Department of Mechanical and Manufacturing Engineering
Schulich School of Engineering,

University of Calgary
Canada

THE FORMATION AND DISSIPATION OF FLAMMABLE MIXTURES FOLLOWING THE RELEASE OF A FIXED MASS OF A BINARY FUEL MIXTURE INTO AIR WITHIN VERTICAL CYLINDRICAL VESSELS

By

P.Cisse,   G.A. Karim*   and   I.Wierzba

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Introduction

The release at zero pressure difference of a certain mass of toxic material /gaseous fuel results in the formation of a rapidly changing hazardous / flammable zones. The initiation, growth and subsidence of such atmospheres are of much

importance.

The current research is mainly focused on examining analytically the evolution of the fugitive gas emissions from the time they are released in a cylindrical open vessel until they find their way into the atmosphere to become dissipated

Interest in finding answers to questions such as:

-What is the configuration/volume of the flammable zone?

-How long does it take before the vessel contents and surroundings are safe?

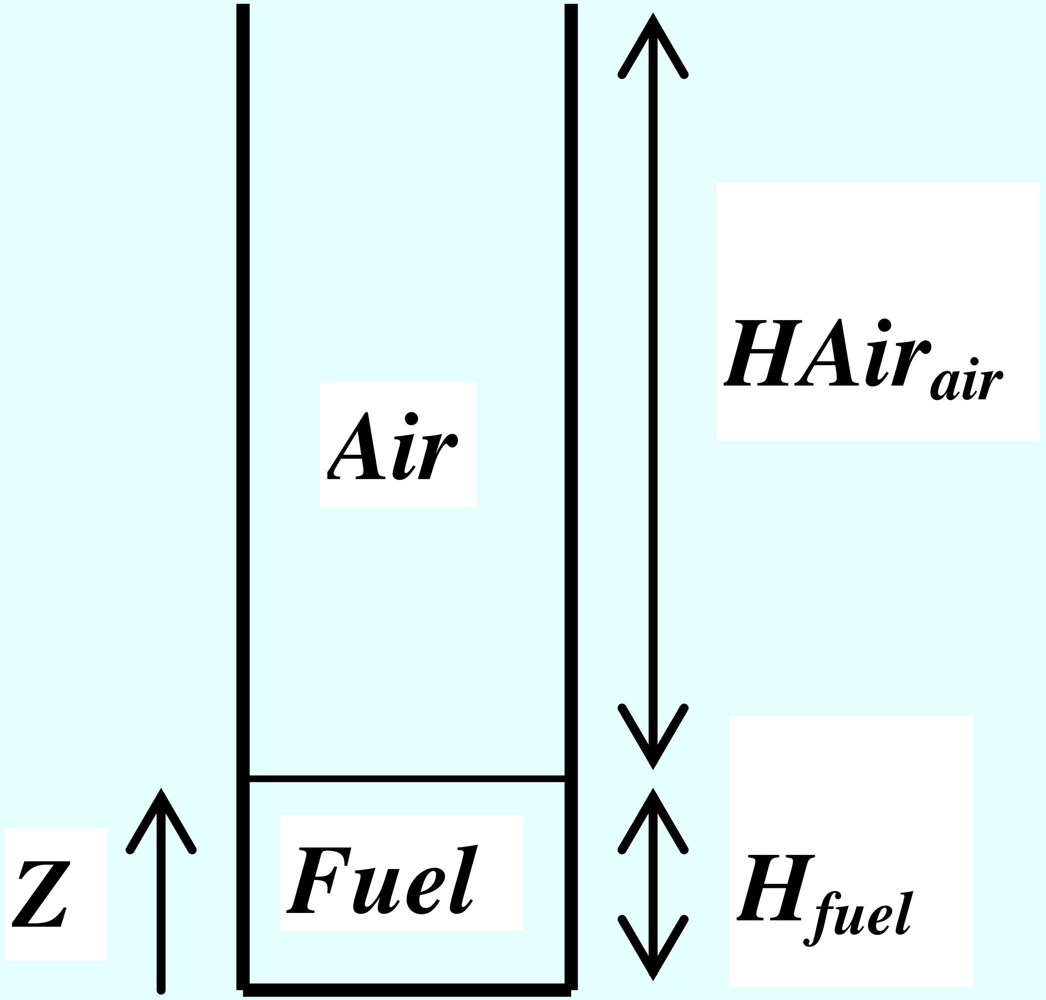
-Where should sensors be placed to detect a fuel release as early as possible?

-What is the rate and pattern of gas discharge into the atmosphere

-How does this dispersion depend on the type of fuel being released, initial conditions and geometry and size of vessel

The Model

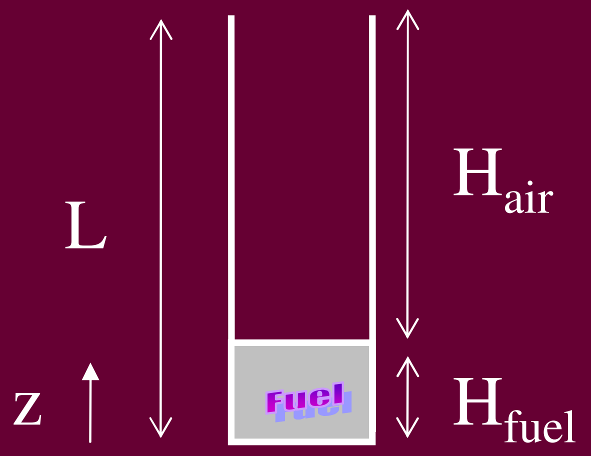
Finite mass of fuel released into air at a negligible pressure difference within a vertical cylinder to establish the temporal and spatial formation and dissipation of flammable zones



Formulation of the problem

Specific Description

(note that a fixed fuel mass released at t=0 at a zero pressure difference)



The cylinder is considered initially to be of two regions

-lower region : mixture of fuels

-upper region : overlaying gas (air, CO2, N2 …),

- outside open stagnant atmosphere of air

The fuels disperse upwards and air downwards. The flow field is set up due mainly to diffusion and bouyancy effects

Task :Determine the flow, concentration and temperature fields and then establish the flammable mixture boundaries and zones.

Approach

- Earlier work examined many features of this situation experimentally with flammable zones detected via a movable intermittent spark. Also the case of liquid fuels was also investigated

- The current predictive treatment extends the calculation domain beyond the physical limits of the vessel.

- Geometry: Axis-symmetric- 2D, (being extended to 3D)

Governing equations:

Equations of continuity, momentum, energy and species conservation when neglecting the viscous dissipation within the gas and any work, solution in in dimensionless form but results displayed here are for specific size and geometry.

The thermodynamic and transport properties as well as flammability limits are taken to change continuously all over the domain of the calculation according to the transient local values of concentration and temperature.

Some Assumptions :

- no chemical reactions.
- gaseous mixture considered as a perfect gas.
- laminar flow
- Boussinesq approximation is applicable.

Physical properties :

The thermodynamic and transport properties are changing instantaneously depending mainly on the local conditions of concentration and temperature.

Conservation equations (2D)

- **Continuity equation**

$$\frac{\partial \bar{\rho}}{\partial \bar{t}}+\frac{1}{\bar{r}}\frac{\partial}{\partial \bar{r}}\left(\bar{\rho}\,\bar{r}\,\bar{\mathrm{v}}_r\right)+\frac{\partial}{\partial \bar{z}}\left(\bar{\rho}\,\bar{\mathrm{v}}_z\right)=0$$

- **Species conservation**

$$\frac{\partial}{\partial \bar{t}}\left(\bar{\rho}\bar{\omega}_i\right)+\frac{1}{\bar{r}}\frac{\partial}{\partial \bar{r}}\left(\bar{\rho}\bar{r}\bar{\mathrm{v}}_r\bar{\omega}_i\right)+\frac{\partial}{\partial \bar{z}}\left(\bar{\rho}\bar{\mathrm{v}}_z\bar{\omega}_i\right)=\frac{1}{\bar{r}}\frac{\partial}{\partial \bar{r}}\left(\frac{\bar{\rho}\bar{D}_i}{R_e Sc_i}\bar{r}\frac{\partial \bar{\omega}_i}{\partial \bar{r}}\right)+\frac{\partial}{\partial \bar{z}}\left(\frac{\bar{\rho}\bar{D}_i}{R_e Sc}\frac{\partial \bar{\omega}_i}{\partial \bar{z}}\right)$$

- **r-momentum equation**

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

- **z-momentum equation**

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

Conservation equations (cont'd.)

