

CFD Simulations of Transient Fuel Gases Mixing, Leakage and Flammability in Air

Rajashekhar Pendyala^{*a}, Jenn Yong^b, Irsyad Ahnaf Azman^c,
 Suhaib Umer Ilyas^a

^aChemical Engineering Department, Universiti Teknologi Petronas, 32610 Bandar Seri Iskandar, Perak Darul Ridzuan, Malaysia

^bShell MDS (M) Sdn Bhd, Tanjong Kidurong, 97008 Bintulu, Sarawak, Malaysia

^cSutera Analytics Sdn Bhd, B2-5-12, Solaris Dutamas, Jalan Dutamas 1, Hartamas Heights, 50480 Kuala Lumpur, Malaysia

rajashekhar_p@petronas.com.my

Dispersion of fuel gases in air is very rapid during accidental release which can lead to minor asphyxiate to major explosion. Leakage of fuel gases poses an unseen threat due to odourless and colourless properties of gas components. A complete understanding of fuel gases mixing behaviours with air is very crucial to develop prevention or mitigation guidelines towards major accident. Various fuel gases transient dispersion behaviours are simulated by using computational fluid dynamics in simple geometries. Transient dispersion behaviour and flammability limits of major fuel gases, which include methane, hydrogen, ethane, propane, carbon monoxide and acetylene are simulated in 2D closed and open-top geometries. Formation of flammability region is predicted and compared for each component of fuel gas in the range of higher and lower flammability limits. It is found that dispersion rate of gases is considerably affected by the density difference between air and fuel gas. Spatial and temporal distributions of fuel gases are compared in closed and open-top geometries.

1. Introduction

Increasing demand of intensified energy in the form of fuel gases also increases the risk of accidental release. Due to odourless and colourless properties, accidental release of fuel gases either due to accidental damage to connecting pipes or storage tanks can form an explosive vapour cloud which can lead to a major disaster to both civilian and industrial sector (Bont et al., 2014). Dispersion studies of fuel gases in air has significant importance towards the advances of prevention guidelines of accidental release as well as the development of standards for design and operation of fuel gases related equipment (Prasad et al., 2012). Computational fluid dynamics (CFD) is an imperative tool to study the dispersion behaviour of fuel gases in air due to complications in conducting physical experiments (Bakar, 2008).

Few studies have been carried out in recent years to study the accidental release of gases in air e.g. hydrogen diffusion due to high pressured storage tanks failure (Liu et al., 2009), natural gas leakage from compressor stations (García et al., 2008) and hydrogen leakage from a fuel cell vehicle (Choi et al., 2013). In a study (Cisse and Karim, 2007), fuel gases dispersion in air was studied and it was found that formation of flammable mixture zones in fuels which are less dense than air is very fast as compared to fuels heavier than air. In a recent study (Hajji et al., 2014), hydrogen accumulation during a leak was studied in a prismatic cavity with ventilation. Hydrogen concentration was found to be increasing with time after leakage and it was observed that the concentration of hydrogen depend on the apex angle. In another study (Vudumu and Koylu, 2009), a computational model was developed to study the transient diffusion of hydrogen in vertical cylinder with open top, partially open top and closed top geometries. Hydrogen dispersion in air was observed to be very rapid due to low density of hydrogen. Zheng et al. (2011) studied the instantaneous leakage of natural gas containing carbon dioxide. The puff dispersion model was analysed to study the upwind dispersion, concentration bifurcation and asymmetry feature.

Transient dispersion of different fuel gases in air using simple geometry is presented, which can be used as benchmark study for practical and complicated geometries with different fuel gas release scenarios. Dispersion behaviour of different fuel gases has been compared and discussed in detail at different time intervals. Formation of flammability region has been studied in between upper and lower flammability limits. Simulations are performed in closed top and open top geometries to study the mixing and flammability envelopes of fuel gases in air.

