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THE CONVECTIVE DISPERSION OF FLAMMABLE MIXTURES WITHIN OPEN CYLINDRICAL ENCLOSURES FOLLOWING THE RELEASE OF A FIXED MASS OF A GASEOUS FUEL

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ABSTRACT

There are many practical situations where a finite mass of a buoyant gas may become suddenly exposed to atmospheric air at a negligible pressure difference within vertical chambers or vessels that are either fully or partially open. The consideration of such situations when a fuel or toxic gas is released is of immense practical importance especially in relation to developing measures for protection against the potential resulting hazards of fire, explosion or toxic emissions. In such situations highly complex transient mixing processes are produced involving the formation and decay of flammable and explosive mixtures within the vessels and may extend with time to their immediate vicinity. Accordingly, the development of suitable predictive models may be effective in producing useful description of the phenomena and may assist in drafting measures for reducing the associated hazards.

In the present work, a fixed mass of a buoyant gaseous fuel is considered to be exposed suddenly with a negligible pressure difference to overlaying air at atmospheric conditions within vertical cylindrical enclosures that are either fully or partially open at the top to the atmosphere. The walls of the containing vessel can be at a different temperature from that of its gaseous contents. The paper describes features of a predictive axis-symmetrical model of the transient convective buoyant mixing viscous processes within the confines of the vertical cylindrical vessel and in its immediate vicinity. Results relating to the releases of a fixed mass of the highly buoyant methane representing natural gas into air are presented. These are then compared with those relating to those of a heavier than air fuel such as propane. The associated complex temporal changes of the spatial concentrations are described. Particular attention is given to the build up and decay of flammable regions within the open-top vessel as well as the release of the fuel gas into the outside atmosphere.

KEYWORDS

Fire Safety, Flammable Mixtures, Gas Mixing, Convective Diffusion

INTRODUCTION

An important source of fire, explosion and toxic hazards is the release of a finite mass of fuel vapour within fuel installations or during various industrial operations. The mixing of fuel 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 would cause serious economic or environmental damage, [1]. Moreover, the exposure of a fuel to the overlaying air constitutes not only a serious safety hazard, but also can be a major source of environmental pollution, [2]. Improvement to our understanding of the mechanism of the processes of gas emission and dispersion will help in developing better guidelines to detect and mitigate hazardous vapour releases.

The isothermal and steady state diffusion of a vaporizing fluid into a gas within a tube, often referred to as Stefan diffusion has been widely investigated. Karim and Tsang [3] investigated the effects of temporally changing concentration gradients of methane-air mixtures on flame propagation. Mastorakos et al [4] performed two dimensional direct numerical simulation of mixing layers of fuel and hotter air. Bunama and Karim [5] developed a numerical model of the formation of flammable atmospheres within vertical enclosures containing a vaporizing liquid fuel. The 2-D axis-symmetrical model pointed out the effects of factors such as fuel properties, ambient conditions, the exposed liquid surface area and the size of the vent area on the transient development and dispersion of flammable atmospheres within vertical cylindrical containers. Ilegbusi et al [6] simulated the mixing of two fluids using fractional step method. They compared the accuracy of different numerical methods for modelling buoyancy driven flows. They also considered the perturbations introduced by valve opening and concluded that especially at large Grashof numbers this effect can not be ignore.

In this work, focus is made on a fixed mass of a buoyant gaseous fuel that is suddenly permitted to spread with a negligible pressure difference into air at atmospheric conditions within vertical cylindrical enclosures that are open at the top to the atmosphere. A predictive axis-symmetrical model of the transient convective buoyant mixing viscous processes within the confines of a vertical cylindrical vessel is described. Results relating to the releases of a fixed mass of the highly buoyant methane representing natural gas into air are presented. These are then compared to those of heavier than air gases. The associated complex temporal changes of the spatial concentrations and velocity fields are described. Particular attention is given to the build up and decay of flammable regions within the open-top cylindrical vessel as well as the release and spread of the fuel gas into the outside atmosphere. The effect of having warm walls on the structure of fluid flow and the dynamics of the flammable zone is examined. Some calculated results were in good agreement with the corresponding set of previously obtained experimental results, [3], and [7].