- **Energy equation**

$$\bar{c}_p\left[\frac{\partial}{\partial \bar{t}}\left(\overline{\bar{\rho}\bar{T}}\right)+\frac{1}{\bar{r}}\frac{\partial}{\partial \bar{r}}\left(\overline{\bar{\rho}\bar{r}\bar{\mathrm{v}}_r\bar{T}}\right)+\frac{\partial}{\partial \bar{z}}\left(\overline{\bar{\rho}\bar{\mathrm{v}}_z\bar{T}}\right)\right]=\frac{1}{\bar{r}}\frac{\partial}{\partial \bar{r}}\left(\frac{\bar{k}}{R_eP_r}\bar{r}\frac{\partial \bar{T}}{\partial \bar{r}}\right)+\frac{\partial}{\partial \bar{z}}\left(\frac{\bar{k}}{R_eP_r}\frac{\partial \bar{T}}{\partial \bar{z}}\right)$$

where the dimensionless group numbers are defined as it follows :

$$R_e=\frac{\rho_0 U_{ref} H_{fuel}}{\mu_0} \qquad P_r=\frac{\nu_0}{\alpha_0}=\frac{\mu_0 c_{p,0}}{k_0} \qquad Sc=\frac{\nu_0}{D_{i,0}}$$

$$Gr_T=\frac{g\left(T_{ref}-T_\infty\right)H_{fuel}^3}{T_\infty \nu_0^2} \qquad Gr_{\omega 1}=\frac{M_2\left(M_1-M_3\right)}{\delta}\frac{g\left(\omega_{1,0}-\omega_{1,\infty}\right)H_{fuel}^3}{\nu_0^2}$$

$$Gr_{\omega 2}=\frac{M_1\left(M_2-M_3\right)}{\delta}\frac{g\left(\omega_{2,0}-\omega_{2,\infty}\right)H_{fuel}^3}{\nu_0^2}$$

❖ Initial conditions :

$$\begin{cases} \bar{z} \le 0 \ : & \bar{\omega}_i = 1, \quad \bar{\mathrm{v}}_r = 0, \quad \bar{\mathrm{v}}_z = 0, \quad \bar{\mathrm{T}} = \bar{T}_{amb} \\ \bar{z} > 0 \ : & \bar{\omega}_i = 0, \quad \bar{\mathrm{v}}_r = 0, \quad \bar{\mathrm{v}}_z = 0, \quad \bar{\mathrm{T}} = \bar{T}_{amb} \end{cases}$$

❖ Boundary conditions :

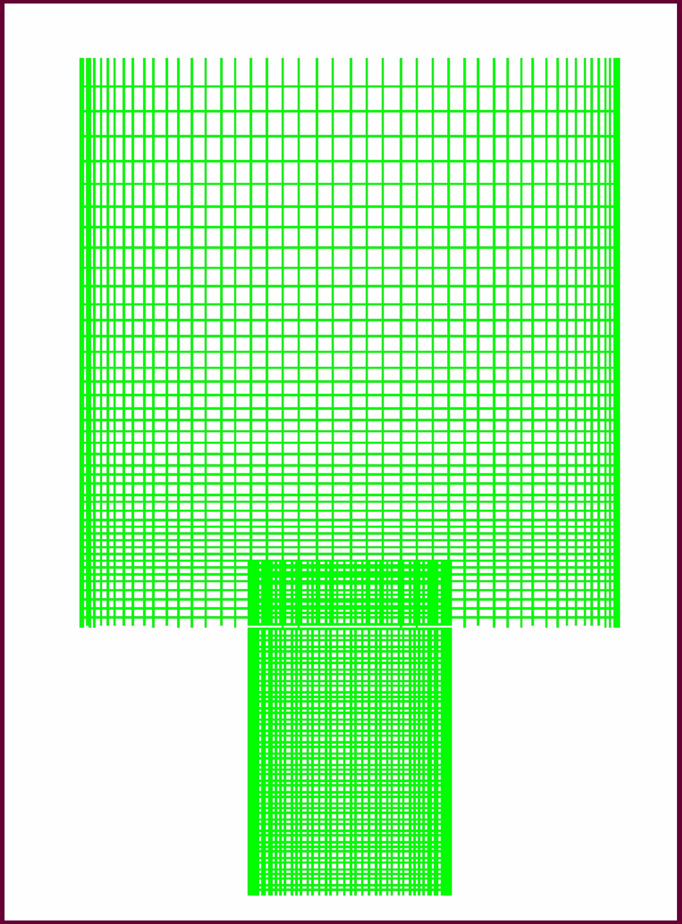
$$\begin{cases} \bar{z} = 0 \ : & \dfrac{\partial \bar{\omega}_i}{\partial \bar{z}} = 0, \quad \bar{\mathrm{v}}_r = 0, \quad \bar{\mathrm{v}}_z = 0, \quad \bar{\mathrm{T}} = \bar{T}_{bot} \\ \bar{z} = \bar{L} \ : & \dfrac{\partial \bar{\omega}_i}{\partial \bar{z}} = 0, \quad \dfrac{\partial \bar{\mathrm{v}}_r}{\partial \bar{z}} = 0, \quad \dfrac{\partial \bar{\mathrm{v}}_z}{\partial \bar{z}} = 0, \quad \dfrac{\partial \bar{T}}{\partial \bar{z}} = 0 \end{cases}$$

$$\begin{cases} \bar{r} = 0 \ : & \dfrac{\partial \bar{\omega}_i}{\partial \bar{r}} = 0, \quad \bar{\mathrm{v}}_r = 0, \quad \dfrac{\partial \bar{\mathrm{v}}_z}{\partial \bar{r}} = 0, \quad \dfrac{\partial \bar{T}}{\partial \bar{r}} = 0 \\ \bar{r} = \bar{R} \ : & \dfrac{\partial \bar{\omega}_i}{\partial \bar{r}} = 0, \quad \bar{\mathrm{v}}_r = 0, \quad \bar{\mathrm{v}}_z = 0, \quad \bar{T} = \bar{T}_{amb} \end{cases}$$

Solution of the governing equations

- Staggered non-uniform control volumes
- QUICK scheme for advection terms with flux limiter ULTRA-SHARP
- SIMPLEC algorithm
- SIP (Strongly Implicit Procedure) to solve the systems of algebraic equations

