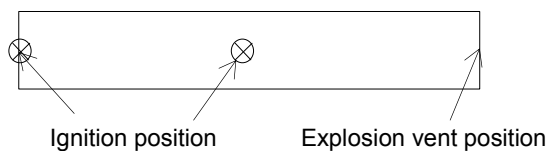


Figure 1: Schematic computation zones for Test vessel 1



Figure 2: Schematic computation zones for Test vessel 2

3. Results and discussion

3.1 The influence of ignition position on Test vessel 1

The influence of ignition position is one of the crucial factors affecting the explosion venting. Thus the detailed investigation of ignition position has been considered because it significantly affects the flame propagation and the relief of internal pressure during a vented explosion. Explosion venting of methane-air and propane-air mixtures were computationally investigated in the cases of rear (end) and central ignition. Computation results of explosion process for open venting explosions were compared with the explosion venting experiment work (Kasmani, 2008). The results of maximum pressure, P_{max} is shown as a function of time for methane and propane explosions with end and central ignition as illustrated in Figure 3 - 5. From Figure 3 and 4, the flame initially shows a good agreement between experimental and computation results in which flame propagated in a slower motion, laminar phase with low pressure and flame speed before the flame approaches the vent. At 100 ms, the pressure attained its maximum peak of 1 barg, whilst the experimental maximum pressure of 0.4 barg was only be reached at 120 ms. It took about 20 ms earlier in computation than experiment. It can be said that, the time taken in simulation result is faster than experiment due to the intensity of combustion in FLUENT is higher than in experiment, this is due the consideration of default hydrocarbon characteristics such as diffusivity and viscosity in simulation (Pederson and Middha, 2012).

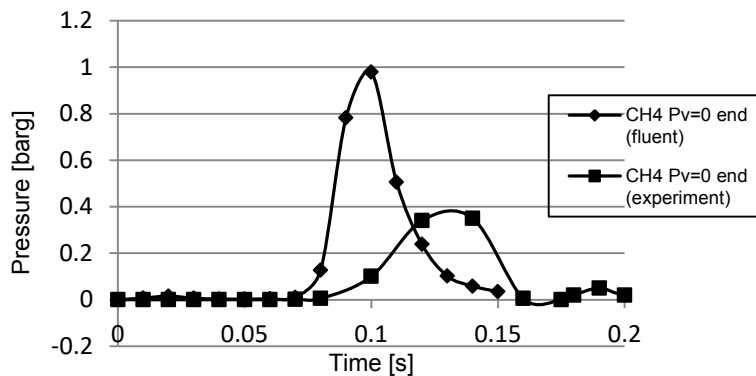


Figure 3: Methane overpressure development data contrast for end ignition

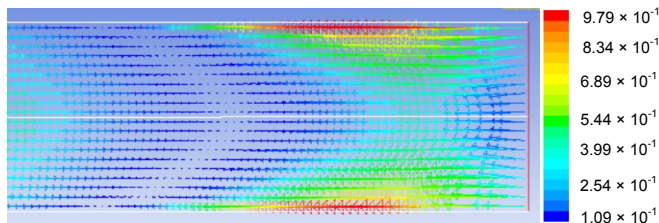


Figure 4: Pressure vector at $t = 0.1$ s

As can be seen in Figure 3 and 4, the maximum pressure at end ignition is slightly higher than central ignition for both computation and experimental results. On the contrary, Bradley and Micheson (1978) reported that the central ignition is considered as the worst case, giving the highest maximum pressure with respect to other ignition positions. Regarding to previous research on vented vessels (Fairweather et al., 2000) the flame initially developed hemispherically from the point of ignition at the end wall, then it elongates towards the vent, in which the unburned gas also being vented out of vessel as shown in Figure 4. The vector direction clearly shown that the unburned gases were also being pushed rapidly towards the vessel with a vigorous interaction between the turbulence and reversal flow from the vent. In contrast, the flame initially moves in spherical flame for central ignition, gradually accelerate on one side towards the vent and also elongate to the opposite direction of vent. From this explanation, it can be said that the end ignition had a larger flame area and thus, gave higher overpressure than the central ignition. Figure 5 illustrates the methane overpressure development data contrast for central ignition.

