

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

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ABSTRACT

The release of a certain mass of gaseous fuel with a negligible pressure difference into enclosures open to the ambient atmosphere whether deliberately or inadvertently results in the formation of rapidly changing flammable mixture zones representing potential fire hazard. The initiation, growth and subsidence of such flammable zones are closely related to the intensity of the mixing processes of the fuel and air due to the combined effects of molecular diffusion and natural convection. The concentration distributions, and consequently the resulting flammable zones, depend on the relative importance of these two effects. A numerical model based on the solution of the equations of conservation of mass, momentum and energy was developed to describe the transient mixing processes and subsequently the development of flammable zones. It was found that for fuels heavier than the overlaying air the concentration gradients are always decreasing upwards. The process is very slow and can be represented fairly well by a one-dimensional simulation. The resulting flammable zones tend to be not fragmented. Fuels lighter than the overlaying air develop with time less organized distributed concentrations within the system. The fuel is dispersed into the air quickly in pulse-like form with a strong dependency on both horizontal and vertical directions. The resulting flammable zones can become fragmented within the system and move much faster than for the corresponding case of heavier than air fuels.

Keywords Fire safety, flammable mixtures, gas mixing

NOMENCLATURE

BF	buoyancy force
$\bar{c}_p, \bar{k}, \bar{D}$	$c_p / c_{p0}, k / k_0, D / D_0$
M	molar weight [g/mol]
\bar{P}	$p / \rho_0 U_{ref}^2$
\bar{r}, \bar{z}	$r / H_{fuel}, z / H_{fuel}$
\bar{T}	$(T - T_0) / (T_b - T_0)$
U_{ref}	reference velocity, $(g H_{fuel})^{1/2}$
\bar{v}	v / U_{ref}
$\bar{\omega}$	mass fraction
$\bar{\omega}_i$	$(\omega_i - \omega_\infty) / (\omega_{0,i} - \omega_\infty)$
$\bar{\rho}, \bar{\mu}$	$\rho / \rho_0, \mu / \mu_0$

$$\tau = t(g / H_{fuel})^{1/2}$$

Subscripts

0	relative to the initial fuel mixture
1,3	relative to the fuel, air respectively
m	relative to the gas mixture
T	due to temperature
ω	due to concentration

INTRODUCTION

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 open to the atmosphere. 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. Highly complex transient mixing process are produced involving the formation and decay of flammable and explosive mixtures within the vessels and may extend to their immediate vicinity. Accordingly, the development of suitable predictive models may be effective in producing useful description of the phenomena and may permit drafting measures for reducing the associated hazards. The isothermal and steady state diffusion of a vaporizing liquid into a gas within a tube, often referred to as Stefan diffusion, is widely investigated. Karim and Tsang [1] and Badr and Karim [2] investigated the effects of temporally changing concentration gradients of methane-air mixtures on flame propagation. Bunama and Karim [3,4] developed a numerical simulation of the formation of flammable atmospheres within enclosures containing a vaporizing liquid fuel. The 2-D axis-symmetrical model pointed out the effects of factors such as the 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. In the present work, a fixed mass of a buoyant gaseous fuel is 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. This paper describes a predictive axis-symmetrical model of the transient convective buoyant mixing viscous processes within the confines of a vertical cylindrical vessel and in its immediate open top vicinity. Results relating to the releases of a fixed mass of highly buoyant methane representing natural gas or hydrogen, into air are

presented. These are then compared with those relating to those of heavier than air. 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 vessel as well as the release of the fuel gas into the outside atmosphere. Some calculated results were in good agreement with a corresponding set of experimental results, [5], [6].