The Grid Used in the Numerical Solution



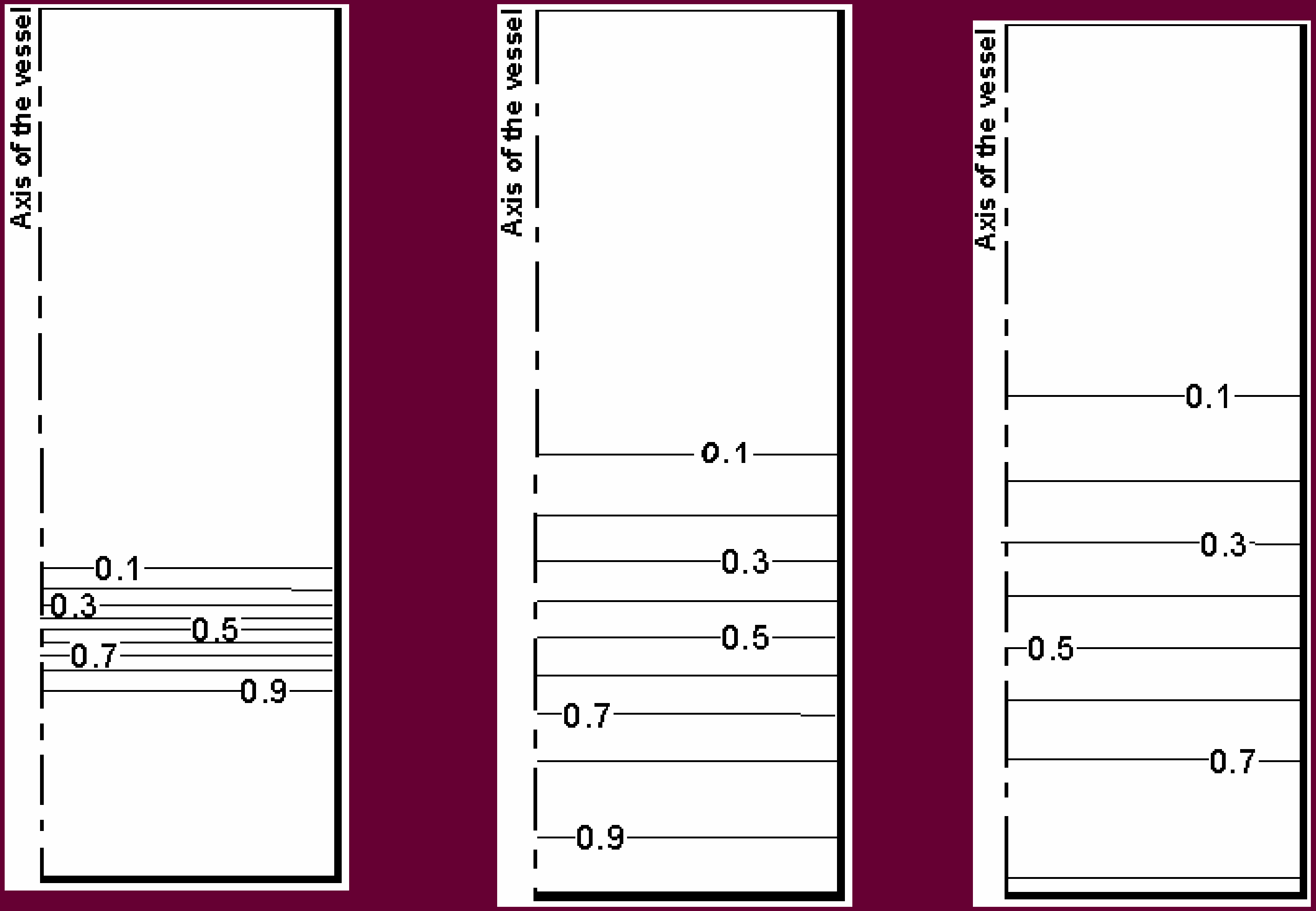
RESULTS & DISCUSSION

The transport processes present are:

- Diffusion-driven processes $\left(\rho_{fuel} > \rho_{atm}\right)$
- Advection-driven processes $\left(\rho_{fuel} < \rho_{atm}\right)$
- Diffusion + Advection of similar importance

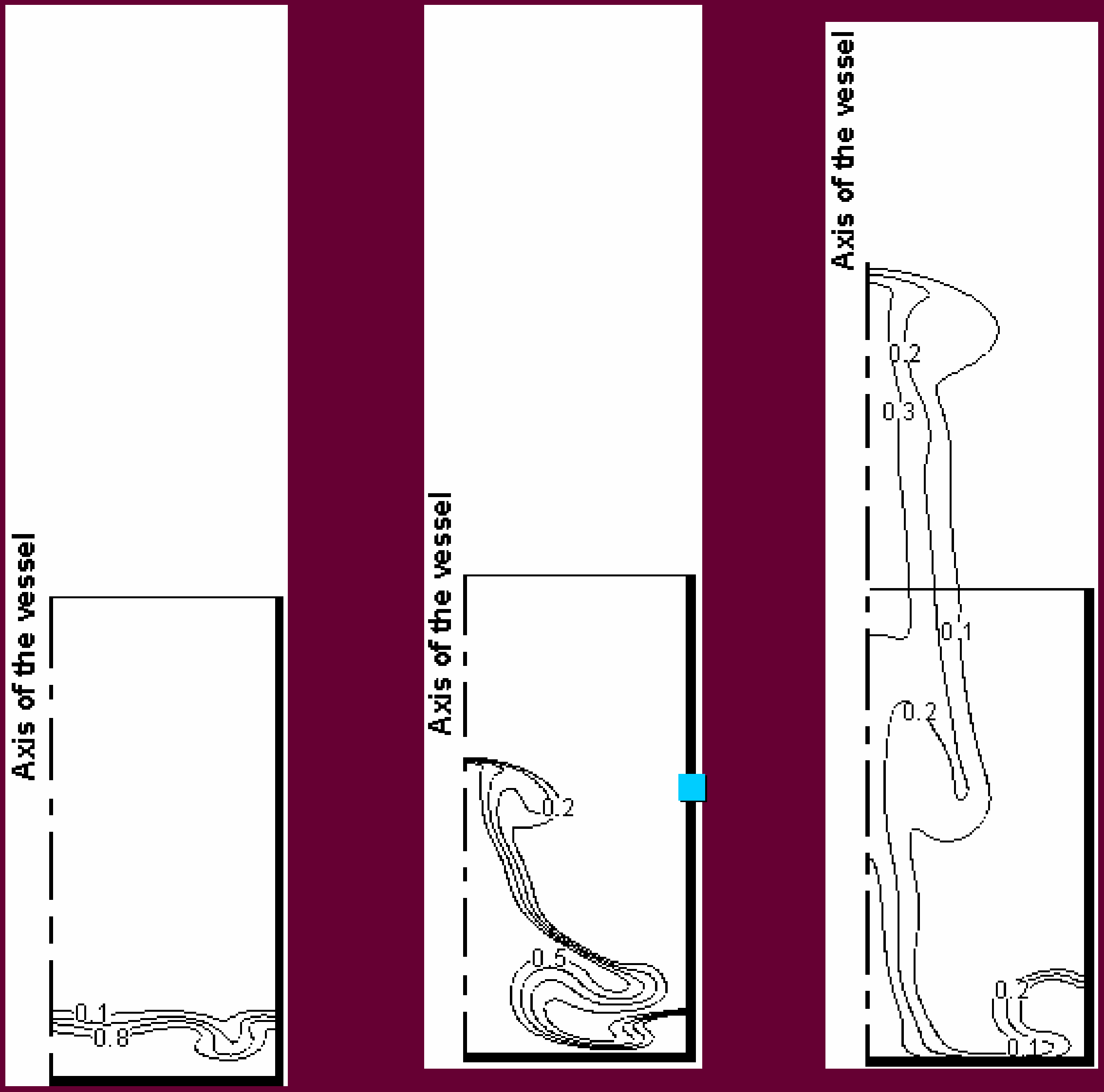
$$\left(\rho_{fuel} \approx \rho_{atm}\right)$$

Heavier than air gases - molecular diffusion driven processes



Molecular diffusion driven processes-Distribution of propane within the vessel of 3 cm diameter, 8cm length, 2 cm initial fuel at time=0.25, 1.25, 4.25

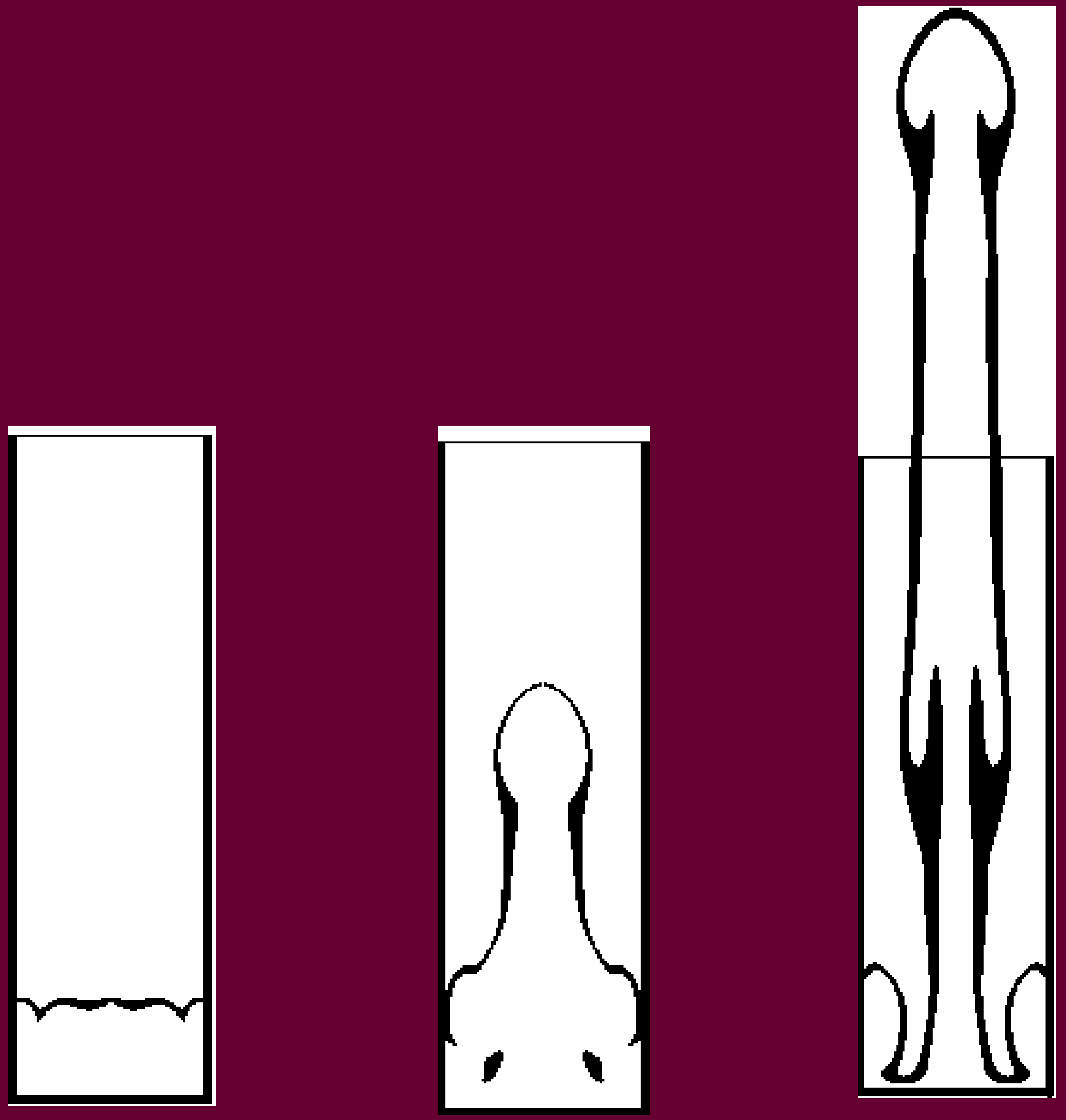
lighter than air gases - a buoyancy driven processes



