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NUMERICAL SIMULATION ON THE RFFECT OF CONCENTRATION ON PREMIXED CH_4/CO_2/AIR EXPLOSION CHARACTERISTICS

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ABSTRACT

In this study, a numerical simulation on the premixed CH_4/CO_2/air (methane/carbon dioxide/air)mixture explosion characteristics was conducted by using the FLame ACcelaration Simulator (FLACs) software. The domain used in the 20 L spherical vessel with 0.808 m diameter. The effect of various equivalence ratios on the explosion characteristics such as the explosion pressure, P_{ex}, maximum explosion overpressure, P_{max}, the maximum rate of pressure rise, $(dP/dt)_{max}$ and gas deflagration index, K_G, were studied. For this purpose, the mixture concentrations range from equivalence ratio (ER) 0.8 to 1.5 (9.6 to 18% vol/vol) were considered. From this study, the explosion pressure, P_{ex}, maximum explosion overpressure, P_{max}, and the maximum rate of pressure rise, $(dP/dt)_{max}$, at various ER was the maximum at a slightly rich concentration (ER=1.2). At lean and rich mixtures, the P_{ex}, P_{max}, $(dP/dt)_{max}$ and K_G decreases. It can be said that, at ER=1.2, the role of thermal-diffusive instability and its effect on the flame speed during the pressure development process had causes the diffused methane, CH_4, to react further into the flame front, which significantly increases the mixture mass burning rate and flame speed thus improving the mixture explosion characteristics. From this study, the flame was also found to propagates the fastest at ER=1.2 due to the incomplete combustion process caused by the insufficient and excess CH_4 present in the lean and rich mixtures. The CH_4/CO_2/air mixtures studied in this study were also found to have the highest level of hazard potential when exploded.

Keywords: Explosion characteristics; FLACs; Numerical simulation; Carbon dioxide; CH_4/CO_2/air mixture

1.0 INTRODUCTION

Explosion is a process where the combustion of a mixture of a flammable gas mixes with oxygen in the air thus resulting in a sudden increase of pressure (Vinnem, 2013).

Gas explosion can occur in various industries and places such as in petrochemical plants, chemical plants, mining industry, offshore module and paint workshops (Addai *et al*., 2015). According to Tang *et al*. (2009), gas explosion contributes 75% of the total losses as compared to fire and toxic release. This makes the prevention of an unwanted explosion such a crucial issue worldwide (Faghih *et al*., 2016) thus raising the awareness to study the explosion characteristics of a fuel/air mixtures among researchers. The explosion characteristics namely the explosion pressure, P_{ex}, maximum explosion overpressure, P_{max}, the maximum rate of pressure rise, $(dP/dt)_{max}$ and gas deflagration index, K_G, are extremely crucial in assessing the hazards of a process, design of relief device against damage from gaseous explosion as well as for design of a safety systems (Tang *et al*., 2009; Zhang and Li, 2017).

Recently, many researchers have successfully studied the explosion characteristics of fuel/air mixtures. Pei *et al*. (2018) studied the carbon dioxide, CO_2, fluid water mist system suppression performance on the methane/air mixture combustion and explosion characteristics. The study was performed by varying the CO_2 pressure and spray time. They reported that the P_{max} and $(dP/dt)_{max}$ decreases by 51.44 and 72%, respectively when the spray time was set for 3 s at CO_2 pressure of 0.4 MPa. According to them, the P_{max} reduces due to the absorbed heat used by CO_2 as well as due to the expansion degree of CO_2. The CO_2 was also reported to have the inhibitory effects on the reaction rate that consequently reduces the $(dP/dt)_{max}$. They also found that the CO_2 causes the average velocity of the flame to decrease by 81.32%. This was due to the suppression effect that CO_2 has on the flame, which significantly reduces the flame propagation speed (Pei *et al*., 2018).

Cui *et al*. (2018) had also studied the effect of low initial temperatures (up to 113 K) and elevated pressures on the methane/air mixture explosion characteristics. Their research showed that as the initial pressure increases, the P_{max} increased significantly while the $(dP/dt)_{max}$ increased linearly. This was due to the increasing flammable mixture density in the vessel as the initial pressure increases. Meanwhile, as the initial temperature increase, the P_{max} was found to increase while the $(dP/dt)_{max}$ was unaffected. According to them, the $(dP/dt)_{max}$ was unaffected because of the combination of the increasing amount of flammable mixture and decreasing flame propagation speed (Cui *et al*., 2018).