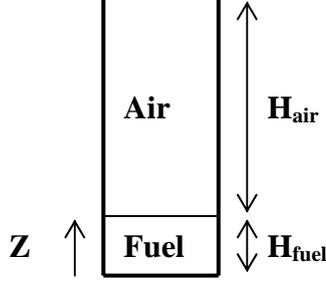


Figure 1. The tube partially filled with fuel

A vertical cylindrical vessel is assumed to contain initially at its base a known finite mass of a gaseous fuel. As shown in Fig. 1, the lower part of the open to atmosphere circular cylindrical vessel contains the fuel while the remaining upper part is considered to be filled with air. It is assumed that at a certain instant of time, (assigned a time of zero), the fuel is let exposed to the air and to commence spreading into it. 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 methane, ethylene or hydrogen.

THE MODEL

$$DF = -\frac{\partial p_d}{\partial z} - \rho g \left[\frac{T_\infty - T}{T_\infty} + \frac{(\omega - \omega_\infty)(M - M_\infty)}{\omega_\infty M_\infty + (1 - \omega_\infty)M} \right] \quad (1)$$

The governing equations of continuity, momentum, energy and species conservation in dimensionless form are:

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

$$\frac{\partial}{\partial t} (\bar{\rho} \bar{v}_r) + \frac{1}{r} \frac{\partial}{\partial r} (\bar{\rho} r \bar{v}_r \bar{v}_r) + \frac{\partial}{\partial z} (\bar{\rho} \bar{v}_r \bar{v}_z) =$$

$$\frac{1}{r} \frac{\partial}{\partial r} \left(\frac{4\bar{\mu}}{3R_e} r \frac{\partial \bar{v}_r}{\partial r} \right) + \frac{\partial}{\partial z} \left(\frac{\bar{\mu}}{R_e} \frac{\partial \bar{v}_r}{\partial z} \right) + S_r$$

$$S_r = -\frac{\partial \bar{p}}{\partial r} - \frac{2\bar{\mu}}{R_e} \frac{\partial \bar{v}_r}{r^2} - \frac{\partial}{\partial r} \left(\frac{2\bar{\mu}}{3R_e} \frac{\partial \bar{v}_z}{\partial z} \right) + \frac{\partial}{\partial z} \left(\frac{\bar{\mu}}{R_e} \frac{\partial \bar{v}_z}{\partial r} \right) - \frac{\bar{v}_r}{R_e} \frac{\partial}{\partial r} \left(\frac{2\bar{\mu}}{3r} \right)$$

$$\frac{\partial}{\partial t} (\bar{\rho} \bar{v}_z) + \frac{1}{r} \frac{\partial}{\partial r} (\bar{\rho} r \bar{v}_r \bar{v}_z) + \frac{\partial}{\partial z} (\bar{\rho} \bar{v}_z \bar{v}_z) =$$

$$\frac{1}{r} \frac{\partial}{\partial r} \left(\frac{4\bar{\mu}}{3R_e} r \frac{\partial \bar{v}_z}{\partial r} \right) + \frac{\partial}{\partial z} \left(\frac{4\bar{\mu}}{3R_e} \frac{\partial \bar{v}_z}{\partial z} \right) + S_z$$

$$S_z = -\frac{\partial \bar{p}}{\partial z} + \frac{1}{r} \frac{\partial}{\partial r} \left(\frac{\bar{\mu}}{R_e} r \frac{\partial \bar{v}_r}{\partial z} \right) - \frac{\partial}{\partial z} \left(\frac{2\bar{\mu}}{3R_e} \frac{1}{r} \frac{\partial}{\partial r} (\bar{r} \bar{v}_r) \right) + \frac{\bar{\rho}}{R_e^2} [Gr_T \bar{T} - Gr_{\omega 1} \bar{\omega}_1 - Gr_{\omega 2} \bar{\omega}_2]$$

