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Analysis of Variation of Thermodynamic and Transport Properties in Flames

Local thermodynamic and transport properties like constant pressure specific heat (c_p), viscosity (μ) thermal conductivity (k). Binary and Multicomponent diffusion coefficients and related quantities like Prandtl (P_r), Schmidt (Sc_{ij}) and Lewis (Le_{ij}) numbers have been calculated for premixed and diffusion flames. The analysis using the properties of mixtures along with the existing experimental results on temperature and concentrations leads to some interesting results like (a) c_p always varies by large amounts. the variation being due to the dual effects of temperature and composition in the case of diffusion flames and due only to the effect of temperature in the case of lean, stoichiometric and near-stoichiometric premixed flames, (b) the quantity $\rho\mu$ (density x viscosity) appears not to vary very much in the case of diffusion flames established in boundary layers and (c) Lewis numbers between species of widely differing molecular weights could be different from 1 by as much as 10-12

Further, some of the conventional assumptions used in analytical studies have been critically reviewed in the light of the various findings of the present work.

Introduction

Realistic analysis of chemically reacting flows involving large enthalpy changes (and so large temperature variations) needs the solution of a large number of coupled set of nonlinear partial differential equations. Reasonably good simplifications using the concepts of similarity will reduce the problem to the solution of nonlinear ordinary differential equations. A number of simplifying assumptions are made on the thermodynamic and transport properties either while converting the partial differential equations to ordinary differential equations or in the solution of the system of ordinary differential equations itself. Obviously one needs to know as to how these approximation influence the resulting solutions. In fact, to be better knowledgeable, it is advantageous to explicitly obtain the effect of each of the approximations separately or in suitable groups.

In order to tackle this situation various methods are possible: (a) The overall characteristics (like Temperature profile etc.) are checked against experimental results obtained

Nomenclature

c_p	Constant pressure specific heat (cal/gm. °K)
D'_{ij}	Binary diffusion coefficient between species i and j (cm²/sec)
D_{ij}	Multi component diffusion coefficient between species i and j for species i diffusing in species j (cm²/sec)
H	Planck's constant
k'	Monatomic thermal conductivity (cal/cm. sec. °K)
k"	Internal thermal conductivity (cal/cm. sec. °K)
k	Total thermal conductivity (cal/cm. sec. °K)
L'_{eij}	Lewis number (based on D'_{ij})
L_{eij}	Lewis number (based on D_{ij})
M	Molecular weight
p	Pressure (atms.)
Pr	Prandtl number $= \mu c_p/k$
R	Universal gas constant (1.987cal/gm-mole.°K)
Sc_{ij}	Schmidt number $\mu/D'_{ij}\rho$ (or $= \mu/D_{ij}\rho$)
T_r	Reduced temperature
T	Temperature (°K)
X_i	Mole fraction of ith species
ρ	Density (gm/cm³)
μ	Viscosity (gm/cm. sec.)
ϕ_{ii}, ψ_{ii}	Functions defined by equations (8, 9 and 11)
$\Omega_{11}(T_r)$ $\Omega_{22}(T_r)$	Collision integrals as a function of reduced temperature
ε_{11}	Reduced characteristic energy of interaction.

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under similar circumstances. (b) Having made an assumption on any property variation (say, c_p = constant), the assumption is checked strictly with in the frame work of the theory by calculating back the variation of the property from the resulting solutions (like using concentrations and temperature for obtaining c_p). It must be noted that such a procedure is not always feasible. For instance, the assumption Lewis number = 1, cannot, at any rate be invalidated by the solutions obtained by using Lewis number = 1, without invoking basic information on kinetic theory. It is, therefore, necessary to take care while using this method to check the accuracies of the solution. (c) The detailed property variations are obtained from basic and standard results of kinetic theory, quantum statistical mechanics and spectroscopy on quantities like collision cross sections, potential energies, specific heats and the experimentally measured values of temperature and concentrations. These are then examined to obtain support for existing approximations or to suggest modifications.

A large number of investigations use the method (a) for the test of the theories. A smaller number of investigations use the method (b) though not explicitly always. Instead, order of magnitude analyses are performed to find out whether certain approximations are valid in the range considered. A relatively small number of investigations use the procedure (c). And the point of view taken in the material to follow is that discussed in (c). There have been a few investigations reported in the literature along these lines.

Fristrom et al [3]* reported detailed measurements of temperature and concentrations in one dimensional methane-air premixed flame and Westenberg and Fristrom [4] made the analysis of this flame for mass and energy conservation. They [4] obtained using conventional formula (see Ref. 5), the diffusional velocities and mass fluxes. The interesting revelation was that diffusional velocities in some regions of flow were as large as the mean flow velocity, so much so, diffusion plays an important role in the structure of the flame. They further calculated the heat release rate distribution through the flame. The various terms in the energy equation, namely, conduction, convection and diffusion were also calculated in an attempt to check the energy balance. It must be noted that they used for the value of thermal conductivity, that of oxygen throughout the flame. The imbalance in the energy equation which they obtained was traced to the arbitrariness of the value of thermal conductivity, particularly to its underestimation.

Structural analysis of stagnation point diffusion flames of methane-air combination was performed by Tauji and Yamaoka [2]. They made an analysis of heat release rates through the flame. The analysis showed the presence of a region where pyrolisis type of reactions took place on the fuel side. There are few other investigations on the structural analysis of one dimensional flames [see, Ref. 7, p. 306]. However, these are oriented essentially towards the determination of kinetic mechanism and are not relevant here.

Though several investigators have used the actual properties in the analysis of flows [see for instance, Refs. 8, 9], the authors know of no study where an explicit analysis of flows has been made for thermodynamic and transport properties. This study, therefore, considers three flows namely, Propane-Air diffusion flame, Methane-Air diffusion flame and Mathane-Oxygen one dimensional premixed flame.

Equations

The properties of the mixture that we compute are, the molecular weight (M), constant pressure specific heat (c_p), density (ρ), viscosity (μ), thermal conductivity (k), Binary diffusion coefficients (D'_{ij}) and Multi component diffusion coefficients (D_{ij}). Other properties derived from these basic data are, Prandtl number (Pr) = $\mu c_p/k$, Schmidt number (Sc_{ij}) = $\mu/D_{ij}\rho$, Lewis number (Le_{ij}) = $D_{ij}\rho c_p/k$, $\rho\mu$, k/c_p, k/T and μ/T. The above properties are obtained by using the well establised relations [see Refs. 5, 6],

$$M = \sum X_i M_i \tag{1}$$

$$c_p = \sum X_i (c_{pi}/M_i) \tag{2}$$

$$\rho = pM/RT \tag{3}$$

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*Numbers in square brackets denote references at the end of paper.

