$$S_u = \sqrt{\frac{C_{i,m}\, X_{f,0} \sum_i k_i\, X_{i,b}\, D_{i,m}}{\theta_m^2\; X_p \qquad B_i}} \tag{9.23}$$

where $X_{f,0}$ = mole fraction of fuel in unburned gas

$\theta_m = 0.7\, T_b/T_u$

$X_{i,b}$ = calculated mole fraction of the $i^{th}$ active species at equilibrium flame temperature $T_b$

$D_{i,m}$ = diffusion coefficient for $i^{th}$ species into unburned gas at mean combustion zone temperature, cm²/s

$B_i$ = dimensionless factor (near unity) that allows for radical recombination.

Another equation has been derived by Manson[11] from an aerodynamic model of the combustion process, viz.,

$$\rho_u - \rho_b = \rho_u S_u^2 \left( \frac{\rho_u}{\rho_b} - 1 \right) \tag{9.24}$$

This equation does not include chemical kinetics. The flame chemistry enters only through $pX_H$, which has been substituted for the flame pressure drop. The final burning velocity equation is as follows

$$S_u = \sqrt{\frac{\rho_b}{\rho_u\,(\rho_u - \rho_b)} \quad \frac{p \cdot X_H\, T_u}{2\, T_b}} \tag{9.25}$$

where $p$ is the pressure (dyne/cm²) and $X_H$ is the mole fraction of H atoms in the burned gas. It is interesting to compare the burning velocities predicted by the Manson equation with that of the Semenov and Tanford-Pease equations. But the burning velocity predictions from the Manson equation are not as consistent as those from the Semenov or the Tanford-Pease equation. Figure 9.12 shows the comparison of predicted and experimental burning velocities.

Most of the experimental behaviour of flame velocities is predicted by the thermal mechanism, but the effect of increased burning velocities in the presence of hydrogen or water in the mixtures not having hydrogen is predicted by the diffusional mechanism. Similarly, the effect of the interchanging argon and helium as diluents is also predicted by the diffusional mechanism only. Both theories have their advantages and drawbacks. A better understanding of the mechanism of flame propagation is obtained by the study of comprehensive theories.

## Comprehensive Theories

In comprehensive theories, an attempt is made to obtain a complete description of the flame, including expressions for the fractional mass transport and concentrations of all chemical species as functions of