Neglecting the viscous dissipation within the gas and any work, the energy equation is:

$$\frac{\partial}{\partial t} (\bar{\rho} c_p \bar{T}) + \frac{1}{r} \frac{\partial}{\partial r} (\bar{\rho} r \bar{v}_r c_p \bar{T}) + \frac{\partial}{\partial z} (\bar{\rho} \bar{v}_z c_p \bar{T}) =$$

$$\frac{1}{r} \frac{\partial}{\partial r} \left(\frac{\bar{k}}{R_e Pr} r \frac{\partial \bar{T}}{\partial r} \right) + \frac{\partial}{\partial z} \left(\frac{\bar{k}}{R_e Pr} \frac{\partial \bar{T}}{\partial z} \right)$$

$$\frac{\partial}{\partial t} (\bar{\rho} \bar{\omega}) + \frac{1}{r} \frac{\partial}{\partial r} (\bar{\rho} r \bar{v}_r \bar{\omega}) + \frac{\partial}{\partial z} (\bar{\rho} \bar{v}_z \bar{\omega}) =$$

$$\frac{1}{r} \frac{\partial}{\partial r} \left(\frac{\bar{\rho} \bar{D}_i}{R_e Sc} r \frac{\partial \bar{\omega}}{\partial r} \right) + \frac{\partial}{\partial z} \left(\frac{\bar{\rho} \bar{D}_i}{R_e Sc} \frac{\partial \bar{\omega}}{\partial z} \right)$$

In the equations above, the dimensionless group numbers (Reynolds, Grashof for heat and mass transfer, Prandtl and Schmidt numbers) are defined as follows :

$$R_e = \frac{\rho_0 U_{ref} H_{fuel}}{\mu_0}, \quad Gr_T = \frac{g(T_{ref} - T_\infty) H_{fuel}^3}{T_\infty \nu_0^2},$$

$$Gr_\omega = \frac{(M_1 - M_3) g(\omega_0 - \omega_\infty) H_{fuel}^3}{\omega_\infty M_3 + (1 - \omega_\infty) M_1 \nu_0^2},$$

$$Pr = \frac{\nu_0}{\alpha_0} = \frac{\mu_0 c_{p,0}}{k_0}, \quad Sc = \frac{\nu_0}{D_{i,0}}$$

SOLUTION OF THE GOVERNING EQUATIONS

The coupled unsteady equations were discretized using a staggered non-uniform control volumes grid. To take advantage of the assumed symmetry, the domain of calculation is based on one half of the cylinder. To accommodate the rapid changes at the interface fuel-air and at the walls, the grid was made finer at these locations. The algorithm SIMPLEX [7,8,9] was used to couple the momentum and continuity equations. 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 [10,11]. The algebraic equations resulting from the discretized equations are solved iteratively using the Strongly Implicit Procedure (SIP) [12,13,14]. As shown on Fig. 2, the boundary is extended beyond the physical limits of the vessel so as to decrease any computational convergence problems around the cylinder outlet, particularly when dealing with very buoyant gases. Also, it gives the subsequent development of flammable zones into the immediate vicinity of the exit.

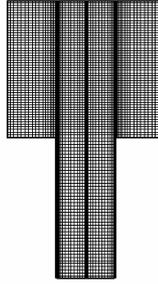


Figure 2: Schematic of the typical domain of calculations showing variable grid distribution

All the results presented in this work are based on the 76x425 grid, unless otherwise specified. Comparison of some calculated results with our own previously obtained experimental data, [5,6] was made. The time of first arrival of flammable mixtures at a given height within the cylinder was experimentally measured following the sudden exposure of rich mixtures of methane-air of different compositions into overlaying air. An electric spark located at the observation height turned on periodically was used to detect the arrival of flammable mixtures. Fairly good agreement between the calculated results and the experimental data were obtained. The following convergence criterion was applied to all dependant variables over the solution domain

$$\frac{\sum \phi_{ij}^n - \phi_{ij}^{n-1}}{\sum \phi_{ij}^n} \leq 10^{-5} \quad (7)$$

where ϕ represents a dependant variable, the indices i, j indicate a grid point and n the current iteration. For the base case, that included regions with 156x525 grid points, the CPU time required for the methane to evacuate the cylinder was approximately 48 hours on the Westgrid High Performance Computing system with allocated RAM up to 1 GB, using double-precision arithmetic and a Fortran 95 compiler.