Another recent study of explosion characteristics was conducted by Kundu *et al*. (2018). This study was conducted using methane/air mixtures under turbulence condition in the 1 m^3 spherical explosion vessel. From this study, the authors reported that the presence of turbulence causes the P_{max} to increase with a significant decrease in explosion time. Besides, the turbulence initiated in the system also causes the $(dP/dt)_{max}$ and K_G to increase. These observations were caused by the evolution of the mixtures laminar burning velocities to turbulent burning velocities as well as due to the increased combustion rate when turbulence was initiated (Kundu *et al*., 2018).

Besides, Mitu *et al*. (2016)have extensively examined the influence of CO_2 addition on the methane/air propagation indices. This study was conducted inspherical vessels with different volumes (i.e. 0.52 and 20 L) at ambient initial conditions with a central ignition. The CO_2 resent in the mixtures was varied from 5 to 40 vol%. They found that both of the P_{max} and $(dP/dt)_{max}$ decreases with increasing explosion time. This was due to CO_2 high heat capacity and its ability to dissociate and to dissipate heat by radiation. Its presence in the mixture decreases the flame temperature that results in a decreasein the overall reaction rate and heat release rate (Mitu *et al*., 2016).

Moreover, Chan *et al*. (2015) and Hinton and Stone (2014) in different studies, have investigated the effect of CO_2 addition on methane/air mixtures flame propagations. Using a flat-flame burner (Chan *et al*., 2015) and a stainless steel spherical vessel with an internal diameter of 160 mm (Hinton and Stone, 2014), the experiments was conducted at various pressure (atmospheric to 18 bar), temperature (298 to 660 K) and equivalence ratio, ER, (0.7 to 1.4). Chan et al. (2015) and Hinton and Stone (2014) used a concentration of 0 to 15 and 40 vol% CO_2 in the mixture. These studies determine that the flame propagates slower with a higher amount of CO_2 present in the mixture. This is becausethe increasing CO_2 concentration in the mixture reduces the reactants' concentrations and decreases the net reaction rate thus reducing the flame speed (Chan *et al*., 2015). Moreover, the also acted as a heat sink which reduces the reaction temperature (Chan et al., 2015) thus causing the mixture flame speed to reduce by 65% when the present in the mixture was 40% (Hinton and Stone, 2014).

While several studies have been conducted using methane/air mixtures, none of the studies using methane/carbon dioxide/air mixtures can be found in the literature. To the author's note, most of these studies only focused on the effect of initial pressure, temperature as well as the range of CO_2 present in the mixtures rather than emphasizing on the effect of mixture equivalence ratio. Apart from that, these studies were also found to focus on obtaining the P_{max} and $(dP/dt)_{max}$ of the mixtures by using an experimental approach instead of numerical analysis. Therefore, the present work aims to provide an understanding of the explosion characteristics (i.e. P_{ex}, P_{max}, $(dP/dt)_{max}$ and K_G) of CH_4/CO_2/air mixtures at various ER using a numerical analysis approach.

2.0 MATERIALS AND METHODS

The software used was the commercial software known as theFLame ACcelaration Simulator (FLACs). This software is developed by GexCon to reckon gas explosions in offshore oil and gas production platforms. The compressible Navier–Stokes equations are solved by FLACs by using a finite volume methodon a 3-D Cartesian grid. The finite volume method employs the finite volume formulation to resolve the Navier–Stokes partial differential equations numerically. The partial differential equations involved are the conservation of momentum, mass, chemical speciesand enthalpy. In FLACs, the turbulence is solved using the k-epsilon model equations. In the combustion model, the flame is contemplated as a collection of flamelets with one-step kinetic reaction. The interaction between the surrounding geometry and the reactive fluid flow is considered through a distributed porosity concept. The flame zone in FLACs is increased by increasing the diffusion by a factor beta. In order to reduce the thickness, the reaction rate is reduced by a factor 1/beta. Beta is chosen such that the flame thickness becomes 3 to 5 grid cells. This is to ensure that the flame propagates directly into the unburned gas mixture with the velocity specifiedfor the flame wrinkling that caused by theflame front instabilities and turbulence level.

