Stretch Effects Extracted from Inwardly and Outwardly Propagating Spherical Premixed Flames

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Unsteady propagation of spherical flames, both inward and outward, are studied numerically extensively for single-step reaction and for different Lewis numbers of fuel/oxidizer. The dependence of flame speed ratio (s) and flame temperature ratio are obtained for a range of Lewis numbers and stretch ($\tilde{\kappa}$) values. These results of s versus $\tilde{\kappa}$ show that the asymptotic theory by Frankel and Sivashinsky is reasonable for outward propagation. Other theories are unsatisfactory both quantitatively and qualitatively. The stretch effects are much higher for negative stretch than for positive stretch, as also seen in the theory of Frankel and Sivashinsky. The linearity of the flame speed ratio vs stretch relationship is restricted to nondimensional stretch of ± 0.1. It is shown further that the results from cylindrical flames are identical to the spherical flame on flame speed ratio versus nondimensional stretch plot thus confirming the generality of the concept of stretch. The comparison of the variation of $(ds/d\tilde{\kappa})_{\tilde{\kappa}=0}$ with $\beta(Lc - 1)$ show an offset between the computed and the asymptotic results of Matalon and Matkowsky. The departure of negative stretch results from this variation is significant. Several earlier experimental results are analysed and set out in the form of s versus $\tilde{\kappa}$ plot. Comparison of the results with experiments seem reasonable for negative stretch. The results for positive stretch are satisfactory qualitatively for a few cases. For rich propane–air, there are qualitative differences pointing to the need for full chemistry calculations in the extraction of stretch effects.

NOMENCLATURE

b_0, c_0	constants in Eq. 21
c_{pu}	specific heat of unburned gas (J/kg/K)
C	constant defined by Eq. 10
E	activation energy (J/mol)
IPF	inward propagating flame
h_r	heat release rate (cal/cm^3 s)
K	stretch defined by Eq. 13
Le*	critical Lewis number
Le	Lewis number of deficient (fuel) species (thermal to mass diffusivity ratio)
OPF	outward propagating flame
q	heat release parameter ($= T_{ad}/T_0 - 1$)
r_f	flame radius (cm)
R	nondimensional flame radius (Eq. 8)
R_g	universal gas constant
S	flame speed (cm/s)
S_u^0	burning velocity relative to unburned gas, with zero stretch (cm/s)
S_u	burning velocity relative to unburned gas, with stretch (cm/s)
S_b^0	flame speed relative to burned gas, with zero stretch (cm/s)
S_b	flame speed relative to unburned gas, with stretch (cm/s)
s	nondimensional flame speed defined in Eqs. 12 and 14
T_{ad}	adiabatic flame temperature (K)
T_f	flame temperature (K)
T_0	unburned temperature (K)

Greek Symbols

α	gradient of s versus $\tilde{\kappa}$ relationship at $\tilde{\kappa} = 0$ (Eq. 1)
β	nondimensional activation energy ($E/R_g T_{ad}$)
δ_0	planar flame thickness ($\lambda_u/\rho_u c_{pu} S_u^0$) (mm)
λ_u	conductivity of unburned gas (J/cm s K)
$\tilde{\kappa}$	nondimensional stretch (Karlovitz number) $= \kappa\delta_0/S_u^0$
κ	stretch rate (s^{-1})
ρ_b	density of burned gas, with zero stretch (kg/m^3)
ρ_u	density of unburned gas, with zero stretch (kg/m^3)

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τ nondimensional temperature, $(T - T_0)/(T_{ad} - T_0)$
ϕ equivalence ratio ((fuel/air)/(fuel/air)$_{stochiometric}$)

INTRODUCTION

Stretch as a phenomenon in enhancing the consumption rate or causing extinction in premixed flames has been explored by several researchers in the last decade. The definition of stretch and its components—curvature, unsteadiness or velocity gradient along the flame surface—have been presented by Buckmaster [1], Matalon [2], Chung and Law [3], and Candel and Poinsot [4]. The problem of stretched premixed flames has been studied in stagnation point geometry using asymptotic techniques by Buckmaster [5], and Durbin [6]. Mendes-Lopes and Daneshyar [7] have in addition conducted experiments and compared his theoretical results with experiments. The results of these theoretical studies based on constant density approximation show a nonlinear behavior of the flame speed with stretch.

The problem of spherically propagating flame has been studied using asymptotic techniques by Sivashinsky [8], Frankel and Sivashinsky [9], and Ronney and Sivashinsky [10], and spherical flame tips on a bunsen flame by Mitani [11]. The asymptotic theory by Matalon and Matkowsky obtains the results for small stretch by utilizing the limits of the activation parameter $\beta \to \infty$($\beta = E/R_g T_{ad}$, E = activation energy, R_g = universal gas constant, T_{ad} = adiabatic temperature), and Le (thermal to mass diffusivity ratio) $\to 1$ in such a way that $\beta(\text{Le} - 1) \sim O(1)$. The theory of Sivashinsky [8] on a converging spherical front and of Ronney and Sivashinsky [10] on an expanding spherical from use the limits $\beta \to \infty$ and $(\text{Le} - 1) \sim O(1)$. Frankel and Sivashinsky [9] have analyzed both outward and inward propagating flames (denoted by OPF and IPF respectively) and have specifically brought out that the stretch effects of these two flames are different because of the reference stationary condition being *cold* in the case of inward flame and *hot* in the case of outward flame. They have also provided expressions for the dependence of flame speed ratio, s, $(= |dr_t/dt|/S_b^0$ for OPF and $= |dr_f/dt|/S_u^0$ for IPF, where r_f = the flame radius, S_u^0 = planar burning velocity relative to unburned gas and S_b^0 = planar flame speed relative to burnt gas) with stretch. Candel and Poinsot [4] have reviewed the definitions of nondimensional stretch or Karlovitz number (denoted by $\tilde{\kappa} = \kappa\delta_0/S_u^0$; δ_0 = planar flame thickness, given by Eq. 9) and compared the results of their two-dimensional computation with the predictions of asymptotic analysis for unity Lewis number and concluded that the comparison is poor for $\tilde{\kappa} > 0.5$. There is however, no evidence in the paper to indicate good comparison for $\tilde{\kappa} < 0.5$.

