Flammable Plumes Dynamics Resulting from the Convective Dispersion of a Fixed Mass of a Gaseous Fuel into Air, Comparison of 3D versus 2D Models Comparison

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1 Introduction

An important source of fire, explosion and toxic hazards is due to releases of fuel vapour within fuel installations or during various industrial operations. The mixing of fuel vapour with the overlaying air produces flammable regions that grow with time and gradually decay as the fuel dissipates into the outside atmosphere. Any source of ignition such as a spark or a sufficiently hot spot within the flammable region can then ignite the mixture to produce a flame that could cause serious economic or environmental damage, [1]. Moreover, the exposure of a fuel to the overlaying air also can be a major source of environmental pollution. Improvement to our understanding of the mechanism of the processes of gas emissions and dispersion will help in developing better guidelines to detect and mitigate hazardous vapour dispersion.

Mastorakos et al [2] performed two dimensional direct numerical simulation of mixing layers of fuel and hotter air. Bunama and Karim [3] developed a numerical model of the formation of flammable atmospheres within vertical enclosures containing a vaporizing liquid fuel. Ilegbusi et al [4] simulated the mixing of two fluids and compared the accuracy of different numerical methods for modelling buoyancy driven flows.

This paper explores the dispersion of a fixed mass of a buoyant gaseous fuel that is suddenly permitted to spread with a negligible pressure difference into overlaying air at atmospheric conditions within vertical cylindrical enclosures that are open at the top to the atmosphere. The results of the 3-D simulation are compared with the corresponding simpler axis-symmetric 2-D computations. The associated complex temporal changes of the spatial concentrations and velocity fields are described. Particular attention is given to the velocity of the lean limit mixture front together with the temporal changes to the total flammable mixtures volume and the changes in the peak concentration of the dispersing fuel. Calculated results were in good agreement with some corresponding set of experimental results and those using other numerical simulations.

2 Problem Description

A vertical cylindrical vessel is assumed to contain momentarily at its base a known finite mass of a gaseous fuel that is buoyant in comparison to the overlaying air. As shown in Fig. 1, the lower part of the open to atmosphere circular cylindrical vertical vessel of diameter D and length L contains the fuel while the remaining upper part is considered to be filled initially with air. It is assumed that at a certain instant of time, assigned time zero, the fuel is permitted to be exposed to the air to commence spreading and dispersing into the overlaying atmosphere under isothermal condition. A transient

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velocity field along with concentration field begins to develop through the coupled transport processes of mass and momentum. Mass is transferred by the combined effects of molecular diffusion and natural convection.

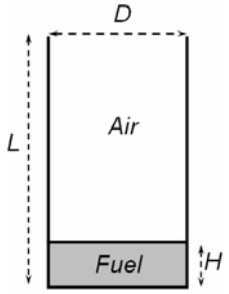

Figure.1 Schematic Diagram of the Problem

Particular interest is focused on the early stages of the evolution of the plume when the diffusion time scale is much larger than the physical time.The flammable region, which represents the mixture portions where the fuel concentration lies between those corresponding to the lean and rich limit values, under the prevailing conditions is then derived from the calculated instantaneous concentration fields.

3 Modeling

The transient equations of the conservation of mass, momentum and energy are the governing equations which are essentially the compressible Navier-Stokes equations coupled with a transport species equation:

$$\frac{\partial \rho}{\partial t} + \vec{\nabla}.\rho\vec{V} = 0 \qquad (1)$$

$$\rho\left[\frac{\partial \vec{V}}{\partial t} + \left(\vec{V}.\vec{\nabla}\right)\vec{V}\right] = -\vec{\nabla}P + \nabla.\tau + \rho\vec{g} \qquad (2)$$

$$\rho\left[\frac{\partial w_i}{\partial t} + \left(\vec{V}.\vec{\nabla}\right)w_i\right] = \vec{\nabla}.\left(\rho D_i \vec{\nabla} w_i\right) \qquad (3)$$

The thermodynamic and transport properties are taken to change continuously all over the domain of calculation according to the transient local values of concentration and temperature The flow of the Newtonian fluid is assumed to be laminar, isothermal and non reactive. The corresponding Rayleigh number was found to be smaller than the turbulent transition value for natural convection in a cavity [5] which tends to justify the laminar flow approximation employed.