RESULTS AND DISCUSSION

Cases of a finite quantity of pure gaseous fuels of different densities diffusing upward into an overlaying atmosphere of air within the vessel of Fig. 1 were considered. All the results presented in this paper were obtained for a cylinder of 6 cm diameter, 20 cm long and an initial fuel height of 2 cm. Focus is made on the effect of relative fuel densities on the rate and patterns of their upward dispersion into the air both within the vessel and in its vicinity just outside. It is known that when the fuel density is smaller than that of the overlaying air, the mixing processes are driven mainly by natural convection with molecular diffusion playing in comparison a very small role. On the other hand, the mixing processes for fuels with density greater than that of the overlaying air are driven by molecular diffusion. From inspection the main controlling parameters are the Reynolds number and the Grashof number due to concentration. Variation in the Schmidt number is negligible.

In situations where the density of the fuel is greater than that of the overlaying air, the upward mixing processes expectedly are relatively very slow and quite ordered. The mixing of the fuel and air starts at the initial interface and expands smoothly both upward and downward from the interface with the corresponding concentration gradient of the fuel remaining always negative in the upward direction. The iso-concentration lines of the fuel are basically horizontal, showing virtually no dependency upon the radial direction.

For a fuel that is less dense than the overlaying air, fast dispersion of the fuel and its subsequent escape into the outside atmosphere as shown typically in Fig. 3, takes place extremely rapidly in comparison to the molecular diffusion controlled cases, often with orders of magnitude time differences. The resulting concentration field then depends strongly on both the radial and axial directions. The upward fuel flow is faster midway between the axis and the walls of the vessel. On this basis, for an early detection of the arrival release of the fuel or a toxic gas at a certain elevation within the confines of a chamber or a vessel, appropriate sensors are better located at about 2/3 of the vessel radius rather than at the walls or the axis. Moreover, the fuel tends to rise initially more of en-masse parcel-like basis. This rapid upward motion entrains the heavier air towards the base of the vessel. Then a plume begins to form at around 2/3 of the radius and later on becomes a puff of fuel that expands and dissipates into the surrounding air as it heads to the top of the vessel. The ascent of an ultra light fuel such as hydrogen or methane escape out of the vessel resembles the dissipation of a transient jet.

From the concentration distribution mapping, information about the transient development and subsidence of flammable regions can be derived, [15]. These regions are assumed to be bound on one side by concentrations that correspond to the local lean flammability limit values and on the other by those corresponding to the rich limit. 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. In the case of molecular diffusion-driven processes, the flammable zones appear horizontal of uniform but thickening bands moving slowly upwards with the flammable zone lingering for a long time. For the natural convection-controlled processes, the flammable region quickly widens, curls outwards towards the upper regions of the vessel, Fig. 4, and fragments into more than one region. Due to the dynamic tumbling fuel spread with 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 and mobile. 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.

The time for the first arrival of a fuel or a toxic gas following its release at a certain location whether within the vessel or its emergence into the outside 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

