Combustion Science and Technology, 1971, Vol. 3, pp. 267–272

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Printed in Belfast, N. Ireland

Effects of Interaction Between Chemical Kinetics and Fluid Mechanics in a Stagnation Point Boundary Layer

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Abstract—In the present study the mutual effects between thin-flame kinetics and fluid mechanics have been studied for a stagnation point flow with boundary layer approximations.

The effects of fluid mechanics on the flame properties have been studied with three models (a) Blasius flow model (or Lees' approximation), (b) Falkner-Skan model and (c) 'Exact' model. It is shown that Blasius flow model overestimates the flame position by a large amount (much larger than 30% over most of the range). The Falkner-Skan model and 'Exact' model overestimate and underestimate, respectively, the flame position by roughly equal amounts (~20–30%). It is, however, shown by heuristic arguments that predictions of flame position will be more accurate provided actual Lewis number values (0.5–0.7) are used with the exact model. The fuel and product concentrations at the wall are under- and overestimated respectively by the Falkner-Skan model compared to the 'Exact' values. Finally, the velocity profile for a realistic case (with temperature profiles due to the experiments of Tsuji and Yamaoka) has been computed and presented.

NOTATION

a = Stagnation velocity gradient (du_e/dx, 1/sec.)
B = Constant defined in the equation (15)
BF = Blasius flow model
C = $\rho\mu/(\rho\mu)_\infty$
c_p = Constant pressure specific heat
E = Exact model for fluid mechanics
F-S = Falkner-Skan model
k = 0 for two-dimensional flows and 1 for axisymmetric flows
H = Heat of combustion of the fuel (cal/gm of fuel)
q_w = Heat transferred into the wall
m_i = Mass concentration of species i
r = Stoichiometric ratio
T = Temperature (°K)
β = Oxidant concentration at infinity
ρ = Density
η = Independent co-ordinate
μ = Viscosity
χ_w = Variable defined by equation (14)

Subscripts

$-$ = Fuel side of the wall
w = Wall condition
n = Non-dimensional quantity
∞ = Free stream
i = 1, fuel; 2, Oxidant; 3, Product

Superscripts

$*$ = Flame position
$'$ = Differentiation with respect to η.

1.0 INTRODUCTION

Studies in fluid mechanics including chemical kinetics generally attempt at or turn out into a reduction in which the effects of kinetics on the fluid mechanics are not considered. Though such a situation can be traced to the simplifying consequences when the coupling (between chemical kinetics and fluid mechanics) is omitted, it continues to be in vogue; this is partly because the primary phenomenon which is more due to chemical kinetics (for e.g. extinction of flames) is thought to be not much affected by fluid mechanics. Also, in some situations the fluid mechanics is not much affected by chemical kinetics. A study in favour of the last statement is that of Lees (1956), wherein the stagnation point heat transfer problem in a hypersonic boundary layer is studied. In this study, Lees showed explicitly that the pressure gradient terms are almost always small compared to other terms and hence they are dropped; along with these terms disappears the coupling between the chemical kinetics and fluid mechanics. Thus the fluid mechanics (momentum equation) remains unaffected by chemical kinetics (species conservation equations) whereas the latter is affected by the former. In the present work, a situation of stagnation point boundary layer wherein the pressure gradient terms become predominant will be considered. Some studies on the effect of fluid mechanics on chemical kinetics (like the effect on extinction conditions) was made earlier by Jain and Mukunda (1968) and Mukunda