2. Materials and methods

Fuel gases mixing in air is studied in a vertical two-dimensional cylindrical geometry with dimensions 1 m x 0.25 m, shown in Figure 1(a). The geometry is filled initially with 10 % of fuel gas and 90% of air at room temperature. At time = 0 s, the fuel gas is released to allow mixing with the overlying air. The initial contour for air and fuel mole fractions is shown in Figure 1(b). Simulations are performed for different fuel gases i.e. hydrogen, methane, acetylene, carbon monoxide, ethane and propane. ANSYS 12.1 (Fluent) is used to simulate transient mixing of fuel gases in air. Fine mesh (0.1 mm element size) is used to predict accurate simulation results. Model setup includes pressure based solver with energy equation, laminar flow model and species transport model. The boundary conditions for the wall are set to be stationary and non-slip. Semi-Implicit Method for Pressure Linked Equations (SIMPLE) algorithm with second order implicit method for unsteady flow equations are used for better accuracy with a time step of 0.01 s. Vudumu and Koylu (2009) have reported that laminar flow analysis is more preferable for safety engineering because over-predicted simulation results are found by using turbulence models in a slow gas release system. Navier-Stokes equation, non-reacting transport equations (two species model) and transient equations for conservation of energy, mass and momentum (Vudumu and Koylu, 2009) are considered in this study.

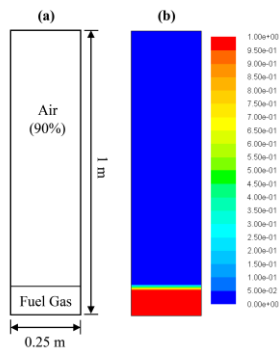


Figure 1: Geometry under consideration with (a) dimensions and (b) mole fraction contour for air and fuel gas

3. Results and discussion

3.1 Dispersion of fuel gases

Mixing behaviour of different fuel gases with air in enclosed geometry has been simulated. At time = 0 s, the vertical geometry is filled with 10 % of the pure fuel gas at the bottom and then allowed to mix with air. Dispersion studies are carried out for 60 s. The simulation results of mole fraction contours of each fuel gas at different time intervals are shown in Figure 2. It is observed that hydrogen and methane starts to disperse in air more rapidly than the other fuel gases due to high density difference and due to this both gases have high diffusion coefficient as compared to other fuel gases.

Table 1: Density ratios, flammability limits and time taken to reach the top for fuel gases

Fuel gases	Density Ratio ($\rho_{\text{Fuel}} / \rho_{\text{Air}}$)	Flammability range (% by volume of Air)	Time taken to reach top (s)
Hydrogen (H ₂)	0.068	4 - 75	4.6
Methane (CH ₄)	0.554	5 - 15	7.9
Acetylene (C ₂ H ₂)	0.906	2.5 - 82	17.8
Carbon monoxide (CO)	0.954	12 - 75	42.9
Ethane (C ₂ H ₆)	1.024	3 - 12.4	-
Propane(C ₃ H ₈)	1.562	2.1 - 10.1	-

Table 1 represents density ratios of fuel gases with air, upper and lower flammability range and time taken for fuel gases to reach the top of enclosed geometry. It is observed that acetylene, carbon monoxide and ethane have also started to disperse after 2 s of mixing with in air. It can be seen from Figure 2 that hydrogen and methane moving rapidly in axial direction of the geometry because less dense gas tends to move upwards.