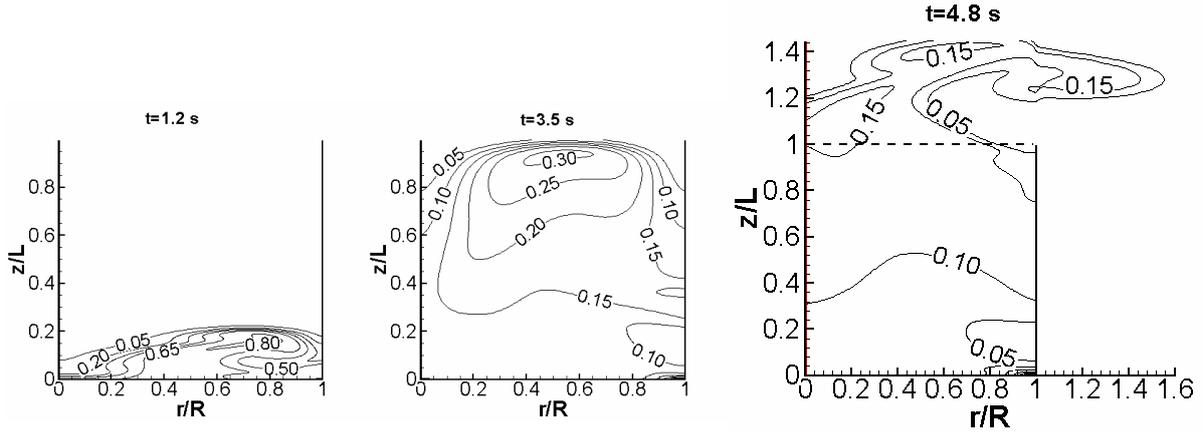


Figure 3: Natural convection-driven processes molar fraction distribution of hydrogen within the vessel at different time instances following its release

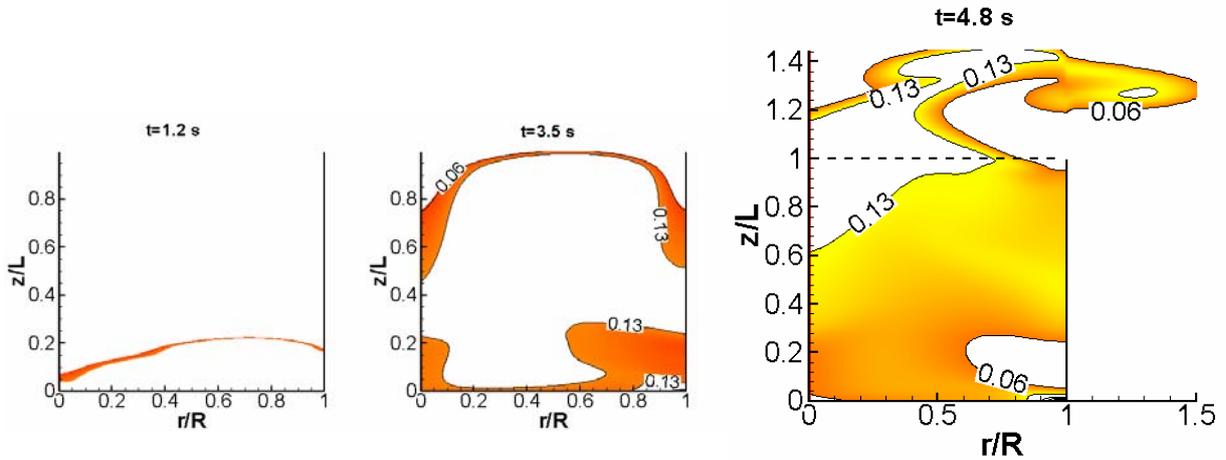


Figure 4: Locations of the flammable zones at different time instances when methane is dispersing into overlaying air

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.

Next, mixtures $\text{CH}_4\text{-CO}_2$ with increasing CO_2 content were considered as the fuel. Figure 6 shows the dispersion times at a given height within the cylinder for different CO_2 content in the initial fuel mixture of $\text{CH}_4\text{-CO}_2$. It can be seen that flammable zones are generated when up to 46% CO_2 is contained in the initial fuel mixture. Within the range of 0 to 46% CO_2 , the dispersion times are very short and similar due to the rapid convective spread of the buoyant gaseous flow. Above the value of 46%, no flammable mixture was formed, [15].

