# NUMERICAL INVESTIGATION ON FLAME PROPAGATION AND PRESSURE DEVELOPMENT IN VENTED EXPLOSION

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# NUMERICAL INVESTIGATION ON FLAME PROPAGATION AND PRESSURE DEVELOPMENT IN VENTED EXPLOSION

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Specially dedicated to my beloved parents, Mohd Zaidi Othman and Salma bt Abdullah, my husband, my siblings, and friends for their continuous support, prayers, encouragement and also understanding during my master programmes.

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#### ABSTRACT

The understanding of the explosion phenomenon is essential for an effective and safe engineering practice, particularly in refinery and chemical plants. Explosion venting technology is one of the effective techniques in protection measures against accidental internal gas explosions by relieving the pressure generated within the volume. The factors governing to the explosion development such as geometry, ignition position and vent burst pressure have been extensively studied. However, the details physical and dynamic mechanism responsible for the generation of significant pressure peaks during vented explosions is insufficient, making it difficult for designing the accurate explosion reliefs in practical situations. The primary motivation of this research was to better understand the turbulent flame propagation in vented gas explosion using modelling approach. Computational Fluid Dynamic (CFD) analyses using ANSYS Fluent is adopted to study the vented gas explosions process. Computations of the deflagrating flames were run in small-scale combustion chambers with two different volume sizes of 0.02 m<sup>3</sup> and 0.0065 m<sup>3</sup>, closed at the one end and open at the opposite face. Only stoichiometric concentration of hydrogen, propane and methane-air mixtures were considered with different ignition positions (end and central ignition) and vent static burst pressure  $(P_v)$ . The condition of the analysis was following experimental data done from previous researcher. From the findings, end ignition gave higher reduced overpressure on simulation results, about 1.4 times higher compared to central ignition due to the larger flame surface area attained. Thus, the time flame needed to reach the venting area became longer. The vents inclusion in the enclosures caused the reduction on the peak overpressure. As the  $P_v$  was further increased, i.e. from 98 mbar to 424 mbar, the venting effectiveness became lesser by 24 % for the methane explosion but not to the vented propane explosion in simulation analysis. This work confirmed that fuel reactivity gave important role on determining the venting effectiveness as stoichiometric hydrogen attained higher reduced explosion pressure (Pred) of 4.150 bar compared that of stoichiometric methane and propane vented explosion, 0.945 and 1.045 bar, respectively, if ignited at central location. It can be said that the distance from the location of ignition to the vent area, the fuel reactivity and P<sub>v</sub> have significant roles to determine the duration of the pressure build up and the amount of vented mass, which describes the external explosion intensity.

### ABSTRAK

Pemahaman asas tentang fenomena letupan adalah penting untuk amalan kejuruteraan yang berkesan dan selamat, terutama dalam loji penapisan dan loji kimia. Teknologi pelepasan letupan adalah salah satu kaedah yang berkesan sebagai langkah perlindungan daripada letupan gas di dalam tangki dengan melepaskan tekanan yang dihasilkan dalam saluran atau paip. Faktor-faktor yang mengawal perkembangan letupan antaranya ialah geometri, kedudukan pencucuh dan tekanan ledakan pelepas telah dikaji secara meluas. Walau bagaimanapun, perincian mekanisma fizikal dan dinamik yang bertanggungjawab dalam penjanaan tekanan puncak bererti semasa pelepas letupan masih lagi tidak mencukupi, menyebabkan kesukaran mereka bentuk alat pelepasan letupan dengan tepat dalam situasi sebenar. Tujuan utama kajian ini adalah untuk mendapatkan pemahaman yang lebih baik dalam perambatan nyalaan yang bergelora dalam pelepasan letupan gas dengan pendekatan pemodelan. Pengkomputeran Dinamik Bendalir (CFD) dianalisa dengan menggunakan ANSYS Fluent untuk mengkaji proses asas pelepasan letupan gas. Proses pengkomputeran mengenai nyalaan deflagrasi gas ini dikaji di dalam kebuk letupan yang berskala kecil dengan dua saiz isipadu yang berbeza iaitu  $0.02 \text{ m}^3$  dan 0.0065 m<sup>3</sup>, yang mana satu di bahagian hujung yang tertutup dan satu di bahagian terbuka yang bertentangan. Hanya campuran hidrogen, propana dan metana pada kepekatan stoikiometri yang dikaji pada kedudukan pencucuh yang berbeza (di hujung dan tengah pencucuh) dan tekanan statik pelepasan letupan ( $P_v$ ). Keadaan analisa ini berdasarkan kajian yang telah dilakukan oleh pengkaji yang lepas. Daripada kajian, kedudukan pencucuh yang berada dihujung saluran memberikan tekanan yang lebih tinggi dalam simulasi, lebih kurang 1.4 kali lebih tinggi berbanding dengan kedudukan pencucuh yang berada di tengah saluran disebabkan oleh penghasilan permukaan nyalaan yang lebih besar. Jadi, masa yang lebih lama diperlukan oleh nyalaan untuk tiba di kawasan pelepasan. Dengan meletakkan pelepasan di dalam saluran menyebabkan pengurangan yang ketara ke atas tekanan. Apabila P<sub>v</sub> meningkat, daripada 98 mbar ke 424 mbar, kecenderungan untuk pengurangan tekanan semakin kurang berkesan sebanyak 24 % untuk letupan metana tetapi tiada kesan terhadap letupan propana di dalam analisis simulasi. Kajian ini membuktikan bahawa keaktifan bahan bakar merupakan faktor penting dalam menentukan keberkesanan pelepasan kerana hidrogen stoikiometrik mencapai tekanan letupan terturun (P<sub>red</sub>) yang tinggi sebanyak 4.150 bar berbanding dengan metana dan propana stoikiometrik, masing-masing, 0.945 dan 1.045 bar, sekiranya dicucuh di tengah saluran. Ini bermakna, jarak dari lokasi pencucuh ke kawasan pelepas, keaktifan bahan bakar dan P<sub>v</sub> memainkan peranan yang penting dalam menentukan tempoh tekanan yang ditokokkan dan jumlah jisim yang dilepaskan, yang mana menyifatkan keamatan letupan luaran.