Experimentally, the effects of stretch on flame speed and temperature have been studied extensively mainly using two classes of flames, such as stagnation and bunsen flames. A large body of work on stagnation flames is reported in the literature as it is subjected to uniform stretch which is easy to quantify, at least in principle. However, the presence of the flame strongly perturbs the flow pattern (as has also been argued by Dowdy et al. [12]) and leads to complex velocity profiles. The definition of flame location becomes an issue as it may not be unique, particularly when the mass flux through the flame changes significantly as can be seen from the difference in the results of Law et al. [13] and Mendes-Lopes and Daneshyar [7]. Law et al. obtain burning velocity from the minimum velocity and get enhanced flame speed with stretch in all cases. Mendes-Lopes and Daneshyar explicitly bring out the contradictory behavior in burning velocity obtained from minimum and maximum velocity points from their experimental data, and Tien and Matalon [14] have confirmed this possibility by asymptotic theory. An examination of the temperature and velocity profiles in the computational study of Kee et al. [15] shows clearly that in a stagnation point flame the mass flux decreases by 50% as one moves from the free stream through the flame to the hot side. This clearly accounts for s being more than unity for the choice of low velocity point and less than unity for the choice of the high-velocity point in the flame. For preserving the trends of extinction in terms of similarity of sharp decrease in flame temperature as well as burning velocity, it appears appropriate that the high velocity point be chosen for the flame location. Hence the results of Mendes-Lopes and Daneshyar for high-velocity point are chosen for comparison here.

Experiments with bunsen flames have been made by Wagner and Ferguson [16] on axisymmetric flames and by Echekki and Mungal [17] on plane two-dimensional flames with negative stretch. The two results differ from each other significantly, as recognized by Echekki and Mungal but they do not provide any insight into the cause of the differences. In the case of bunsen flame, the presence of flow divergence causes difficulties in the measurements of flame speed. But the spherical propagating flame in comparison to both bunsen flame and stagnation flame has advantages in terms of characterizing both flame speed and stretch. Even though spherical propagating flame has been studied by several researches including Ronney [18, 19], Dixon-Lewis [20], and Sloane [21] particularly on the measurement of the flame speed, none of the studies have extracted the effects of stretch. Palm-Leis and Strehlow [22] have conducted the experiments on expanding spherical flame and presented results of the rate of the flame propagation dr_f/dt with flame radius, r_f. Carrier et al. [23, 24] have constructed a theory for single step reaction with varying equivalence ratio and compared their results on the variation of dr_f/dt with flame radius with those of Palm-Leis and Strehlow [22]. Some of the deficiencies of this work [23, 24] are that (1) the choice of the activation energy is arbitrary and unrelated to heat release behavior with full chemistry and (2) it falls short of using the results to obtain the influence of stretch. There are arguments in the paper indicating that in the case of spherical propagation there are no stretch effects as long as flame thickness is small compared with the radius of curvature (p. 241 of Ref. 24). This obviously cannot be true since the stretch effects are directly derived from the flame surface area variation whether the flame is thin or thick. The asymptotic theories have indeed made use of the thinness of the flame to extract the results of flame speed vs stretch. It must be also be pointed out that Palm-Leis and Strehlow and Dixon-Lewis [20] have recognized that expanding flames experience stretch. In a recent study, Dowdy et al. [12] have solved the spherical propagating H_2–air flame and presented the results of Markstein length as a function of composition from experiments and computations on full chemistry. The accent in this article is more on the measurement of flame speed than on stretch. The data is processed using a model which can only provide the linear behavior of s versus $\tilde{\kappa}$ relationship.

The present work reports calculations on a propagating spherical flame and presents a comprehensive set of results on the dependence of flame speed ratio, s, and flame temperature ratio, T_f/T_{ad}, (T_f = flame temperature) with both positive (expanding flame) and negative (converging flame) stretch. When the work began, the initial efforts were on two-dimensional flames. However, it transpired that the unsteady one-dimensional spherical flame has not been adequately explored. Since stretch effects, due to both nonuniform tangential velocity along the flame and unsteadiness, are accounted for in the expression for stretch, one should be able to extract the effects from a study solely of the one-dimensional unsteady flame. A summary of the earlier results, the computational aspects, the results and comparison with asymptotic theories as well as experimental data are presented.

PRINCIPAL RESULTS OF ASYMPTOTIC THEORY

The analysis of Matalon and Matkowsky [25] involving a limit process of $\beta \to \infty$, $(\mathrm{Le} - 1) \to 0$ in such a way that $\beta(\mathrm{Le} - 1) \sim O(1)$ leads to

$$s = 1 - \alpha\tilde{\kappa}, \tag{1}$$

$$\frac{T_f}{T_{ad}} = 1 - \frac{1}{1+q}(\mathrm{Le} - 1)\tilde{\kappa}I(q), \tag{2}$$

where

$$\alpha = \frac{1}{2}\beta\frac{(\mathrm{Le} - 1)}{(1+q)}I(q) + \left(1 + \frac{1}{q}\right)\ln(1+q), \tag{3}$$

$$I(q) = \int_0^\infty \ln(1 + qe^{-x})\,dx, \tag{4}$$

$$q = \frac{T_{ad}}{T_0} - 1. \tag{5}$$

The critical Lewis number, Le*, at which α changes sign is given by

$$\mathrm{Le}^* = 1 - \frac{2}{\beta}(1+q)\frac{(1+1/q)\ln(1+q)}{I(q)} \tag{6}$$

The analyses of Sivashinsky [8] for converging flames and of Ronney and Sivashinsky [10] for expanding spherical flames refer to a different limit process namely, $\beta \to \infty$, Le ~ 1 and lead to an equation for the flame speed as a function of nondimensional flame radius given by

$$\frac{ds}{dR} = -s^2 \ln s^2 + \frac{2s}{R}, \tag{7}$$

where

$$R = \frac{r_f}{\delta_0 \beta I_1(q)} = \frac{2s}{\tilde{\kappa}}\frac{\rho_u}{\rho_b}\frac{1}{\beta I_1(q)} = C\frac{s}{\tilde{\kappa}} \tag{8}$$

$$\delta_0 = \lambda_u / (\rho_u c_{pu}, S_u^0) \tag{9}$$

In the above equation, $C = 2\rho_u/(\rho_b \beta I_1(q, \mathrm{Le}))$and

$$I_1(q) = \int_e^1 \left[\left(\frac{x-e}{1-e}\right)^{(\mathrm{Le}-1)} - 1\right]\frac{dx}{x} \tag{10}$$

where $e = 1/(1+q)$. It is possible to convert the equation relating s and R into one ralating s and $\tilde{\kappa}$. This is obtained as

$$\frac{ds}{d\tilde{\kappa}} = \frac{s}{\tilde{\kappa}}\left(\frac{Cs^2 \ln s^2 - 2\tilde{\kappa}}{Cs^2 \ln s^2 - \tilde{\kappa}}\right). \tag{11}$$

The Taylor series expansion in the $s - R$ space gives the small stretch result as $s = 1 + 1/R$. The corresponding result in $s - \tilde{\kappa}$ coordinates is $s = 1 + \tilde{\kappa}/C$.