(1968). In the earlier work, comparisons of the three models namely (a) potential flow, (b) Falkner-Skan flow and (c) Lees' approximation (or Blasius flow) were made with regard to extinction conditions. It was shown that all the three models are fairly accurate in obtaining the extinction velocities. However, the earlier study is incomplete to the extent that comparisons with the 'Exact' model were not made. In the present work, we consider three models namely (a) Lees' approximation (or Blasius flow, *BF*), (b) Falkner-Skan flow (*F–S*) and (c) 'Actual coupled set of equations' which has been termed 'Exact' in the sense that fluid mechanics is described accurately. So far as the chemical kinetic part is concerned, the thin-flame approximation or Burke-Schumann Kinetics is invoked. This is thought to be sufficient for considering the interaction between chemical kinetics and fluid mechanics as the finite kinetics alters the thin-flame only to the order $D_1^{-1/3}$ (D_1 = First Damkohler number $\sim 10^4$ or more) in the near equilibrium regime (we are studying any way an equilibrium flow). With this approximation, we lose the information on extinction phenomenon which is essentially due to finite kinetics. Since an earlier study (1968) has already considered such a problem, though, in a restricted sense (as stated above), we limit ourselves to thin-flames kinetics.

The governing equations of momentum and conserved property are integrated to obtain velocity, temperature and conserved property profiles. The thin-flame position as obtained by the three models are compared with the experimental results of Tsuji and Yamaoka (1967). The concentration profiles for the *F–S* approximation are compared with those of 'Exact'.

2.0 FORMULATION

The geometry under consideration is a stagnation point flow in which air flows past a body through the pores of which, a gaseous fuel is injected at a specific rate. Under certain conditions, a flame is established near the stagnation point when ignition is effected. The principal assumptions under which the study is performed are that

(a) Reaction is single step
(b) Thin-flame approximation (or Burke-Schumann kinetics) is invoked
(c) Molecular weights and constant pressure specific heats of all the species are same
(d) Prandtl (Pr) and Schmidt (Sc) numbers are each equal to unity
(e) $C = (\rho\mu)/(\rho\mu)_e = 1$
(f) Fourier's law of heat conduction and Fick's law of diffusion are valid

It is believed that the principal conclusions arrived at in this paper would not be affected seriously by the above assumptions.

2.1 GOVERNING EQUATIONS

The momentum, conserved property, enthalpy and fuel conservation equations can be written down for a stagnation point boundary layer with the thin-flame approximation as (Lees, 1956; Mukunda, 1968).

$$f''' + ff'' + \frac{1}{(k+1)}\left(\frac{\rho_e}{\rho} - f'^2\right) = 0 \quad (1)$$

$$F'' + fF' = 0 \quad (2)$$

$$\frac{d^2h}{dF^2} = \frac{d^2m_i}{dF^2} = 0, \qquad (i = 1, 2, 3) \quad (3)$$

along with the conditions at the thin-flame front given by (Mukunda, 1968; Tsuji and Yamaoka, 1966)

$$m_1(F^*) = m_2(F^*) = 0$$
$$m_3(F^{*-}) = m_3(F^{*+}) \quad (4)$$

$$\left(\frac{dm_1}{dF}\right)_{F=F^{*-}} = -\frac{1}{r}\left(\frac{dm_2}{dF}\right)_{F=F^{*+}} = \frac{1}{r+1}\left[\left(\frac{dm_3}{dF}\right)_{F=F^{*+}} - \left(\frac{dm_3}{dF}\right)_{F=F^{*-}}\right] \quad (5)$$

$$T(F^{*+}) = T(F^{*-}) \quad (6)$$

$$\left[\left(\frac{dT}{dF}\right)_{F^{*+}} - \left(\frac{dT}{dF}\right)_{F^{*-}}\right] = -\frac{H}{c_p r}\left(\frac{dm_2}{dF}\right)_{F^{*+}} \quad (7)$$

In the above set of equations, an equation in terms of *F* has been arbitrarily introduced in order to facilitate the study. It has been so defined that (a) it has a range from zero to unity and (b) the kinetic/enthalpy equations when transformed using *F* as the independent variable instead of η, have a simpler form (the first derivative terms are absent). It is called a conserved property variable since its governing equation does not have a source term.

The enthalpy *h* is defined by

$$h = c_p T + \frac{u^2}{2} - \sum m_i h_i^0 \quad (8)$$

where H_i^0 = heat of formation of i^{th} species. In the equations to follow, the kinetic energy term is neglected as it is small compared to chemical enthalpy terms.