In this study, the geometryof the vessel was first constructed (labelled "domain") as shown in Figure 1. The domain used for the simulation was assumed to be a 20 L spherical vessel that was constructed in a big box (marked by the blue line) that represents the surroundings where the diameter was assumed to be 0.808 m. The ignition point was set at the centre of the sphere (marked by a greencircle). The fuel/air mixture used was the premixed CH_4/CO_2/air mixture, at concentrations range from equivalence ratio (ER) 0.8 to 1.5 (9.6 to 18% vol/vol). The monitor point was set at one coordinate denotes as M1 (marked by a pink circle).Euler was chosen as the boundary condition used in themodel. In this model, the outer part of the boundary was assumed to be the atmospheric pressure. The initial temperature and pressure are set to be at atmospheric pressure condition.

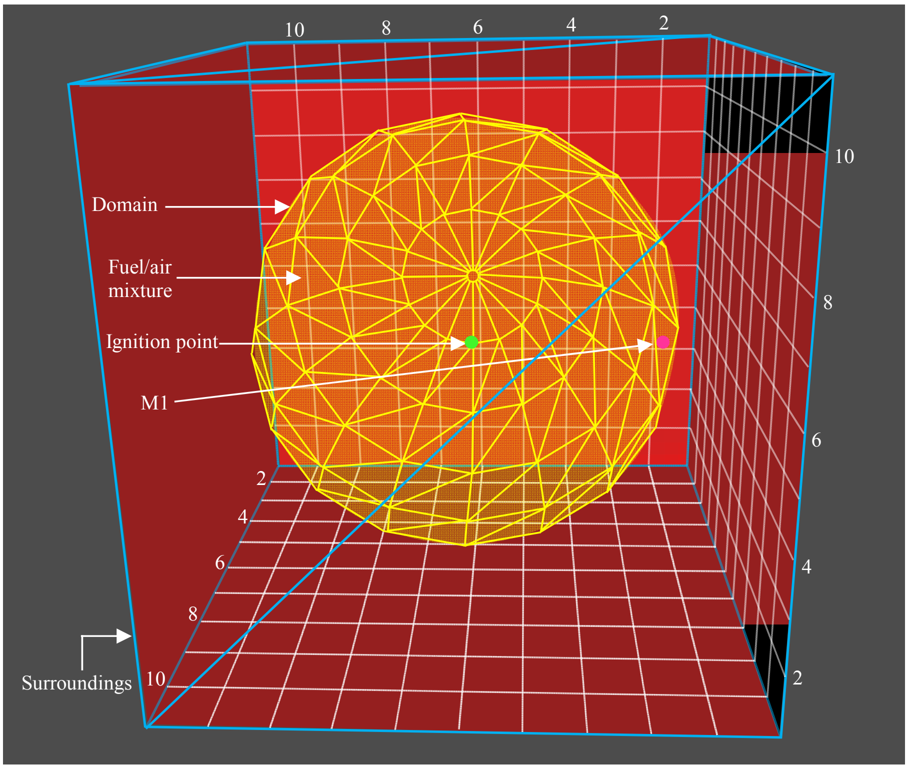

Figure 1: The geometry of the domain constructed in theFLACs simulation.

3.0RESULTS AND DISCUSSION

3.1 Explosion pressure, P_{ex}

Figure 2 shows the explosion pressure, P_{ex}, development obtained from the FLACs simulation at various equivalence ratios, ER.From Figure 2, the trend of the P_{ex} development in FLACs stabilized once it reaches its maximum value. This was suspected due to the exclusion of the quenching effect in FLACs code (Arntzen, 1998; Sulaiman, 2015). In FLACs code, all the fuel present in the mixture was assumed to be fully reacted during the combustionprocess. This stops the flame propagation since no more fuel could react to supports the combustion process hence causing the $P_{ex}$to stabilize once it reaches its maximum value. Additionally, it can also be observed that the P_{ex} in FLACs increases as early as 0.71 ms. According to Li *et al.*(Li et *al.*, 2018), this phenomena occurred due to the high initial burning rate of flame in FLACs simulation which was also reported by Ma *et al.* (2014) and Pedersen and Middha (2012).