$$\mu_i = 2{\cdot}6693 \times 10^{-5}\ (M_i T)/(\sigma_i^2\, \Omega_{22}\, (T_{r,\, ij}) \quad (4)$$

$$k_i' = 15R\, \mu_i/4M_i \quad (5)$$

$$k_i'' = 0.88\, k_i'(2\, c_p/5R - 1) \quad (6)$$

$$\mu = \sum_i - \mu_i(1 + \sum_{j,\, j \neq i} \phi_{ij}\, X_j/X_i)^{-1} \quad (7)$$

$$\phi_{ij} = \left[\ 1 + (\mu_i^2\, M_j\, /\, \mu_j^2\, M_i)^{0{\cdot}25}\right]^2 \times$$

$$\{2\sqrt{2}(1 + M_i/M_j)^{0{\cdot}5}\}^{-1} \quad (8)$$

$$\phi_{ji} = \phi_{ij}\, \mu_j\ M_i/\mu_i M_j \quad (9)$$

$$k' = \sum_i k_i'\ (1 + \sum_{j,\, J \neq 1} \Psi_{ij}\, X_j/X_i)^{-1} \quad (10)$$

$$\Psi_{ij} = \phi_{ij}[1 + 2.41\, (M_i - M_j)\, (M_i - 0{\cdot}142\, M_j)$$

$$(M_i + M_j)^{-2} \quad (11)$$

$$k''_{mix} = \sum_i k_i''\ (1 + \sum_{j,\, j \neq 1} \phi_{ij}\ X_j/X_i)^{-1} \quad (12)$$

$$k = k' + k'' \quad (13)$$

$$D'_{ij} = 2.628 \times 10^{-3}\, T^3\, (M_i + M_j)/(2M_i\, M_j)^{1/2} \times$$

$$\left\{p\, \sigma_{ij}^2\ \Omega_{11}\, (T_{r,\, ij})\right\}^{-1} \quad (14)$$

$$D_{ij} = \frac{M}{M_j}\, \frac{K^{ji} - K^{ii}}{K} \quad (15)$$

$$K_{ij} = \frac{X_i}{D'_{ij}} + \frac{M_i}{M_k} \sum \frac{X_k}{D'_{ik}},\ K_{ii} = 0 \quad (16)$$

K is the determinent of K_{ij} and K^{ji} are the minors,

$$K^{ji} = (-1)^{i+j} \begin{vmatrix} 0 & \cdots\ K_{1,i-1} & K_{1,i+1} & \cdots\ K_{1,n} \\ \vdots & & & \\ K_{j-1,1} \cdots & K_{j-1,i-1} & K_{j-1,i+1} \cdots & K_{j-1,n} \\ K_{j+1,1} \cdots & K_{j+1,i-1} & K_{j+1,i+1} \cdots & K_{j+1,n} \\ \vdots & & & \\ K_{n,1}\ \cdots & K_{,i-1} & K_{n,i+1} & \cdots\ K_{n,n} \end{vmatrix} \quad (17)$$

where,

$T_{r,i} = (HT|\varepsilon_i)$, $T_{r,ij} = (HT/\varepsilon_{ij})$,
$\varepsilon_{ij} = \sqrt{\varepsilon_i\, \varepsilon_j}$,

$\sigma_{ij} = \frac{1}{2}\ (\sigma_i + \sigma_j)$, X_i = Mole fraction of i^{th} species,

ε_i = Energy characteristic of intermolecular attraction

ε_{ij} = Reduced energy
σ_i = Zero energy collision diameter
k_i' = Monatomic thermal conductivity
k_i'' = Internal thermal conductivity.
H = Planck's constant.

The details about the flames considered are summarised in Table I. Figs. 1, 2, 3 show the geometry and the detailed temperature and concentration profiles as taken from Refs [1, 2 and 3].

It is worthwhile noting that in the chemical analysis of Propane-Air flame, the concentration of water vapour has not been obtained. However, in the case of Methane-Air flames the complete information is available. (It is complete in the sense that the concentration of most of the stable species have been obtained.)

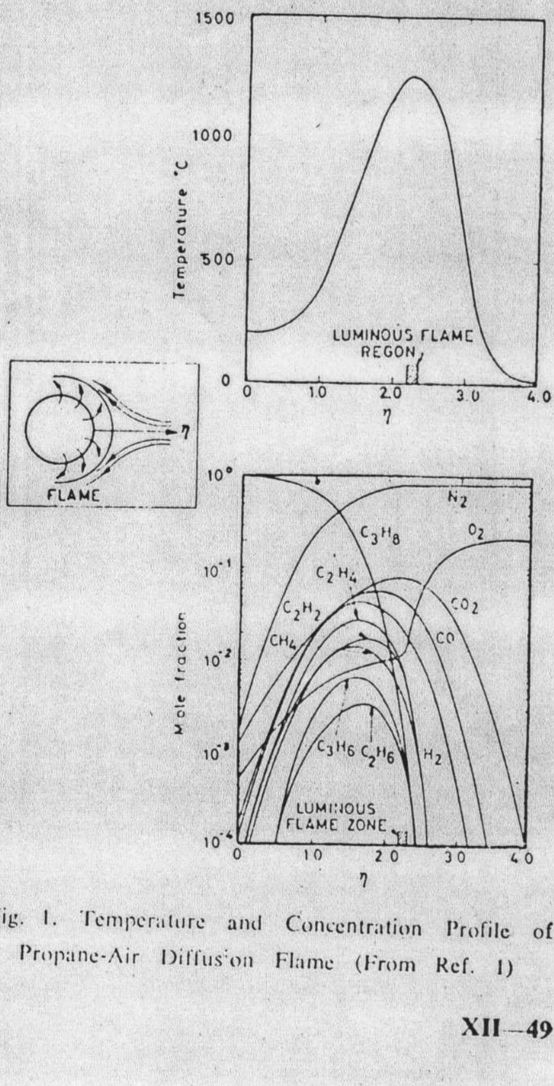


Fig. 1. Temperature and Concentration Profile of Propane-Air Diffusion Flame (From Ref. 1)

TABLE I

No.	Flame	Geometry	Fuel-Oxidant combination	Pressure and other conditions
1.	Diffusion (Ref. 1)	Stagnation point flow	C_3H_8 (Propane) – Air	1 atm Injection rate $(f_w) = -0.8$
2.	Diffusion (Ref. 2)	Stagnation point flow	CH_4 (Methane) – Air	1 atm. Injection rate $(f_w) = -1.5$
3.	Premixed (Ref. 3)	One dimensional flow	CH_4 (Methane) – O_2 (Oxygen)	0.1 atm ; Initial composition (moles): CH_4 : 0.078 O_2 : 0.915 N_2 : 0.001 CO_2 : 0.002 Ar : 0.003

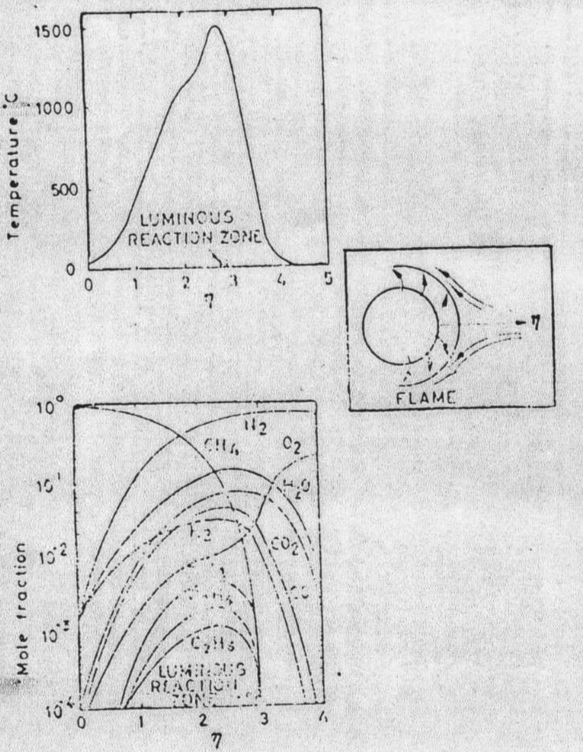


Fig. 2. Temperature and Concentration Profile of Methane-Air Diffusion Flame (From Ref. 2).

