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FREE CONVECTIVE COMBUSTION WITH VARIABLE PROPERTIES

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This paper treats the problem of free convective combustion of near vertical fuel surfaces in quiescent oxidant atmosphere, both theoretically and experimentally. The theory improves on existing theories in terms of taking into account variable thermodynamic and transport properties. The locally similar solutions obtained numerically are compared with earlier predictions as well as experiments on mass burn rate, flame stand off and other features. While comparison in the case of some fuels seems bettered by the use of variable properties, the not-too good a comparision in other cases is traced to experimental inaccuracies more particularly related to the non-achievement of steady combustion. To remedy this, an experimental apparatus was carefully designed and the results of these experiments show good comparison with theoretical predictions in all cases considered.

Introduction

Free convective combustion of near vertical fuel surfaces has been treated by several workers.[1–5] Kosdon et al[1] have solved the conservation equations for the burning of vertical plates using the similarity hypothesis. The predictions have been compared with experimental results on vertical cellulosic cylinders. While the flame stand-off is shown to behave qualitatively in the same way ($y_f \sim x^{1/4}$) in both the cases, quantitative comparison has called for suitable adjustment of wall mixture properties. The experimental stand-off behaves as

$$y_f \sim 0.0085\, x^{1/4} \quad (x, y \text{ in } m)$$

whereas the constant property theory gives

$$y_f \sim 0.0135\, x^{1/4}$$

The correct prediction of mass burn rate calls for the use of 700 cal/gm as effective heat of vaporization (L) and this is reported by Kosdon et al to be reasonable for α-cellulose. Consistent adjustment of transport parameters to yield better comparison of flame stand-off will in turn affect the mass burn rate. In fact, it is not possible to choose any meaningful set of parameters which permit simultaneous correct prediction of mass burning rate and flame stand-off within the frame work of the constant property theory.

Subsequently, Kim et al[2] formulated the problem in a similar manner and carried through the solutions as a function of various parameters by treating the Lewis numbers, $\rho\mu$ and $\rho\kappa$ as constants in the field. They also developed an expression for mass burn rate using a profile technique. This development has generally been accepted in combustion literature. The authors obtained similarity solutions for various cases and compared their results with experiments[3]. Table 1 summarizes the comparisons drawn from Fig 2 which is based on Ref 2.

As can be noticed, the predictions are different from theory by 45-80% in the case of benzene and toluene. In the case of methanol, the comparison is more satisfactory, with a deviation of about 20%. In the case of PMMA—O_2 and α-celluose—air, the theoretical predictions are coupled with experiments to determine the parameters B and L and to see if these are reasonable. In the case of PMMA—O_2, B and L are obtained as 4.18 and 714.5 cal/gm. In performing these calculations, the authors[2] use a fuel surface temperature of 325°C and a viscosity at wall equal to that of nitrogen at 395°C. These arbitrary choices of parameters are hard to justify. The parameters B and L from the literature[6] for plexiglas are about 8 and 325 cal/gm, respectively. Thus the estimates made by Kim et al[2] are substantially in error. Stated differently, the predictions of burn rates for plexiglas based on its known properties would be in significant error by a factor of $\ln(8 + 1) / \ln(4.18 + 1) = 1.34$

Kim et al[2] argue that their markedly higher

TABLE 1
Comparison of earlier theories and experiments.

Fuel	Benzene		Toluene		Methanol	
Method	*Gr'*	*A*	*Gr*	*A*	*Gr*	*A*
Expt.	4.8×10^8	167	8.5×10^8	150	10^8	100
Theory	4.8×10^8	244	8.5×10^8	271	10^8	120
Variation (%)	—	46	—	80	—	20

$Gr' = g_o\rho_w^2 x^3/\mu_w{}^2$; $A(x) = \frac{1}{\mu_w}\int_o^X m''\, dz$; see Fig 2 also.

burn rate predictions for heavy fuels like benzene and toluene are related to the low Lewis numbers in the fuel rich region. In discussing this point, they make several statements which do not explain the reasons for the discrepancy. Thus, the two principal features of the experiments, namely, the mass burn rates and flame stand-off are inadequentely explained by the current theories. In a work on liquid droplet combustion, Raghunandan and Mukunda[17] have shown that a substantial part of the discrepancies can be overcome by accounting for the variable property effects, particularly with respect to flame stand-off. Later, Paul et al[18] showed that in the case of forced convection boundary layers, the burn rate dependence on fuel could be predicted only if the variable density effects of the boundary layer are properly accounted for. In the present case also, it is felt that a consistent theory which accounts for variable thermodynamic and transport properties would remove the ambiguities connected with the choice of properties at several places, as well as improve the predictions.