From Figure 2, the maximum value of the P_{ex} from FLACs increases from lean concentration (ER = 0.8) to slightly rich concentration (ER = 1.2) and then decreases as the ER increase. This shows that P_{ex} development is highly dependent on the ER. This is attributed to the thermal-diffusive instability, which alters the mixture mass burning rate, and this reflects the P_{ex} development and its maximum value. It can be said that in the very lean mixture (ER=0.8), the combustion process was limited by the methaneoxidizer reaction due to the insufficient amount of methane, CH_4, present in the mixture (Tang *et al*., 2014) that limits the flame front stretch effect towards the unburned gas mixture. This led to the slowest flame propagation and hence the lowest P_{ex}. At the stoichiometric concentration (ER=1.0), the CH_4 and oxygen, O_2, present in the mixture are enough to react with each other. Therefore, no excess $CH_4$was left to further diffuse into the flame front and reacted. However, the increasingfuel concentration(Tang *et al*., 2014) in the mixture resulted in the higherheating value of the fuel mixture thus causing the P_{ex} at ER=1.0 to be higher than the P_{ex} at ER=0.8 by 1.1 times. Meanwhile, at the slightly rich concentration (ER=1.2), the flame was suspected to have the highest surface area due to the highly corrugated flame front resulting from the thermal diffusive instability. This causes the excess CH_4 present in the mixture to diffuse into the flame front and reacted further giving the highest P_{ex}. Beyond ER=1.2, the flame front stretch effect was also limited due to the incomplete combustion process (Tang *et al*., 2014). The excess CH_4present and diffused into the flame front had resulted in a lower heat release and mass burning rate. Therefore, as the mixture concentration increases, the flame propagates slower at the mixture of ER=1.4 and ER=1.5 with 1.0 times lower P_{ex} than the mixture at ER=1.2.

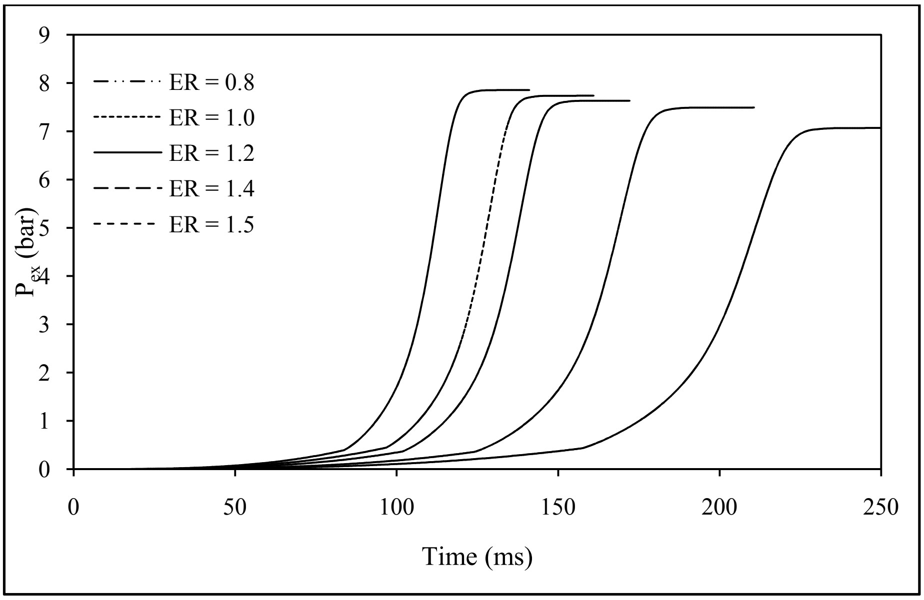

Figure 2: Pressure history for CH_4/CO_2/air explosion at various equivalence ratios (ER)