Frankel and Sivashinsky [9] have derived two different expressions of flame speed for positive and negative stretch flames in the limit of $\beta \to \infty$ and Le $\to 1$ as given below.

$$s = \frac{S_b}{S_b^0} = 1 + \left[\frac{\ln \sigma}{1-\sigma} + \beta(1-\mathrm{Le})I(\sigma)\right]\tilde{K}, \tag{12}$$

where

$$K = \frac{2\delta_0}{r_f}\sigma = \frac{\rho_u}{\rho_b}. \tag{13}$$

S_b^0 is the burning velocity with respect to burned gas. The flame speed with respect to burned gas, S_b, is used for outward propagation since the hot end is stationary. For inward propagating flame, a separate relationship between s and $\tilde{K}$ is given below.

$$s = \frac{S_u}{S_u^0} = 1 + \frac{1}{\sigma}\left[\frac{\ln \sigma}{1-\sigma} + \beta(1-\mathrm{Le})I(\sigma)\right]\tilde{K}. \tag{14}$$

In these studies, the $\tilde{K}$ is defined as $2\delta_0/r_f$. The above expressions, converted to s versus $\tilde{\kappa}$, give

$$s = \frac{1+\sqrt{1+4C_f\tilde{\kappa}\sigma}}{2} \quad \text{(Outward)} \tag{15}$$

where

$$C_f = \frac{\ln \sigma}{1-\sigma} + \beta(1-\mathrm{Le})I(q)$$

and

$$s = \frac{1+\sqrt{1+4C_f\tilde{\psi}}}{2} \quad \text{(Inward).} \tag{16}$$

In order to make comparisons, a set of values is chosen for q, Le, and β. The chosen parameters for the single step reaction are for the CH_4–air system. The only way the composition enters the calculations would be through T_{ad}, β, and Le, which are considered to be variables.

THE CHOICE OF PARAMETERS

The value of adiabatic flame temperature (T_{ad}) is based on equilibrium calculations and the corresponding heat of reaction adjusted to satisfy the value of T_{ad}. In the case of a lean flame (CH_4–air), the adiabatic flame temperature was obtained without any adjustment of the heat of reaction. Most of the results presented are for this case. The thermodynamic and transport properties are considered variable and the choice of the diffusion coefficient of any species is calculated from the thermal conductivity with the Lewis number for the species (Le_i) set to a particular value. In the case of lean mixtures typical values may be chosen to be unity for all species except the deficient reactant. In the case of CH_4, the principal species have unity Lewis number. However, for parametric variations, $Le = Le_f$, (Lewis number of the fuel) is varied over a wide range from 0.4 to 2.0 to cover both propane-air and hydrogen-air mixtures. In the case of stoichiometric composition, it is not obvious what is the most appropriate value of Le. The appropriate value of Le is therefore chosen as stated above. The nominal values of β are obtained from comparison of the heat release profiles with full chemistry as follows. The heat release rate for the second-order single-step reaction can be represented as [26]

$$h_r/h_{r,\max} = (1-\tau)\left(\frac{1}{\phi}-\tau\right)\exp(-E/RT), \tag{17}$$

where h_r is the heat release rate and $h_{r,\max}$ is the maximum value of h_r. The temperature at the peak h_r, denoted by $T_{\max}$, can be shown to be related to the activation energy, E by

$$E = \frac{\left(1+\frac{1}{\phi}-2\tau_m\right)}{\left(\frac{1}{\phi}-\tau_m\right)(1-\tau_m)}\frac{R_g T_m^2}{(T_{ad}-T_0)} \tag{18}$$

where $\tau_m = (T_m - T_0)/(T_{ad} - T_0)$, T_m being the temperature at maximum reaction rate. Thus determination of the temperature at peak heat release from full chemistry calculations along with the above relations gives the activation parameter. Figure 1 shows the variation of heat release rate with nondimensional temperature, τ for stoichiometric and lean CH_4-air compositions [26]. It can be seen that the fit is reasonable for the lean case, but poor for the stoichiometric case at the high-temperature end. The tail of the spatial distribution of temperature is very long at the hot end for full chemistry in comparison to the single step case. This situation is not unique to CH_4, but appears to be general for a series of hydrocarbons as the calculations on C_3H_8 show. This

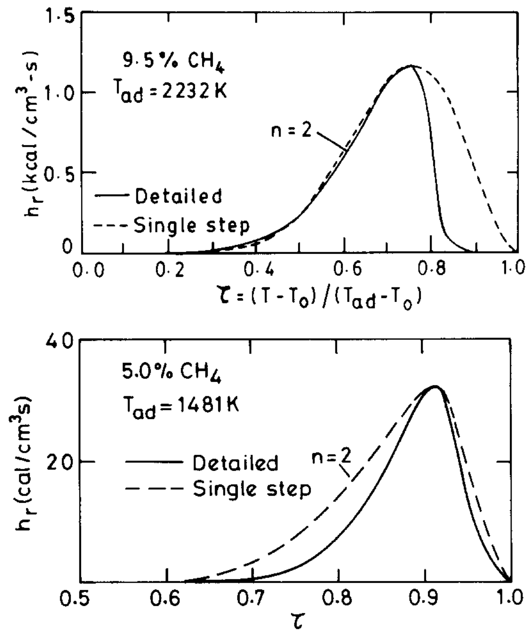

Fig. 1. Heat release rates with full chemistry and single step reaction for CH_4–air system.

implies that stoichiometric hydrocarbon flames are not easy to replicate in terms of heat release distribution using single step chemistry. The parameters for the lean case are T_{ad} = 1481 K, β = 15.3, and Le nearly unity. For the stoichiometric case, T_{ad} = 2224.0 K, β = 6.3, and Le_i values are nearly unity. In the calculations β is varied from 5 to 15.3, and Le from 0.4 to 2.0 for the lean case.