NOMENCLATURE

C_p (J/kg.K)	Constant pressure heat capacity
$\overline{c_p}, \overline{k}, \overline{D}$	$c_p / c_{p0}, k / k_0, D / D_0$
D (m²/s)	Diffusion coefficient
g (m/s²)	Gravitational acceleration
Gr_w Gr_T	Mass transfer and thermal Grashof no.
H_{fuel} (cm)	Height of the fuel in the vessel
K (W/m.K)	Thermal conductivity coefficient
L (cm)	Vessel length
M (kg/kmol)	Molecular weight
R (cm)	Cylinder radius
P (Pa)	Pressure
$\overline{P}$	$P / \rho_0 U_{ref}^2$
p_r	Prandtl number
r, z	Cylindrical coordinates
$\overline{r}, \overline{z}$	$r / H_{fuel}, z / H_{fuel}$
Re	Reference Reynolds number
Ra	Rayleigh number
S_r	Source term, equation (4)
S_z	Source term, equation (5)
S_c	Schmidt number
T (K)	Temperature
$\overline{T}$	$(T - T_0) / (T_b - T_0)$
t (s)	Time
U_{ref} (m/s)	$\sqrt{gH_{fuel}}$
V_r (m/s)	Radial velocity
V_z (m/s)	Axial velocity
$\overline{V_r}, \overline{V_z}$	$V_r / U_{ref}, V_z / U_{ref}$
w	Mass fraction
$\overline{w}$	$\overline{w_i} = (w_i - w_\infty) / (w_{0i} - w_\infty)$
μ (Pa.s)	Viscosity
ρ (kg/m²)	Density
$\overline{\rho}, \overline{\mu}$	$\rho / \rho_0, \mu / \mu_0$
Subscripts	
0	Relative to the initial fuel mixture
1	Relative to the fuel
2	Relative to the air
m	Relative to the mixture
T, w	Due to temperature & concentration

THE PROBLEM

A vertical cylindrical vessel is assumed to contain initially at its base a known finite mass of a gaseous fuel that may be highly buoyant in comparison to air. As shown in Fig. 1, the lower part of the open to atmosphere circular cylindrical vessel of radius R and length L contains the fuel while the remaining upper part is considered to be filled with air. The side walls of the container are assumed to be isothermal and may be either at a similar or a different temperature to that of the gaseous mixture components at the beginning of the mixing process.

It is assumed that at a certain instant of time, assigned time zero, the fuel is permitted suddenly to be exposed to the air and to commence spreading into overlaying atmosphere. A transient flow field and a concentration distribution begin to develop through the coupled transport processes of mass, momentum and energy. Mass is transferred by the combined effects of molecular diffusion and natural convection. Molecular diffusion is driven by the local concentration gradients while the convective mass transfer is due to the bulk flow of the moving gaseous mixture which is greatly controlled by buoyancy effects for lighter than air gases such (M=16 kg/kmol) or hydrogen (M=2 kg/kmol)

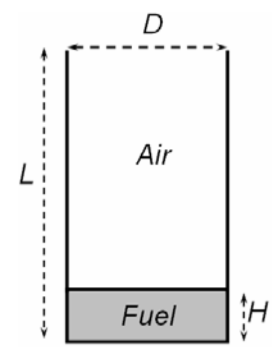


Figure.1 Schematic Representation of the Problem

It is necessary to determine the variation of the concentration field of the different species within the vessel at any time instance and location. The flammable region, which represents the portions where the fuel concentration lies between those corresponding to the lean and rich limit values, is then derived from the calculated concentration fields.

MODEL DESCRIPTION

The transient equations of conservation of mass, momentum and energy are the governing equations. 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, axis-symmetrical and satisfies the Boussinesq approximation. The corresponding Rayleigh number was found to be around 10^6. This is smaller than the transition value of Rayleigh number for natural convection in a cavity ($\approx 10^9$), [8] which tends to justify the laminar flow approximation employed. The Soret and Dufour aspects are considered to be negligible. Within the vertical open topped cylinder, the spread of the gas into the overlaying air and the inherent flow are driven mainly by the buoyancy forces resulting from the density differences. The driving buoyancy force in the vertical direction when treating the mixture as a perfect gas can be represented as:

$$DF = -\frac{\partial p}{\partial z} - \rho g\left[\frac{T_\infty - T}{T_\infty} - \frac{(w_\infty - w)(M - M_\infty)}{w_\infty M_\infty + (1 - w_\infty) M}\right] \qquad (1)$$