In the next section, a theory is based on free convection under diffusion limited conditions with thin flame approximation is presented. A single step reaction is assumed allowing for the possibility of five or six species. For most of the cases considered the elements are C,H,O and N. N_2 is treated as inert and the products considered are CO, CO_2 and H_2O. It is assumed that C goes to equal molar fractions of CO and CO_2. This is done so that the temperatures obtained from the thin flame approximation are not unrealistic in the case of hydrocarbon—O_2 systems. In the case of hydrocarbon—air flames, the problem is not serious and one can take the stoichiometric reaction leading to CO_2 alone since the temperatures predicted from the thin flame approximation are quite realistic. The assumed stoichiometry has less effect on mass burn rate than on flame temperature. The effect of fuel cracking, which is relevent in a few of the cases considered, has been ignored because the effects felt through thermodynamic and transport property variation are expected to be small.

Two models for diffusion have been tried, namely, the trace diffusion and the multicomponent formulation of diffusion fluxes.

The governing equations are treated by the similarity hypothesis and the various thermodynamic and transport property effects appear as variable co-efficients of the terms.

The question of similarity of solutions has been discussed earlier by Kosdon et al[1] in response to a question by Sirignano. The present work departs from the earlier work only to the extent of variable properties. Since the thermodynamic and transport properties are functions of dependent variables which follow similarity, it can be expected that similarity of solutions is as good an approximation to reality as in the earlier works[1,2].

Theory:

The model is a burning surface that is semi-infinite in *x* and *y* directions and infinite in the *z*-direction, like in the models described in Refs 1 and 2. The essential assumptions are that:

(1) Two-dimensional laminar boundary layer approximations are valid; (2) reaction rates are large compared to diffusion rates resulting in thin flame, and all further implications are assumed to hold; and (3) the inclination of the surface to the vertical (ϕ) is small enough to render normal (*y*-direction) momentum equation trivial. (An order of magnitude analysis of momentum equations reveals that the presently reported methodology is valid for about $\phi = \pm 10°$. Though this kind of limit is somewhat tentative the authors believe that the methodology can not be valid for angles as large ± 87° as suggested in an earlier work[2]).

Further, negligible temperature and pressure gradient diffusion, single step chemical reaction and negligible radiant heat transfer are assumed.

Under the above conditions the governing equations of conservation can be written as[13]

mass:

$$(\rho u)_x + (\rho v)_y = 0 \qquad (1)$$

momentum (x − direction):

$$\rho u(u)_x + \rho v(u)_y = [\mu\ (u)_y]_y + g_o \cos\phi\ (\rho_\infty - \rho) \qquad (2)$$

energy:

$$\rho u\ c_p\ (T)_x + \rho v\ c_p\ (T)_y = [k\ (T)_y]_y + \Sigma c_{pi} D_i\ \rho(Y_i)_y(T)_y \qquad (3)$$

species:

$$\rho u(Y_i)_x + \rho v(Y_i)_y = [D_i\ \rho(Y_i)_y]_y \qquad (4)$$

where subscripts x and y refer to partial differentiation with respect to x and y.

The equation of state is,

$$\rho T/M = \rho_\infty T_\infty / M_\infty \ (5)$$

The single step reaction is represented by

$$\nu_F F + \nu_o O + \nu_I I \rightarrow \nu_P P + \nu_I I + Q \qquad (6)$$

The boundary conditions which the solution of these equations should satisfy are:

At the wall ($y = 0$), $u = 0$, $T = T_s$ (constant known) (7)

at infinity ($y = \infty$)

$$u = 0,\ T = T_\infty,\ Y_O = Y_{O\infty},\ Y_I = Y_{I\infty} \qquad (8)$$

at the flame ($y = y_f$),

$$Y_F = Y_O = O \text{ (thin flame)} \qquad (9)$$

the surface gradient conditions

$$\rho D_F(Y_F)_y\}_{\,y\,=\,0} = \dot{m}''\ [Y_F(0^+) - Y_F(0^-)] \qquad (10)$$

$$\rho D_I(Y_I)_y\}_{y=0} = \dot{m}''\ Y_I(0^+) \qquad (11)$$

$$\dot{m}''\ (\rho v)_{\,y=0} = \tfrac{1}{L}\ k(T)_y\}_{\,y=0} \qquad (12)$$

and the flame interface conditions

$$-D_F\rho(Y_F)_y\Big\}_{y_f^-} = \frac{D_0\rho}{i}(Y_0)_y\Big\}_{y_f^+} \qquad (13)$$

$$k(T)_y\Big\}_{y_f^-}^{y_f^+} = -\frac{Q}{i}D_0\rho(Y_0)_y\Big\}_{y_f^+} \qquad (14)$$

In order to obtain a complete solution to the problem, equations (1) through (5) have to be solved for ρ, u, v, T, Y_F, Y_O and Y_I subject to the boundary conditions mentioned above. This is accomplished by employing the similarity hypothesis.