COMPUTATIONAL ASPECTS

The computations were made with a standard code, developed in the laboratory for plane one-dimensional flames [27–29] modified to account for cylindrical and spherical geometries. Unsteady one-dimensional equations of motion in the appropriate coordinate system using the following initial and boundary conditions were solved. For outward propagating flames the conditions are

$$\text{at } t=0: \begin{cases} r < r_{f,0}: T = T_{ad},\, T_i = Y_{i,ad} \\ r > r_{f,0}: T = T_u,\, Y_i = T_{i,u} \end{cases}$$

$$\text{for } t>0: \begin{cases} r = 0: \partial Y_i/\partial r = 0,\ \partial T/\partial r = 0 \\ (r \to \infty): Y_i \to Y_{i,u},\, T \to T_u \end{cases} \tag{19}$$

and for inward propagating flame

$$\text{at } t = 0: \begin{cases} r < r_{f,0}: T = T_u, Y_i = Y_{i,u} \\ r > r_{f,0}: T = T_{\text{ad}}, Y_i = Y_{i,\text{ad}} \end{cases}$$

$$\text{for } t > 0: \begin{cases} r = 0: \partial Y_i/\partial r = 0,\ \partial T/\partial r = 0 \\ (r \to \infty): \partial Y_i/\partial r \to 0,\ \partial T/\partial r \to 0, \end{cases} \tag{20}$$

where $r_{f,0}$ is the initial flame radius. Results for different Lewis numbers were obtained for single-step chemistry treating the specific heats and thermal conductivity as variables and calculating diffusivities from the desired values of constant Lewis number of each species. The flame radius, f_f, is identified by the location at which the temperature is equal to either (1) $(T_{\text{ad}} + T_0)/2$ (definition 1) or (2) $0.8T_{\text{ad}} + 0.2T_0$ (definition 2). This choice was made to examine the variability in the experiments that depends on the location of the flame surface. The various quantities that are obtained in the computation for spherical OPF are set out in Fig. 2 for different starting conditions and Lewis numbers. There will be transients due to the initial conditions, the time scale of which is of the same order as the flame transit time defined by δ_0/S_u^0. The r_f versus will be a unique function of the parameters after the transient time has elapsed. The computational time required to overcome the transient for nonunity Lewis numbers is much larger than that for unity Lewis number. In order to cover a larger range of stretch, one must start the calculations with a smaller initial radius. However, if the radius is too small, the flame may not even begin propagation because for some parameters the flame may quench at the larger stretch which arises at small radii.

The flame speed, dr_f/dt, is S_b in the case of an outward propagating flame and, because the unburned gas is at rest, is S_u in the case of an inward propagating flame. The hot side is stationary for outward propagation and the cold side is stationary for inward propagation. Figure 2 shows the various features of the spherical flame propagation for two Lewis numbers. The portion marked "transient effects" is because of the effect of initial conditions. These effects vanish beyond a certain

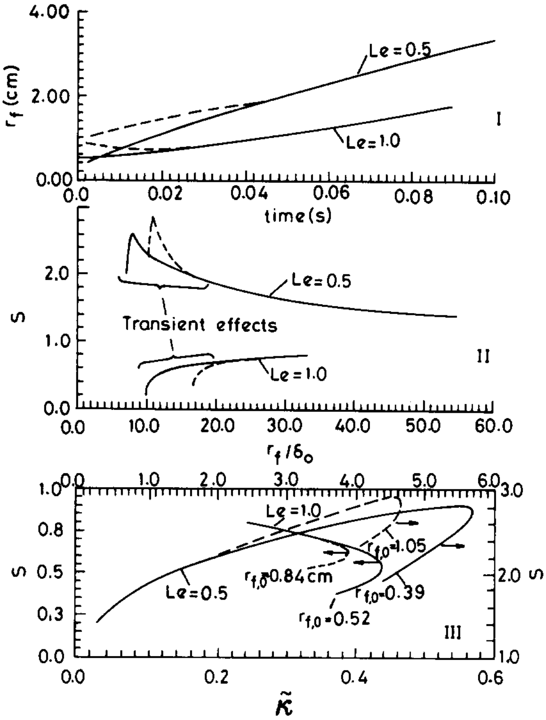

Fig. 2. Influence of different variables on s versus $\tilde{\kappa}$ of spherical propagating flames ($\beta = 15.3$). I: r_f versus time, II: s versus R_F/Δ_0, III: s versus $\tilde{\kappa}$.

time and the plot of s versus r_f/δ_0 will be unique for a particular flame. These effects are eliminated by making calculations with different initial radii and retaining the common region of the variation of s with $\tilde{\kappa}$. For Le = 0.5, the flame speed ratio decreases from values larger than unity to the planar value of unity but for Le = 1 increases from values less than unity towards the planar value. The curves in Fig. 2(II) are similar to those obtained by Palm-Leis and Strehlow [22] in their experiments. Stretch is evaluated from the r_f versus time data as $\kappa = (2/r_f)(dr_f/dt)$ for spherical flames and $\kappa = (1/(dr_f/r_f)dt)$ for cylindrical flames. The nondimensional stretch is $\tilde{\kappa} = \kappa\delta_0/S_u^0$. A further check was made on the dependence of s with $\tilde{\kappa}$ on the choice of the value of S_u^0 by varying the reaction rate pre-exponential factor. Figure 3 shows the results to be identical when the transient effects were eliminated. The choice of a lower burning velocity permits the coverage of a larger stretch range. Though the results in Fig. 3 are for positive stretch, the statements made here are

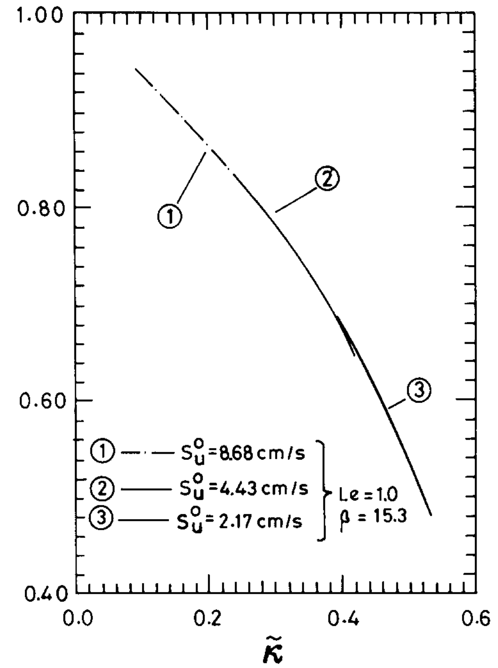

Fig. 3. Effect of burning velocity on s versus $\tilde{\kappa}$.

