New Formulation for One-Dimensional Premixed Flames

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Abstract

A NEW formalism that brings out the wave character of flame propagation of one-dimensional flames has been explicitly presented for simple as well as complex kinetics and realistic diffusion. While the combustion literature has accepted the idea of a combustion wave, this is the first time that the equations expressing this feature mathematically have been presented. The governing equations are shown to have a strong conservation form suitable for numerical computation. They are solved for a single-step reaction using the two-step MacCormack explicit scheme and are shown to be very fast compared to the unsteady computational technique. Compared to the unsteady technique, application of the same numerical scheme to complex kinetics seems to be numerically less efficient.

Contents

For the case of a single global step, the equation to be solved for obtaining flame speed and flame structure can be shown to be

$$\frac{\partial T}{\partial t} = \frac{k}{\rho c_p} \frac{\partial^2 T}{\partial x^2} + \frac{\dot{w}'''}{\rho} \frac{H}{c_p} \tag{1}$$

where T is the temperature, H the heat of reaction, $\dot{w}'''$ the reaction rate, ρ the density, $k/\rho c_p$ the thermal diffusivity, and t and x the time and distance coordinates, respectively. The boundary conditions are that $T(x \rightarrow -\infty, t) - > T_{-\infty}$ and $T(x \rightarrow \infty, t) \rightarrow T_\infty$. In the laboratory-fixed coordinates, integration of Eq. (1) gives a propagating flame.[1] The crux of the present method is in transforming the variables $(T; x,t)$ into $(P = dT/dx; T, t)$.

By using the theory of partial differentials, Eq. (1) can be transformed to

$$\frac{\partial}{\partial t}\left(\frac{1}{P}\right) + \frac{\partial G}{\partial T} = 0 \tag{2}$$

$$G = \frac{k}{\rho c_p}\left(\frac{\partial P}{\partial T}\right)_t + \frac{\dot{w}'''}{\rho c_p} \frac{H}{P} \tag{3}$$

The boundary conditions on P are,

$$P = 0 \text{ at } T = T_{-\infty} \text{ and } T = T_\infty \tag{4}$$

The above transformation implicitly takes note of the monotonic variation of temperature from $T_{-\infty}$ to T_∞, a feature valid in adiabatic freely propagating flames. The steady-state analog of the method was presented by Spalding.[2]

Equation (2) is the one being sought and G represents the local speed of propagation of the flame. Under steady condi-

tions, $(\partial G/\partial T) = 0$ leads to constant G. This is identified with the flame speed S_u as follows. Assuming that Eq. (1) admits a steady propagating solution, we set $T = g(x - S_u t)$.

Observing that

$$\frac{\partial T}{\partial t} = -S_u g' = -S_u \frac{\partial T}{\partial x}$$

and

$$\frac{\partial^2 T}{\partial x^2} = g''$$

Eq. (1) reduces to

$$S_u g' = \frac{k}{\rho c_p} g'' + \frac{\dot{w}'''}{\rho c_p} H$$

Defining $P = g'$ and writing $g'' = P(dP/dg)$, the above equation gives

$$S_u = \frac{k}{\rho c_p} \frac{dP}{dg} + \frac{\dot{w}''' H}{\rho c_p P} \tag{5}$$

which is the same as Eq. (3).

The approach for treating complex kinetics is similar. The equations are

$$\rho \frac{\partial Y_i}{\partial t} = \dot{w}_i''' - \frac{\partial}{\partial x}(\rho V_i Y_i), \quad i = 1, \ldots NOS \tag{6}$$

and

$$\rho \frac{\partial h}{\partial t} = \frac{\partial}{\partial x} k \frac{\partial T}{\partial x} - \frac{\partial}{\partial x} \sum_1^{NOS} \rho V_i Y_i (h_i + h_i^0)$$

$$- \sum_1^{NOS} \rho \frac{\partial Y_i}{\partial t}(h_i + h_i^0) \tag{7}$$

where V_i is the diffusional velocity,

$$h = \sum_1^{NOS} (h_i + h_i^0) Y_i$$

the total enthalopy of the mixture.