Define a similarity variable η such that

$$\eta = K_1 x^{-1/4}\int_0^y \rho\, dy$$

$$\text{where } K_1 = \left[\frac{Lg_0 \cos\phi}{4c_{pw} T_\infty \rho_w^2 \mu_w^2}\right]^{1/4} \qquad (15)$$

and a similarity function f, such that

$$\psi = K_2 x^{3/4} f(\eta)$$

$$\text{where } K_2 = 2\left[\frac{4Lg_0 \cos\phi \mu_w^2}{c_{pw} T_\infty \rho_w^2}\right]^{1/4} \qquad (16)$$

where ψ is the stream function such that

$$\rho u = \rho_w \frac{\partial\psi}{\partial y}, \quad \rho v = -\rho_w \frac{\partial\psi}{\partial x}. \qquad (17)$$

Further, defining similarity functions for temperature and mass fractions,

$$(T - T_\infty)/T_\infty = g(\eta)$$

$$Y_i = s_i\ (\eta), \qquad (18,\ 19)$$

the equations and boundary conditions can be transformed. Now the boundary condition at the flame becomes

$$s_F(\eta_f) = s_O\ (\eta_f) = 0 \qquad (20)$$

where

$$\eta_f = K_1\ x^{-1/4} \int_O^{y_f} \rho\ dy \qquad (21)$$

and y_f determines the flame position at any x.

The difficulty arising out of the boundary condition being set at an apriori unknown position (since y_f should come out as a solution of the equations) is obviated by a further linear transformation $\xi = \eta/\eta_f$.

The transformed equations are:

$$f''' + cf'' + 3a\eta_f ff'' - 2a\eta_f (f')^2 + \eta_f^3 \frac{b}{M}(gM_\infty + M_\infty - M) = 0 \quad (22)$$

$$g'' + 3\,\mathrm{Pr}\, a\eta_f fg' + dg' + \sum_{i=F/O,I,P} \frac{c_{pi}}{c_p} Le_i \zeta_i' g' = 0 \quad (23)$$

$$s_i'' + 3Sc_i f\, S_i' + e_i\, S_i' = 0 \quad (24)$$
$$i = F/O,\ I$$

where the prime denotes the differentiation w.r.t.ξ& a, b, c, d, e_i are given by

$$a = \frac{(\rho\mu)_w}{\rho\mu}, \quad b = a\frac{c_{pw}T_w}{L}, \quad c = \frac{d}{d\xi}(\ln \rho\mu),$$
$$d = \frac{d}{d\xi}(\ln \rho k), \quad e_i = \frac{d}{d\xi}(\ln \rho^2 D_i) \quad (25)$$

Further, the transformed boundary conditions become

$$f'(0) = f'(\infty) = g(\infty) = 0,\ g(0) = (T_s - T_\infty)/T_\infty$$
$$s_F(1^-) = s_0(1^+) = 0,\ s_0(\infty) = y_{0\infty}\ s_I(\infty) = Y_{I\infty}$$
$$s'_F(0) = -3\eta_f\, Sc_{Fw} f(0)\, \{s_F(0^+) - s_F(0^-)\}$$
$$s'_I(0) = -3\eta_f\, Sc_{Iw}\, f(0)\, [s_I(0^+)],\ g'(0) = -\frac{3\mu_w L}{k_w T_\infty}\eta_f\, f(0) \quad (26)$$

and the interface conditions would be,

$$s_F'(1^-) = -\frac{D_0}{iD_F} s_0'(1^+)$$
$$g'(1^+) - g'(1^-) = -\left[\frac{D_0 \rho Q}{ikT_\infty}\right]_f s_0'(1^+) \quad (27)$$

Now the task is to solve the transformed equations and then obtain from them the physical variables. This has been accomplished by numerical computation.

Numerical Solution:

As can be readily seen, the problem is a non-linear β-point boundary value problem. The method of solution employed in the present work is similar to Radbill's[7]. The equations and boundary conditions are linearized and then solved iteratively as a linear boundary value problem. The non-linear terms involving η_f are also linearized. As can be noted, the total order of equations is 9 (counting only one equation for fuel and oxidizer) and there are ten boundary conditions available; the extra condition leads to calculation of η_f.

The numerical integration was carried out using the Gill modification of the Runge-Kutta method. The initial solution was estimated, based on known solutions for simpler cases. The thermophysical and transport properties were obtained from available methods of estimation[8,10].

It was found that the solution was weakly oscillating and diverging. This was remedied by relaxing the newly obtained solution by a factor of 0.5, that is a new iterate = 0.5 (previous iterate) +0.5 (present solution). On a convergence criterion of 0.1% on $f(0)$, the iteration scheme converged in about 20 iterations taking a CPU time of about 50 seconds on the Dec-1090 system.