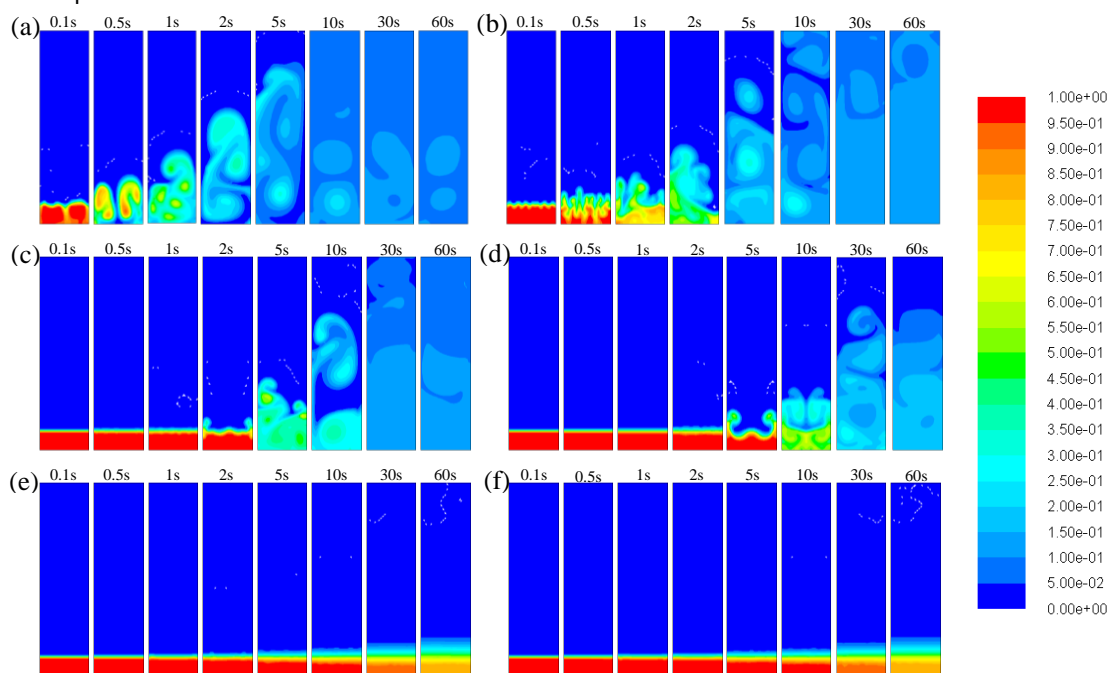


Figure 2: Dispersion behaviour of fuel gases mixing with air at different time intervals. (a) hydrogen, (b) methane, (c) acetylene, (d) carbon monoxide, (e) ethane and (f) propane

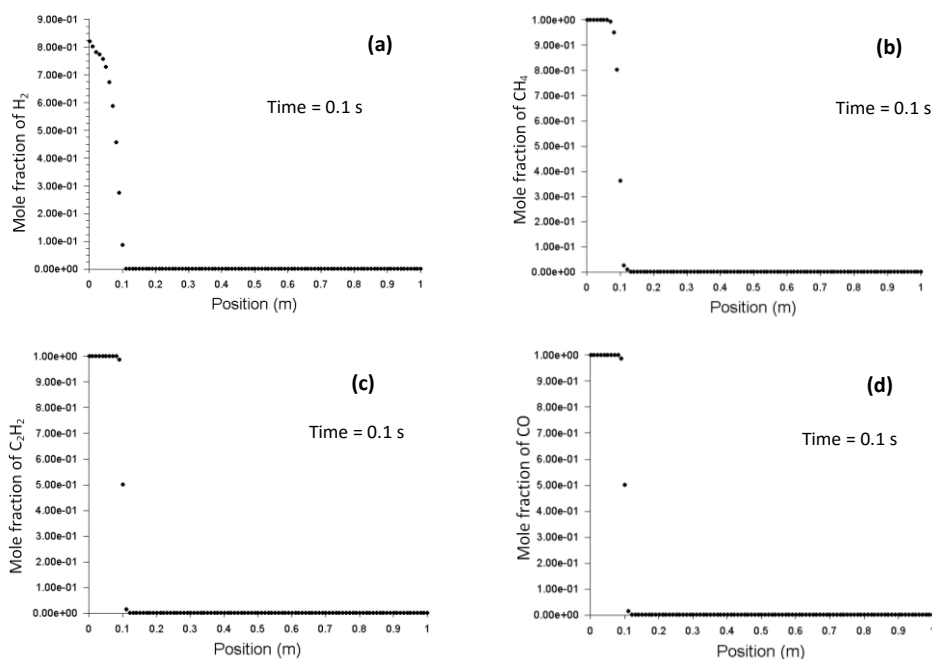


Figure 3: Mole fraction of (a) hydrogen, (b) methane, (c) acetylene and (d) carbon monoxide at 0.1 s along centreline of geometry

It is found that after gas leakage, hydrogen, methane, acetylene and carbon monoxide reach to the top of enclosed geometry in 4.6 s, 7.9 s, 17.8 s and 42.9 s. The results have shown similar performance with the previous literature (Vudumu and Koylu, 2009). Slow mixing behaviours are seen in ethane and propane dispersion in air and both gases does not managed to reach to the top in 60 s due to higher density than air. These gases are observed to be dispersing majorly in radial direction. To study the distribution of mole fraction along centreline of the geometry for hydrogen, methane, acetylene and carbon monoxide, graphs are plotted at initial and final time to reach to the top of the geometry, shown in Figure 3 and Figure 4.