The diffusional velocities are calculated from expressions given in Hirshfelder et al.[3] If we use the transformations

$$d\bar{t} = (\rho_u/\rho)dt, \quad \tau = (T - T_{-\infty})/(T_\infty - T_{-\infty})$$

$$P_i = (\partial Y_i/\partial x)_t, \text{ and } P_{NOS+1} = (\partial \tau/\partial x)_t$$

the vector equations of flame propagation become

$$\frac{\partial U}{\partial \bar{t}} + \frac{\partial F}{\partial \tau} = 0 \tag{8}$$

where

$$U = [P_i/P_{NOS+1}, \ P_{NOS}/P_{NOS+1}, \ 1/P_{NOS+1}]^T \tag{9}$$
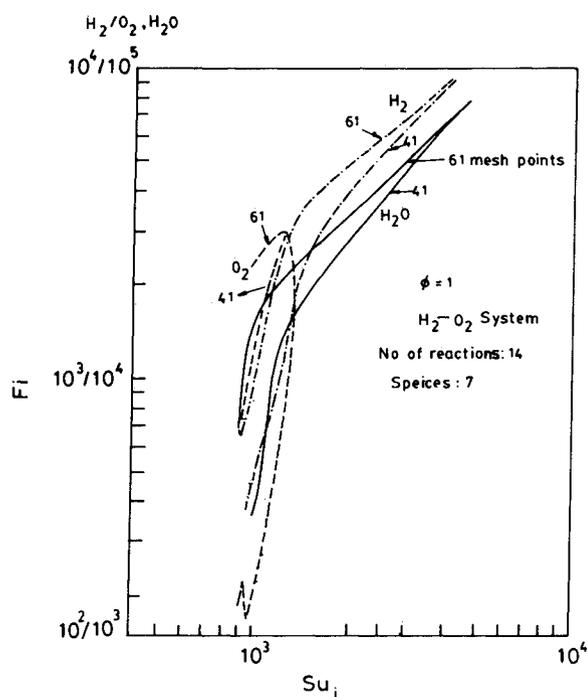
Fig. 1 F_i vs Su_i for 41 and 61 mesh points in τ.

$$F = [F_1, \ F_2..F_{NOS+1}] = [P_1(G_{NOS+1} - G_1),...P_{NOS}$$

$$\times (G_{NOS} - G_{NOS+1}), G_{NOS+1}]^T \tag{10}$$

$$G_i = \frac{1}{P_i}\left[\frac{\dot{w}_i'''}{\rho_u} - \frac{P_{NOS+1}}{\rho_u}\frac{\partial}{\partial \tau}(\rho V_i Y_i)\right] \tag{11}$$

$$G_{NOS+1} = \frac{1}{\rho_u c_P}\left[\frac{\partial}{\partial \tau}\left\{kP_{NOS+1} - \sum_1^{NOS} \rho V_i Y_i \frac{(h_i + h_i^0)}{(T_\infty - T_{-\infty})}\right\}\right]$$

$$- \sum_1^{NOS} \frac{(h_i + h_i^0)}{c_p(T_\infty - T_{-\infty})}\frac{P_i}{P_{NOS+1}}G_i \tag{12}$$

with

$$\tau = 0, \quad Y_i = Y_i^{-\infty}, \quad P_i = P_{NOS+1} \equiv 0 \tag{13}$$

$$\tau = \phi, \quad Y_i = Y_i^\infty \ (\text{equilibrium}), \quad P_i = P_{NOS+1} \equiv 0 \tag{14}$$

As in the earlier case, P_i and G_i are the dependent variables and t and τ independent variables. Steady state is obtained at $(\partial U/\partial t) = 0$ and, thus, $[F] = \text{const}$. These give $G_{NOS+1} = \text{const}$ and $P_i(G_{NOS+1} - G_i) = \text{const}$. The only general solution is

$$G_1 = G_2 = --- = G_{NOS+1} = S_u, \ \text{the flame speed} \tag{15}$$

In the classical numerical schemes, the flame speed S_u is obtained through integration of the steady equations of species from $-\infty$ to ∞ as

$$S_u = \int_{-\infty}^{\infty} \frac{\dot{w}_i'''}{\rho} \, dx / (Y_i^\infty - Y_i^{-\infty}) \tag{16}$$

Similar treatment of Eq. (11) gives

$$\int_0^1 V_i G_i d\tau = S_u(Y_i^\infty - Y_i^{-\infty}) = G_i(Y_i^\infty - Y_i^{-\infty}) \tag{17}$$

Thus, the equivalence between S_u and G_i is established at steady state.