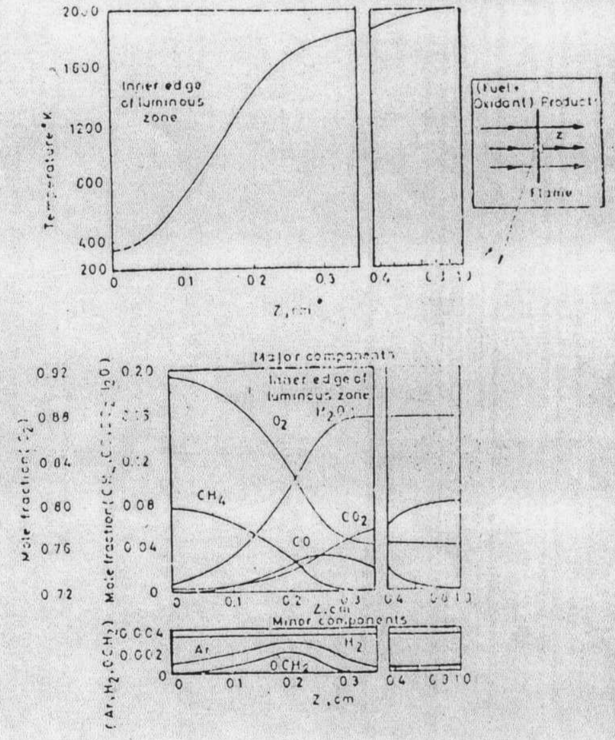


Fig. 3. Temperature and Concentration Profiles of Methane-Air Primixed Flame (From Ref. 3)

The reason why both diffusion and premixed flames were considered was because the basic mechanism and structure would be different in both the cases. Also the thermodynamic properties can be expected to show differenrces between the flame structures because the fuel-oxidant combinations are unmixed in the former and completely mixed in the latter (these are discussed subsequently)

A programme was written in Fortran IV for IBM-360(44) computer to calculate the properties using the following data σ_i=collision diameter, ε_i=characteristic energy, M_i=molecular weight. Ω_{11} $(T_{r,i})$, Ω_{12} $(T_{r,i})$ = collision integrals as a function of reduced temperature, obtained from Refs. [5 and 6], c_{pi}= constant pressure specific heat as a function of temperature and the concentrations and temperature at any given station.

Discussion

Constant pressure specific heat (c_p, *cal/gm/°K*)

The results of c_p vs. η (or z) are shown in Figs.4, 6 and 8. It is seen from Fig.4 (Propane-Air diffusion flame) that the approximation c_p = constant is violated to a great extent. In fact it varies from 0.574 near the wall through 0.72 to 0.24 ,near the free stream. The maximum value of specific heat does not occur near the maximum temperature zone, but occurs well inside of it, The explanation for this behaviour lies in the dependence of c_p on both composition and temperature. In the case of diffusion flame, we notice that the two extreme states in the flow are essentially composed of either propane or air. The specific heat at the same temperature for C_3H_8 is more than one and

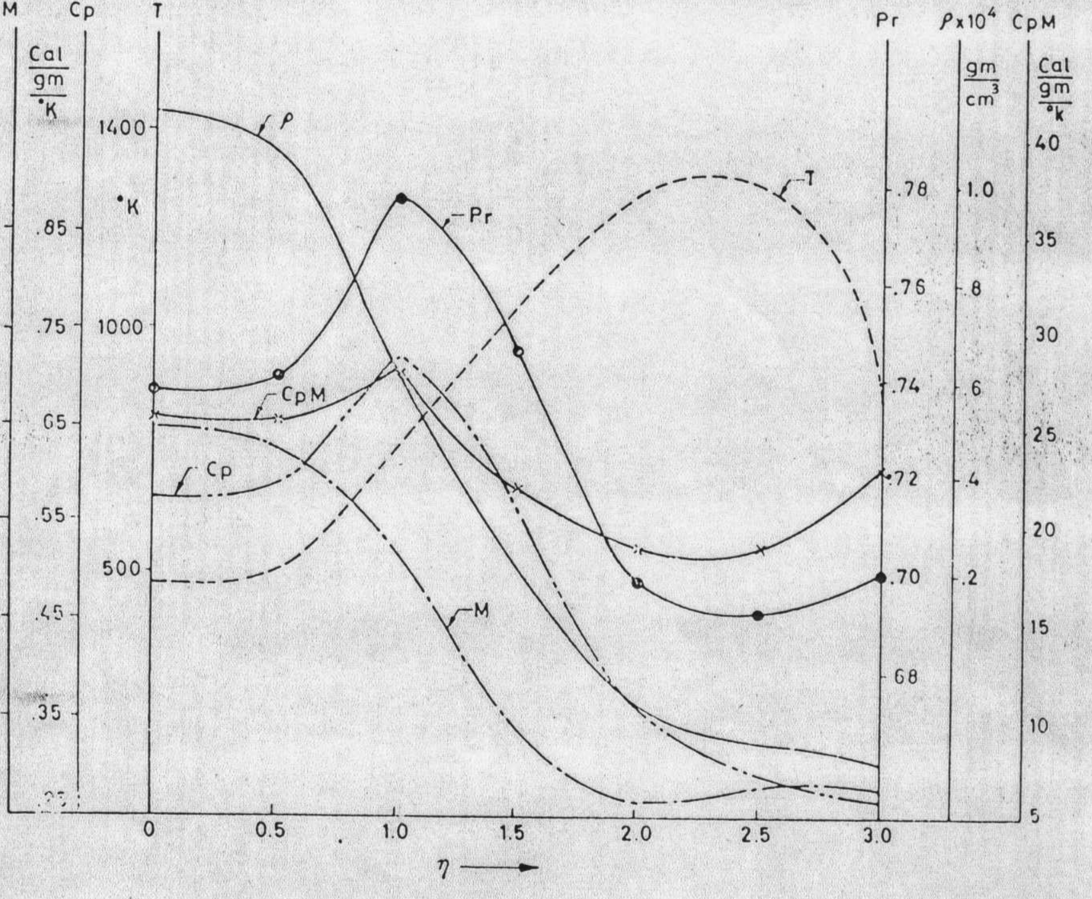


Fig. 4. Variation of Properties in C_3H (Propane)- Air Diffusion Flame.