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## LIST OF ABBREVATIONS

AFSW	-	Algebraic flame surface wrinkling
CFD	-	Computational Fluid Dynamics
DDT	-	Deflagration-to-detonation transition
EDM	-	Eddy Dissipation Model
EN	-	European Standard
LFL	-	Lower Flammability Limit
NFPA	-	National Fire Protection Association
UFL	-	Upper Flammability Limit

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### **CHAPTER 1**

### INTRODUCTION

### 1.1 Background of Research

In vented gas explosions, the turbulent flow field, vessel geometry and unsteady interaction of flame propagation drives the mechanisms and phenomena in order to determine the explosion damage at different initial/operating conditions and geometrical parameters. In a chemical industries and processing plant, the accidental explosion of pressure vessel often occur in a confined area within the vessel, pipes, channels or tunnels. That equipment was used as a transportation of the reactive or combustible material from one section to another section for storage purposes. Zubaidah (2015) reported that, the explosive accidents in pipes or vessels can be caused by uncontrolled leaks; even a very tiny pin hole leak of combustible material into air could leads to the development of internal gas explosions.

The understanding of the explosion phenomenology explosions is important for an effective and safe engineering practice, i.e., for selecting the key conditions and parameters in the design and operation of refinery and chemical plants. In order to prevent the destructive damage to plants in industries, several techniques have been developed such as venting. Explosion venting technology is one of the effective and widely used methods in protection and mitigation measures against accidental internal gas explosions, by discharging hot burned gases out of vessel and relieving the pressure generated within the volume, thus minimizing the vessel or pipe from explosion impact (Bauwens *et al.*, 2011).

The technique of studying discharge technology in vessel have extensively been studied by experimental works (Chippett, 1984; Jun *et al.*, 2001; Daubech et al., 2013; Kasmani *et al.*, 2013 and Zhao and Zheng, 2015), theoretical analysis (Simpson, 1986 and Li *et al.*, 2012) and numerical simulation (Xilin *et al.*, 2009; Bingyan *et al.*, 2012 and Skjold, 2014). There are numerous influencing factors governing to the explosion development that have been carried out includes the type of hydrocarbon/fuel-air mixture, vessel geometry, ignition position, vent burst pressure, initial pressure and ignition temperature (Molkov *et al.*, 2000; Kasmani *et al.*, 2013; Fakandu *et al.*, 2015 and Guo *et al.*, 2015). However, the study on mechanism of combustion, physical and dynamic process of explosion is still scarce due to insufficient information on the main parameters and of mechanism involved contributing to explosion hazards.

The experimental investigation is constrained with site condition and test methods as there are great difficulties on theory analysis. Analytical models and empirical correlations (Bradley and Mitcheson, 1978; Tamanini, 1993 and Molkov, 1999) also often have conflict agreements among the practitioners due to the nature complexity, and influencing factors that could affect the peak overpressure, i.e. geometry of the enclosure, the mixture reactivity, type of vent and congestion or obstacle inside the chamber. The comparison of Computational Fluid Dynamics (CFD) simulations of vented explosions with experimental data (Bimson *et al.*, 1993; Watterson *et al.*, 1998; Molkov *et al.*, 2006 and Tulach *et al.*, 2015), have shown that it is a challenge to adequately model the major physical phenomena involved in vented gas explosion.