If we invoke the boundary layer approximation $\partial p/\partial y = 0$, the term (ρ_∞/ρ) can be replaced by $T/T_\infty = T_n$. With this, the momentum equation becomes,

$$f''' + ff'' + \frac{1}{(k+1)}(T_n - f'^2) = 0 \quad \text{(1a)}$$

2.2 BOUNDARY CONDITIONS

The boundary conditions for the problem in the dimensionless form are (Mukunda 1968).

$$\eta = 0; \quad F = 1, \quad f = f_w, \quad f' = 0, \quad h = h_w$$

$$\frac{dm_1}{dF} = \chi_w(m_1 - 1), \quad \frac{dm_i}{dF} = -\chi_w m_i, \quad i = 2, 3 \quad (9)$$

$$\eta = \infty; \quad F \to 0, \quad f' = 1, \quad h = h_\infty, \quad m_2 = \beta,$$

$$m_1 = m_3 = 0 \quad (10)$$

The boundary conditions for m_i at $\eta = 0$ describe the convective-diffusive balance at the wall; the other boundary conditions are the usual ones and are self-evident.

3.0 SOLUTIONS

The solutions for the enthalpy and kinetic equations (3) can be obtained using the conditions (4–7) and the boundary conditions (9) and (10) and they are

$$m_1 = 0$$
$$m_2 = \beta - \chi_w(\beta + r)F/(1 + \chi_w)$$
$$m_3 = (r + 1)\chi_w F/(1 + \chi_w)$$
$$T_n = 1 + \{T_{n,w} - 1 + B(r\chi_w/\beta - 1)/(1 + \chi_w)\}F$$
$$0 \leqslant F \leqslant F^* \quad (11)$$

$$m_1 = \chi_w(1 + \beta/r)F/(1 + \chi_w) - \beta/r$$
$$m_2 = 0$$
$$m_3 = \beta(r + 1)[1 - \chi_w F/(1 + \chi_w)]/r$$
$$T_n = T_{n,w} + (1 + B - T_{n,w})(1 - F)$$
$$F^* \leqslant F \leqslant 1 \quad (12)$$

$$F^* = (1 + \chi_w)/[\chi_w(1 + r/\beta)] \quad \text{(13a)}$$

$$T_n^* = \frac{(1 + B)(\chi_w - \beta/r) + \beta(1 + \chi_w)T_{n,w}/r}{\{\chi_w(1 + \beta/r)\}} \quad \text{(13b)}$$

where

$$\chi_w = f_w/F'(0, f_w) \quad (14)$$

$$B = H\beta/(rc_p T_\infty) \quad (15)$$

For most gases under reasonable levels of injection ($V_w/U_\infty \sim 0.1 - 0.3$), temperature T_n varies in the boundary layer by a large amount (of the order of 1–6). Due to this fact, it is unreasonable to expect the pressure gradient terms to become insignificant as was the case with Lees (1956). Hence we have now to integrate a coupled set of equations (1a) and (2) using the temperature profiles as given by (11) and (12). The scheme of solution for a given fuel will be

1. To fix a value of f_w
2. To assume a value of χ_w
3. To obtain F^* using equation (13a)
4. To obtain T_n profiles from equations given in (11) and (12)
5. To integrate equations (1a) and (2) to satisfy boundary conditions given in (9) and (10) on f' and F and in this event determining $f''(0)$ and $F'(0)$
6. To find $\chi_w = f_w/F'(0, f_w)$
7. To repeat the operations (3–6) till satisfactory convergence is obtained
8. To obtain η^* from the converged F vs. η profiles by locating the value of η corresponding to $F = F^*$.