3.2 Maximum explosion overpressure, P_{max}, and maximum rate of pressure rise, $(dP/dt)_{max}$

Figure 3 gives the maximum explosion overpressure, P_{max}, and the maximum rate of pressure rise, $(dP/dt)_{max}$, at different equivalence ratio, ER, when the initial temperature and pressure is at ambient condition. The basis of CH_4/CO_2/air concentration used is 60% methane, CH_4,and 40% carbon dioxide, CO_2. In Fig.3, the P_{max} and the $(dP/dt)_{max}$ fromFLACs simulation was found to be the highest at a slightly rich concentration (ER=1.2). A similarobservationwas also observed by Mitu and Brandes (2017) and Mitu and Brandes (2015). At both lean (ER=0.8) and rich concentrations (ER>1.2), the value of P_{max} and the $(dP/dt)_{max}$ reduces. This was due to the role of thermal-diffusive instability that affects the flame speed and the pressure development process (Tang *et al*., 2014). At ER=0.8 and ER>1.2, the limit flame front stretch effect towards the unburned gas mixture had limitthe CH_4 present in the mixture to diffused and reacted.

This causes the mixture mass burning rate to decrease resulting in a lower P_{max} and $(dP/dt)_{max}$. Meanwhile, for mixture at ER=1.2, the highest amount of excess CH_4 diffused and reacted at the flame front had significantly increased the mixture mass burning rate. This had also resulted in the highest P_{max} and the $(dP/dt)_{max}$. On the other hand, the presence of CH_4 and oxygen, O_2, that are enough to react with each other in the mixture at the stoichiometric concentration (ER=1.0) had also failed to increase the mixture mass burning rate. This causes the P_{max} and the $(dP/dt)_{max}$ for the mixture at ER=1.0 to be lower by 1.0 and 1.2 times respectively than the mixture at ER=1.2.

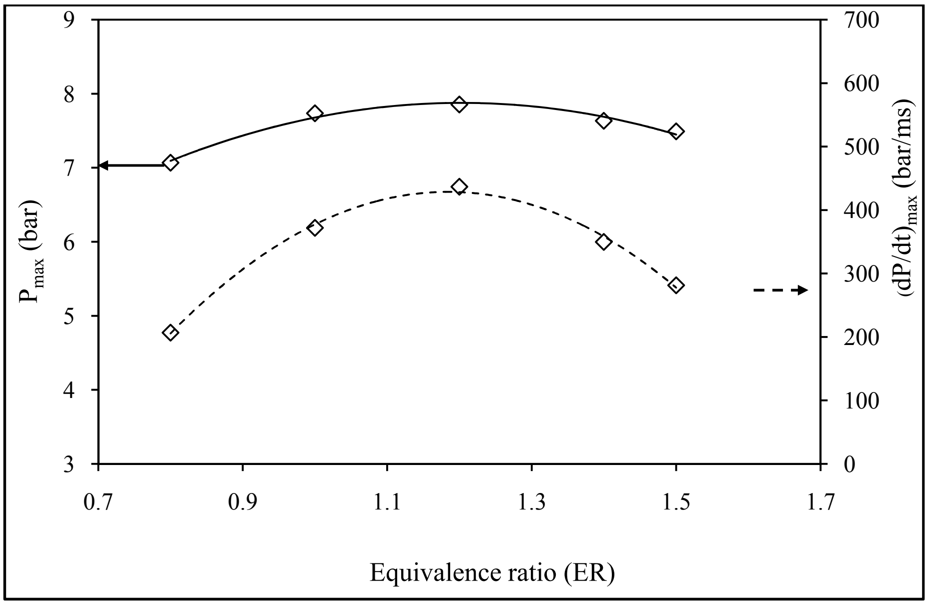

Figure3: Maximum explosion overpressure and maximum rate of pressure rise for CH_4/CO_2/air explosion at variousequivalence ratios (ER)

3.3 Gas deflagrations index, K_G

Apart from the explosion pressure, P_{ex}, the maximum explosion overpressure, P_{max}, and the maximum rate of pressure rise, $(dP/dt)_{max}$, gas deflagration index, K_G, was also used to characterize the severity of an explosion. In order to calculate the value of K_G, Eq. (1) was used (Cesana & Siwek, 2000).According to Rodgers and Morrison (2007), the K_G is classified into three hazard classes as shown in Table 1.

$$K_G = 0.27144 \times \left(\frac{dP}{dt}\right)_{max} \tag{1}$$

Table 1: Deflagration index hazard classes (Rodgers and Morrison, 2007)

Hazard class	**The range of K_G (bar.m/ms)**
St-1	≤ 0.2
St-2	$0.2 < K_G \leq 0.3$
St-3	> 0.3

Figure 4 shows the K_G development obtained from the FLACs simulation at various equivalence ratios, ER. The trend of K_G are found to be similar with the trend ofthe maximum explosion overpressure, P_{max}, and the maximum rate of pressure rise, $(dP/dt)_{max}$, as shown in Figure 3. From Figure4, the deflagration index, K_G, was also found to increase in the lean side and stoichiometric and decreases in the rich side.