Buoyancy driven processes, molar fraction distribution of methane within the vessel of 6cm diameter, 20cm length, 2cm initial fuel at time=0.5, 1.0, 1.5

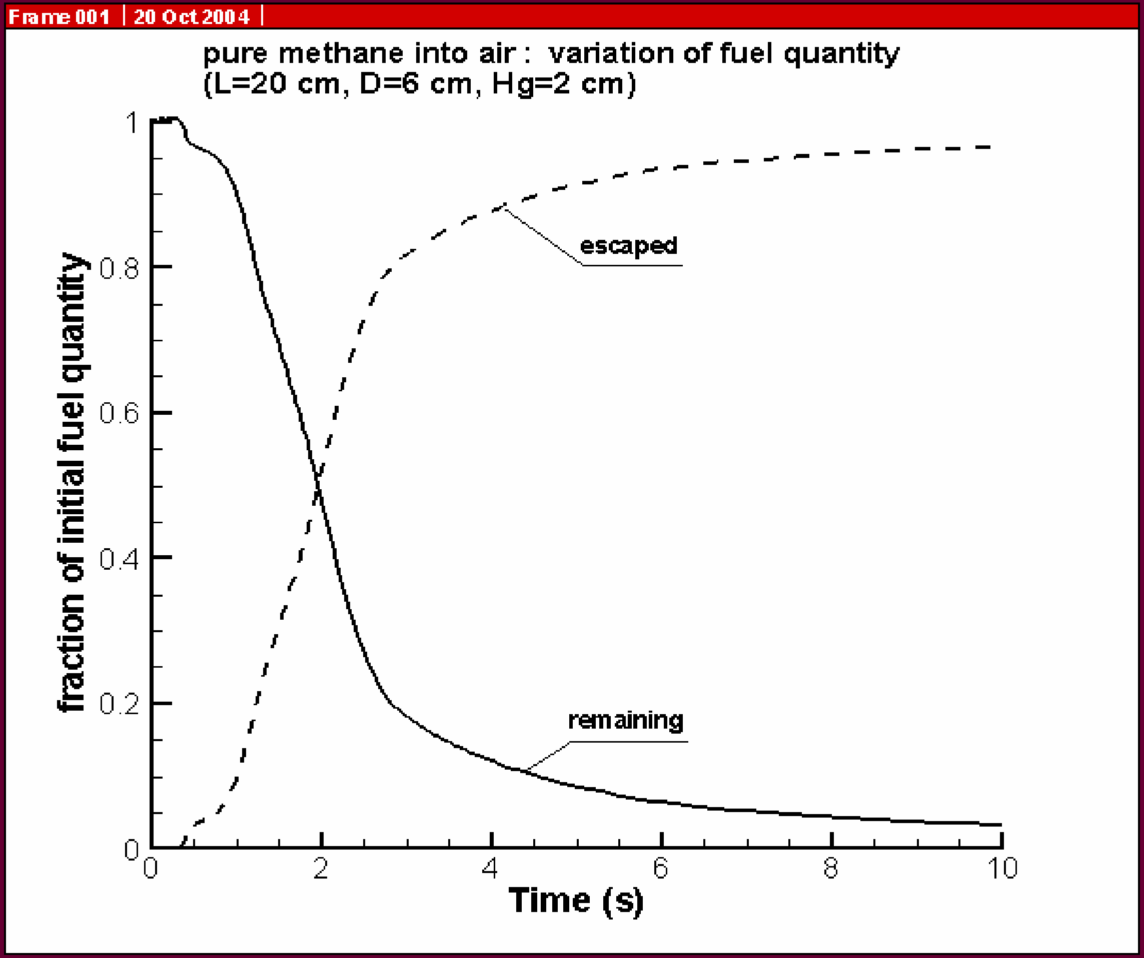
Flammable zones evolution

Methane released into air

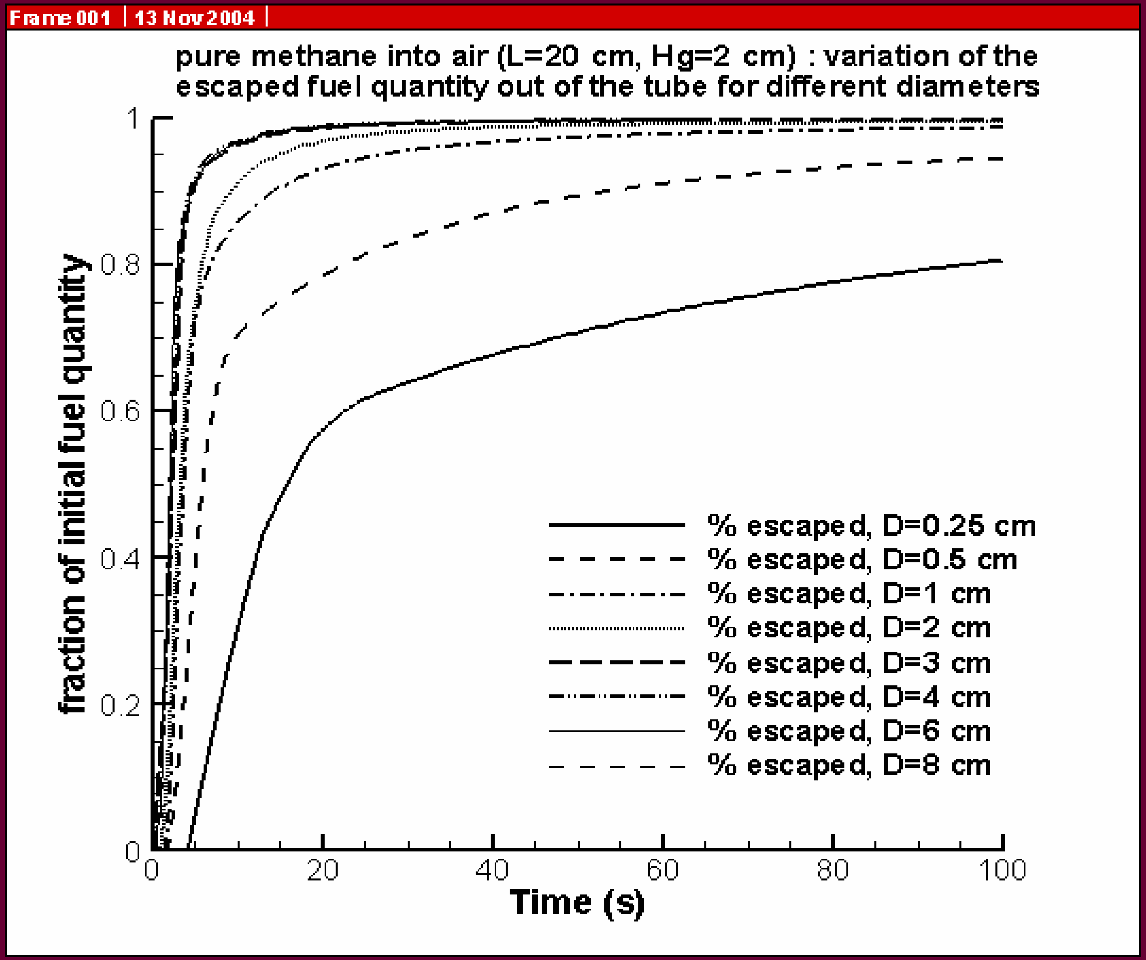


Temporal variation of the methane fraction escaping into the atmosphere and that remaining in the vessel,