Results and Discussion:

Table 2 shows the various thermodynamic and transport parameters chosen for computation. As stated earlier, the product is assumed to consist of CO, CO_2 in equal molar fractions and H_2O. Calculations have also been made in some cases with CO_2 as the only product of oxidation of carbon. The models used for diffusion are (*i*) trace diffusion approximation and (*ii*) strict multicomponent diffusion. The use of trace diffusion approximation yielded negative mass fractions for products near the surface (~−0.1). It was therefore discarded and the model with a single term in the Sonine polynomial expansions was used and all results presented here are based on this method. A careful examination showed that a trace diffusion model should be used with care especially when the number of species is small. (Heimerl and Coffee[20] note that for the computation of flame speeds in HNO systems the choice of the diffusion model does not seem critical. This has also been the experience in H_2-O_2 systems[21].)

The various results of computation, the results of present experiments and their comparison with the earlier experiments and present theory are shown in Table 3. For the constant property case, $\mu = 3.0 \times 10^{-5}$ kg/m.s, $\rho = 0.55$ kg/m^3 $Pr = 0.73$ and $cp = 0.36$ kcal/kg K have been used which roughly corresponds to properties of nitrogen at 300°C. As can be noticed from the table, the wall density varies by a factor of two, wall viscosity is not very different from 1.1×10^{-5} kg/m.s in most cases, excepting for α-cellulose—air and PMMA-O_2 systems; the transfer number varies by a factor of five for the systems considered.

Variable properties do not alter the predictions on mass flux for methanol but they do for benzene, as can be seen from Table 3 (columns 8 and 10). The burn rate predicted is 30%

TABLE 2
Thermodynamic and Transport Properties and References.

Fuel	Q Kcal/Kg	L Kcal/Kg	i	T_s, K	ϵ/K	σ	$c_{p,\text{ gas}}$
Methanol	3712[14]	285.2[3]	1.25	337.6[3]	507.0[8]	3.58[8]	9
Ethanol	4950[14]	235.2[23]	1.74	351.4[23]	391.0[8]	4.45[8]	9
Acetone	5083[14]	140.5[3]	1.79	329.8[3]	379.0*	4.90*	11
Benzene	7010[14]	115.7[3]	2.46	353.2[3]	440.0[9]	5.27[9]	9
Toluene	7128[14]	117.0[3]	2.52	383.6[3]	447.3*	5.58*	11
Xylene	7288[14]	123.1[3]	2.57	403.1[3]	463.6*	5.79*	*T*
Gasline	8408[3]	133.5[3]	2.89	423.1[3]	486.6*	6.07*	*T*
Kerosene	7876[3]	175.5[3]	2.91	523.5[3]	601.6*	6.73*	*E*
PMMA-air	4265[15]	325.0[6]	1.52	600.0[6]	430.1*	5.50*	*T*
α-cellulose	3053[1]	700.0[1]	0.8	648.0[1]	507.0[M]	3.58[M]	*M*

T, E, M = > close to the values of Toluene, Ethanol, Methanol respectively.
* Estimated from approximate formulas available in Ref.8.
Numbers on the top of the values indicate references.

lower in the case of variable properties compared to constant properties; the flame stand off is also smaller in the variable property theory. To determine the probable cause, the various quantities in the equations are plotted against distance in Fig 1. One notices that except for specific heat, the variation of properties for benzene is much greater than for methanol. The Lewis number diverges from unity significantly. It has been argued[2] that low Lewis numbers of heavy fuels are responsible for the discrepancy between measurements and theory. The Lewis number for heavy fuels seen in Fig.1 is, in fact, more than unity in some regions and goes below unity near the flame. The peculiarity is due to the multicomponent environment provided by inerts and products generally tending to increase the diffusivities of the heavier fuels. Thus the interpretation that lower Lewis numbers are responsible for the reduced burn rate would not be correct. All that can be stated is that the combined variation of Lewis numbers and other mixture properties are responsible for the observed behaviour.

Figure 2 and Table 3 (columns 8, 10 and 11) show a comparison between the predictions of the present theory and some experimental result[2,3], along with the results of earlier theory[2]. The computed burn rates and other parameters were nondimensionalised, using the density and viscosity of nitrogen at the wall temperature, since this seems to be the procedure used in Ref.2. to prepare the plots. (The original data were unavailable to us as they seem to result from work by Kanury Murty, privately communicated to the authors of Ref.2) The predictions of the present theory compare very well with the data for PMMA-O_2 and methanol-air, and are indisputably better than those of earlier theory in the case of benzene and toluene. As can be readily seen from Table 3, the results of the constant property theory compare reasonably well with experiments only for lighter fuels like methanol and acetone. For other fuels, the experimental results are much'lower- as low as half of the theoretical predictions in some cases. Even with the variable property predictions, the comparisons with experiments of Perry et al[3] are not very satisfactory for heavier fuels. After a careful review of the theoretical predictions and experimental results, it was thought that the experimental results could be in error particularly for heavier fuels.

