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On the Theory of One-Dimensional Flame Propagation

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Seemingly contradictory results have been obtained for the dependence of linear burning velocity on heat transfer to the flame holder (1, 2).[2] Although the analysis of Emmons and collaborators does not allow a solution involving zero heat transfer to the flame holder, the Hirschfelder, Curtiss, et al., development gives, explicitly, a solution for this case. Detailed analysis of this problem shows, however, that the results are different only because different mathematical descriptions of the cold boundary condition are involved. We shall demonstrate this result for flame propagation without diffusion,[3] using the notation of Hirschfelder, Curtiss and collaborators.

Assuming a unimolecular decomposition, $A \rightarrow bB$, and using the appropriate equations for conservation of mass and energy, it can easily be shown that

$$\lambda/M(d^2T/dx^2) = (w_A C_{P_A} + w_B C_{P_B} - \frac{1}{M}(d\lambda/dx))(dT/dx) + [(h_B - h_A)/M] M_A B^0 \eta_A \exp(-A^0/RT) \quad [1]$$

where λ is coefficient of thermal conduction; M, mass flow (ρv); T, temperature, η_A, moles of A per cc. of mixture; B^0, frequency factor; A^0, activation energy; C_{PA} and C_{PB}, heat capacity at constant pressure of A and B; h_A and h_B, enthalpy per gram of A and B; ρ density; and $w_A = M_A\eta_A/\rho$, $w_B = M_B\eta_B/\rho$, where M_A and M_B = molecular weight of A and B.

From [1] we can obtain two different results depending on the formulation of the cold boundary conditions. The assumption used by Emmons and collaborators,

$$(dT/dx)_c = (d^2T/dX^2)_c = 0 \quad [2]$$

where the subscript c stands for cold boundary, implies,

$$M = \infty \quad [3]$$

since $M_A B^0(\eta_A)_c \exp(-A^0/RT_c) > 0$ and $(h_B)_c - (h_A)_c \neq 0$ for $b \neq 1$, i.e., for the only type of unimolecular reaction which can lead to flame propagation. In fact, for all reasonable reactions $b > 1$ and $h_B < h_A$.

If it is assumed that

$$(dT/dX)_c = 0 \quad [4]$$

Then finite values are obtained for M if and only if

$$(d^2T/dX^2)_c = [((h_B - h_A)/\lambda)B^0\eta_A \exp(-A^0/RT)]_c \quad [5]$$

This is essentially the boundary condition adopted by Hirschfelder and collaborators for the case of no heat input to the holder. It should be noted that the limiting conditions involved in [3] and [5] can be obtained without confusing the problem by division of dw_B/dx by dT/dx for cases in which either or both of these derivatives vanish.

From the preceding discussion, it is apparent that the boundary conditions imposed by these two groups of authors differ, and hence the results also differ. Physically, we see that Emmons and his collaborators analyzed the case of premixed gases flowing through a channel, with a reaction taking place all along the duct and combustion occurring at the region of very great reaction rate. Hirschfelder and his group, however, analyzed the case of gases instantaneously mixed at the flame holder.

An alternate set of boundary conditions which may merit a detailed study is the following:

$$(d^2T/dX^2)_c = 0, \quad (dT/dx)_c \neq 0, \quad (dw_B/dx)_c \neq 0 \quad [6]$$

Equation [6] implies, for unimolecular decomposition and constant specific heats, the relation

$$(dT/dx)_c = [(1 - C_{P_B}/C_{P_A})T_c B^0/v] \exp(-A^0/RT_c) \quad [7]$$

if the initial gas mixture contains pure component A. These boundary conditions will also give finite flame speed.

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[2] Refers to References at end of letter.

[3] The results are similar for flame propagation with diffusional transfer.

References

1 "Theory of Propagation of Flames," Part I by J. O. Hirschfelder and C. F. Curtiss; Part II by M. Henkel, W. Spaulding and J. O. Hirschfelder; Part III by N. Henkel, H. Hummel and W. Spaulding, Third Symposium on Combustion Flames and Explosion Phenomena, Williams and Wilkins, Baltimore, 1949, pp. 121–140.

2 "Thermal Flame Propagation," by H. W. Emmons, J. A. Harr and Peter Strong, Harvard University, Contract no. AT(30-1)-497, February 1950.