Equation (2) for global kinetics and Eq. (8) for complex kinetics are expressions consistent with strong conservation form and numerical treatment of such forms is well understood in fluid flows. Further, the integration space is bounded between $\tau = 0$ and 1 in the transformed space. This is of

benefit in situations where adiabatic flame propagation is treated.

MacCormack's two-step explicit scheme is adapted for the numerical scheme. Initial tests were conducted on Eq. (2) with a choice of reaction rates such as

$$(\dot{w}_i'''/\rho)(H/c_p) = C_1 \sim \tau(1 - \tau^{n-1}) \tag{18}$$

For this case of functions, one can show that

$$P = \sqrt{C_1 (c_p\rho/k)}(1 - \tau^{n-1}) \tag{19}$$

and

$$S_u = \sqrt{(k\rho/c_p)C_1} \tag{20}$$

The expression for the reaction rate is realistic with n characterizing the activation energy parameter. It was first presented by Spalding.[2]

Computation starts with arbitrary profiles of P vs τ satisfying $P = 0$ at $\tau = 0$ and 1. Values of n of 2-10 have been tested. Calculations were made on a small microprocessor with a computational speed of 1/20th that of a main frame speed (DEC1090). Convergence to exact solution was always acquired in about 150-300 steps as long as the number of steps chosen is about 1½ times n with a minimum of about 7 steps. When the same problem was programmed as an unsteady integration scheme in the x coordinate [based on Eq. (2)], a DEC1090 was needed because of the storage requirements and the CPU time was 10 times longer. This is what prompted consideration of the complex reaction scheme problem using the same technique. The calculations showed several problems, including oscillations of profiles in time and the need for using a Schumann filter to eliminate the spurious oscillations and long integration times. Typically, 2000-2500 steps were required to obtain reasonable convergence and the CPU times for the schemes turned out to be probibitively large compared to the integration of the equations in the time-space coordinate. While the former needed about 60 min (CPU) for a 28 specie reversable reaction (14×2), a 7 specie H_2-O_2 system needed only 25 min. The latter technique used an operator split scheme with an implicit integration scheme for reaction and explicit for diffusion. Integration with the explicit scheme even for chemistry led to convergence, but an oscillatory of one in about 20 min CPU time.

A typical march toward steady state is shown in Fig. 1 where F_i, the error in the approach to steady state, is plotted against the flame speed of each of the species. It is seen that F_i decreases by orders of magnitude before the flame speed approach each other to near-constant values. The values of G_i along the flame are nearly constant in a region of $\tau = 0.2$-0.9 and are different beyond this range. Use of different initial profiles leads to differing values in the region beyond the range and has no effect on overall features such as flame speed, peak mass fractions of radicals, etc.

In conclusion, this work has presented a way of casting conservation equations for one-dimensional flames into wave propagation form. Coupled with MacCormack explicit scheme, the formulation leads to fast computation of the flame structure of a single-step reaction. The numerical scheme applied to problems of complex chemistry does not appear efficient compared to other techniques and there is need to explore other numerical schemes for this class of formalism.

References

[1]Emmons, H. W., "Fluid Mechanics and Combustion," *Thirteenth Symposium (International) on Combustion*, The Combustion Institute, Pittsburgh, PA, 1971, pp. 713-721.

[2]Spalding, D. B., "Predicting the Laminar Flame Speed in Gases with Temperature Explicit Reaction Rates, Parts I and II," *Combustion and Flame*, 1957, pp. 287-307.

[3]Hirshfelder, J. O., Curtiss, C. T., and Bird, R. B., *The Molecular Theory of Gases and Liquids*, John Wiley & Sons, New York, 1954.