In the experiments of Perry et al[3] the burn rate measurements were made with fuel soaked

TABLE 3

Results of computations and comparison with experiments

1	2	3	4	5	6	7	8	9	10	11	12	13
						Variable properties		Constant properties		previous experiment	present experiment	%error present theory & expt. in $\dot{m}''_{av}$
Fuel	$-f(o)$	ρ_w	$\mu_w \times 10^5$	$k_w \times 10^6$	B	$y_f/x \times 10^3$	$\dot{m}''_{av} \times 10^3$	$y_f/x^{1/4} \times 10^3$	$\dot{m}''_{av} \times 10^3$	$\dot{m}''_{av} \times 10^3$	$\dot{m}''_{av} \times 10^3$	
Methanol	0.30	1.08	1.35	6.40	2.57	12.0	13.0	14.4	13.1	16.7[3]	15.00	−13.30
Methanol ($\alpha = 0$)	0.315	1.10	1.33	6.30	2.75	13.3	13.6	—	—	—	15.00	− 9.30
Ethanol	0.291	1.32	1.27	5.90	2.73	12.1	13.0	16.9	15.3	—	15.00	−13.30
Acetone	0.370	1.73	1.10	4.80	4.61	12.8	15.6	18.7	20.2	19.0[3]	15.90	− 2.00
Benzene	0.370	2.02	1.13	4.50	5.58	13.9	16.7	21.4	24.4	15.8[3]	16.50	1.20
Benzene ($\alpha = 0$)	0.384	2.08	1.11	4.40	6.14	15.0	16.9	—	—	—	16.50	2.50
Toluene	0.361	2.03	1.20	5.30	5.38	13.4	16.4	21.6	24.5	14.8[3]	15.70	4.50
Xylene	0.344	2.08	1.26	5.40	5.10	13.6	15.4	21.7	23.5	12.8[3]	14.30	7.70
Kerosene	0.286	1.73	1.47	6.90	3.15	11.6	14.1	21.2	20.1	10.0[3]	16.50	−14.50
α-Cellulose	0.157	0.53	2.55	14.10	1.08	8.2	8.0	10.2	9.4	7.5	—	—
PMMA—O_2	0.416	1.32	1.87	10.70	7.79	10.9	23.1	20.1	29.0	24.0[2]	—	—
PMMA—air	0.204	1.06	2.14	10.60	1.69	10.2	11.2	15.6	12.1	10.4[19]	—	—

[average mass flux over 0.1 m height on liquid experiments $\alpha = 0$ refers to oxidation to CO_2 only]

Numbers in the top right corner of column 11 indicate references from which data are drawn.

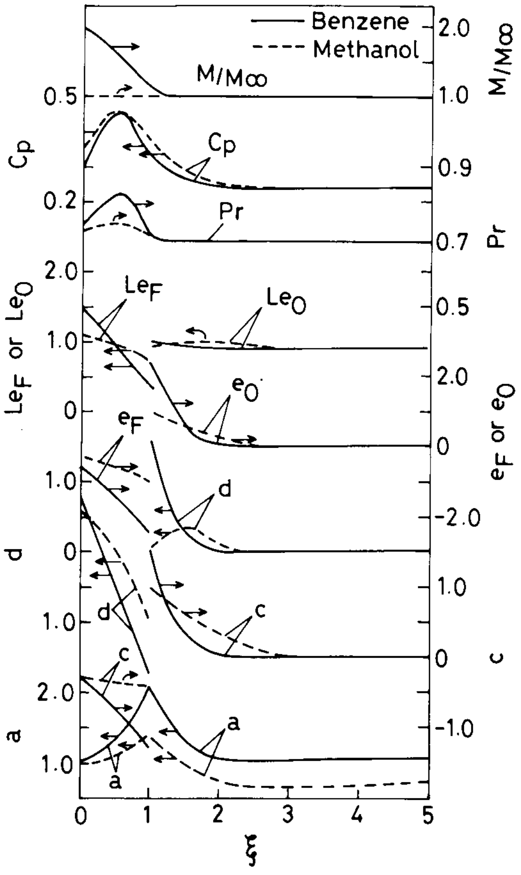

FIG. 1. Variation of mixture properties with normalized distance.

wicks simply held in air. The thickness of the wick is not specified. In a few trial experiments on 10mm thick porous wick made to appreciate the situation, the observable change in the flame shape was found to take about 6–8 minutes when the fuel supply was completely cut off. Hence one cannot assert that the burning surface was kept wet throughout the six minutes period. If one were to wait a reasonable time to reach steady-state conditions, such a state would be reached when the surface region carry only vapors and the measurements belong to a lower transient burn rate. It was, therefore, decided that careful experiments be conducted to establish steady-state behavior.