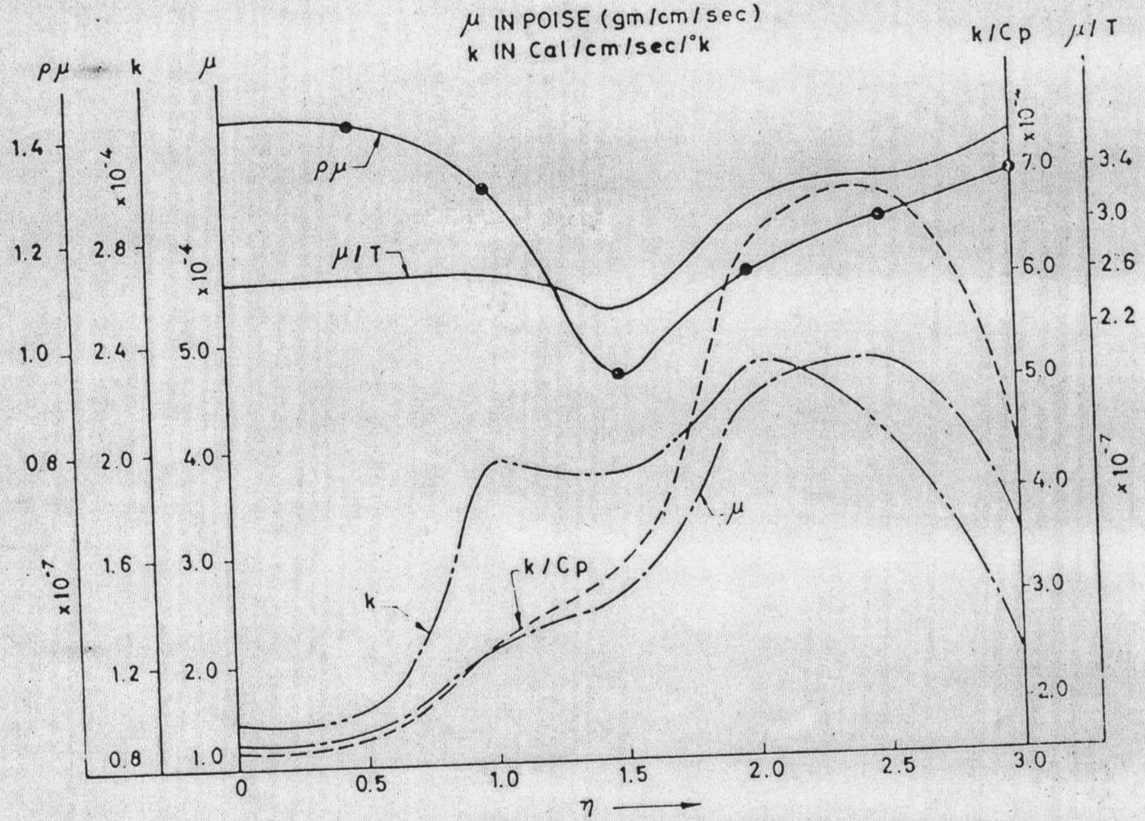


Fig. 5. Variation of Properties in C_3H_8 (Propane)- Air Diffusion Flame.

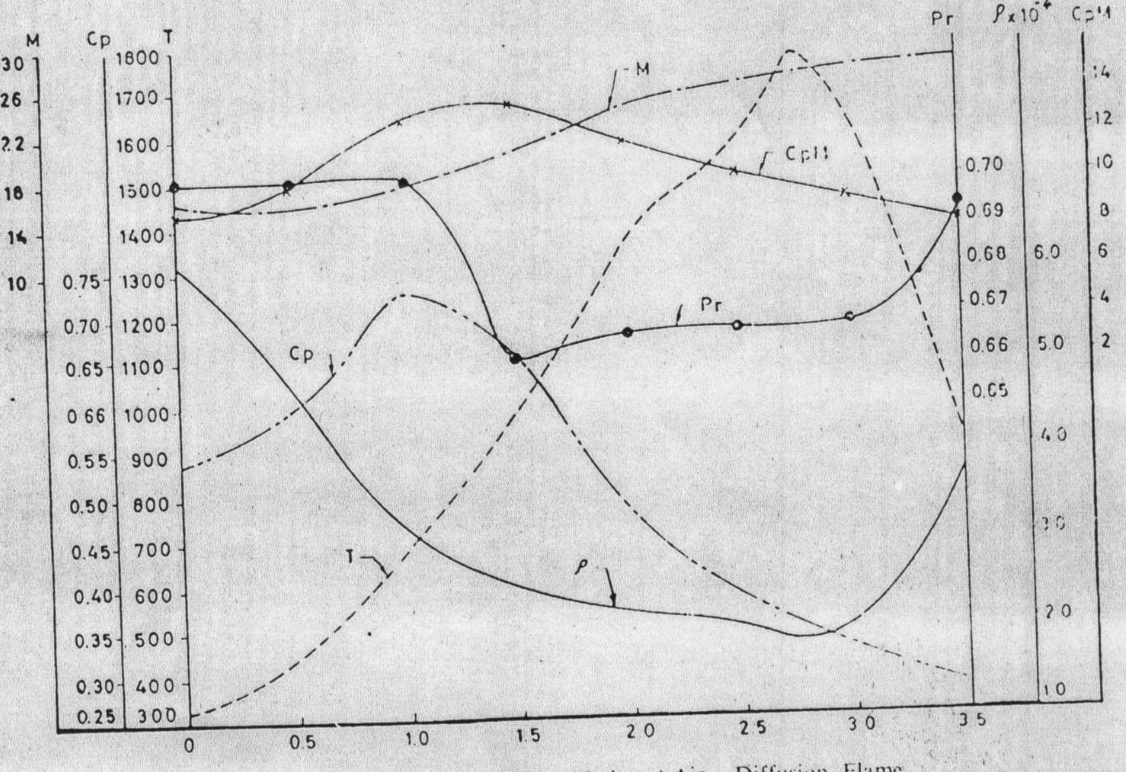


Fig. 6. Variation of Properties in CH_4 (Methane)-Air Diffusion Flame.

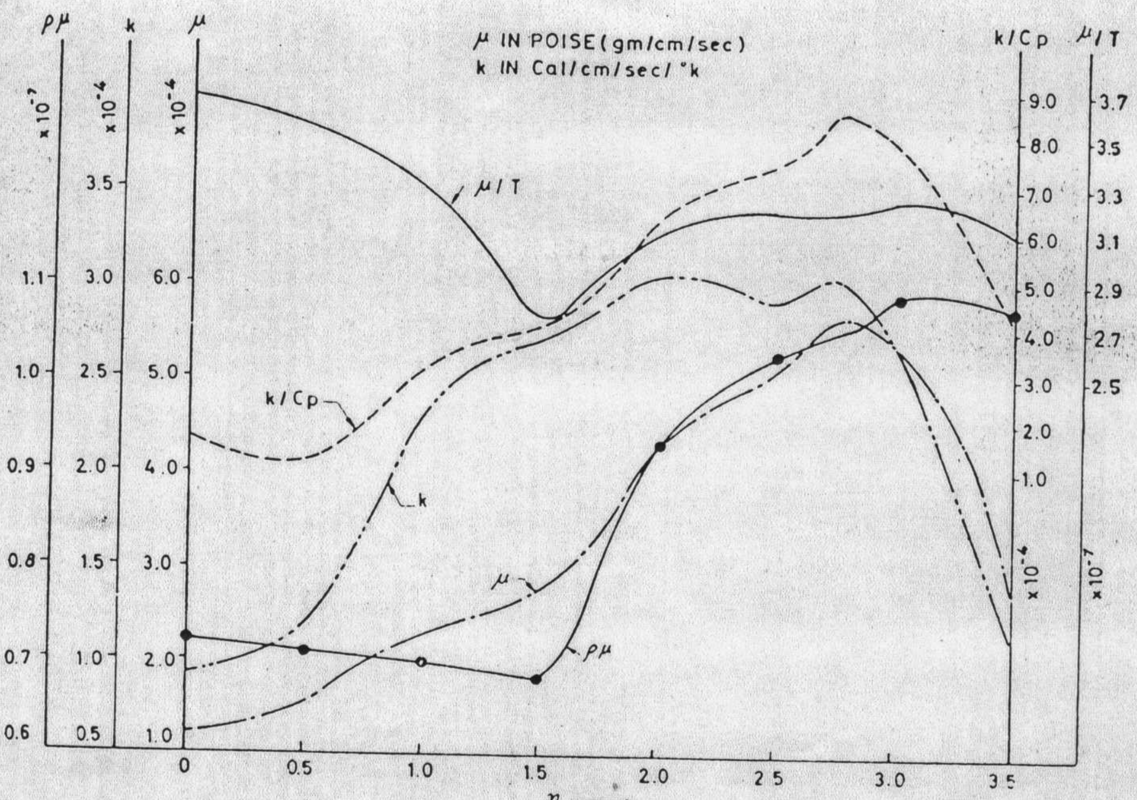


Fig. 7. Variation of Properties in CH_4 (Methane)-Air Diffusion Flame.