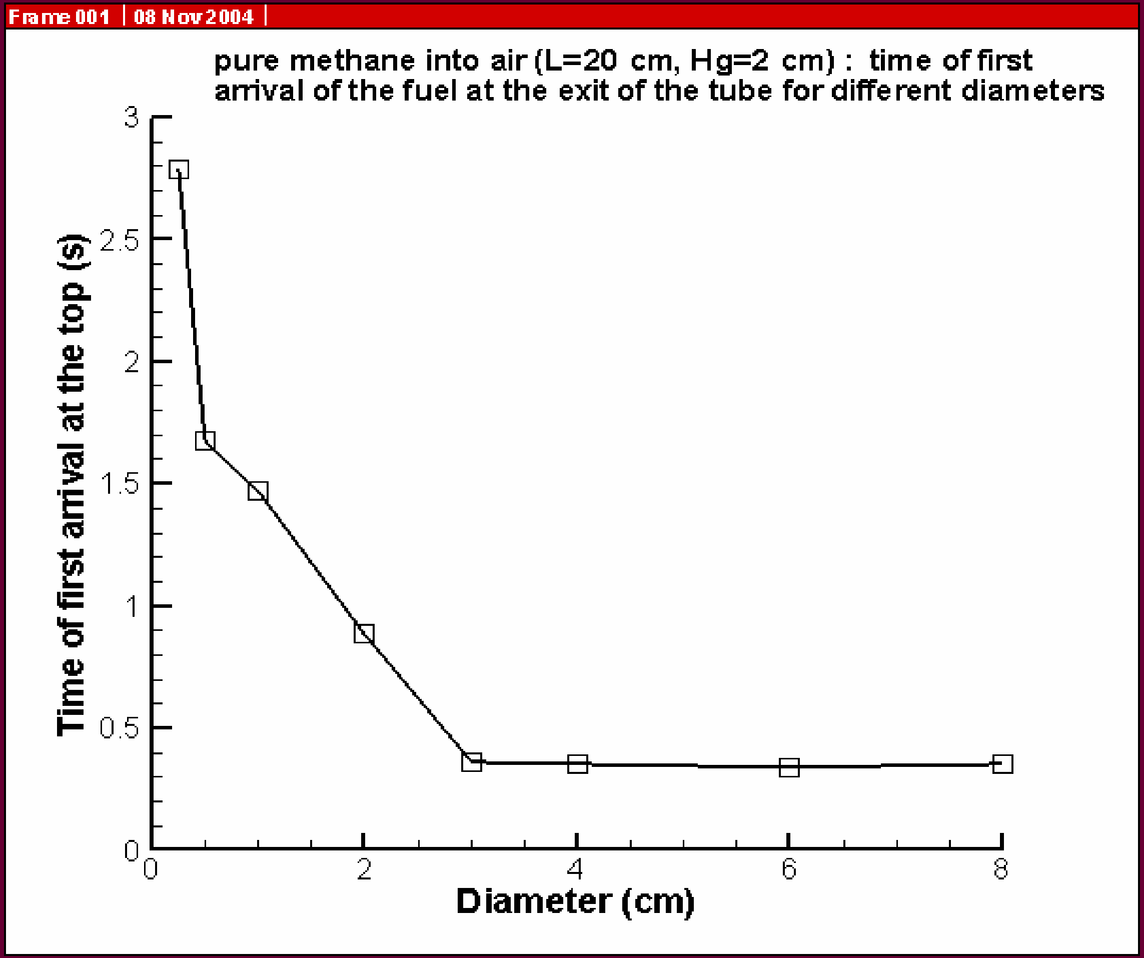
methane diffusing upward into air.



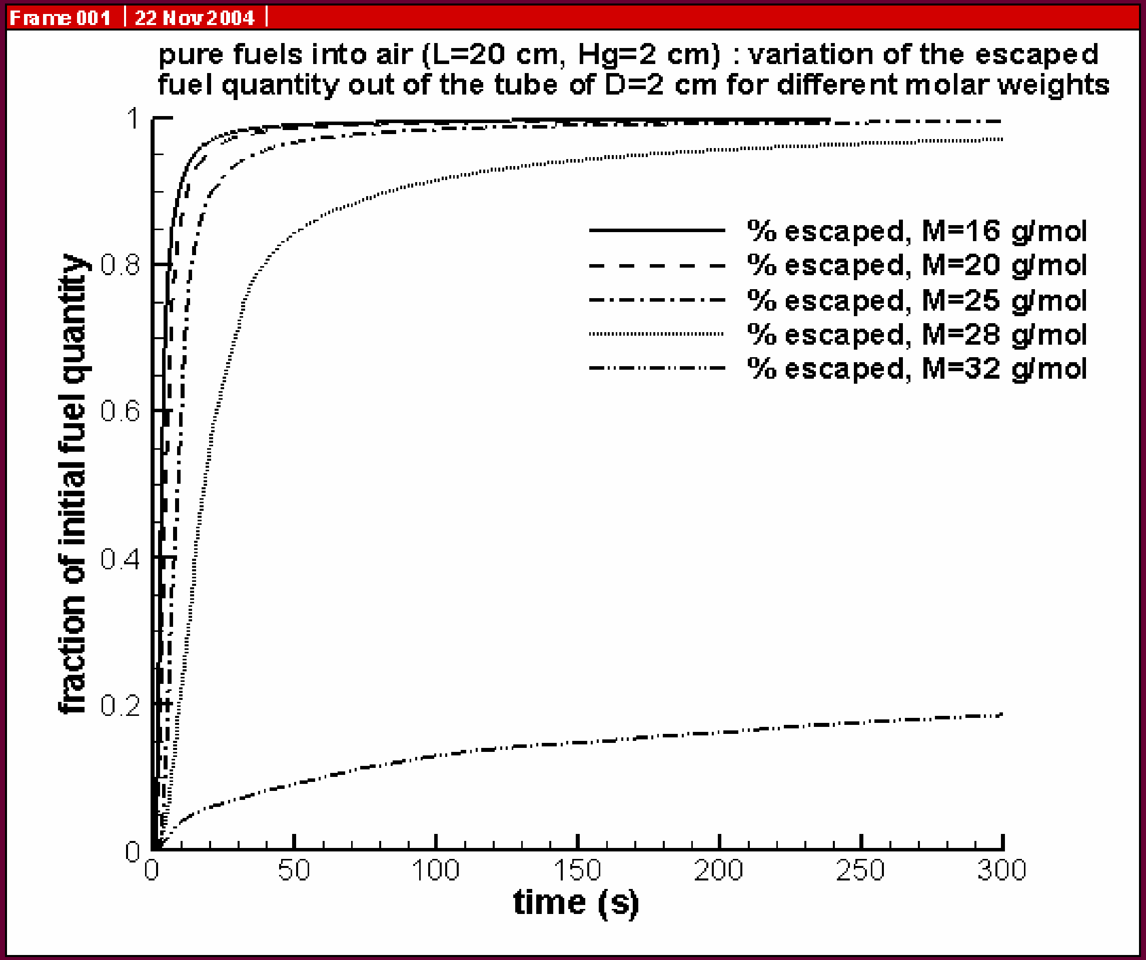
Variation of the fraction of methane escaping with time for different diameter cylinders.