Present Experiments

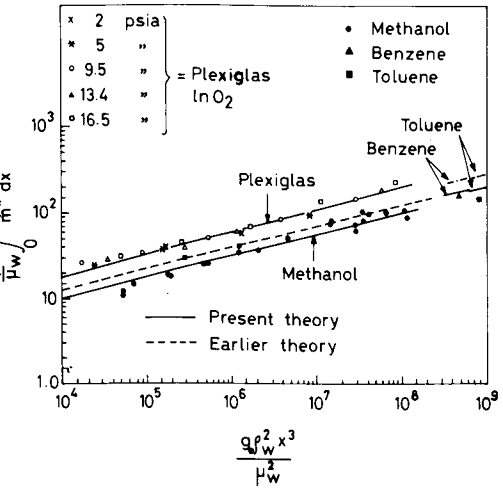

FIG. 2. Comparison with earlier theory, experiment and present theory. 1. Comparison with earlier theory and experiment. 2. Thermodynamic and transport properties and references. 3. Results of computations and comparison with experiments.

After several initial trials, it was decided that the apparatus must be chosen so that any change in flow rate would show an effect in a minute or a minute and a half. It would have been difficult to visually assess the steady nature otherwise, this would call for a thin wick. It was also clear that it should be made of ceramic to withstand reasonably high surface temperatures. Based on these considerations, a 3mm thick ceramic wool pack in a metallic open box, 120mm high and 60mm wide was chosen. The metallic plates were backed with asbestos sheet to prevent heat loss and the whole structure was imbedded in a large asbestos sheet in order to prevent curving of the flame at the edges. Fuel was supplied at controlled rates from the back, at the top through nine thin tubes. The flame reached a steady state in about five minutes. The observable response time of the system to a step disturbance was about one and a half minutes. Measurement of steady flow rates indicated that it could be found in a range, the lower limit of which corresponded to a state where the wick is just burning full; the higher limit corresponding to a condition when the fuel is just about to flow past the wick. In the case of heavier fuels like Xylene, obtaining steady conditions of combustion turned out to be more difficult. To facilitate obtaining good steady conditions, the fuel was fed through 9 tubes at two levels—one at 5-cm height, the other at 11.5 cm height, both flow rates were independently controllable. With this change, the combustion behavior could be well controlled towards obtaining steady conditions.

Measurements using a 0.1 mm chromel-alumel thermocouple showed that at the upper limit of the burn rate, the surface temperature is about 5°C below the boiling point of the liquid. At the lower limit, the surface reached values as much as 30°C-40°C above the boiling point. The upper limit was characterized by the flame curving at the lower end of the wick. Also, at this flow rate the color of the flame would be reddish yellow, whereas it would be bluish yellow at the lower limit. Because of the finite resistance of the wick to downward flow of the liquid, the surface would be "superwet" at the upper region of the wick, resulting in slight loss of the two-dimensionality of the flame. This was clearly observed in the case of benzene, toluene and xylene, when the fuel was fed only at one level. The fuel would "prefer" to burn at the top rather than flowing down. The above facts which are an average of the two end values were taken as the steady burn rate. The present experimental results on mass flux are included in Table 3. It is clear that the mass flux values from the present experiments are much higher than the earlier ones. The present theoretical values show much better agreement with the experiments. This is an interesting observation, when one notes that the constant property theory shows an increase in burn rate, and in the earlier experiments, the burn rate of fuels of higher molecular weight decreased. The present results which show near-independence of the burn rate with respect to fuel characteristics are a consequence of the influence of a combination of different properties.

While the average difference between the present theory and experiments is less than 10%, the worst difference amongst the cases examined is 15%.

A comparison for PMMA cylinders burning in air is also shown in Table 3. Using the results available in Ref(19), m''_{av} is obtained for a typical cylinder of length 0.1m (and diameter = length/3) by logarithmic interpolation. The prediction agrees well with the experiment with the prediction, being 7% higher than the measured value. A final comparison is for the flame stand-off distance in the case of α-cellulose. The effective value of L has been estimated, using the burn rates of Kosdon et al(1), as 770 cal/g. The corresponding flame stand off is predicted by the present theory as $y_f = 0.0082\ x^{1/4}$ (x,y in m) and the photographic measurements[1] suggest $y_f = 0.0085\ x^{1/4}$. The constant property prediction[1] is $y_f = 0.0135\ x^{1/4}$. The flame stand-off distance prediction of the variable property theory is not new and has been strikingly demonstrated much earlier out in the case of liquid droplet combustion theory.[17]

Conclusions

Inclusion of the Lewis number and variable property effects into the model is marked by improved predicted burn rates, especially in the case of fuels of higher molecular weight. It is shown that the reduction in burn rates from constant property theory to variable property theory in the case of heavier fuels is due to the difference in mixture properties. The predicted burn rates diverge from the measured burn rates by a maximum of about 15%.