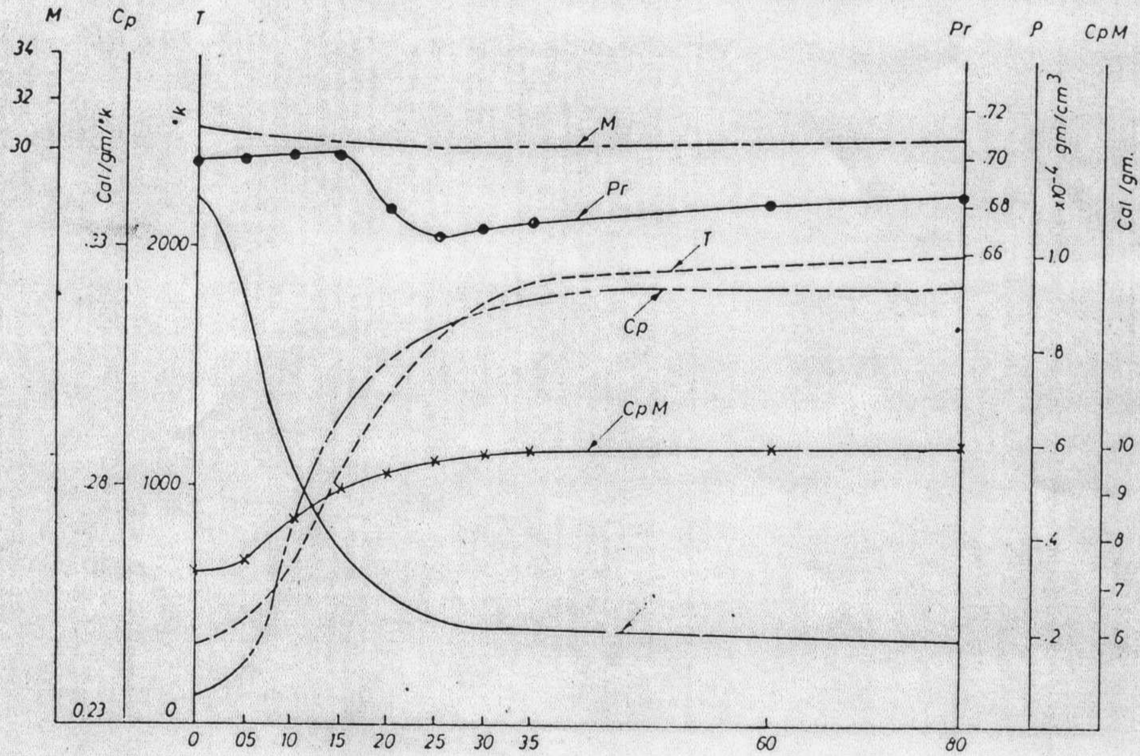


Fig. 8. Variation of Properties in CH_4 (Methane)-Air Premixed Flame

half times that of air due to the number of degrees of freedom of C_3H_8 molecule being much larger than that of oxygen or Nitrogen (and so of air). Hence we notice that with regard to the composition changes, the value of c_p should in fact decrease as we proceed outwards from the wall to the free stream. However, the effect of temperature would be such as to increase the value of c_p from the wall outwards up to the maximum temperature point. The combined effects of composition and temperature leads to the observed behavior.

It is noted from Fig. 6 that the situation is equally bad in the case of Methane-Air diffusion flame. c_p varies from 0.53 through 0.73 to 0.24 near the free stream. The maximum occurs again inside of the maximum temperature region. It appears, therefore, that in both the above cases the assumption c_p=constant is violated quite strongly. Even if we stated that variation of c_p with respect to temperature could be taken care of by an averaging procedure, we still would have to tackle the variation of c_p with respect to compusition which we notice, from the above, can be quite strong. The true representation of c_p either through the flow or in the critical regions (like a specific location-the thin flame position) is directly connected with the accurate prediction of flame temperature and temperature profiles.

Thus it appears that the approximation c_p= constant could be poor in predicting the overall characteristics of a diffiusion flame when hydrocarbon type fuels are used with the conventional oxidant namely, air (simply because it is hard to find a hydrocarbon fuel having c_p values comparable to that of oxidant at the same temperature).

It was thought that c_pM ($=C_p$, cal/gm-mole/°K) would probably have a more regular (or smaller) variation through the flame since molecular weight itself changes through the flame. That this is not so is seen from Figs. 4 and 6. Though the variation is reduced in the case of Methane-Air diffusion flame, no importance can be attached to it.

In order to stress the fact that the assumption $c_p = c_p(T)$ alone is incorrect, in principle, c_p's at various stations have been plotted as a function of local temperature in Fig.10 (B). The multivaluedness of c_p vs. T curve reveals that there must be other factors determining c_p: these, as we know very well, are the concentrations of various species.

c_p in the case of a premixed flame shown in Fig. 8, appears to be monotically increasing with increasing distance. This suggests that the effect of composition could be minimal and as such c_p vs. T is plotted in Fig. 10(A). It is observed that c_p indeed varies nearly linearly with temperature. The reason for this is not far to find. Table I shows that the initial composition is of lean fuel-air mixture kind. The composition variation through the flame does not show any significant quantities of species having large specific heat (see Fig. 3). Hence the mixture all through the flame acts as a single species as far as specific heat is concerned. A such any variation in c_p will essentially be due to temperature variations,

Molecular weight

As is expected, molecular weight variations both with Propane-Air and Methane-Air diffusion flames are considerable., It varies from 44 to 29 (from wall to free stream) and 16 to 29 monotonically with C_3H_8- Air and CH_4--Air flames respectively. Any variation in the molecular weight directly affects the equation of state (of course, it affects diffusion coefficients also as will be seen subsequently). Quite often, the approximation $\rho\ T$ = constant is made use of in constant pressure flames. It is seen this will be strongly affected in the cases similar to those we have considered herein. The same is not true with premixed flames, at least, with lean, stoichiometric and near-stoichiometric compositions. In such cases the molecular weight variation are very small (see Fig. 8) and the above approximation ρT = constant is valid.

Viscosity, thermal conductivity and some related quantities

It can be seen from Figs. 5 and 7 that viscosity varies considerably through the flame. In the analysis of flows, viscosity enters in two forms, (a) Prandtl number and (b) $C = (\rho\mu / \rho_\infty \mu_\infty)$. The plot of $\rho\mu$ through the flame shows that its variation is not large ($\backsim$ 30-40 % with respect to the free stream value). The conventional assumption regarding C in boundary layer type of flows is that $C = 1$. It appears that this assumption is not bad, after all.

It is seen that thermal conductivity also varies over a wide range through the flame. Westenberg and Fristrom [4] in their analysis of energy balance of $CH_4 - O_2$ pre mixed flame, used thermal conductivity of oxygen for that of the mixture, This is also plotted in Fig. 9. The plot shows that in the region where the discrepancy was observed (in the region $z = 0.2 - 0.4$, see Fig, XIII-16, p. 316 of Ref. 4), the thermal conductivity is over estimated in the assumed case in comparison with the actual variation. This in fact worsens the balance of the terms in the energy equation. That the worsening of the balance of the terms has occurred even after including H_2, one of the high energy species, is a significant point to note. Thus it appears that the energy balance ean be improved only if the highly energetic species (like H, O, OH etc.) are included in the evaluation of conduction term. Thermal conductivity enters the analysis of flows through the non-dimensional numbers, Prandtl and Lewis numbers.