Two distinct numerical codes were employed to solve the above equations to ensure that the results are independent of the computational method. Ansys-CFX Commercial software and a number of modifying subroutines were used for 3-D and 2-D axis-symmetrical simulations. The calculation domain was extended beyond the physical limits of the vessel to examine the consequences of the emergence of the fuel into the immediate vicinity of the vessel which has also important practical safety implications. The 2-D axis-symmetric simulations were performed using both a FORTRAN and the Ansys-CFX code. A 80×150 structured mesh was used inside the vessel with the same amount of grid points in the surrounding atmosphere which was extended to five diameters in the radial direction and five tube lengths in the vertical direction outside of the vessel. The time step was chosen to be 1ms to ensure a stable solution. The two sets of calculated results were in good agreement with each other. The processes were also resolved in 3-D simulations. A structured mesh of 200,000 grid nodes inside the vessel and the same amount in the outside atmosphere was employed with the same time step of 1ms. A series of mesh independence tests were carried out.

4 Results and Discussions

Cases of a finite quantity of the pure gaseous fuel, methane diffusing upward into an overlaying atmosphere of air within the vessel of Fig. 1 were considered. The typical representative results to be shown were obtained for a cylinder of 4cm diameter and 5cm long with an initial undisturbed fuel height of 1cm. This configuration would result in the following values of the key dimensionless numbers involved: Grashoff: 106, Reynolds: 100 and Schmitt: 0.8. Cylinder diameter sizes of less than

4 cm for this configuration ensure the free evolution of the plume as a single finger, reducing the complexities of multiple plumes,[2]. However, calculations for a 10cm diameter showed the dynamics of the transient flammable zone were still not significantly affected by the walls.

Fig. 2 shows 3-D simulation results of a certain mass of methane dispersion into air. The resolved concentration fields appear of much more complexity in the 3-D results than the 2-D simulations. This would indicate that forcing the symmetry in the 2-D simulations is unjustified in general for such a 3-D phenomenon. However, the 2-D simulations tend to be sufficiently accurate in some situations where the 3-D results display near symmetrical behaviour. As an example, the dispersion of the fuel from relatively small diameter vessels or under small gravitational acceleration and for small density difference between the fuel and air is adequately resolved by 2-D axis-symmetric modelling.

Fig.3 shows examples of how the flammable zones which are bounded outwardly by the lean limit concentration and inwardly by the corresponding rich limit, grow from initially very thin confined to a narrow region along the interface between the fuel surface and air to thickening later on while moving upwards. It is evident that the evolution of the flammable zone is dominated by the growth and mobility of the rising fuel and the fingering structure. The flammable region which does not necessarily always extend over the whole cross-sectional area of the vessel is of irregular shape and develops both inside and outside the vessel. Moreover, the flammable zone can become fragmented into parcels. This would have an important implication about the spread of the fire hazard.

The growth and spread pattern of the fuel-first-arrival boundary (1% fuel molar fraction contours) are shown in Fig.4 for both 3-D and 2-D simulations. This boundary appears to accelerate at the beginning to reach a limiting vertical velocity. The 3-D prediction of this velocity appears to be in good agreement with earlier corresponding theoretical and experimental results, [6]. The 2-D models appear to underestimate this velocity by up to 15% for the cases examined.

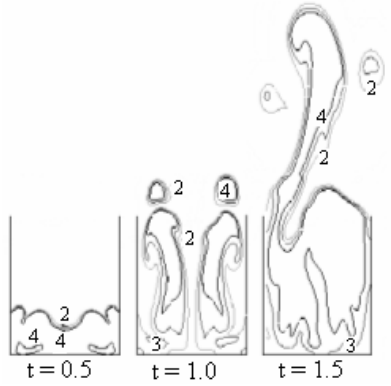

Figure.2 Molar fractional distribution,(3-D & 2-D) of methane within the vessel of d=4cm, L= 5cm, Z= 1cm , (1), (2), (3), (4) represent 0.0, 0.1, 0.2 and 0.3 fuel molar fraction respectively

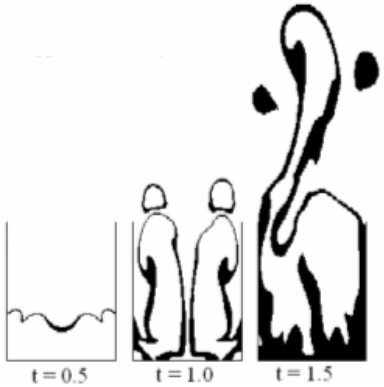

Figure 3 Locations of the flammable zones following methane release into a cylinder for 2D and 3D simulation, (d= 4cm, L= 5cm&H=1cm)