This trend of the dispersion time shown in Fig. 6 is in good agreement with the experimental observations reported by us in previous work [5, 6]. As the initial concentration of CO_2 increases, the density of the mixture $\text{CH}_4\text{-CO}_2$ in the lower part of the cylinder increases towards the density of the air and consequently, the buoyancy effects become less important. Close to the concentration value of 46% of CO_2 , the buoyancy effects become negligible resulting in mixing processes less intense governed by molecular diffusion and then, the fuel

surrounded by such quantity of CO_2 cannot find anymore enough air to generate flammable mixtures. Replacing the CO_2 by nitrogen in the initial fuel mixture in the lower part of the cylinder leads to a different configuration since the fuel mixture of methane and nitrogen irrespective of their proportion will remain always lighter than the overlaying air. The buoyancy effects will be always present producing faster dispersion of the fuel into the air. Beyond a concentration of around 40% N_2 there is insufficient time to form a combustible mixture. However, should the diluent be applied to the overlaying air while keeping the fuel in the lower portion on its own can produce distinctively different trends. Then, a heavy air- CO_2 mixture descends while mixing with the rising light methane reducing the likelihood of forming a flammable zone and representing a more effective application of a diluent to eliminate a fire hazard. However when nitrogen is applied homogeneously to the overlaying air within the vessel the buoyancy effect will be always present. Beyond a certain nitrogen concentration in air the ascending methane cannot form flammable mixtures. However, it was found that under certain conditions a seemingly safe mixture combination can be associated with some flammable zones due to the possible infiltration of fresh pure air from well outside the vessel to replace the escaping buoyant gases. This is an area that needs further research and identification.

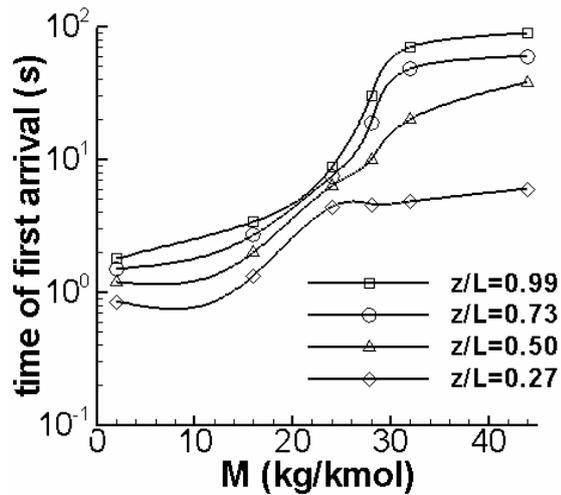


Figure 5: Time of first arrival of the fuel at different heights within the vessel as a function of the molar weight of the released fuel.

CONCLUSION

The predicted results of the transient spatial changes in fuel concentrations when a fixed mass of fuel is released with a negligible pressure difference upward 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 time of the fuels within the vessel are very much longer representing a lingering hazard.

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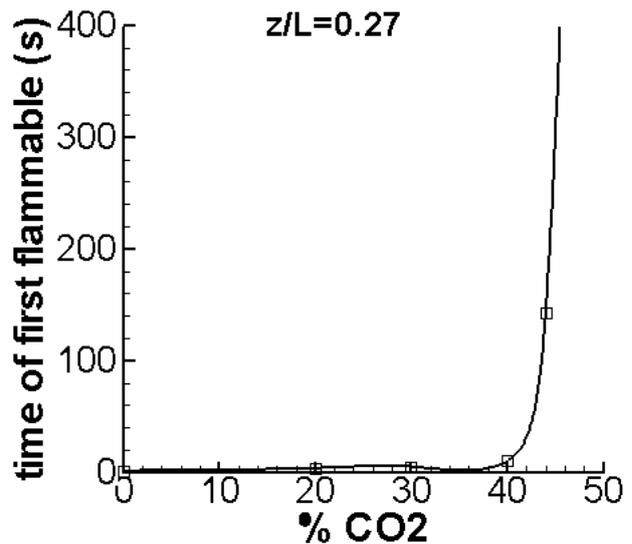


Figure 6: Time of arrival of first flammable mixture at height $z/L=0.27$ when different mixtures of CH_4 and CO_2 are dispersing into atmospheric air within the cylinder.

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