Numerical simulation by computational fluid dynamics (CFD) is finite volume software and one of the alternative methods of studying vessel explosion and design criteria instead of experimental and theoretical. CFD could give better understanding on the micro mechanism instead of macro perspective on experimental work. Besides, the advantage of using numerical simulation is easily control and repetitive simulation. Thus, the numerical simulation on venting explosion process in this project was built based on Computational Fluid Dynamic analyses using ANSYS Fluent software in order to fulfil the primary motivation of this research; to acquire extensive understanding of turbulent flame propagation associated with vented gas explosion, with a view to develop better models and techniques for assessing explosion risks in the process industries. Computational Fluid Dynamic (CFD) analyses using ANSYS Fluent was adopted in order to investigate the phenomenology underlying vented gas explosions.

#### **1.2 Problem Statement**

The potential gas explosion hazard caused by the deflagration to detonation transition of gas in processing system has raised a crucial concern among the researchers and practitioners in order to improve the safer inherent design plants and the process equipment. If this potential hazard is not properly addressed, the impact would be catastrophic to life, equipment and properties. Explosion venting is one of the effective method or protective techniques applied widely in industry to protect equipment, pipes, and buildings, by relieving the high pressure burned and unburned gas to the external air for avoiding internal gas explosions (Bauwens, *et al.*, 2011 and Guo *et al.*, 2015). Thus, it is crucial to forecast the mode of flame propagation and combustion behaviour and pressure development along the pipe or vessel in order to recognize the worst-case explosion phenomenon, which would correspond to the installation of appropriate protection and mitigation measures systems.

Explosion venting is commonly installed to minimize gas explosion risk due to deflagration to detonation transition, and has been widely studied experimentally and numerically, by given correlations offered in NFPA 68 and European Standard as references for sizing the vent. A research was performed extensively from laboratory scale tests (Cooper *et al.*, 1986) and to large-scale tests (Zalosh, 1980;

Wingerden, 1989; and Bimson *et al.*, 1993). Numerical studies of vented explosions have been reported by several researchers such as Watterson *et al.* (1998); Molkov *et al.* (2006); Xilin *et al.* (2009); Bauwens *et al.* (2011); Bingyan *et al.* (2012) and Skjold, (2014). Meanwhile, the empirical correlations have been developed by Bradley and Mitcheson (1978a, b); Molkov, (1999) and Molkov *et al.* (1999).

However, the studies on the physical and dynamic process of explosion development during the venting to ambient air is yet not well understood since it involved many parameters governing to the overall mechanism. In this study, the understanding of the flame propagation in vented gas explosion will be explored by carrying out the numerical simulation using ANSYS Fluent and the result will be compared to experimental data (Kasmani, 2008) for validation. The aim of this work is to numerically predict the pressure development profiles, flame acceleration behaviour of fuel-air mixtures explosion and possible event for transition to detonation using ANSYS Fluent.

#### **1.3** Objective of Research

The research work is involved only the simulation work, using software Ansys FLUENT version 14. The objectives of the work research are:

- i. to correlate the explosion parameters such as maximum reduced overpressure,  $P_{max}$ , flame propagation and combustion behaviour in different length of vessel with the influence of fuel concentration and fuel reactivity to experimental data (Kasmani, 2008).
- ii. to determine the influence of volume vessel and vent bursting pressure,  $P_v$  on physical and dynamic of vented explosion mechanism.

#### 1.4 Scopes of Study

The scopes of this research cover:

- i. Two different length, L and diameter, D of pipe were used; L = 1.000 m, D = 0.162 m (Test vessel 1) and L = 0.315 m with D = 0.162 m (Test vessel 2). This configuration was based on experimental work done by Kasmani (2008) in order to validate the numerical investigation for this vented explosion analysis.
- The numerical explosion test was simulated in a vented vessel using ANSYS Fluent at ambient condition. The ignition source was allocated at end and centre of vessel for Test vessel 1 and only end ignition was considered for Test vessel 2.
- iii. Different premixed fuel-air mixture of hydrogen, propane and methane-air mixtures with different concentrations or equivalence ratio, $\Phi$ , were used to quantify the explosion characteristics to the explosion development.
- iv. The value of vent bursting pressure from experimental data (Kasmani, 2008) which  $P_v = 0.098$ , 0.178, 0.209 and 0.424 bar were used to investigate the effect of different  $P_v$  on maximum overpressure.

#### 1.5 Research Limitation

ANSYS Fluent has its own limitation which is, the result did not show a good agreement for reactive fuel like hydrogen. In this case, ANSYS CFX would be

recommended rather than normal ANSYS Fluent operation. The model in ANSYS Fluent did not include the significant parameters such as the complete kinetic mechanism of the hydrocarbons/fuels in order to get the best result for complex hydrocarbon such as hydrogen and propane.

#### 1.6 Significance of Study

The study focuses on quantifying the vented gas explosion mechanism on two different vessel configurations. The factors influencing the explosion development have been emphasised by quantifying the explosion parameters to its physic and dynamics mechanisms. Simulation results obtained from this work gave valuable information on the dynamics of explosion mechanism in term of different vessel sizes, fuel reactivity and concentration and ignition locations.

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