The variation of Prandtl number through the diffusion flames is shown in Figs. 4 and 6. It can be noticed that its variation is rather negligible (of the order of 5-8% with respect to the value of air = 0.73). Thus the assumption of Prandtl number = constant = Prandtl number for air appears to be excellent in diffusion flames.

In the case of one-dimensional premixed flames (deflagrations) the viscous terms are rarely important. In fact the momentum equation amounts to the statement that pressure is consatant in the flow field. As such, these plots are not discussed any more; except to note that most of the remarks noted earlier are generally valid even in this case.

In the expression for the flame speed of a one dimensional premixed flame [10], the term k/c_p appears explicitly. With the intension of finding a reference state for the evaluation of an average k/c_p, the variation of k/c_p with z (or η) is plotted in Figs. 9, 5 and 7. It appears that k/c_p varies so widely, all the way from 2×10^{-4} to 8×10^{-4} in the case of diffusion flames and from 4×10^{-4} to 10×10^{-4} in the case of premixed flame, that it is difficult to define a reference state for evaluating an average k/c_p.

Lewis numbers (L'_{eij}, L_{eij})

Since Schmidt numbers can be defined by $Sc_{ij} = Pr/Le_{ij}$, any discussion of the variation of Prandtl and Lewis numbers can be used to discuss the variation of Schmidt numbers. Particularly in view of the fact that Prandtl number is sensibly constant, variation of one would imply inverse variation of the other. Let us therefore limit our discussion to Lewis numbers. We can define two different kinds of Lewis numbers, $L'e_{ij}$ and L_{eij} by using Binary diffusion coefficients and Multicomponent diffusion coefficients respectively.

Figs. 11, 12 show the plots of L'_{eij} vs, η for a number of pairs of gases in C_3H_8 - air and CH_4 air flames. In these plotes O_2 is taken to be diffusing into each one of the other gases. It appears that the range of Lewis numbers all lie within 0·6—3·0 with C_3H_8—air flame and 0·4—1·6 with CH_4—air flame except for Lewis numbers between H_2 and other species. Since it is well known that large moleculer weight differences lead to large diffusion coefficients, Lewis numbers based on H_2 and other species have been plotted. It appears that these Lewis numbers are in the range of 10-12. Such large Lewis numbers certainly affect the flame structure, most certainly, the concentration profiles. But it is not clear what strong influences they have on the overall flame properties. Some studies of differing Lewis numbers on flame speeds of premixed flames have been performed by Campbell et al [11]. These studies on effects of non-normal diffusion are more concerned with the effects on the steady state approximation used in chain

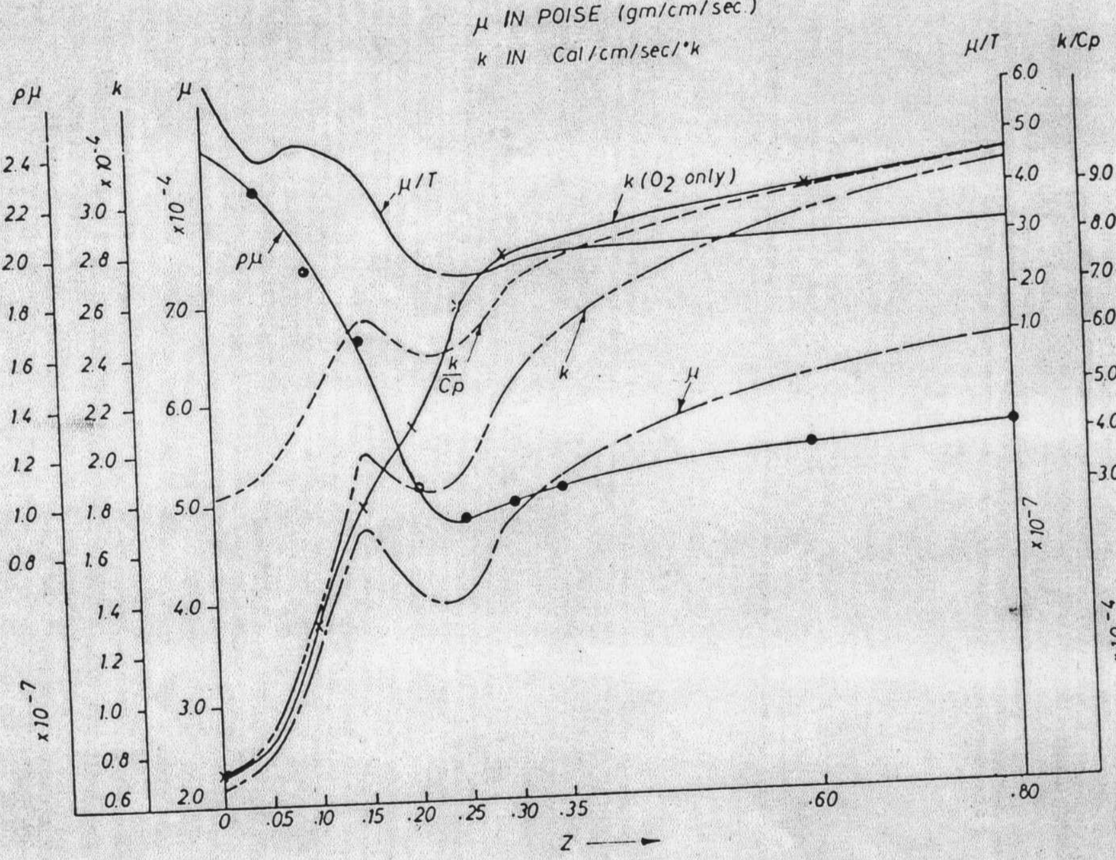


Fig. 9. Variation of Properties in CH_4 (Methane)

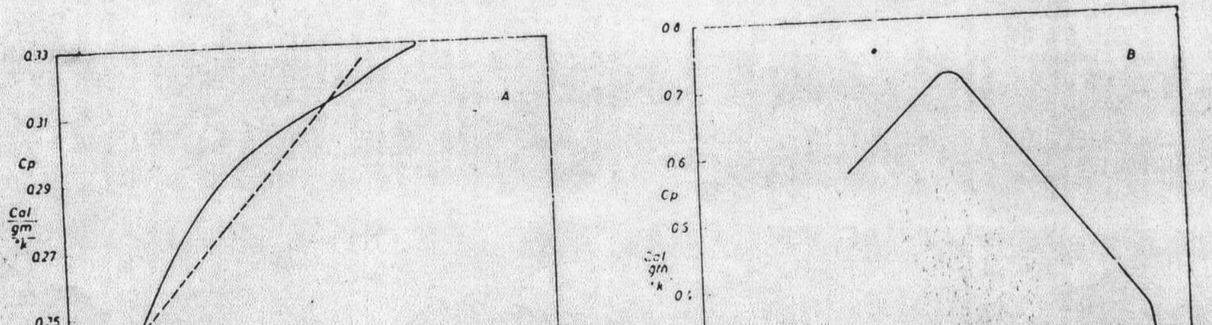


Fig. 10. Variation of Specific Heat with Temperature in
(A) Premixed Flame (CH -Air)
(B) Diffusion Flame (C_3H_8-air)

reactions rather than on the flame structure. In fact, in this particular paper by Campbell, there is not even a discussion of the effects of diffusion on flame speeds which they have obtained from numerical integration of the governing equations.