The fifth order set of equations was integrated using Runge-Kutta-Gill procedure and a double iteration scheme to determine $f''(0)$ and $F'(0)$. The double iteration scheme involved the following procedure. For a fixed f_w and assumed $F'(0)$, the value of $f''(0)$ was iterated upon to satisfy $f'(\infty) = 1$ using the bisection technique [irrespective of what happens to $F(\infty)$]. Later, $F'(0)$ would be iterated upon to satisfy $F(\infty) = 0$, using, again, the bisection technique. It may specifically be noted that the use of thin-flame T_n profile in the momentum equation caused no convergence difficulties; partly the reason is that the T_n profile is continuous (though it possesses a gradient discontinuity). Convergence would be obtained in about 3×10 iterations [the first number indicates the number of iterations on χ_w and the second number, the number of iterations on $f''(0)$ and $F'(0)$] upto injection rates of about $f_w = 0.5$. Beyond this range the number of iterations on $f''(0)$ and $F'(0)$ would increase anywhere upto 25.

TABLE I

$-f_w$	$f''(0)$ BF	$f''(0)$ $k = 0$ F S	$f''(0)$ $k = 0$ E	$-F'(0)$ BF	$-F'(0)$ $k = 0$ F S	$-F'(0)$ $k = 0$ E	z_* BF	z_* $k = 0$ F S	z_* $k = 0$ E
0.2	0.370	1.121	1.820	0.370	0.450	0.550	0.60	0.445	0.363
0.3	0.323	1.050	1.675	0.323	0.395	0.536	1.10	0.760	0.559
0.4	0.276	1.018	1.580	0.276	0.343	0.489	1.97	1.165	0.817
0.5	0.233	0.980	1.480	0.233	0.295	0.438	3.40	1.680	1.140
0.6	0.191	0.922	1.375	0.191	0.251	0.390	6.20	2.400	1.538
0.7	0.151	0.880	1.265	0.151	0.210	0.343	14.34	3.470	2.041
0.8	0.110	0.835	1.165	0.110	0.175	0.318	59.70	4.560	2.520

BF = Blasius, $F\ S$ = Falkner-Skan, E = Exact, $T_w = T_e = 300$ K.

4.0 RESULTS AND DISCUSSION

The calculations were performed using the following data:

Fuel = Propane, $H = 10$ Kcal/gm of fuel.

$r = 3.636$, $\beta = 0.232$, $T_e = T_w = 300$ °K,

$c_p = 0.32$ cal/gm °K. Nitrogen is treated as inert.

The results are shown in Tables I–III and Figures 1–4.

a) *Skin friction*

Table I has been constructed from the calculations made in this paper and using the tables of Emmons and Leigh (1953). The results of $F\ S$ ($k = 0$) have been partly reported by Tsuji and Yamaoka (1966). Examination of Table I reveals that at each injection rate the value of $f''(0)$ is much larger with flame than without. The skin frictional force which is proportional to $C_w \times f''(0)$, $C_w = (\rho\mu)_w/(\rho\mu)_e$, is seen to be larger with flame than without because $C_w = 1$ here. However, this cannot be asserted in general, since, $f''(0)$ would in fact depend on the C profile to be used in the momentum equation. Figure 1 shows the velocity and temperature profiles for a particular injection rate. It appears that the velocity inside the boundary layer exceeds that of free stream by as much as 35%. This is certainly possible since the large decrease in density by as much as one sixth must reflect in a considerable increase in velocity. In fact this increase in velocity beyond the free stream velocity well inside the boundary layer is responsible for the increased skin friction values. Similar results have been obtained by Liu and Libby (1971).

b) *Realistic case*

In order to compute the velocity profile for a realistic case, the temperature profile $T_w(\eta)$ was taken from the experimental plots of Tsuji and Yamaoka (1967) and used in the equation

$$f''' + ff'' + [T_w(\eta) - f'^2] = 0 \qquad (16)$$

This equation was integrated with the boundary conditions (9) and (10) by using techniques simpler than those used in the earlier case [as this is a single third order nonlinear differential equation with only one unknown, $f''(0)$]. The resulting velocity and temperature profiles are shown in Figure 2. The velocity overshoot inside the boundary layer seems to be of the order of 30%. It appears worthwhile to measure velocity profiles and compare them with the above calculations.

c) *Heat transfer*

The heat transfer into the wall is given by (Chung 1965),

$$q_w = \frac{\mu}{P_r}\left(\frac{\partial h}{\partial y}\right)_w + (\rho v)_w \sum (m_i h_i - m_{i-} h_{i-}), \qquad (17)$$

where q_w = heat transferred into the wall, and conditions with subscript '_' indicate that these are evaluated on the fuel side of the wall.