The governing equations of continuity, momentum, energy and species conservation when neglecting the viscous dissipation within the gas and any work, in dimensionless form are:

$$\frac{\partial \bar{\rho}}{\partial \bar{t}} + \frac{1}{\bar{r}}\frac{\partial}{\partial \bar{r}}(\bar{\rho}\bar{r}\bar{V}_r) + \frac{\partial}{\partial \bar{z}}(\bar{\rho}\bar{V}_z) = 0\,, \qquad (2)$$

$$\frac{\partial}{\partial \bar{t}}(\bar{\rho}\bar{V}_r) + \frac{1}{\bar{r}}\frac{\partial}{\partial \bar{r}}(\bar{\rho}\bar{r}\bar{V}_r\bar{V}_r) + \frac{\partial}{\partial \bar{z}}(\bar{\rho}\bar{V}_r\bar{V}_z) = \frac{1}{\bar{r}}\frac{\partial}{\partial \bar{r}}\left[\frac{4\bar{\mu}}{3\,\mathrm{Re}}\bar{r}\frac{\partial \bar{V}_r}{\partial \bar{r}}\right] + \frac{\partial}{\partial \bar{z}}\left[\frac{\bar{\mu}}{\mathrm{Re}}\bar{r}\frac{\partial \bar{V}_r}{\partial \bar{z}}\right] + S_r\,, \qquad (3)$$

$$S_r = -\frac{\partial \bar{P}}{\partial \bar{r}} - \frac{2\bar{\mu}\bar{V}_r}{\mathrm{Re}\,\bar{r}^2} - \frac{\partial}{\partial \bar{r}}\left[\frac{2\bar{\mu}}{3\,\mathrm{Re}}\frac{\partial \bar{V}_z}{\partial \bar{z}}\right] + \frac{\partial}{\partial \bar{z}}\left[\frac{\bar{\mu}}{\mathrm{Re}}\frac{\partial \bar{V}_z}{\partial \bar{r}}\right] - \frac{\bar{V}_r}{\mathrm{Re}}\frac{\partial}{\partial \bar{r}}\left[\frac{2\bar{\mu}}{3\bar{r}}\right]\,, \qquad (4)$$

$$\frac{\partial}{\partial \bar{t}}(\bar{\rho}\bar{V}_z) + \frac{1}{\bar{r}}\frac{\partial}{\partial \bar{r}}(\bar{\rho}\bar{r}\bar{V}_r\bar{V}_z) + \frac{\partial}{\partial \bar{z}}(\bar{\rho}\bar{V}_z\bar{V}_z) = \frac{1}{\bar{r}}\frac{\partial}{\partial \bar{r}}\left[\frac{\bar{\mu}}{\mathrm{Re}}\bar{r}\frac{\partial \bar{V}_z}{\partial \bar{r}}\right] + \frac{\partial}{\partial \bar{z}}\left[\frac{4\bar{\mu}}{3\,\mathrm{Re}}\frac{\partial \bar{V}_z}{\partial \bar{z}}\right] + S_z\,, \qquad (5)$$

$$S_z = \frac{-\partial \bar{P}}{\partial \bar{r}} - \frac{2\bar{\mu}\bar{V}_r}{\mathrm{Re}\,\bar{r}^2} - \frac{\partial}{r\partial \bar{r}}\left[\frac{\bar{\mu}}{\mathrm{Re}}\bar{r}\frac{\partial \bar{V}_r}{\partial \bar{z}}\right] - \frac{\partial}{\partial \bar{z}}\left[\frac{2\bar{\mu}}{3\,\mathrm{Re}}\frac{\partial \bar{r}\bar{V}_r}{r\partial \bar{r}}\right] + \frac{\bar{\rho}}{\mathrm{Re}^2}\left[Gr_T\,\bar{T} - Gr_{w_1}\overline{w_1} - Gr_{w_2}\overline{w_2}\right]\,, \qquad (6)$$

$$\frac{\partial}{\partial \bar{t}}(\bar{\rho}\overline{c_p}\,\bar{T}) + \frac{1}{\bar{r}}\frac{\partial}{\partial \bar{r}}(\bar{\rho}\bar{r}\bar{V}_r\overline{c_p}\,\bar{T}) + \frac{\partial}{\partial \bar{z}}(\bar{\rho}\bar{V}_z\overline{c_p}\,\bar{T}) = \frac{1}{\bar{r}}\frac{\partial}{\partial \bar{r}}\left[\frac{\bar{k}}{\mathrm{Re}\,P_r}\bar{r}\frac{\partial \bar{T}}{\partial \bar{r}}\right] + \frac{\partial}{\partial \bar{z}}\left[\frac{\bar{k}}{\mathrm{Re}\,P_r}\frac{\partial \bar{T}}{\partial \bar{z}}\right]\,, \qquad (7)$$