Klein [see Ref. 7, p. 317] has shown that if the complex flame, has a single set of 'fuel' and 'oxidizer' with which heat release can be connected, then it is this Lewis number which is significant in the prediction of overall properties. In support of this idea Westenberg and Fristrom [4] plotted the concentrations of the significant species CH_4 and CO - (with which energy release could be connected, as being in two steps) against the dimensionless temperature, the corresponding adiabatic flame temperature being defined at the 'disappearance' of each of the species CH_4 and CO. The linearity of this plot was taken as a good check of the unity Lewis number approximation. In order to gain more insight into this aspect, the Lewis numbers $L'e_{ij}$ and Le_{ij} for this flow have been plotted in Fig. 13. It can be noticed that most of the Lewis numbers lie between 0.5 and 1.6. And in particular, Lewis numbers between CH_4 - O_2 and CO - O_2 lie between 1.0 - 1.25 and 0.75 to 1.0. This possibly, implies that the overall effects could siill be described sufficiently satisfactorily with Lewis number = 1 approximation.

In this particular plot (Fig. 13), it is further noticed that the Le_{ij} are almost equal to the $L'e_{ij}$, This is mostly because of the fact that the average moleculer weight is constant in the flow (the variation is less than 0.8% in the flow).

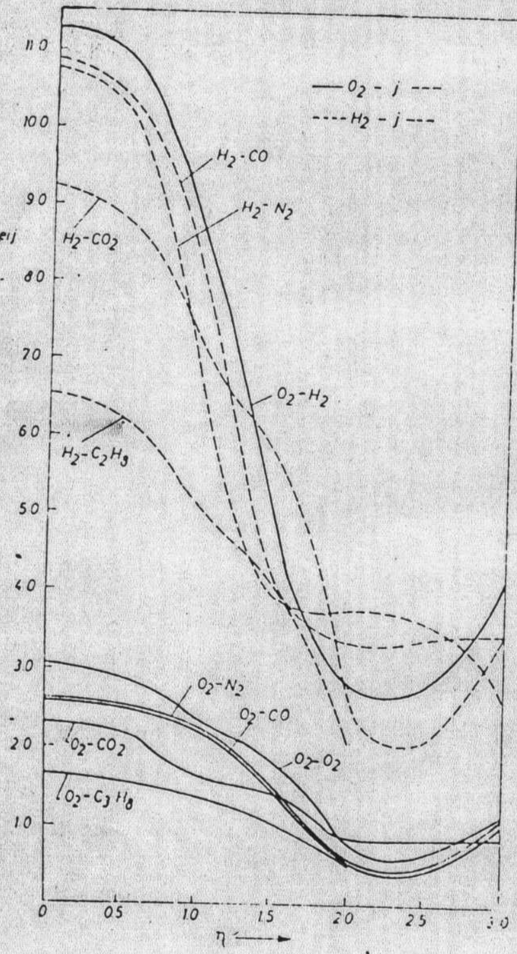


Fig. 11. Variation of Lewis Numbers Based on Binary Diffusion Coefficients in C_3H_8-Air Diffusion Flame.

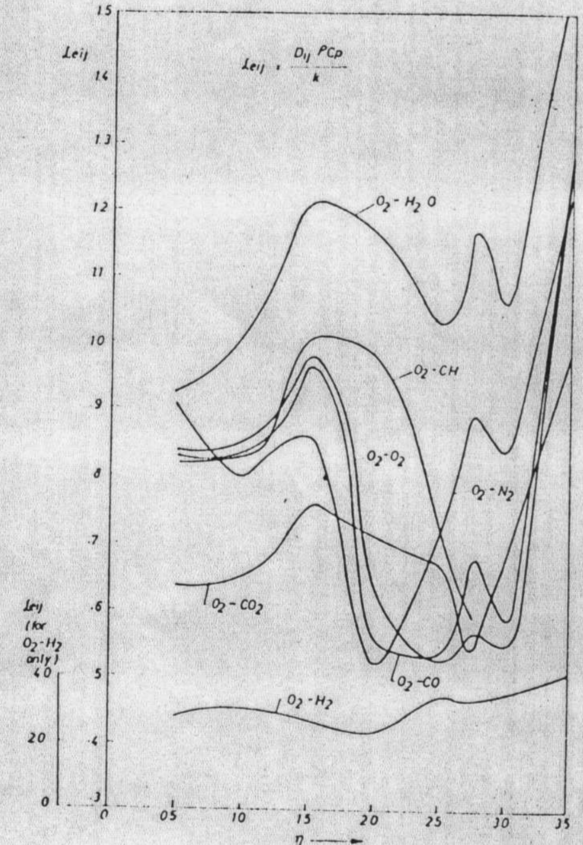


Fig. 12. Variation of Lewis Numbers Based on Binary Diffusion Coefficients CH_4-Air Diffusion Flame.

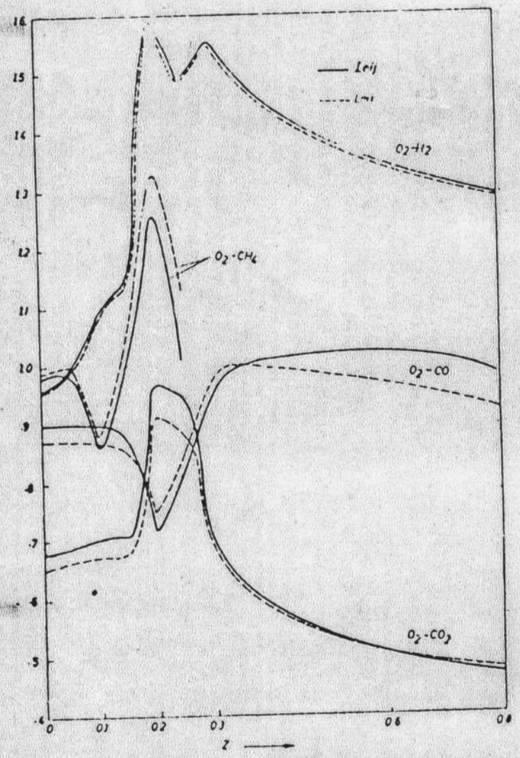


Fig. 13. Variation of Lewis Numbers CH_4-Air Premixed Flame.

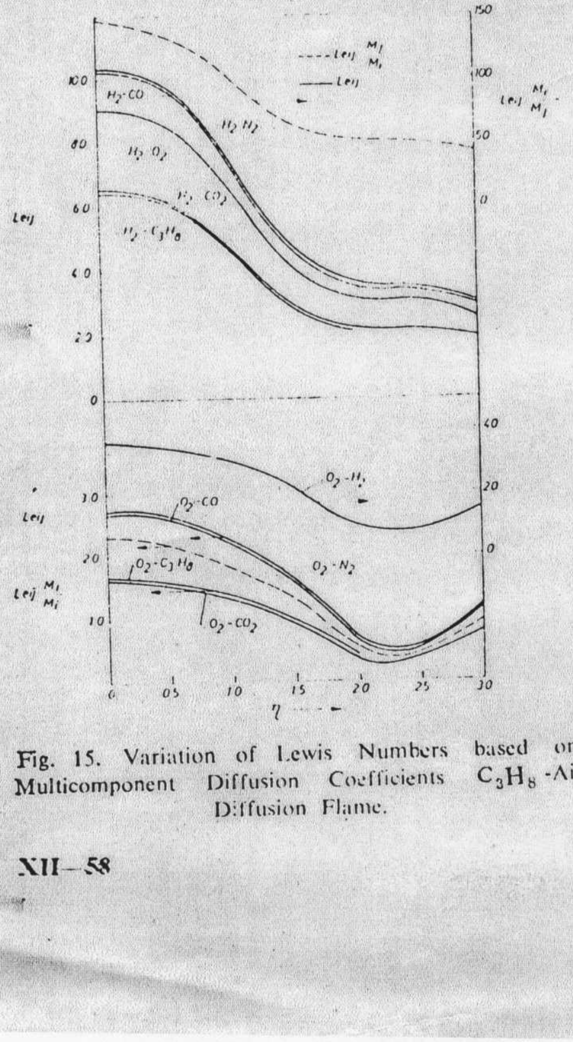


Fig. 15. Variation of Lewis Numbers based on Multicomponent Diffusion Coefficients C_3H_8 -Air Diffusion Flame.