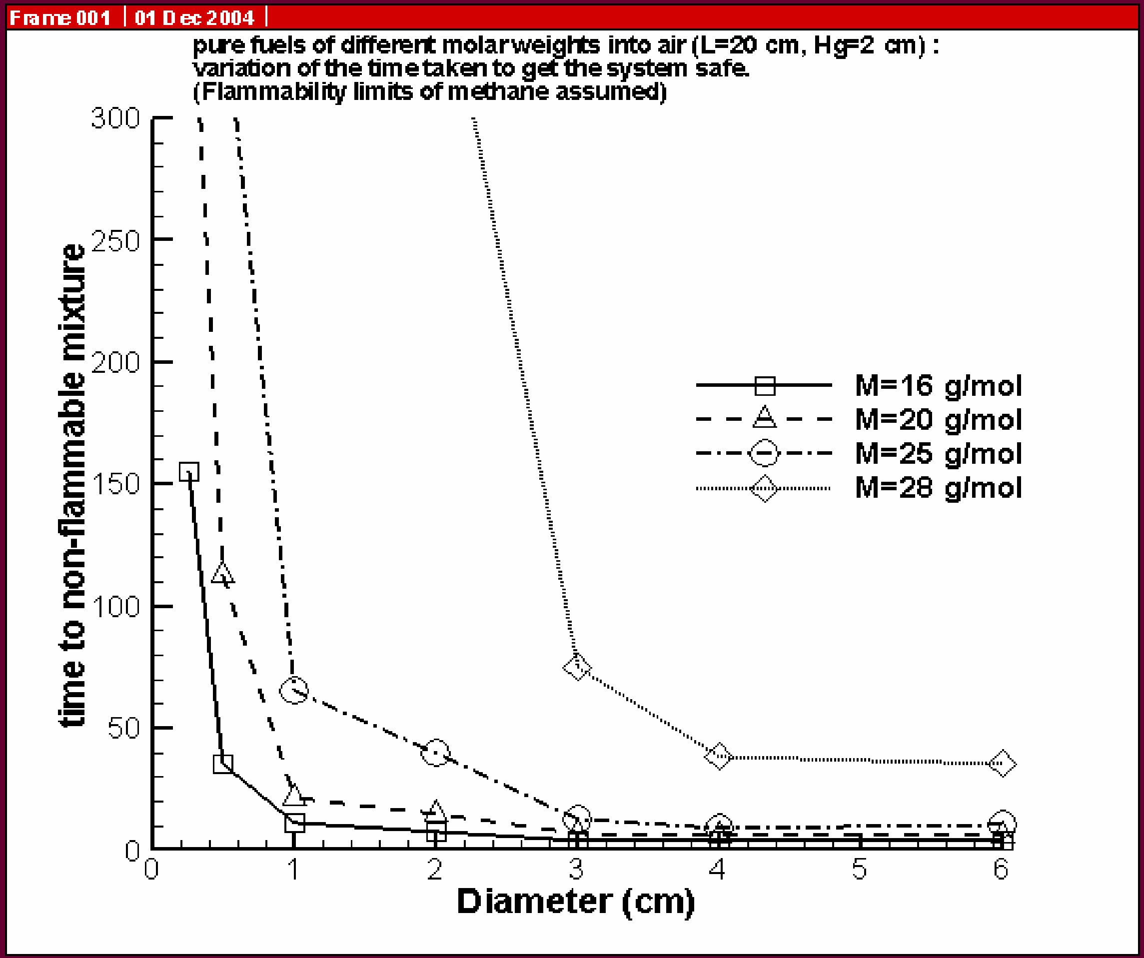
Variation in the time taken for the first arrival of fuel outside the vessel with the diameter of the vessel, methane into air



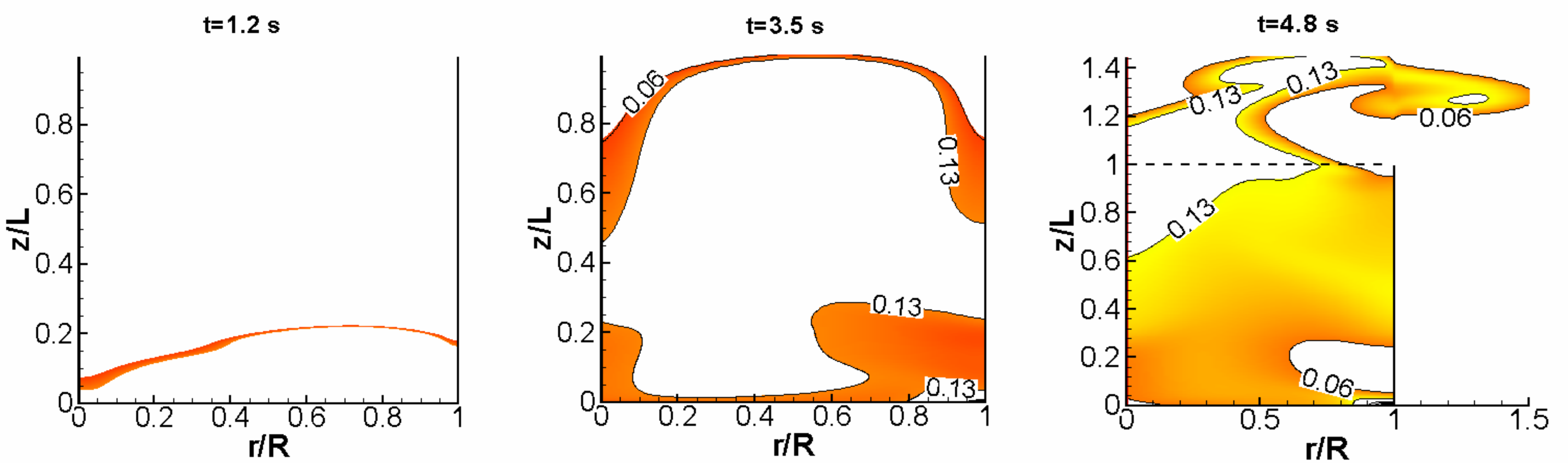
The corresponding variation of the fuel fractional mass escaping with time for various fuels of different molecular weights



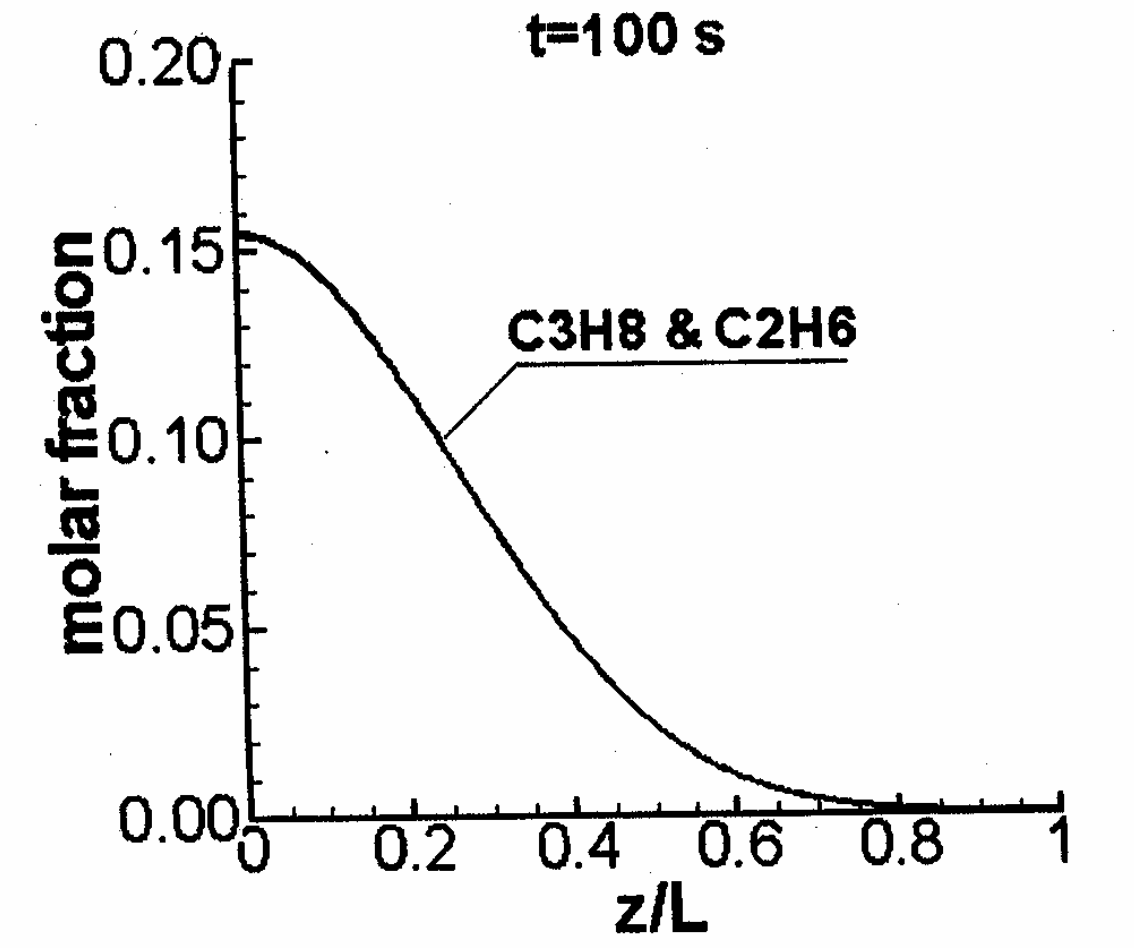
Time needed to render the contents non-flammable as a function of the cylinder diameter for various fuels with different molecular weights