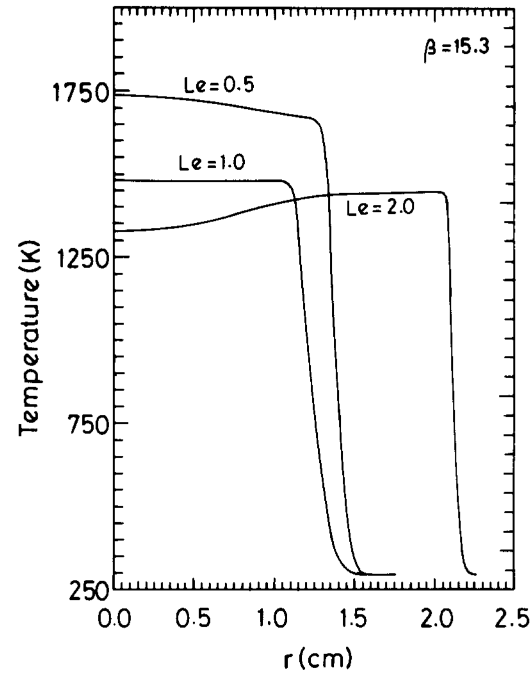

Fig. 4. Instantaneous temperature profiles for different Le.

also valid for negative stretch. Figure 4 shows the variation of temperature with distance for several Lewis numbers. It is seen that the flame temperature is the same as adiabatic flame temperature for Le = 1, greater for Le < 1, and less for Le > 1, with $\tilde{\kappa} > 0$. The temperature varies by up to 150 K on the burnt side and it was necessary to identify a criterion for determining the flame temperature, T_f, when $T_f > T_{ad}$ for outward propagation and $T_f < T_{ad}$ for inward propagation. After some trials it was found that the criterion of 1% peak reaction rate as the location for T_f was reasonable. The flame radius required to obtain the near-planar conditions is large for nonunity Le cases (typically, for Le = 0.5, the range of computation is up to a radius of 30–40 mm and the radius required for s to attain unity is as much as 200 mm).

To assess the sensitivity of the results to the location of r_f, calculations were made with definitions 1 and 2 (most results are reported with definition 1). The choice of these values was motivated by the observation that in full chemistry calculations, the radicals producing luminosity occur in this temperature range. The results are plotted in Fig. 5. These show differences of less than 3% for positive stretch and less than 6% for negative stretch. If results for a different definition in this range are required the results can be scaled appropriately. Further, the flame location set by the

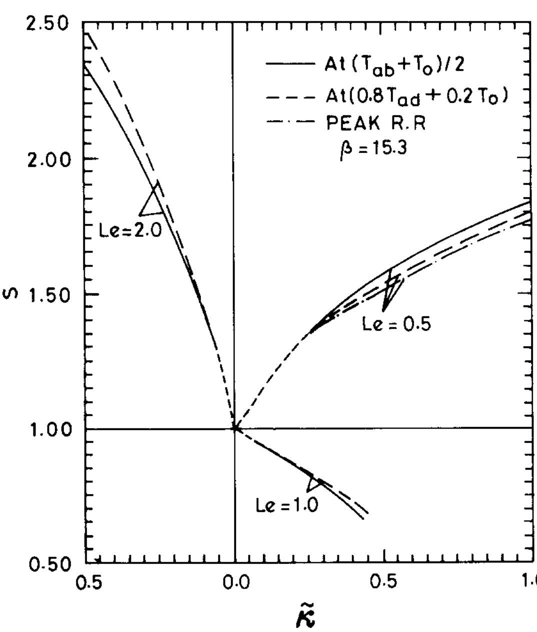

Fig. 5. Sensitivity of s versus $\tilde{\kappa}$ plot to the definition of r_f.

peak reaction rate is considered and the results of this definition are also seen (peak R.R) in Fig. 5 for the case of Le = 0.5. The results depart from those of other definitions only very slightly. There is difficulty in obtaining results based on peak reaction rate and very fine gridding is required to avoid oscillations due to interpolation of the location of the peak reaction rate of CH_4. Because of this, only the results of temperature definitions of r_f are reported in the results.

RESULTS AND DISCUSSION

Comparison with the Asymptotic Theories

A comparison between the three theories [8–10, 25] and the present calculations for specific values of q, Le, and β is presented in Table 1.

There are significant differences with the results of the two asymptotic theories. The choice of Lewis numbers has been made such that they are close enough to unity for all the theories to be valid. The results of Matalon [2] indicate Le* = 0.45 at $\beta = 15.3$ and -0.757 with $\beta = 6.3$, while Sivashinsky's theory leads to Le* = 1. The unrealistic negative value for Le* at $\beta = 6.3$ obtained from Matalon's asymptotic theory [2, 25] may be due to β being insufficiently large and the kinetic effects being significant. Ronney and Sivashinsky [10] indicate that for Le > 1 their theory may be unsatisfactory and second order terms may have to be considered. However, even in the region of Le < 1, the two theories do not match, as is evident from Table 1. The results of Frankel and Sivashinsky [9] show that they are different from those of other theories, but will be shown to compare well with numerical results for outward propagating flames (see later). It is evident from the relations shown above that qualitatively, the results of the predictions of T_f/T_{ad} are the same in the theories as well as the present computations (this will be explicitly discussed later).