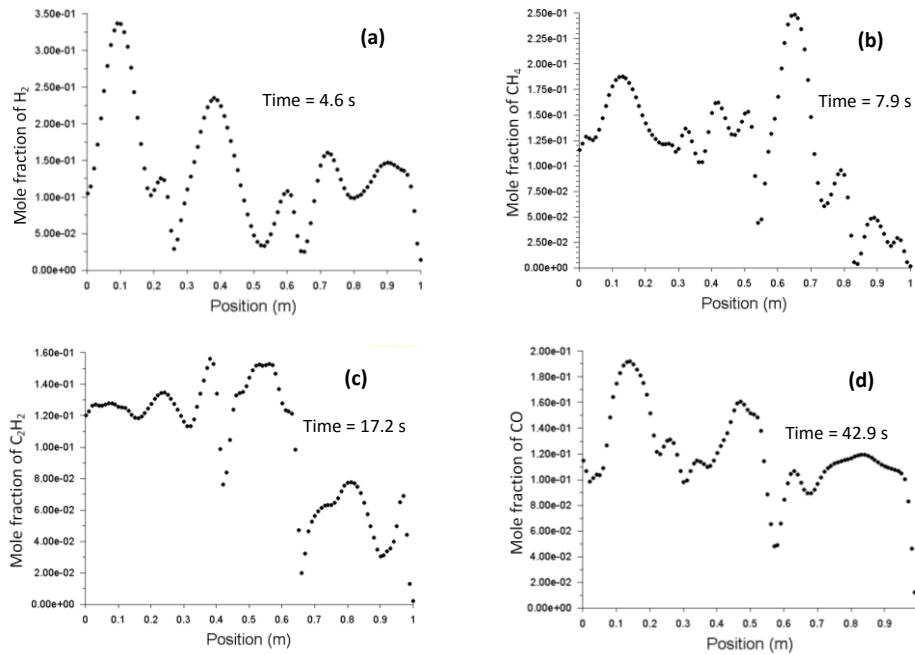


Figure 4: Mole fraction of (a) hydrogen, (b) methane, (c) acetylene and (d) carbon monoxide at the time to reach to the top along centreline of geometry

3.2 Development of flammability region

Flammable region mark an area where the fuel gases will create fire even if there is tiny spark. The region is bounded by the upper flammability limit and lower flammability limit for each gas, shown in Table 1. Simulations are performed without consideration of jet-momentum effect and wind effect to predict more accurate results. It can be seen from Figure 5 that in-case of hydrogen dispersion, a rapid flammable region is formed. After 2 s of dispersion, half of the container is taken by the flammable region. It is observed that the geometry is completely prone to fire within 10 s of hydrogen leakage. Hydrogen has the second widest range of flammability region next to acetylene which is 4 - 75 %vol in air. It is observed that the formation of flammability region for methane (i.e. 5 - 15 %vol) is faster than acetylene (2.5 - 82 %vol) because of the reason that methane disperses more rapidly than acetylene. It can be seen that after 5 seconds, flammability region of methane is exceeding half of the geometry while acetylene flammability regions reaches only quarter of the geometry. Simulation results show that carbon monoxide release in air posture less threat within 60 s as it does not reach to the top of geometry. It is found that the formation of flammability region for heavy fuel gases i.e. ethane and propane poses less threat than light fuel gases because of low dispersion rate and narrow range of flammability region. The flammability region for ethane and propane is found to be limited to the area of first contact of air and fuel gas.

3.3 Comparison of open top and enclosed geometry

Simulations have been performed in open top and enclosed geometries for various fuel gases. Dispersion behaviour of hydrogen and methane in open-top and enclosed geometries is presented in Figure 6. It is found that mixing behaviour of fuel gases for the first few seconds is similar however, enclosed geometries exhibits faster dispersion behaviour. It is observed that hydrogen and methane escape from the top of the geometry after 60 s while in enclosed geometry concentration distribution of fuel gases is found to be evenly spread throughout the whole geometry.

The rapid upward movement of Hydrogen and methane is because both gases has high diffusion coefficient when mixed with air and low density than air. The distribution of hydrogen and methane concentration is effected by the convective mass transfer and molecular diffusion driven by buoyancy and local concentration difference respectively. It can be seen that hydrogen and methane dispersion starts in axial and radial direction at very short time.