$$\frac{\partial}{\partial \bar{t}}(\bar{\rho}\bar{w}) + \frac{1}{\bar{r}}\frac{\partial}{\partial \bar{r}}(\bar{\rho}\bar{r}\bar{V}_r\,\bar{w}) + \frac{\partial}{\partial \bar{z}}(\bar{\rho}\bar{V}_z\,\bar{w}) = \frac{1}{\bar{r}}\frac{\partial}{\partial \bar{r}}\left[\frac{\overline{\rho D_i}}{\mathrm{Re}\,Sc}\bar{r}\frac{\partial \bar{w}}{\partial \bar{r}}\right] + \frac{\partial}{\partial \bar{z}}\left[\frac{\overline{\rho D_i}}{\mathrm{Re}\,Sc}\frac{\partial \bar{w}}{\partial \bar{z}}\right]\,, \qquad (8)$$

where:

$$\mathrm{Re} = \frac{\rho_0 U_{ref} H_{ref}}{\mu_0}\,, \qquad Gr_T = \frac{g(T_{ref} - T_\infty)H_{ref}^3}{T_\infty v_0^2}\,,$$

$$Gr_w = \frac{(M_1 - M_3)}{w_\infty M_3 + (1 - w_\infty) M_1}\,\frac{g(w_0 - w_\infty)H_{ref}^3}{v_0^2} \qquad (9)$$

$$P_r = \frac{v_0}{\alpha_0} = \frac{\mu_0 c_{p0}}{k_0}\,, S_c = \frac{v_0}{D_{i,0}}\,.$$

The governing equations were discretized using a staggered non-uniform grid. The advection terms are approximated using the QUICK scheme combined with the flux limiter ULTRA-SHARP to eliminate the numerical diffusion errors and the non-physical oscillations [9]. The enhanced SIMPLE algorithm, [10], is used to couple the momentum and continuity equations. The algebraic equations resulting from the discretized equations are solved iteratively using the Strongly Implicit Procedure (SIP). A special treatment extended the calculation domain 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 implications.

RESULTS AND DISCUSSION

Cases of a finite quantity of a pure gaseous fuel diffusing upward into an overlaying atmosphere of air within the vessel of Fig. 1 were considered. All of the results being presented in this paper were obtained for a cylinder of 6 cm diameter and 20 cm long with an initial fuel height of 2 cm. The values of the dimensionless numbers are: Thermal Grashoff:10^6, reference Reynolds:500, Prandtl:0.7 and Schmidt: 0.8.

It is well known that the vertical mixing processes for fuels with densities greater than that of the overlaying air are purely driven by molecular diffusion. Thus, there is no bulk fluid motion and the mixture velocity is zero everywhere within the vessel. As shown typically for the dispersion of propane in Fig.2, mixing starts at the initial interface of the fuel and air and expands smoothly both upward and downward with the corresponding concentration gradient of the fuel remaining always negative in the upward direction. The iso-concentration lines of the fuel remain basically horizontal, showing virtually no dependency upon the radial direction. The flammable zone is composed of horizontal, thickening bands moving slowly upwards and lingers for a long time.