Flame Speed and Temperature Ratios

The flame speed ratio s versus $\tilde{\kappa}$ for both inward and outward propagating flames for various Lewis numbers and $\beta = 15.3$ are plotted in Fig. 6. It can be seen that for positive

TABLE 1

A Comparison of $(ds/d\tilde{\kappa})_{\tilde{\kappa}=0}$

β	T_{ad}	q	Le	$-\alpha$ [2]	1/C [10]	$(ds/d\tilde{\kappa})_{\tilde{\kappa}=0}$ Ref. [9]	Present
			Outward Propagating Flame (Positive Stretch)				
15.3	1481.0	3.94	2.0	5.63	–	−4.0	−4.1
			1.3	3.06	−0.79	−1.48	−1.7
			1.2	2.71	−0.58	−1.12	−1.5
			1.0	2.00	–	−0.4	−0.68
			0.8	1.29	0.96	0.32	0.0
			0.7	0.93	1.71	0.68	0.57
			0.5	0.19	–	1.4	1.48
6.3	2224.0	6.41	1.3	2.71	−0.28	−0.85	−1.1
			1.2	2.58	−0.21	−0.7	−1.0
			1.0	2.31	–	−0.4	−0.68
			0.8	2.05	0.36	−0.11	−0.25
			0.7	2.58	0.65	0.04	−0.15
			Inward Propagating Flame (Negative Stretch)				
15.3	1481.0	3.94	2.0	5.63	–	−19.9	−5.2
			1.3	3.06	−0.79	−7.38	−4.1
			1.2	2.71	−0.58	−5.59	−3.8
			1.0	2.00	–	−2.01	−3.3
			0.8	1.29	0.96	1.58	−2.7
			0.7	0.93	1.71	3.37	−2.3
			0.5	0.19	–	6.95	−0.075

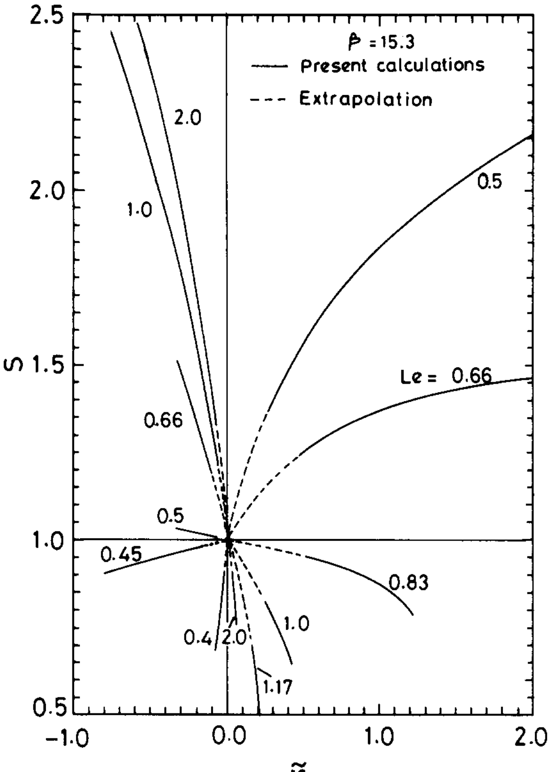

Fig. 6. Flame speed ratio versus $\tilde{\kappa}$ for both inward and outward propagating flames for various Lewis numbers.

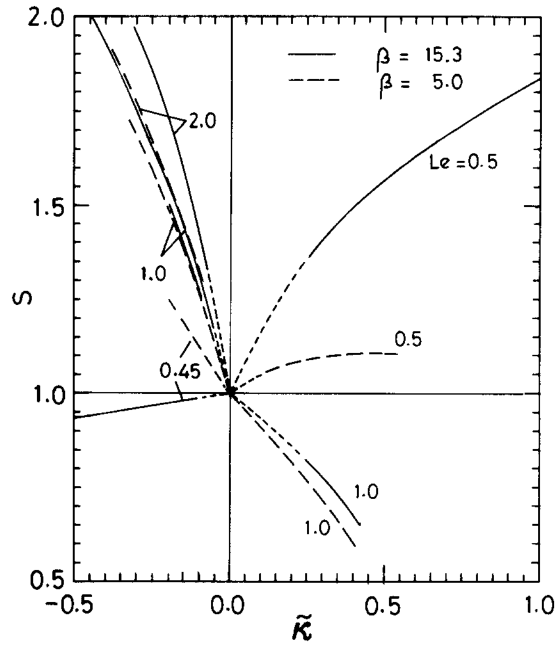

Fig. 7. Dependence of flame speed ratio versus $\tilde{\kappa}$ on activation parameter.

stretch $s = 1$ must lie between Le = 0.66 and 0.83. The actual value of Le* is estimated to be 0.8. The linearity of the curves, particularly for positive stretch, is restricted to $\tilde{\kappa} = \pm 0.1$, although the linear approximation may be made with an error of less then $+5\%$ up to $\tilde{\kappa}$ of 0.5. Figure 7 shows the effect of the activation parameter, β on the s versus $\tilde{\kappa}$ plot. The activation parameter does play a role, though it is not significant at a Lewis number of unity. According to the theory, at Le = 1 there is no effect of β on s versus $\tilde{\kappa}$ relationship. The calculated results for this value of Lewis number are almost identical at $\beta = 15.3$ and 10 but are some what different at $\beta = 5$, implying that kinetic effects become important at low β. The results for nonunity Lewis number show significant variation with β; these are not inconsistent with the expectations of asymptotic theory [2]. Most of the results on the flame speed ratio and comparisons with theory are shown in Table 1. The results of Frankel and Sivashinsky [9] compare well with the numerical results for positive stretch, but not so well for negative stretch.

In order to make comparisons, the slopes of s versus $\tilde{\kappa}$ at $\tilde{\kappa} = 0$ have been obtained and plotted in Fig. 8 as a function of $\beta(\mathrm{Le} - 1)$, the parameter in Eqs. 3, 13, and 14 that appears in the asymptotic theories. The data from the present calculations for different values of β and q fall on a straight line for positive stretch, as expected from the theory. The results of Frankel and Sivashinsky compare well with the present results for positive stretch. But Matalon and Matkowsky's theory [25] gives a parallel line which is displaced as shown in Fig. 8. The results for negative stretch fall on a curved line and asymptotic theories do not compare well with the present results. Further, the influence of β seems significant and it is fortuitous that the results for small β fall close to the results from the asymptotic theory of Matalon and Matkowsky which is expected to be valid for large β.

Figure 9 shows the variation of the temperature ratio with stretch. The trends regarding $T_f/T_{ad} \lessgtr 1$ for Le $\gtrless 1$ are consistent with the expectations of asymptotic theory. The strong curvature in the variation of the temperature is

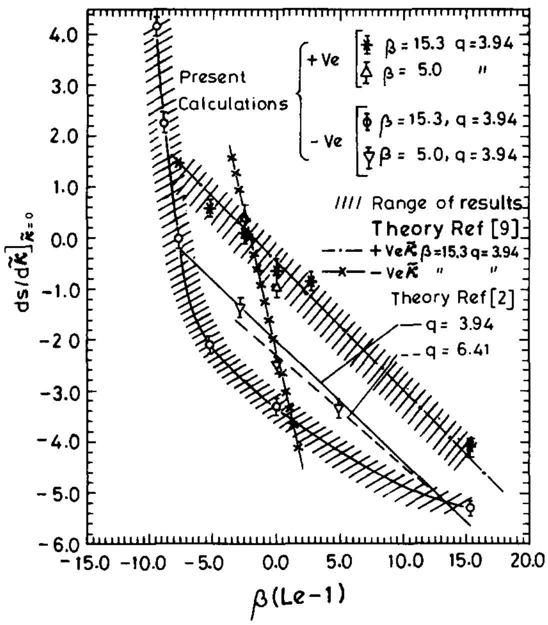

Fig. 8. Comparison of α (the slope of the curve s versus $\tilde{\kappa}$ at $\tilde{\kappa} \approx 0$) with $\beta(\mathrm{Le} - 1)$ between present calculations and asymptotic theories.