Flame stand-off also is predicted quite accurately by the present theory. Thus the importance of including variable property effects in vertical free convective burning is evident.

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Nomenclature

Symbol	*Meaning*	*Units*
B	Transfer number $(Y_{o\infty}Q/iL) - (h_{vap}/L)$	—
c_p	Specific heat of the gas mixture	kcal/kg K.
c_{pi}	Specific heat of i^{th} component	kcal/kg K
D_i	Multicomponent diffusion co-efficient of i^{th} species	m^2/sec
g_o	acceleration due to gravity	m/sec^2
Gr	Grashof number $g_o x^3 \rho^2 (T - T_\infty)/\mu^2 T_\infty$	—
h	Specific sensible enthalpy of gas mixture (Ref. 298. 15°K)	kcal/kg
h_i	Specific sensible enthalpy of i^{th} component	kcal/kg
h_{vap}	Specific sensible enthalpy of gas mixture at vaporising temperature	kcal/kg
h_{fg}	latent heat of phase change from liquid to gas	kcal/kg
k	Thermal conductivity (gas phase)	kcal/m sec K
i	Stoichiometric ratio $- M_o\nu_o/M_F\nu_F$	
L	Effective heat of vaporization $= h_{fg} + c_{pi}(T_s - T_\infty)$	kcal/kg
L_{ei}	Lewis number $= D_i\rho c_p/k$	—
M	Molecular weight	
$\dot{m}''$	Burn rate per unit area	Kg/m^2 sec
P	Pressure	N/m^2
Pr	Prandtl number	—
Q	Heat of combustion per unit mass of fuel	kcal/kg
R	Universal gas constant	kcal/mole K
S_c	Schmidt number	—
T	Temperature	K
u	Velocity in x-direction	m/sec
v	Velocity in y-direction	m/sec
x	Parallel co-ordinate (along vertical)	m
y,z	Normal and transverse co-ordinates	m
Y_i	Mass fraction of i^{th} species	—
y_f	Flame stand-off	m

Greek Symbols:

ρ	density	kg/m^3
μ	obsolute viscosity	kg/m sec
ν	stoichiometric co-efficients	—
τ	$= h_{vap}/L$	—
ϕ	angle of inclination of the surface to the vertical	—
η_f	non-dimensional flame stand-off	—

Subscripts:

f	flame
i	i^{th} component
w	Wall
s	surface (same as wall)
∞	ambient
I	Inert
F	Fuel
O	Oxidizer
P	Product

COMMENTS

M. M. Hirschler, B.F. Goodrich, USA. In some work we have done on flows down a corridor, we have been able to determine that there is mass transfer from the upper layer to the lower layer (F. M. Galloway and M. M. Hirschler, ASTM Symp. on Mathematical Modeling of Fires and Related Test Methods, Dec. 1986, New Orleans, LA.). I wonder why you did not include mass transfer down in your model.

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M. A. Delichatsios, Factory Mutual Research, USA. One may consider the case of abrupt change of ambient temperature from 25° C to 200° C. In that case, one expects that a negative velocity will be developed at the edge of the boundary layer near the transition region. Do your boundary layer equations and their solution allow for negative velocities?

Author's Reply. Our mathematical model does indeed allow flow reversal and temperature inversion in the boundary layer. In case of the step (two-layer) stratification, velocity profiles show negative vertical velocities and the temperature dips below the ambient value in the outer region of the boundary layer *above* the lower layer. The temperature inversion region is narrower than the flow reversal region. However, mass transfer from the upper layer to the lower layer cannot be handled by this "boundary layer" model because the equations are parabolic and therefore disturbances in flow or temperature cannot be "felt" upstream. The boundary conditions far away from the wall are always maintained at $u = O$ and $T = T_\infty(x)$.

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R. G. Gann, National Bureau of Standards, USA. In developing this type of model, especially the "upper layer" portion, it is critical to keep in mind the impact of *realistic* materials combustion properties.

As oxygen is consumed in the lower part of the flame, the fuel pyrolyzed above will burn slower, extending the flame front both in thickness and in distance from the wall. In addition, as the oxygen decreases, the nature of the combustion products changes (e.g., less CO_2, more CO and partially burned fuel) and the effective heat of combustion will drop. I expect these factors will dominate the rates of fuel consumption, energy release and chemical species generation.

The latter is especially important in predicting the onset of upper layer burning and flashover.

Author's Reply. Our model takes into account the effect of changes in the ambient oxidizer concentration due to stratification on the burning rate and flame stand-off distance from the wall, as long as (a) the chemical reaction rate remains much higher than the oxidizer diffusion rate and (b) the combustion products remain unchanged. When there is incomplete combustion and/or relatively slow chemical reaction rates, these factors can significantly affect the overall wall fire characteristics as pointed out in the question. With minor modifications in the model, the effects of these factors can be studied. However, we also discovered in this analytical study that the convective transport of the oxidizer from the lower, oxidizer-rich layer, is strong enough to continue the fire vigorously up to a certain distance downstream, shielding the effect of the oxidizer-lean upper layer. Of course, the model is laminar, and therefore the actual extent to which the upstream memory (in terms of oxidizer concentration) will last needs to be investigated further, which is currently in progress.