From Table 1, the value of the calculated $K_G$at all involved conditions are found to fall into the highest levelof hazard class (St 3) as it is higher than 0.3 bar.m/ms. This proves that the CH_4/CO_2/air mixture has a high explosion hazard potential that would have resulted in a deadly explosion and causes loss of life as well as severe properties damaged (Tang *et al*., 2009; Xie *et al*., 2016).

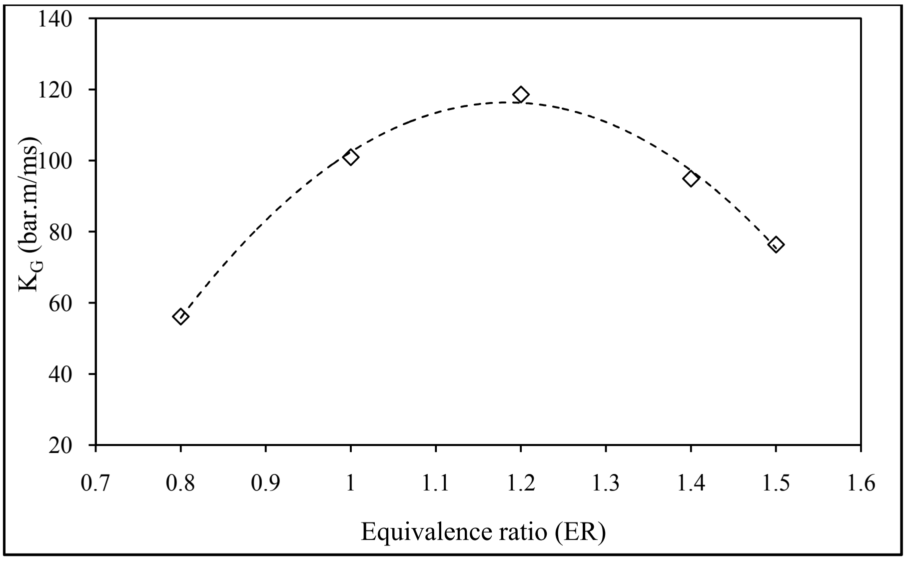

Figure4: Deflagration index for CH_4/CO_2/air explosion at various equivalence ratios (ER)

4.0 CONCLUSIONS

The numerical studies on the explosion characteristics of CH_4/CO_2/air mixtures were performed. The simulation was carried out using the FLACs simulator where the explosion characteristics of the mixtures were studied at various equivalence ratios, ER (ER=0.8 to 1.5). From this study, the main findings are listed as follows:

1. The fastest flame propagation was observed at a slightly rich concentration (ER=1.2). The flame propagates slower at lean (ER=0.8) and rich mixture (ER>1.2) due to the incomplete combustion process caused by the insufficient and excess methane, CH_4, presence in the mixture respectively.

2. The explosion pressure, P_{ex}, maximum explosion overpressure, P_{max}, and the maximum rate of pressure rise, $(dP/dt)_{max}$, at various ER, shows the same trend. These characteristics show the highest value for the mixture at ER=1.2. This was due to the role of thermal-diffusive instability and its effect on the flame speed during the pressure development process. This phenomenon had caused the diffused CH_4 to react further into the flame front, which significantly increases the mixture mass burning rate and flame speed.

The CH_4/CO_2/air mixture at various ER is found to fall into the highest levelof hazard class (St 3) with the mixture at ER=1.2 being the most severe when exploded.

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REFERENCES

Addai, E.K., Gabel, D. and Krause, U. (2015). Explosion characteristics of three component hybrid mixtures. *Process Safety and Environmental Protection, 98*, 72–81.

Arntzen, B. J. (1998). Modelling of turbulence and combustion for simulation of gas explosions in complex geometries.