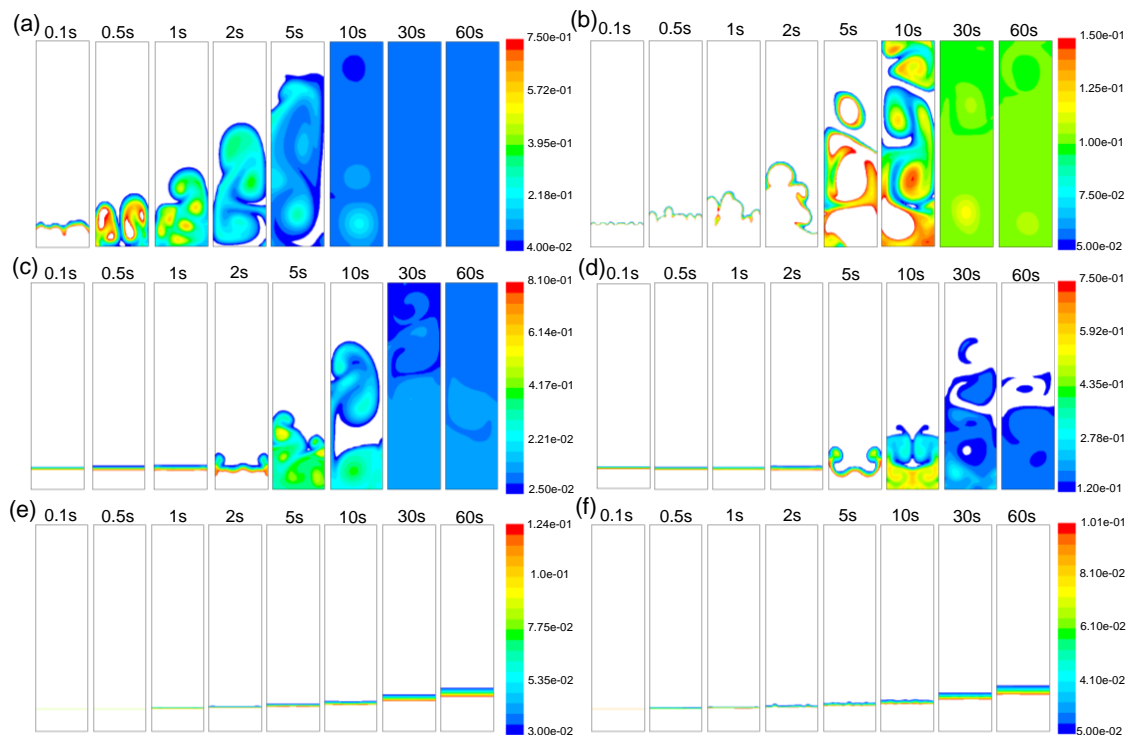


Figure 5: Formation of flammability region for (a) hydrogen, (b) methane, (c) acetylene, (d) carbon monoxide, (e) ethane and (f) propane

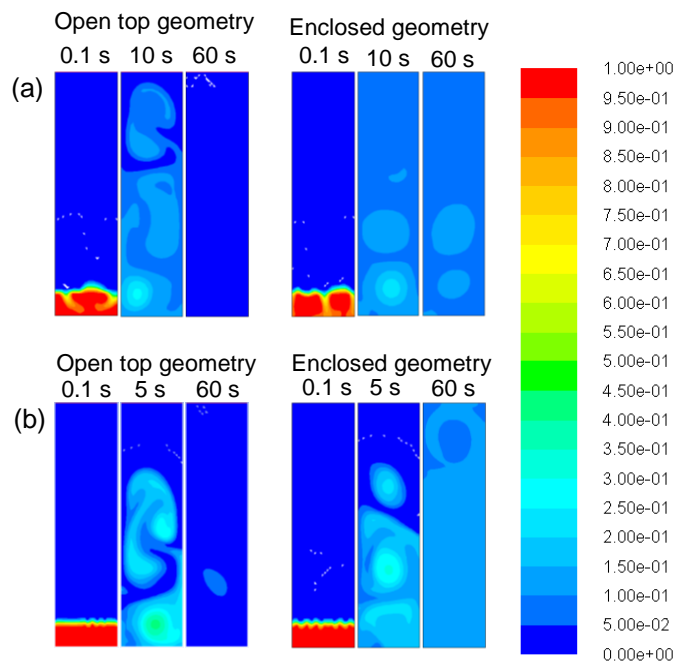


Figure 6: Comparison of dispersion behaviour of (a) hydrogen and (b) methane in open-top and enclosed geometries