TABLE II

Schmidt No. (Sc)	0.5	1.0	1.5	2.0
$\eta^*(f_w = -0.5)$	2.904	2.380	2.135	1.970

TABLE III

	$-f_w$	0.2	0.4	0.6	0.8
T_w^*	BF	6.60	7.05	7.15	7.37
	F-S	6.35	6.90	7.10	6.99
($T_{w,e} = 1$)	E	6.12	6.77	6.99	7.10

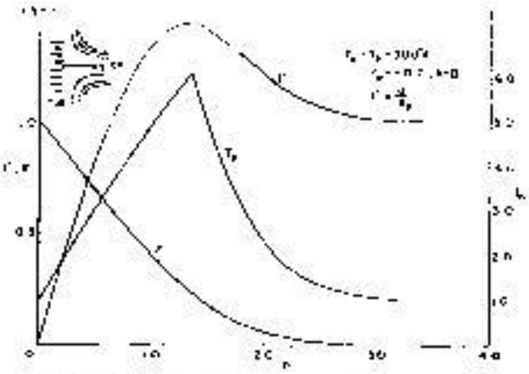

FIG. 1. Plot of velocity, conserved property and temperature profiles with η for stagnation point flow.

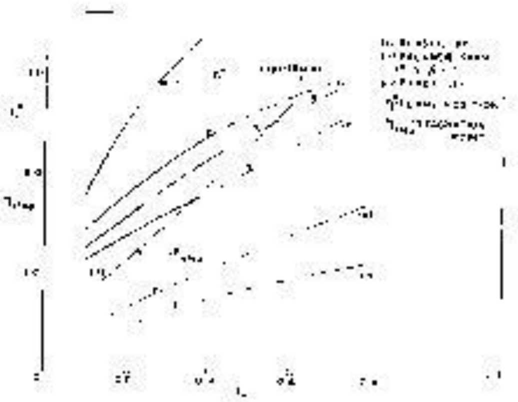

FIG. 3. Variation of flame position and stagnation plane with injection rate

If we rewrite the above expression in dimensionless form for Prandtl and Schmidt numbers equal to unity, we get

$$\frac{q_w}{\sqrt{\rho_e \mu_e a(k+1)}} = [-T_{w,n} + (1+B)]\{-F'(0)\} \tag{18}$$

Thus for a fixed fuel, wall and free stream conditions, the heat transferred into the wall is proportional to $F'(0)$. The errors in the estimation of heat transfer rate will likewise be proportional to errors in the estimation of $F'(0)$. If we now use the results presented in Table I, we can conclude that the heat transfer estimates as obtained by Lees' and Falkner-Skan approximations will be roughly 50–60% and 30–40% less compared to 'Exact' values.

d) *Thin-flame position*

Figure 3 shows a comparison of the thin-flame position and stagnation plane position as given by the three models. Also the experimental results of Tsuji and Yamaoka (1967), have been plotted on the figure. It may be observed that the Lees approximation (*BF*) overestimates the flame position by a large amount. The Falkner-Skan (*F–S*) values overestimate and 'Exact' values underestimate by roughly the same amount (about

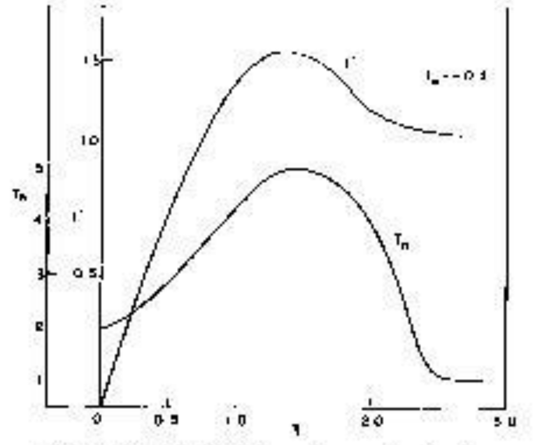

FIG. 2. Velocity and temperature profile for the experimental situation of Ref. 4.