Cesana, C. and Siwek, R. (2000). *Operating Instructions 20 L Apparatus* (6th ed.). Birsfelden, Switzerland: Kuhner AG.

Chan, Y.L., Zhu, M.M., Zhang, Z.Z., Liu, P.F. and Zhang, D.K. (2015). The effect of co2 dilution on the laminar burning velocity of premixed methane/air flames. *Energy Procedia, 75*, 3048–3053.

Cui, G., Wang, S., Liu, J., Bi, Z. and Li, Z. (2018). Explosion characteristics of a methane/air mixture at low initial temperatures. *Fuel, 234*, 886–893.

Faghih, M., Gou, X. and Chen, Z. (2016). The explosion characteristics of methane, hydrogen and their mixtures: A computational study. *Journal of Loss Prevention in the Process Industries, 40*, 131–138.

Hinton, N. and Stone, R. (2014). Laminar burning velocity measurements of methane and carbon dioxide mixtures (biogas) over wide ranging temperatures and pressures. *Fuel, 116*, 743–750.

Kundu, S. K., Zanganeh, J., Eschebach, D., Badat, Y. and Moghtaderi, B. (2018). Confined explosion of methane-air mixtures under turbulence. *Fuel, 220*, 471–480.

Li, J., Hao, H., Shi, Y., Fang, Q., Li, Z. and Chen, L. (2018). Experimental and computational Fluid Dynamics study of separation gap effect on gas explosion mitigation for methane storage tanks. *Journal of Loss Prevention in the Process Industries, 55*, 359–380.

Ma, G., Li, J. and Abdel-jawad, M. (2014). Accuracy improvement in evaluation of gas explosion overpressures in congestions with safety gaps. *Journal of Loss Prevention in the Process Industries, 32*, 358–366.

Mitu, M. and Brandes, E. (2015). Explosion parameters of methanol-air mixtures. *Fuel, 158*, 217–223.

Mitu, M. and Brandes, E. (2017). Influence of pressure, temperature and vessel volume on explosion characteristics of ethanol/air mixtures in closed spherical vessels. *Fuel, 203*(Supplement C), 460–468.

Mitu, M., Prodan, M., Giurcan, V., Razus, D. and Oancea, D. (2016). Influence of inert gas addition on propagation indices of methane–air deflagrations. *Process Safety and Environmental Protection, 102*, 513–522.

Pedersen, H. H. and Middha, P. (2012). Modelling of vented gas explosions in the CFD tool FLACS. *Chemical Engineering Transaction, 26*, 357–362.

Pei, B., Yang, Y., Li, J. and Yu, M.-g. (2018). Experimental study on suppression effect of inert gas two fluid water mist system on methane explosion. *Procedia Engineering, 211*, 565–574.

Rodgers, S.A. and Morrison, L. S. (2007). *NFPA 68 - Standard on Explosion Protection by Deflagration Venting*. National Fire Protection Association Retrieved from http://gazkhodro.ir/wp-content/uploads/2015/11/NFPA-68-2007-Standard-on-Explosion-Protection-by-Deflagration-Venting.pdf.

Sulaiman, S. Z. (2015). *Gas Explosion Characteristics in Confined Straight and 90 Degree Bend Pipes*. Universiti Teknologi Malaysia.

Tang, C., Huang, Z., Jin, C., He, J., Wang, J., Wang, X. and Miao, H. (2009). Explosion characteristics of hydrogen–nitrogen–air mixtures at elevated pressures and temperatures. *International Journal of Hydrogen Energy, 34*(1), 554–561.

Tang, C., Zhang, S., Si, Z., Huang, Z., Zhang, K. and Jin, Z. (2014). High methane natural gas/air explosion characteristics in confined vessel. *Journal of Hazardous Materials, 278*, 520–528.

Vinnem, J.E. (2013). *Offshore Risk Assessment Vol. 1: Principles, Modelling and Applications of QRA Studies*: Springer London.

Xie, Y., Wang, J., Cai, X. and Huang, Z. (2016). Pressure history in the explosion of moist syngas/air mixtures. *Fuel, 185*, 18–25.

Zhang, Q. and Li, D. (2017). Comparison of the explosion characteristics of hydrogen, propane, and methane clouds at the stoichiometric concentrations. *International Journal of Hydrogen Energy, 42*(21), 14794–14808.