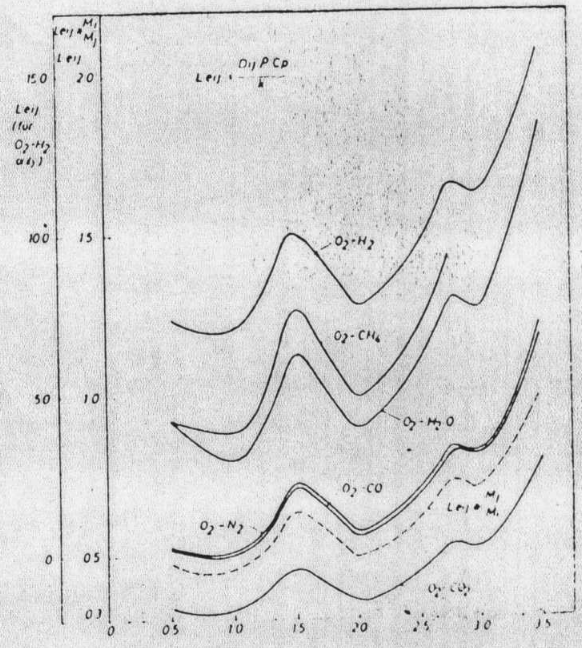
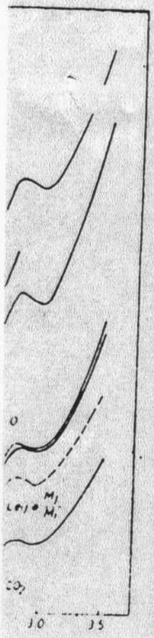


Fig. 14. Variation of Lewis Numbers based on Multi-Component Diffusion Coefficients CH_4-Air Diffusion Flame.

In Fig. 14 has been plotted Le_{ij} for CH_4-air diffusion flame. A surprising feature about the curves is that all of them have similar shapes Suspecting the effect of molecular weight on the differences in the curves, $Le' = Le_{ij} \times (M_i/M_j)$ have been plotted in the same figure. It is observed that all the curves collapse into a single curve. This interesting feature is again repeated in the case of C_3H_8 - air diffusion flame as is evident from Fig. 15. However, CH_4 - air premixed flame does not have this feature. Further no explanation of this behaviour seems possible since the multicomponent diffusion coefficients themselves have a rather complicated dependence on the molecular weights and binary diffusion coefficients.

In making the conventional approximations, the most usual assumption concerning diffusion coefficients is that binary diffusion coefficients are used instead of multicomponent diffusion cofficients because of the complicated dependence of the latter on the flow changes (X_i's). These quantities appear in the nondimensionalised form of the equations as Lewis numbers. A fur-



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ther assumption regarding the Lewis number will be that they are all equal and equal to unity.

In order to examine this aspect we consider Lewis numbers based on binary diffusion coefficent [Figs. 11, 13]. They seem to have rather awkward variations in the flow, without any apparently simple relation amongst themselves. If we consider, however, the Lewis numbers based on multicomponent diffusion cofficients, these seem to have a simple correlation amongst each other. If we make a further approximation that the modified Lewis number, Le' $(= Le_{ij}\, M_i/M_j)$ is a constant throughout the flow, it leads us to the following situation: Even in a flow with a large number of species, one can define a single Lewis number $(= Le_{ij}\, M_i/M_j)$ which can be treated a constant (not necessarily unity) and the analysis carried out. However if one does not wish to make an approximation of constant Le' one still can derive benefit out of the simple correlation between the various species. The usefulness of this correlation merits careful examination as, we believe, it may have far reaching consequences in the analysis of diffusion flames with complex structure.

Conclusions

Analysis of earlier experiments on diffusion and premixed flames leads us to the following significant conclusions:

1. Constant pressure specific heat varies fairly widely through the flow and this probably will affect the calculation of some overall characteristics quite strongly.

2. Prandtl number remains sensibly constant and it appears that $Pr = 0.73$ (near to that of air) will be an excellent approximation for reacting flows.

3. The quantity $C \ (= \rho\mu/\rho_\infty \mu_\infty)$ appears to vary not very strongly and the approximation $C = 1$ will not be very bad.

4. Lewis numbers based on binary diffusion coefficients vary rather oddly through the flow and they lie within $0.5 - 3.0$ for most pairs of gases. The Lewis numbers between species in which one is a very light component compared to the other (like H_2 — any other species, like O_2.) Lewis numbers will indeed be very large $\sim 10 - 12$

5. It appears suggestive that a single value of Lewis number $(= Le_{ij}\, M_i/M_j)$ can be assigned for analysis of flows of complicated structure in the case of diffusion flames.

The discussions noted above open up a few lines of investigation. It appears necessary to perform theoretical analysis of, for instance, wall supported diffusion flames, to determine the accuracy of prediction of heat transfer rates by the approximations $c_p =$ constant and other assumptions on the transport properties. If constant values are to be assigned to those quantities, then what is the reference state that should be chosen for them? What differences between the structure of diffusion flames and premixed flames are responsible for the remarkable behavior of Lewis numbers based on multicomponent diffusion coefficients in the case of diffusion flames in contrast to those of premixed flames? Would actual Prandtl number variations through the flow have insignificant effects on heat transfer? and so on. These and other related questions will be considered subsequently for detailed study.

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ZUSSAMMENFASSUNG

Thermodynamische Eigenschaften wie spezifische Wärme bei konstantem Druck c_p, Zähigkeit μ und Wärmeleitfähigkeit (k) sowie Diffusionskoeffizienten mit Binär- und Mehrfachkomponenten und damit zusammenhängende Grössen wie Prandtl- Schmidt- und Lewiszahlen sind für vorgemischte Flammen und Diffusionsflammen berechnet worden. Die Analyse, die auf den Eigenschaften von Gasgemischen und auf vorgegebenen, experimentell ermittelten Temperaturen und Konzentrationen beruht führt zu einigen interessanten Ergebnissen, wie z.B.: (a) c_p ändert sich immer sehr stark; wobei diese Änderung auf die Doppelwirkung von Temperatur und Zusammensetzung im Falle der Diffusionsflamme zurückzuführen ist, während im Falle verdünnter, stöchiometrischer oder faststochiometrischer Flammen, die Temperatur alleine die Ursache ist. (b) Die Grösse (Dichte mal Zähigkeit) scheint sich bei Diffusionsflammen in Grenzschichten nicht sehr stark zu ändern, und (c) Lewiszahlen fur Proben mit sehr unterschiedlichen Molekulargewicht können um das 10-12 Fache von 1 abweichen. Ferner sind in Anbetracht der verschiedenen Ergebnisse der Vorliegended Arbeit einige der normalerweise getroffenen Annahmen neu durchdacht worden.