The observed slower evolution of mixing in 2-D simulation is consistent with the known tendency of large scale features to grow more rapidly in a 3-D domain than in a 2-D one. The corresponding rates of growth of the flammable fronts (5% and 15% fuel molar fraction contours) are also shown in Fig.4. The growth of the rich flammable front does not appear as smooth as that of the fuel-first-arrival or lean limit boundaries. This is because the rich flammable front falls into the wake mixing zone and is affected by the vortices displaying a more chaotic behavior. Its movement was observed to be more complex and a function of a number of other parameters such as the initial amount of the fuel to be dispersed. This behavior of the rich limit has important safety implications on the size and growth rates of the flammable zones. As an example our numerical simulations showed that immediately following a methane spillage into air, the lean flammable front would travel at around 16cm/s, in the vertical direction.

The maximum variation in the value of the concentration of the fuel anywhere in the domain is shown in Fig.5a. This value decreases rapidly with time with the dissipation of the fuel to approach a near

zero value after some considerable time and could be estimated reasonably well both by the 2-D and 3-D simulation approaches. Similarly, the temporal changes in the total volume of the flammable zone development normalized relative to the maximum possible flammable volume that could be produced on mixing homogeneously the available fuel with air in lean limit proportion are shown in Fig.5b. This parameter is of practical significance as it could represent a gross measure of the immediate energy release following ignition. Similar trends are exhibited for the two simulation approaches.

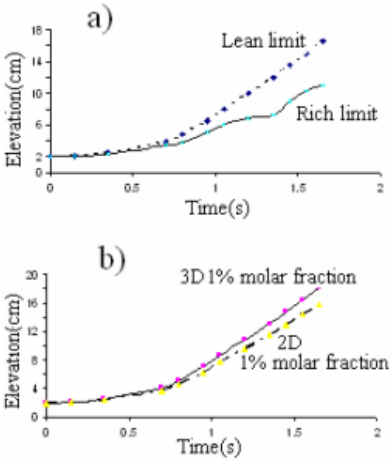

Figure 4. Elevation of the methane finger as a function of time, (L=5cm, Z= 2cm) a) Lean limit compared to b) rich limit, for3-D and 2-D

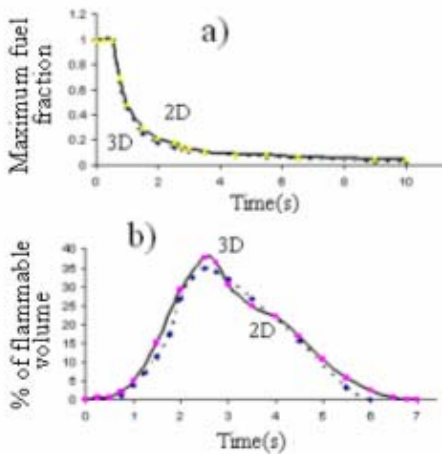

Figure 5. (a) Maximum fuel mole fraction in the domain, (b) Percent of flammable volume to the maximum possible flammable volume as a function of time, D=4cm, L=5cm, Z=1cm

On this basis, it can be suggested that although the 3-D simulated structure of the fuel mixing processes, appears to display some notable differences with that obtained on the basis of 2-D simulation, the transient changes in the gross values of some of the key safety parameters such as the maximum fuel concentration and the relative flammable mixture volume tend to be relatively small.

6 Concluding Remarks

For fuels that are less dense than air the temporal changes in the fuel concentration field and hence the formation and decay of the flammable mixture zones is strongly dependant on the dynamics of the fuel fingering. The fuel concentration contours travel at approximately a constant rate at the initial stages of the dispersion. The predictions of such a rate are better made with 3-D modelling. The lean-flammable boundary (5% fuel molar front for methane in air) appears to travel approximately at a constant velocity of around 16cm/s.

The rich flammable front which fell into the mixing zone displayed a chaotic and less smooth behavior compared to the lean flammable front. Although the 3-D simulated structure of the fuel mixing processes appears to display some notable differences with that obtained on the basis of 2-D simulation, the transient changes in the gross values of some of the key safety parameters such as the maximum fuel concentration and relative flammable mixture volume tend to be relatively small.

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