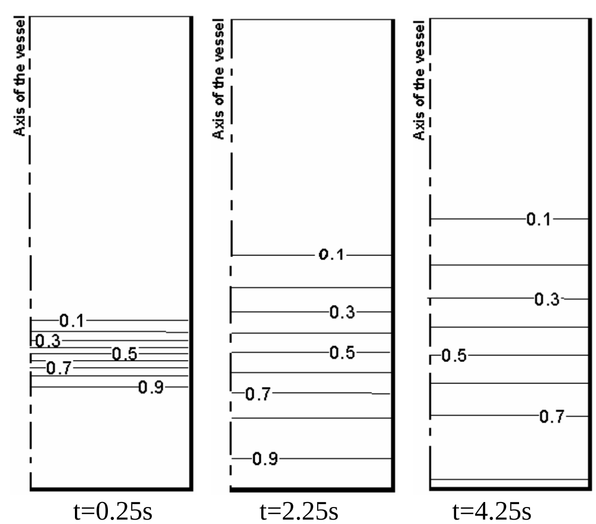
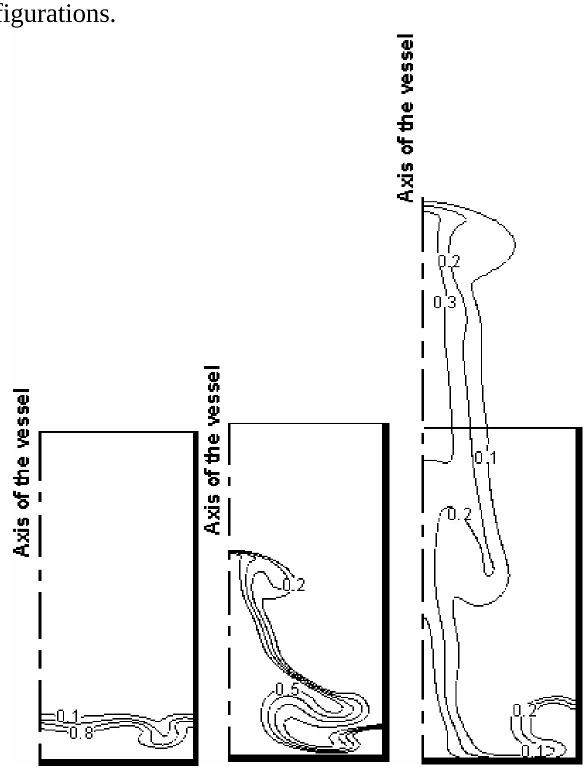


Figure.2 Molecular diffusion driven processes-molar fraction distribution of propane within the vessel of 3 cm diameter, 8cm length, 2 cm initial fuel at different time instants

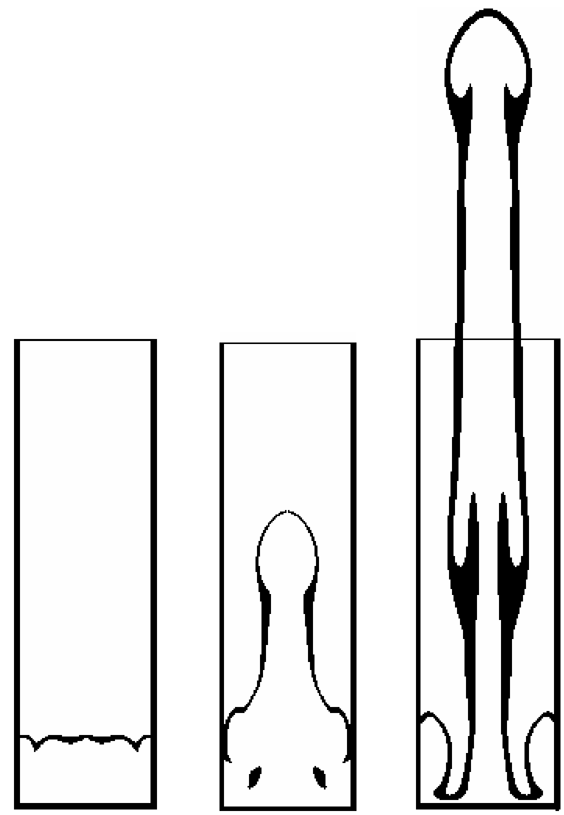
When the fuel density is smaller than that of the overlaying air, the mixing process is mainly driven by natural convection with molecular diffusion playing a smaller role. Under such a condition dispersion of the fuel takes place extremely rapidly in comparison to the molecular diffusion controlled cases. The resulting concentration field depends strongly on both the radial and axial directions and the fuel tends to rise on bulk basis. As shown typically in Fig.3 for methane dispersing into air, some wrinkles appear on the interface in both the fuel and air in a fingering like manner. These instabilities grow and may neck at some point and release a batch of the fuel to the atmosphere. Then a plume begins to form and later to become a puff of fuel that heads to the top of the vessel. There would be some fuel lingering by the walls which will migrate towards the central region as it progresses within the cylinder and it may produce another puff that expands and dissipates into the surrounding air. This will continue till the remaining fuel gas in the vessel becomes so much diluted that it can no longer produce buoyancy driven flow. For instance, four puffs were observed when methane was investigated in the prescribed geometrical configurations.



t=0.50s t=1.00s t=1.50s

Figure.3 Buoyancy driven processes, molar fraction distribution of methane within the vessel of 6cm diameter, 20cm length, 2cm initial fuel at different time instants