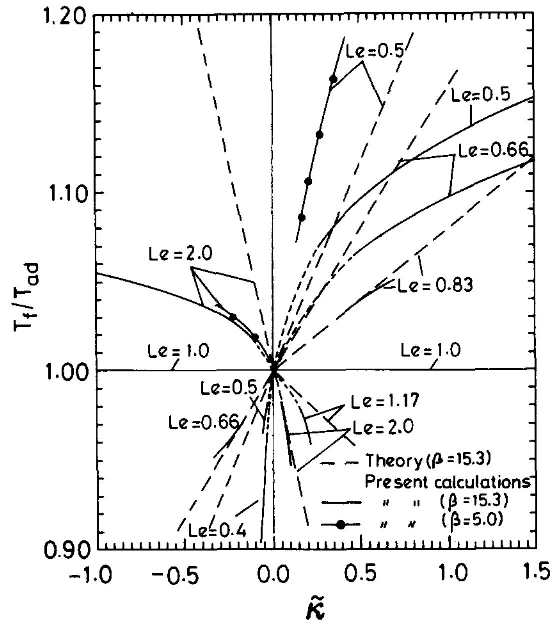

Fig. 9. Variation of temperature ratio with stretch for various cases considered along with theoretical results [25].

similar to that of s. The theoretical results of Matalon [2] also are shown. The differences between the two are significant. One set of results on the effect of β for Le = 0.5 shows clearly the dependence on β, whereas the asymptotic theory suggests no dependence on β. To assess the expectation of dependence of $T_f/T_{\mathrm{ad}} - 1$ on $\tilde{\kappa}(\mathrm{Le} - 1)$ as in Ref. 2, the computed data were expressed in terms of these coordinates (see Fig. 10). These show the single-step chemistry results to correlate on this plot, as do the s versus $\tilde{\kappa}$ data at relatively small stretch ($\tilde{\kappa} < 0.2$). The negative stretch data follow a different trend.

Comparison with Experimental Results

The experimental results available for comparison are those of Palm-Leis and Strehlow [22], Mendes-Lopes and Daneshyar [7], Echekki and Mungal [17], and Wagner and Ferguson [16]. The results of Palm-Leis and Strehlow [22], are in terms of dr_f/dt versus r_f. These need to be converted into s versus $\tilde{\kappa}$ plots. For this, the burning velocity at zero stretch, S_u^0 is required. To obtain this, a curve-fit of the data is made in terms of

$$\frac{dr_f}{dt} = S_b^0 + \frac{b_0}{r_f^m} + \frac{c_0}{r_f^{2m}} \tag{21}$$

The burning velocity, S_u^0 is obtained from S_b^0 by multiplying it with the unstretched density ratio, ρ_b/ρ_u. The exponent m was varied to determine a fit with minimum standard error. It transpired that $m = 1$ provided a good enough fit and the contribution of the quadratic term in r_f was insignificant ($< 2\%$). The data for both CH_4–air and C_3H_8–air were analyzed. These curve-fits show the burning velocity, S_u^0, to be lower than values reported by other authors by 10% in two cases and to be an overestimate in one case. Since there are no means of establishing the causes for this behavior, the value of S_u^0 obtained in this way was used for data reduction. The two results for negatively stretched CH_4–air flames at bunsen flame tips reported by Wagner and Ferguson 1[6] with an axisymmetric burner and Echekki and Mungal [17] using a two-dimensional burner are quite different (see Fig. 12); the results of Ref. 17 shows a much stronger dependence of s on $\tilde{\kappa}$ compared with those of Ref. 16. In order to check if geometry would make a difference in the s versus $\tilde{\kappa}$ relation-

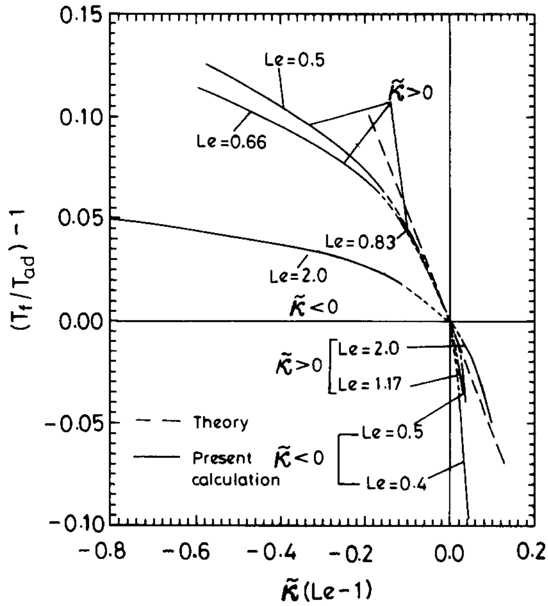

Fig. 10. Plot of $(T_f/T_{ad} - 1)$ against $\tilde{\kappa}(\text{Le} - 1)$, as expected by asymptotic theory [25] and the results from present calculations.