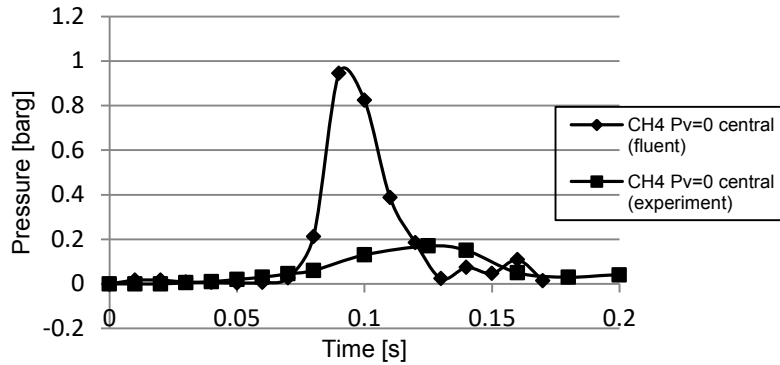


Figure 5: Methane overpressure development data contrast for central ignition

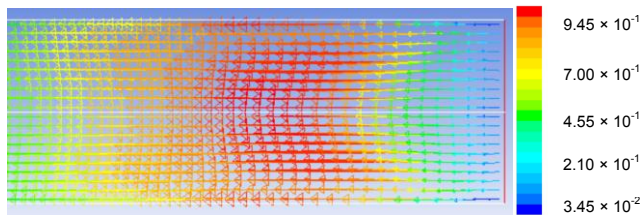


Figure 6: Pressure vector at $t = 0.09$ s

The different flame propagation between end and centrally ignited mixtures can be discussed based on the residual amounts of unburned gases left inside the vessel at the time the flame reaches the vent as shown in Figure 4 and 6. When mixtures are centrally ignited, the flame is stretched on both directions; substantially pushed out only small amount of burned gases from vessel. It can be postulated that combustion is still far from completion as there is larger amount of unburned gases left inside the vessel with respect to the almost complete combustion if mixtures ignited at the end wall ignition, leading to higher P_{max} . Propane gas has higher reactivity than methane gas; vessel pressure of propane was slightly higher than methane as shown in Figure 7. The vessel pressure reached to its maximum pressure at 100 ms and 90 ms for end and central ignition.

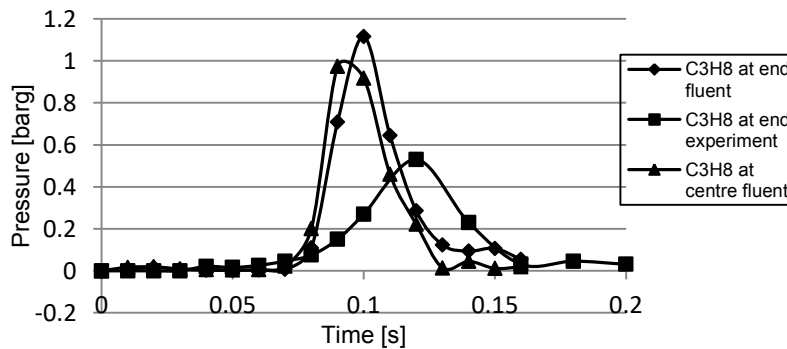


Figure 7: Propane overpressure development for end and central ignition

3.2 The influence of P_v on P_{max} for Test vessel 2

The presence of opening/breaking vent as an obstacle in vessel would delay or hinder the venting process. It would also generate turbulence effects and pressure wave which interacts with the flame front to distort it. As the flame front was distorted, it would increase the flame surface area compressed towards the vent, causing the increment of pressure inside the vessel, and hence, increase the maximum mass burning rate. According to McCann et al. (1985) lower breaking pressure, P_v resulted to lower P_{max} due to smaller flame elongation in vessel and hence, smaller flame area. In contrast, as the breaking pressure is high, it takes longer time to break, reduces the effect of flame distortion and thus, would result on higher P_{max} . The flame at higher P_v

become cellular flame prior to removal of the relief panel. The effect of vent burst pressure, P_v has been studied widely (Cooper et al., 1986) in order to know at what extent this parameter will influence the magnitude of P_{max} . Four different static burst pressures, P_v of 0.098 bar, 0.178 bar, 0.209 bar and 0.424 bar were used. From the investigation, it was found that P_{max} increased with the increase of P_v . Figure 6 and 7 show the variation of maximum overpressure, P_{max} with static bursting pressure, P_v on stoichiometric methane-air and propane-air for 0.315 m length.