Fig.4 shows examples of how the flammable zone grows from being initially very thin and confined to a narrow region along the interface between the fuel surface and air to later on thickening while moving upwards in the inner regions. For the natural convection-controlled processes, the flammable region quickly widens, curls outwards towards the axis of the vessel and fragments into more than one region. Due to the dynamic tumbling spread of the lighter than air fuel, the changing flammable region does not necessarily always extend over the whole cross-sectional area of the vessel and it is of irregular shape. Moreover, these flammables zones can become fragmented into parcels within the vessel. This would have an important implication about the characteristic spread of a fire within such confines, should it develop.



t=0.50s t=1.00s t=1.50s

Figure.4 Locations of the flammable zones at different time instances when methane is released into a vessel of 6cm diameter, 20cm length, 2cm initial fuel

The time for the first arrival of the flammable zone following its release at a certain location is of practical importance. The knowledge of such times for any configuration is needed when planning safety measures such as for reducing the fire hazard, evacuation of compartments or establishing the transient rate of fugitive gas emissions into the surroundings. Fig. 5 shows for the same conditions of the earlier examples how such times vary very widely with the molecular weight of the gas for different elevations within the vessel. These times become exceedingly long for the heavier than air fuels indicating both a longer period for taking remedial action with a lingering of the hazard.

Consideration is now given to the effect of warm walls on the corresponding motion pattern of the fluid. These numerical simulations were performed using the FLUENT commercial software for comparison. The advection terms were again approximated using the QUICK scheme. PISO algorithm, [10], was used for pressure-velocity coupling. The pressure term discritization was done by the body force weighted scheme, [10], which is more suitable for buoyancy driven problems.

First order Eulerian method was employed to deal with the transient terms. Calculated results using the predictive model developed were in good agreement with the corresponding set of results obtained by FLUENT. As an example, table 1 shows the good level of agreement of the calculated times for the first arrival of the flammable zone when using the two approaches.

Hot walls warm up the fuel and air layers adjacent to them and make them more buoyant compared to the gas at the inner region. Thus, there is no sign of lingering fuel layer at the walls and the fuel would disperse much faster. In the absence of any methane and early after the beginning of simulation, warm walls would create a circulation zone within the vessel which would produce an upward motion at the walls and a downward motion at the axial region of the vessel as shown in fig.6.

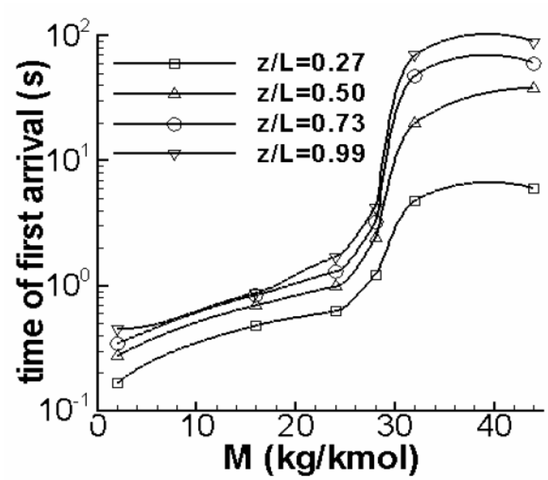


Figure 5: Time of first arrival of the flammable zone at different heights within the vessel of 6cm diameter, 20cm length, 2cm initial fuel as a function of the molar weight of the released fuel

Table.1
First arrival of the flammable zone at different elevations obtained by Fluent in comparison with calculated results

	$Z/L=0.27$	$Z/L=0.50$	$Z/L=0.73$	$Z/L=1.0$
Fluent	0.51s	0.76s	0.88s	0.95s
Calculated Results	0.48s	0.74s	0.85s	0.9s

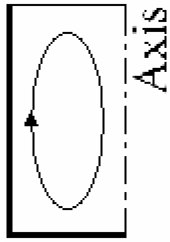


Figure.6 Schematic representation of the recirculation zone produced by warm walls

This is in contrast to mass transfer effects which tend to induce an upward motion and away from both the walls and the central region. The net effect of the combined heat and mass transfer effects, as shown in fig.7 was to have a puff of fuel which rises from the walls, but will move towards the center after leaving the vessel. This rapid upward motion entrains the heavier air towards the base of the vessel and enhances the rate of growth of the volume of the flammable zone and the time for fuel evacuation from the vessel.