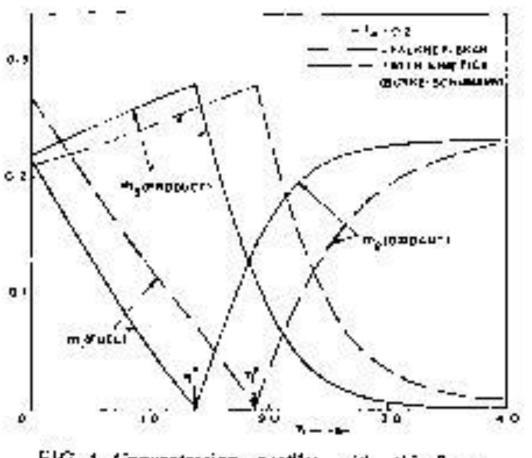

FIG. 4. Concentration profiles with thin-flame approximation.

15–20%). Qualitatively the inclusion of temperature effects in the momentum equation seems to correct the predictions in the right direction, though the correction happens to be larger than necessary. These are perhaps solely due to $C \neq 1$ and $Sc \neq 1$ in the actual case. Computations of the thin-flame position for the wall jet with various Schmidt numbers and the potential flow approximation lead to results as below. Lees (1958), estimates the value of Schmidt number to vary between 0.5 to 0.7 for atom-molecule mixtures where the light gas component is not large in flows of the kind we are considering. The experimental study of Tsuji and Yamaoka (1969) on the concentrations of various species (except the unstable species like atoms H, O, etc.) seems to belong to the case where the light gas component is not large. In such a case the corrections due to change in Schmidt number will be in the right direction and quite possibly of the right magnitude (as may be inferred from the Table II).

e) *Concentration profiles*

Figure 4 shows the concentration profiles for the *F–S* and 'Exact' models. One significant observation is that the values of fuel and product concentration at and near the wall are overestimated and underestimated (respectively) by the *F–S* approximation when compared to the 'Exact' model. These are essentially because the value of χ_w is overestimated by the *F–S* model compared to the exact model (See Table I). Further, due to this overestimation of χ_w, the maximum flame temperatures are also overestimated by the *F–S* model; the overestimation of the maximum flame temperature being of the order of 2–3% by the *F–S* model and 6% by the *BF* model, as can be seen from Table III. Thus the maximum flame temperature seems to be little affected by the kind of fluid mechanical approximations.

5.0 CONCLUSIONS

The stagnation point boundary layer with chemical reactions in a subsonic environment has been considered. The effects of the three fluid mechanical models, Blasius (*BF*) or Lees' approximation, Falkner-Skan (*F–S*) and Exact (*E*) on various flame characteristics have been studied.

Some findings are:

1. The maximum thin-flame temperatures are estimated to within 6% by both the models *BF* and *F–S* when compared with 'Exact'.
2. The heat transfer rates into the wall are largely underestimated (by as much as 50–60%) by both the models when compared with 'Exact'.
3. The thin-flame position is predicted with large errors by the *BF* model. However, the errors in the overestimation of flame position by the *F–S* model seems not to be large. With Schmidt number equal to unity the Exact model underestimates the thin-flame position. Further, with consideration of $Sc \neq 1$, there is a possibility of good estimation of the thin-flame position by the Exact model.
4. The fuel and product concentration profiles are under and overestimated (respectively) by both the approximations when compared with the 'Exact' one.

It is a pleasure to thank Dr. H. R. Nagendra for many helpful discussions on the numerical part of the study. Thanks are due to Mr. N. Ramani and Mr. A. G. Marathe for the heplful suggestions on the manuscript. Thanks are also due to the authorities of Indian Institute of Science for the sanction of computer grants.

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Received April 26, 1971