Figure 8 illustrates that all the present computation results were well below the experimental data. The computation result from FLUENT gave a similar trend as the experimental result, only at different value, which is smaller in P_{max} . This is due to the assumption adopted in FLUENT. The combustion model used in FLUENT only considered the turbulence-chemistry interaction by neglecting the chemical kinetics rate of reaction. As can be seen, the results at $P_v = 0.098$ bar for end and central ignition are at least 2 and 3 times lower than experimental P_{max} . The trends of computation result of methane are far from consistent and it is apparent that the effects of vent are different for end and central ignition. It should be noted that there was no significant increase in P_{max} for $P_v = 0.209$ bar and 0.424 bar at central ignition. It can be said that, the influence of P_v on P_{max} for centrally ignited was smaller compared to end ignition.

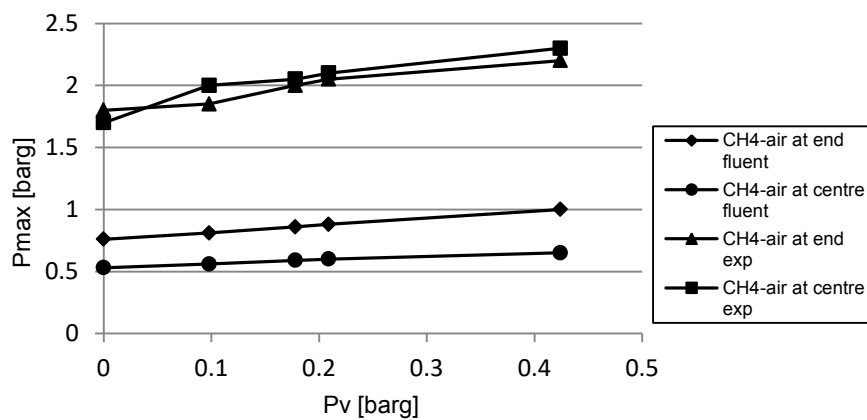


Figure 8: P_{max} versus P_v on stoichiometric methane-air for $L = 0.315$ m of vessel

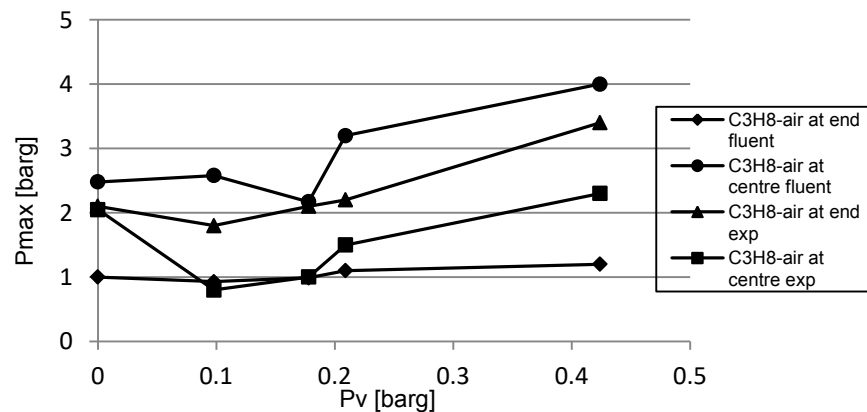


Figure 9: P_{max} versus P_v on stoichiometric propane-air for $L = 0.315$ m of vessel

There was a decrease in P_{max} with P_v for propane at 0.098 bar and 0.178 bar for end and central ignition. Figure 9 shows that the influence of P_v on P_{max} for stoichiometric propane-air explosion was smaller for end ignition in FLUENT result. It was the opposite observation on the stoichiometric methane-air vented explosion. It can be said that, at higher P_v , the explosion is vented at later stage, when the flame is nearer to the walls. It would give a small increase in flame area, resulting to a small increase in burning rate and hence, the overpressure inside the vessel (Ponizy and Leyer, 1999). However, at centrally ignited, both experimental and simulation gave similar trend, giving a lower P_{max} at P_v of 0.209 barg, and an increase of P_{max} afterwards. It can be said that, the simulation model could predict the mechanism of the vented explosion with the presence of the vent, providing all the assumption should be made consideration on the kinetic reaction mechanism.

4. Conclusions

The performed experimental measurements served for the initial setting of the boundary conditions for numerical calculation of methane-air and propane-air combustion. The venting explosion process of flammable gas in closed vessel was simulated by $k-\varepsilon$ turbulence model and Eddy-dissipation turbulent combustion model of FLUENT software. Initially, the results of the experiment and simulation are in a good agreement, but after the opening of bursting disc, the pressure from simulation is higher ~ 2 to 3 times than experiment either at end or central ignition. The different value of static burst pressure, P_v affects the maximum overpressure, P_{max} . The higher the static burst pressure, the higher maximum overpressure obtained, and particularly on more reactive fuel such as propane.

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