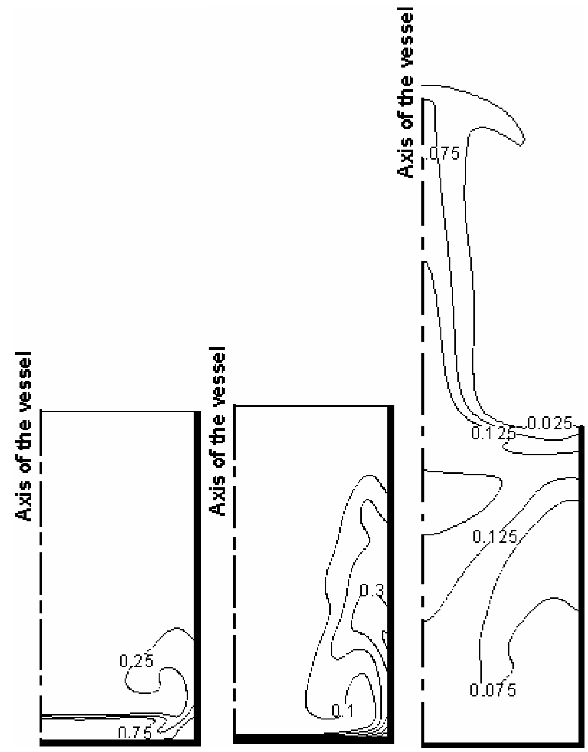


Figure.7 Buoyancy driven processes with warm walls, molar fraction distribution of methane within the vessel of 6cm diameter, 20cm length, 2cm initial fuel at 300K, isothermal walls at 350K and at different time instants

The volume of the flammable zone and its temporal development either within the vessel or its emergence into the outside atmosphere is of practical importance as it represents a measure of the immediate energy release on ignition. Such knowledge is needed for planning safety measures such as for reducing the fire hazard, evacuation of compartments or establishing the transient rate of fugitive gas emissions into the surroundings. Fig. 8 shows for the same conditions of the earlier examples how the growth of this volume increases with the wall temperature.

Obviously, the volume of the flammable zone depicts an oscillatory behavior with the unheated walls which is due to pulsating nature of the phenomenon. Each puff would enlarge the flammable zone as it detaches from the rest of the fuel and would decrease the flammable volume as it leaves the domain. On the other hand with warm walls, the flammable zone grows faster and then decays much earlier and does not appear to show a similar oscillatory behavior. The maximum flammable volume is much larger which represents a greater hazard that lasts a shorter time.

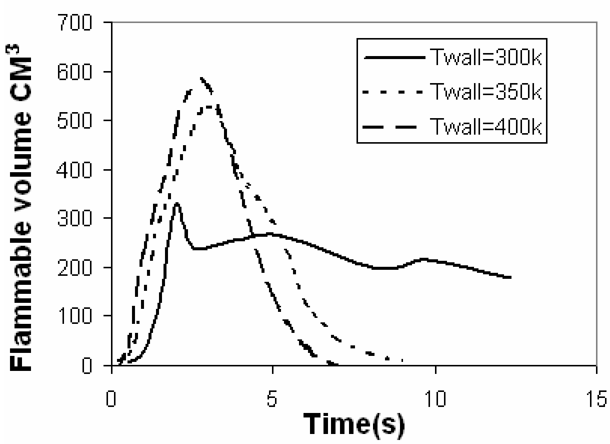


Figure.8 Volume of the flammable zone as a function of time following the release of 2cm methane at 300K in a vessel of 6cm diameter, 20cm length with walls at 300K, 350K, 400K

CONCLUSIONS

The predicted results of the transient spatial changes in fuel concentrations when a fixed mass of fuel is released with a negligible pressure difference into the atmosphere of an open enclosure showed the importance of the fuel density relative to that of air. For fuels that are less dense than air, the temporal changes to the fuel concentration field and hence the formation and decay of flammable mixture zones is strongly dependant on both the radial and axial coordinates. For heavier than air fuels, the mixing processes are very much slower in comparison and the residence times of the fuels within the vessel are very much longer representing a lingering hazard. In Addition, warm walls have a pronounced effect on the dynamics of the fuel plume and the flammable region. Warm walls would enhance the growth of the flammable zone and will increase the maximum flammable volume, but will drastically decrease its life time.

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