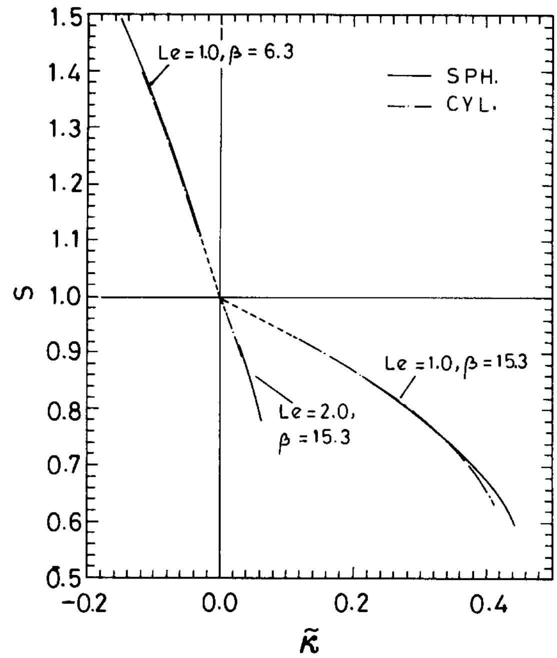

Fig. 11. Comparison of s versus $\tilde{\kappa}$ for cylindrical and spherical geometries.

ship, calculations were made for the cylindrical geometry as well as the spherical geometry and the results compared. The results are shown in Fig. 11 for both positive and negative stretch. The fact that the curves are virtually coincident shows the generality of the definition of stretch to be valid and the explanation for the differences between Refs. 16 and 17 must lie elsewhere. The discrepancy is caused possibly by the choice of flame location and, consequently, the radius of curvature of the flame. The measured values are in the range 0.36–0.55 mm in Ref. 17 and 0.5–1 mm in Ref. 16. These are indeed small and comparable to the flame thickness itself. Echekki and Mungal state that the curvature is measured at the centre of the bright zone. The flame zone in the experiments is quite thick at the centre and if a slightly upstream region was chosen, the radius of curvature could be much less then reported. The present calculations were made for the range of $r_f > 3$ mm and hence the results are much less sensitive to the exact flame location. Thus the difference in r_f could possibly explain the discrepancy.

All the experimental results discussed in this section along with the present computational results for the corresponding cases using estimated parameters for single-step chemistry are shown in Fig. 12. The estimated parameters for these cases and the slopes of s versus $\tilde{\kappa}$ curves from both experiments and calculations are set out in Table 2.

It can be seen from Fig. 12 and Table 2 that the comparison between the experimental results and the calculations is poor for most cases. A reasonable match is obtained only in case of lean CH_4–air flame. For the case of stoichiometric CH_4–air, it is seen that the $ds/d\tilde{\kappa}_{\tilde{\kappa}=0}$ from Palm-Leis [22] and Strehlow is -2.82 and from Mendes-Lopes and Daneshyar [7] about -3.47. The difference is not small but not significant if we note that in the case of stagnation point geometry, the value strongly depends on the choice of flame location. For the rich C_3H_8–air mixture, it appears that the slopes do not agree even in sign. This implies that single-step reaction may be inadequate in describing the effects of stretch on flame speed. This will call for a consideration of full chemistry effects on the flame speed-stretch behavior and will be the subject of a later publication.

TABLE 2

Estimated Parameters for Experimental Conditions

Case	ϕ	Le	β	$\beta(\mathrm{Le}-1)$	$(ds/d\tilde{\kappa})_{\tilde{\kappa}=0}$		Nature of Stretch
					Experimental	Calculated	
CH_4–air	1.0	1.0	6.3	0.0	−6.46 [17]	−3.3	−ve
CH_4–air	1.0	1.0	6.3	0.0	−2.8 [16]	−3.3	−ve
CH_4–air	1.0	1.0	6.3	0.0	−2.82 [22]	−0.75	+ve
CH_4–air	0.5	1.0	15.3	0.0	−1.22 [22]	−0.68	+ve
C_3H_8–air	0.775	1.9	7.0	6.3	−3.8 [22]	−2.5	+ve
C_3H_8–air	1.55	1.04	8.0	0.32	+0.97 [22]	−0.725	+ve
H_2–air	1.65	0.574	3.0	1.72	−5.7 [12]	−1.225	+ve
CH_4–air	1.0	1.0	6.3	0.0	−3.47 [7]	−0.75	+ve

CONCLUDING REMARKS

This article has treated the problem of flame propagation in a spherical geometry (also cylindrical geometry to a limited extent) in an attempt to extract the flame speed and flame temperature variations with both positive and negative stretch.

One of the principal results is that the response of the flame is very different to positive and negative stretch (as also seen in asymptotic theory of Frankel and Sivashinsky). For the flames considered (and for most practical flames), consistent with the asymptotic theory of Frankel and Sivashinsky, it appears that response to negative stretch is stronger than to positive stretch. For most hydrocarbon–air flames near stoichiometric (for which β is expected to be about 6–9), and hydrogen–air flames (for which β is expected to be about 3–5), kinetic effects on the flame speed ratio–stretch relationship can be significant. Consistent with earlier studies on stagnation point flames [5–7] the stretch effect becomes nonlinear beyond a value of 0.1. The behavior of the flame temperature seems similar, with clear kinetics effect beyond that predicted in asymptotic theory. The results of positive stretch indicate consistency between the present and those of the asymptotic theory in displaying a linear behavior of $ds/s\tilde{\kappa}_{\tilde{\kappa}=0}$ versus $\beta(\mathrm{Le}-1)$ and T_f/T_{ad} versus $\tilde{\kappa}$ $(\mathrm{Le}-1)$ plots. An examination of most of the available experimental data along with the present numerical calculations suggests that the single-step theory may be inadequate to explain the effects of stretch on flame speed.

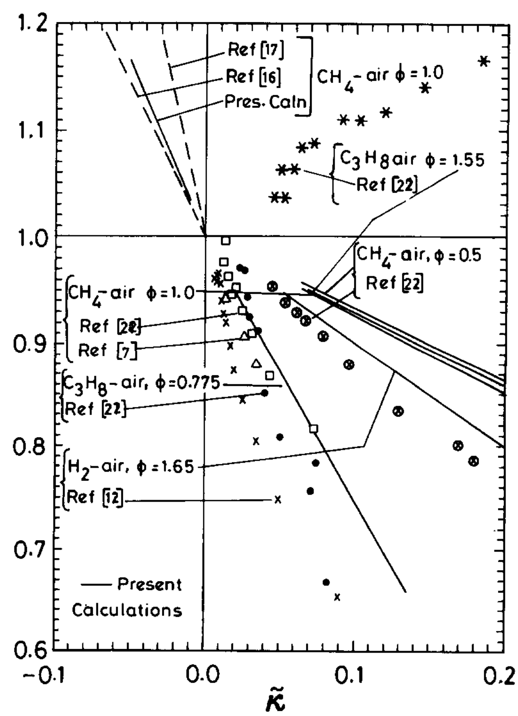

Fig. 12. Comparison of s versus $\tilde{\kappa}$ from present calculations with available experimental data.

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