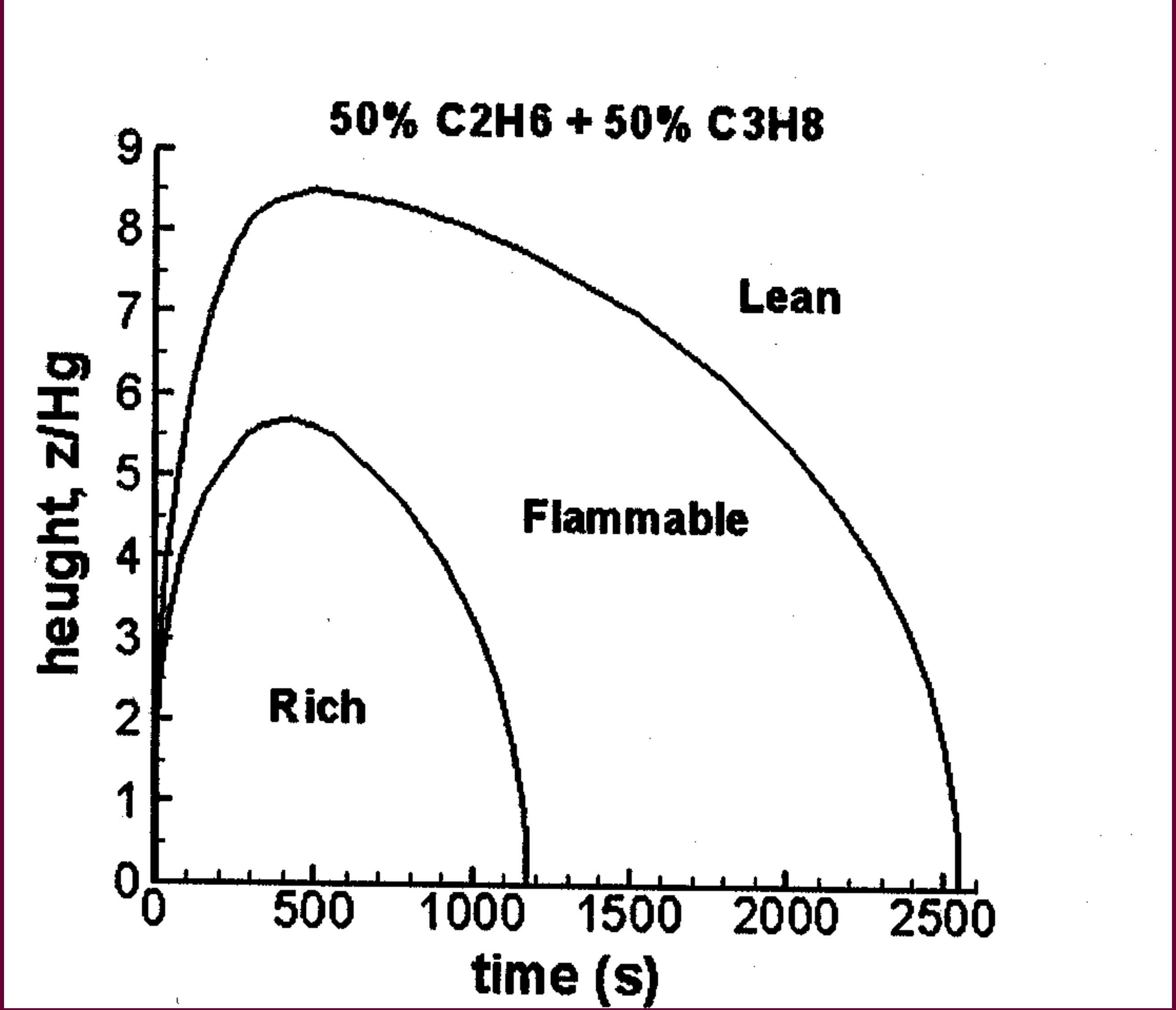
Flammable zones formation and spread following the dispersion of methane into air



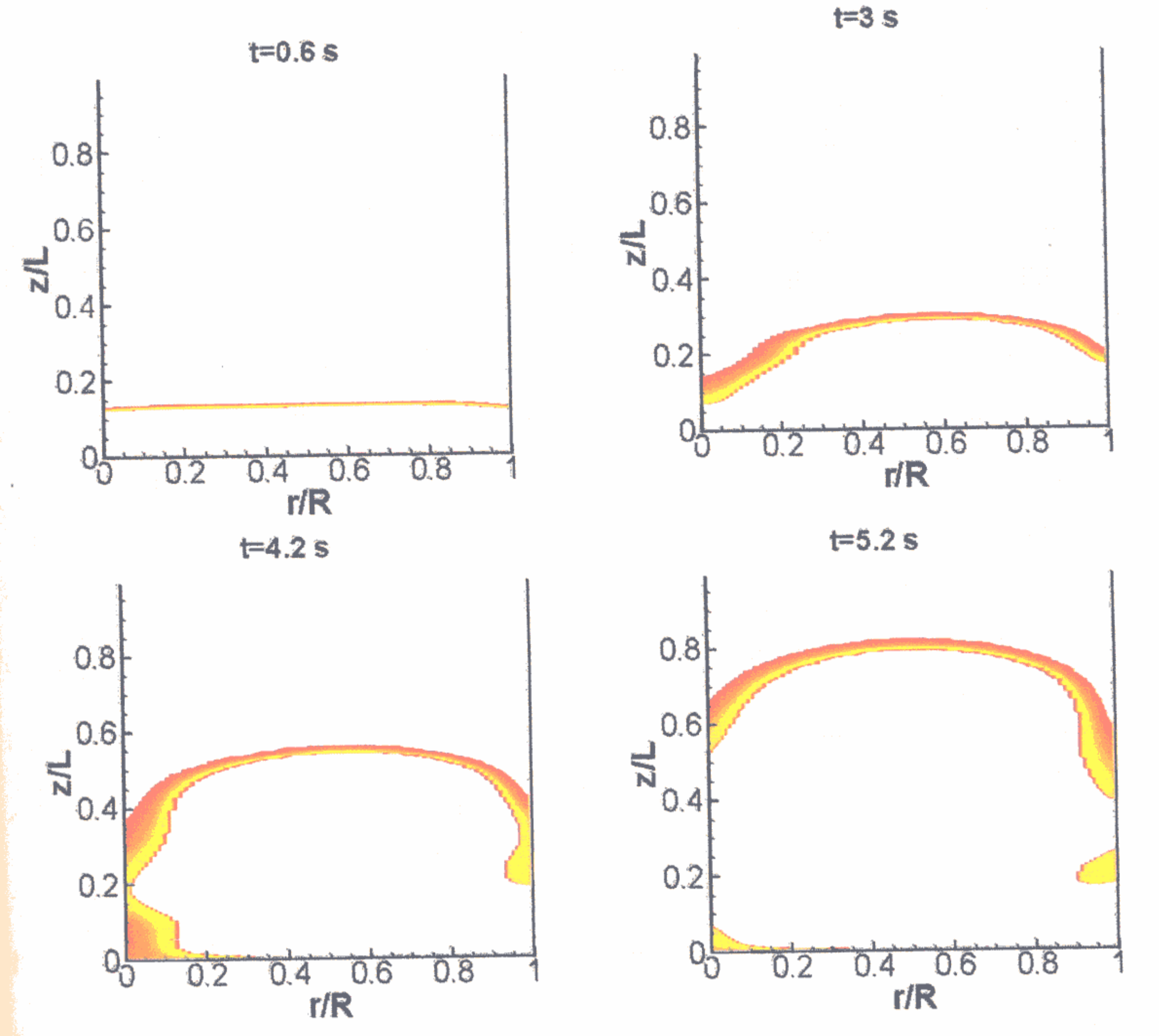
The molar fraction variation along the height of the vessel after 100s following the dispersion of a homogeneous mixture of ethane and propane , (heavier than air), at ambient temperature and pressure