4. Conclusions

Simulations of transient fuel gases mixing and flammability in air are studied. The findings have significant importance towards development of safety and mitigation guidelines. It is found that density difference and buoyancy play significant role towards mixing of fuel gases in air. Hydrogen and methane are found to be highly dispersed in air in less time which poses high risk and danger while transportation or using in other applications. Light fuel gases (hydrogen, methane, acetylene and carbon monoxide) tend to disperse faster than dense gases (ethane and propane). After slow release, it is observed that ethane and propane showed minimum dispersion in air. It is found that hydrogen reaches top of the geometry in 4.6 s followed by methane, acetylene and carbon monoxide with the time 7.9 s, 17.8 s, and 42.9 s. Ethane and propane display low mixing behaviour and does not reached to the top because of higher density than air. The formation of flammability regions exhibit that light gases pose more threat than heave gases despite of limited range of flammability. Hydrogen and methane occupied whole geometry within 10 s to form flammability region while the heavier fuel gases (ethane and propane) tend to concentrate at the bottom of the geometry. It is found that concentration distribution of hydrogen and methane in enclosed geometry is evenly spread throughout the whole geometry while in case of open top geometry, both gases escape from the top of the geometry within 60 s.

Acknowledgment

This work is supported by Chemical Engineering Department, Universiti Teknologi PETRONAS.

References

- Bakar R.A., 2008, A technical review of compressed natural gas as an alternative fuel for internal combustion engines. *Am. J. Eng. Appl. Sci.*, 1, 302-311.
- Bont R.D., Inaudi D., Walder R., 2014, Detection and localization of leakages in toxic/flammable chemicals pipelines using distributed fibre optic sensor. *Chemical Engineering Transactions*, 36, 31-36.
- Choi J., Hur N., Kang S., Lee E.D., Lee, K.-B., 2013, A CFD simulation of hydrogen dispersion for the hydrogen leakage from a fuel cell vehicle in an underground parking garage. *Int. J. Hydrogen Energ.*, 38, 8084-8091.
- Cisse P., Karim G.A., 2007, The rapid formation and dispersion of flammable zones within cylindrical vertical enclosures following the release of a fixed mass of hydrogen and other gaseous fuels into air. *Int. J. Hydrogen Energ.*, 32, 630-636.
- García J., Migoya E., Lana J.A., Crespo A., 2008, Study of the dispersion of natural gas issuing from compressor stations through silencers with upper cover. *J. Hazard. Mater.*, 152, 1060-1072.
- Hajji Y., Bouteraa M., Cafsi A.E.L., Belghith A., Bournot P., Kallel F., 2014, Dispersion and behavior of hydrogen during a leak in a prismatic cavity. *Int. J. Hydrogen Energ.*, 39, 6111-6119.
- Liu Y.-L., Zheng J.-Y., Xu P., Zhao Y.-Z., Bie H.-Y., Chen H.-G., Dryver H., 2009, Numerical simulation on the diffusion of hydrogen due to high pressured storage tanks failure. *J. Loss Prevent. Proc.*, 22, 265-270.
- Prasad K., Pitts W.M., Fernandez M., Yang J. C., 2012, Natural and forced ventilation of buoyant gas released in a full-scale garage: Comparison of model predictions and experimental data. *Int. J. Hydrogen Energ.*, 37, 17436-17445.
- Vudumu S.K., Koynu U.O., 2009, Detailed simulations of the transient hydrogen mixing, leakage and flammability in air in simple geometries. *Int. J. Hydrogen Energ.*, 34, 2824-2833.
- Zheng Y., Wang B., Zhang Y., 2011, Numerical simulation of instantaneous dispersion of natural gas highly containing carbon dioxide and its reliability analysis. *IEEE 3rd International Conference on Communication Software and Networks (ICCSN)*, Xi'an, China, 534-537.