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C. Fernandez-Pello, University of California, Berkeley, USA. I am concerned about how realistic is the present formulation of the model, in particular the boundary conditions at the boundary layer edge, in its attempt to describe the burning of the back wall in a compartment fire. In a practical case, it is very unlikely that a still stratified layer will be formed at the back wall (or for that matter at any wall) of the compartment. For example, the recirculation flow in the compartment will generate an upward flow near the wall that will influence the character of the boundary layer (from free to mixed convection), and will disturb the temperature and composition distribution. Other potential sources of disturbances are the entrainment of gas by the boundary layer flow and effects related to buoyancy-generated local recirculations.

Author's Reply. While it is true that in the realistic case of a compartment fire there will be recirculation patterns instead of a quiescent atmosphere in the interior, the actual flow direction and magnitudes will depend on a number of parameters which can differ drastically from case to case. There can be an upward flow near the wall as pointed out in the comment above, or a negatively buoyant downward flow mentioned by other investigators. Therefore, we believe the problem of a wall fire in a stratified atmosphere must be first understood for the simple case of a quiescent atmosphere, and then it may be extrapolated to a specific case. Furthermore, the recirculation flows in the compartment interior, which are usually buoyancy-driven, will not be very high velocity flows. Under those circumstances, the boundary layer structure of the wall fire will be preserved and the low velocity external flow will not have a great effect on some of the important characteristics, such as the local burning rate, as long as the ambient stratification is not significantly disturbed. We made some preliminary calculations for the wall fire with an external upward flow. When the upward velocity ouside the boundary layer was 10% of the maximum velocity inside the boundary layer, the burning rate changed by less than 1.5%. The effect of the nonzero velocity boundary condition on the stratification (temperature and composition distribution) is beyond the scope of the present investigation; however, it is an important related problem.

T. Kashiwagi, National Bureau of Standards USA. The existence of a similar solution is assumed in the model. This is only true when $\dot{m} \sim 1/x^{1/4}$. Was $\dot{m} \sim 1/x^{1/4}$ demonstrated in your experiments with various fuels?

Author's Reply. No measurements of the mass burning rate as a function of x have been made in our experiments; only the average burn rates were obtained. Measurements of $\dot{m}''$ vs x in some of the earlier experiments (Ref. 2 of the paper) show $\dot{m}'' \sim x^{-0.25}$. The flame stand-off measurements of Kosdon et al. (Ref. 1 of the paper) also show $Y_f \sim x^{0.25}$.

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J. deRis, Factory Mutual Research, USA. Could you explain in simple terms the principal reason why your predicted variable property mass transfer rates are smaller for higher molecular weight fuels.

It should be pointed out that aromatic fuels such as benzene, toluene, and xylene have highly radiative flames—even for small, laminar situations. In the case of simple candle flames burning in air at their smoke point, the flames typically release 30% of their energy in the form of radiation. It would be both interesting and important to know how much this flame radiation is reduced by the presence of an adjacent, vaporizing wall.

For larger scale turbulent flames, the presence of a vaporizing wall significantly reduces the flame radiation.

Author's Reply. Efforts to trace the effects of variable property to one of the features like the diffusivity of fuel show that no one property is responsible; they are due to a combination of effects. A related point quite often not appreciated in combustion investigations is that the effects of Lewis number are complex. It is found in this study as well as in the case of droplet combustion (Ref. 17 of the paper) that increasing fuel Lewis number causes a decrease in burn rate rather than the opposite. Also, the Lewis number itself varies from values larger than unity to less than unity. In light of this, it is appropriate to conclude that a combination of effects of thermodynamic and transport properties is responsible for the results obtained.

The radiant heat flux to the surface can be estimated if the flame emissivity (ϵ) and the mean effective temperature at which radiation is emmited (T_m) are known. For the situation under consideration, the data presented by Yuen and Tien[1] indicates an emissivity of about 0.0012 for a flame thickness of 1 mm and a mean temperature (T_m) of about 1500 K. This is confirmed by Markstein[2] also. However, Blackshear and Murthy (Ref. 3 of the paper) report a measured ϵ ranging from 0.0026 to 0.0039 for benzene. This is in reasonable agreement with the total emissivity for gas-soot mixtures presented by Taylor and Foster[3]. Taking the higher of the values, $\epsilon = 0.004$ and $T_m = 1500$°k, the radiative flux would be about 15% of the convective heat flux, and this would alter the mass burn rate by about 6%, which lies within the range of uncertainties in measurements and predictions of mass burn rate.

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