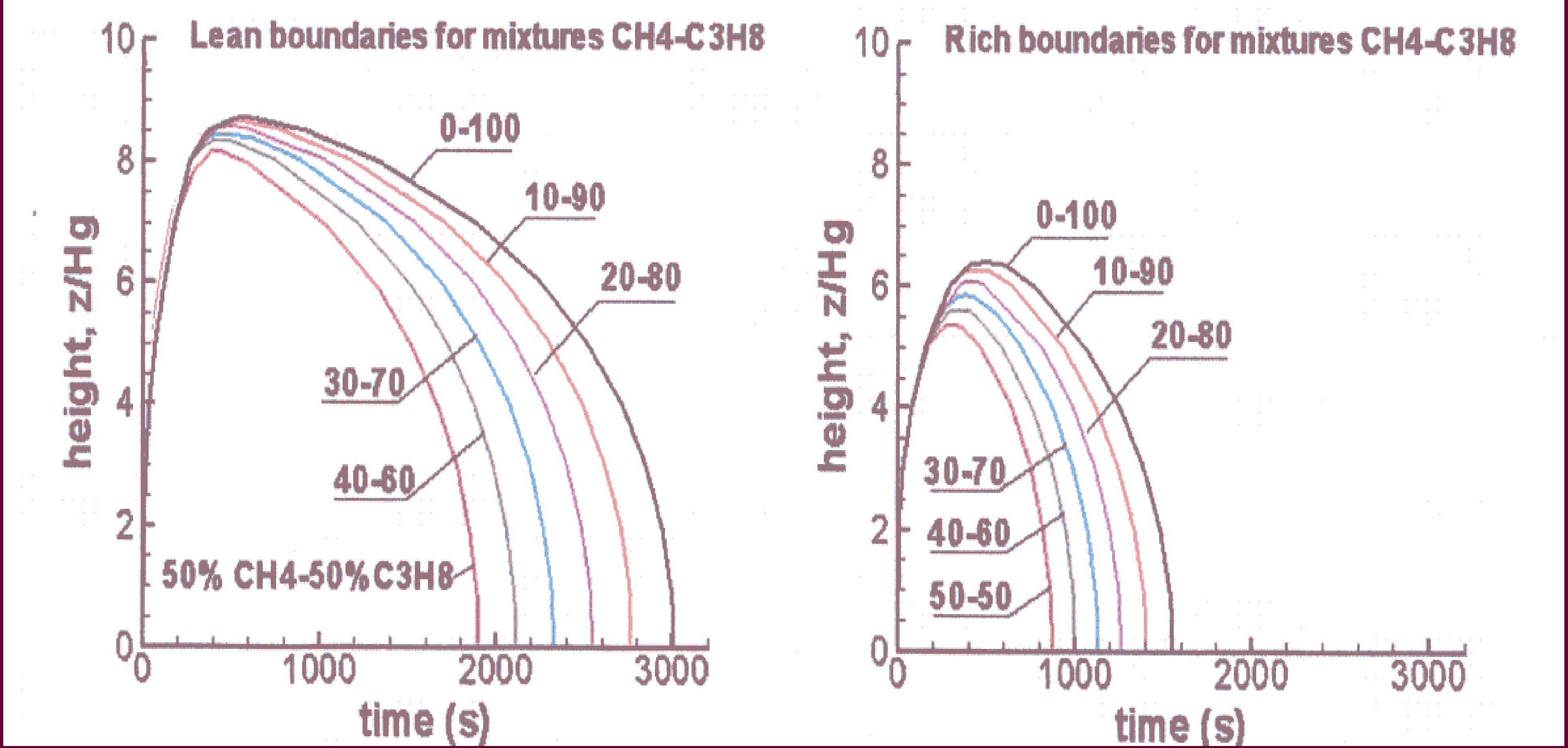
Variation of the lean and rich limits boundaries along the vessel with time following the release of a mixture of ethane and propane into air



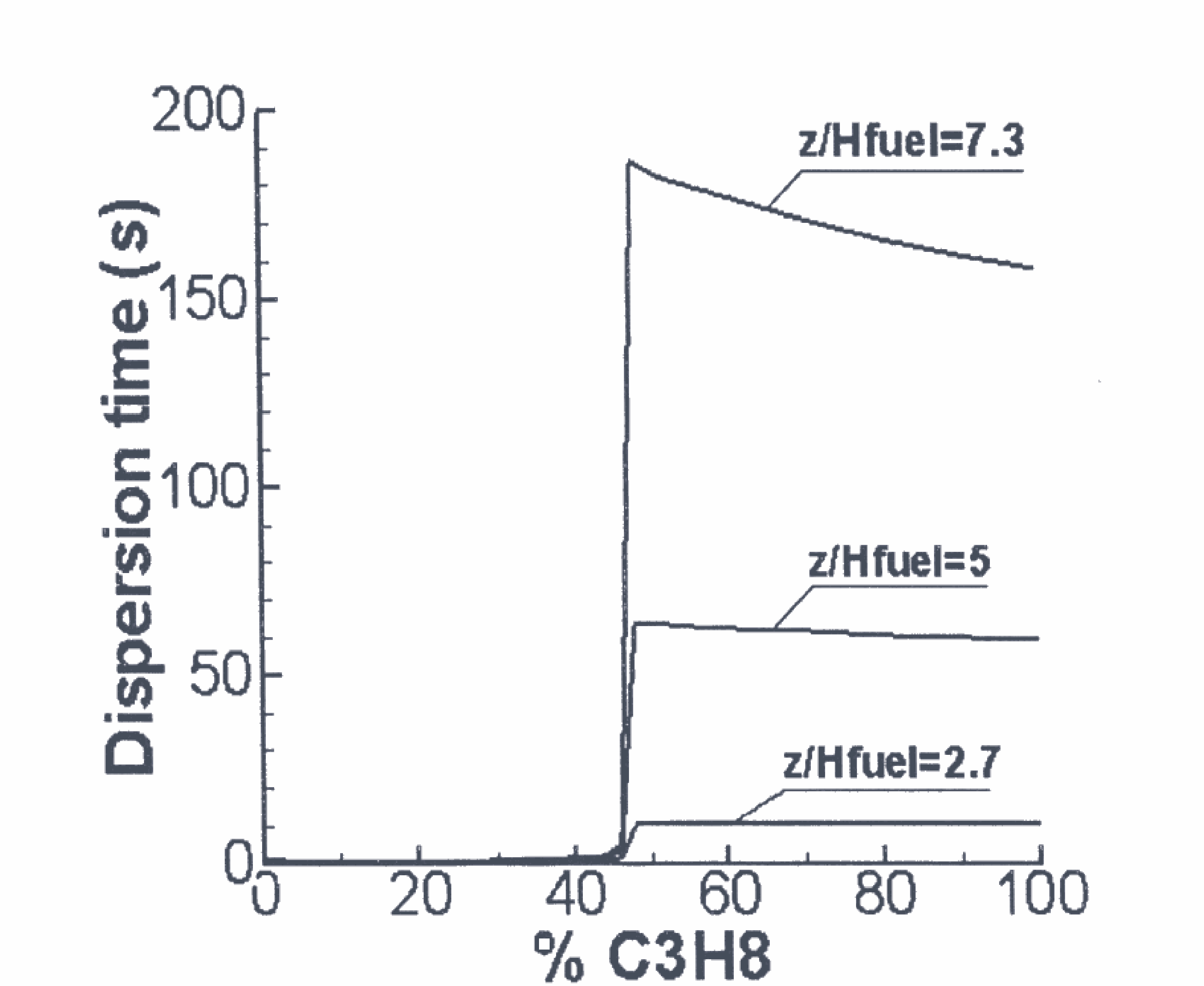
Location of flammable zones at different times following the release of a fuel mixture of 50% methane and 50% ethylene, (lighter than air) by volume into air



Variation in the locations of the lean and rich limit boundaries of the flammable zones for various heavier than air mixtures of propane and methane dispersing upwards into air, (numbers refer to percentages of methane and propane)



The minimum time to form a flammable mixture at different locations along the vessel with changes in the concentration of propane in mixtures with methane



Conclusion

- The release with a negligible pressure difference of a fixed mass of heavier than air fuel into overlaying air within vertical cylindrical vessel is diffusion controlled producing slow fuel dispersion.
- The flammable zones formed are regular in shape and their eventual decay in the overlaying air takes much time
- The corresponding dispersion of lighter than air fuels is buoyancy controlled and in comparison is extremely rapid.
- The flammable zones formed tend to be less regular, changing in shape and would not linger long.
- Stratification of the fuel produces less flammable volumes than the corresponding homogeneous case.

Conclusion

- The exposure of a binary fuel mixture of a heavier and lighter than air components to the overlying air within an open cylindrical vessel displays significantly different behavior depending on the type of the two fuels and their initial concentrations.

- When the composition of the initial fuel mixture is such that its homogeneous density is greater than air the dispersion processes and the associated formation and dissipation of flammable mixtures formed are very slow and molecular diffusion driven despite the presence of the very buoyant component gas.

Conclusion

- Likewise, for fuel mixtures of composition such that the homogeneous density is lighter than air the resulting processes are very fast and buoyancy driven despite the presence of a much heavier than air fuel component.

- With fuels having significantly different flammability limits values, such as methane and propane the longest time observed for the first formation of a flammable mixture at any specific location within the vessel is associated with fuel mixtures having density heavier than air but not with the heavy fuel component.

Acknowledgements

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