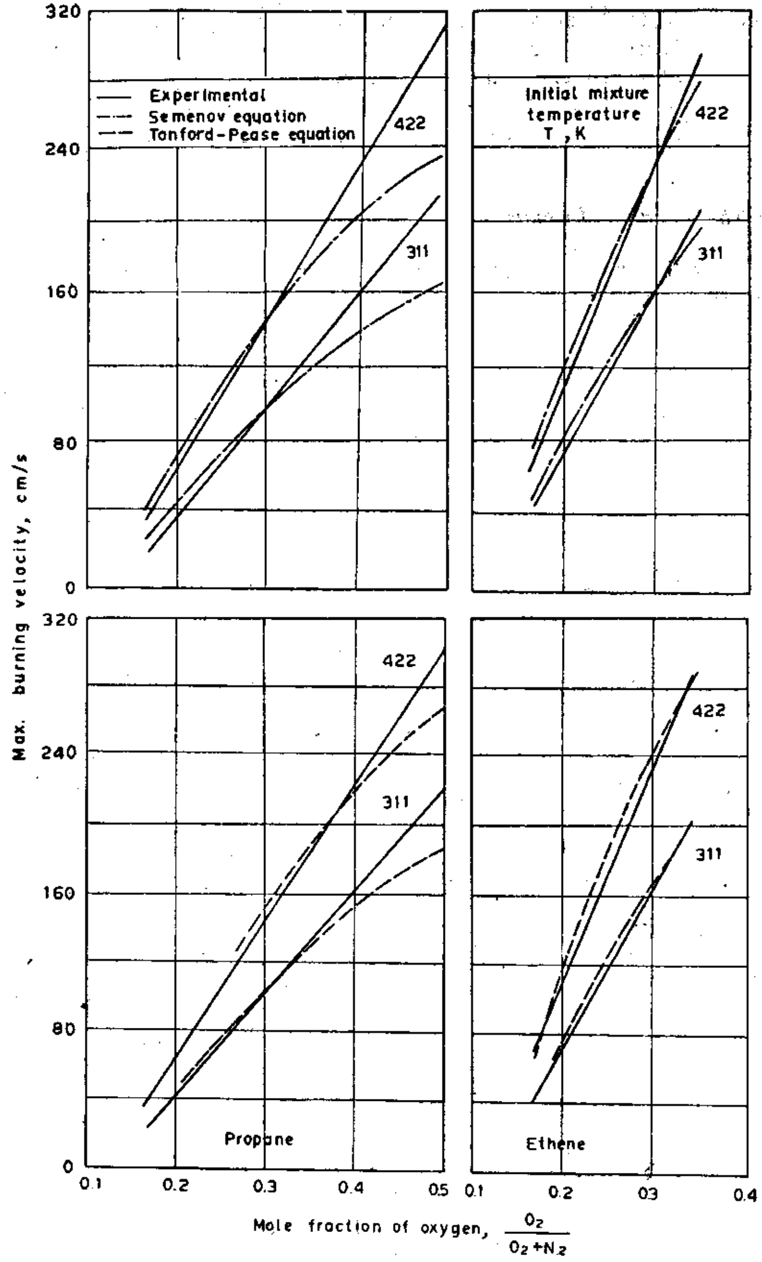

Fig. 9.12 Comparison of predicted and experimental burning velocities (With permission of the Combustion Institute, from *Fourth Symposium (International) on Combustion*, 1953).

distance or temperature, without introducing the assumption that either energy or mass transport are of primary importance.

A rigorous mathematical treatment of flame propagation has been attempted by Hirschfelder et al.[18], which includes both the thermal and diffusional effects. The basic equations presented are as follows:

### (a) The Equation of Continuity

The overall equation of continuity for a one-dimensional steady state condition is

$$\frac{d}{dx}(\rho U)=0 \tag{9.26}$$

where $\rho$ is the density of the fluid and $U$ is the mass average velocity. The equation may be integrated to give

$$G=\rho U \tag{9.27}$$

The constant of integration, $G$ is identified as the mass rate of flow (per unit cross section in the $y=z$ plane) and is independent of the co-ordinate $x$.

Similarly, each individual chemical component $i$, has a separate equation of continuity. If $n_i$ is the number of molecules of the $i$th species per cm$^3$, $U_{d,i}$ is the diffusion velocity of the $i$th species relative to the mass average velocity, and $I_i$ is the number of molecules of the $i$th species which are produced by chemical reaction per second per cm$^3$, then

$$\frac{d}{dx}[n_i\,(U+U_{d,i})]=I_i \tag{9.28}$$

### (b) The Equation of Energy Balance

$$\frac{d}{dx}\left(k\,\frac{dT}{dx}\right)-\frac{d}{dx}[\sum_i n_i\,G_i\,H_i(U+U_{d,i})]=0 \tag{9.29}$$

### (c) The Equation of State

$$n=\sum_i n_i=\frac{P}{RT}$$

or

$$P=nRT \tag{9.30}$$

The concept of one-dimensional steady state flame propagation is an idealization of the behaviour of gases in a small segment of a Bunsen burner flame zone. In the solution of the one-dimensional problem, the concept of a flame holder is introduced with two properties: (i) it prevents the back diffusion of product molecules formed in the chemical reaction and (ii) it serves as a heat sink extracting an amount of heat from the flame:

$$q_0=-k\left(\frac{dT}{dx}\right)_0 \tag{9.31}$$

Equations (9.26) to (9.30) are formulated in terms of individual species. Therefore, it is necessary to identify each chemical species in the combustion reaction as also the enthalpy, molecular weight, and other properties of the species. Further, the specific rates of chemical production for a sufficient number of species must be known so that the remaining may be calculated from the chemical equations relating the various species. In order to do this the rate constants for each independent step in the reaction scheme must be established. However, this information is completely lacking for hydrocarbon-air flames.

The equations describing the propagation of a flame are one dimensional steady state equations of change and the diffusion equations along with their boundary conditions possess a solution for only one value of the mass rate of flow $G$. The solution describes the boundary conditions at both $x=\infty$ (the hot boundary) and $x=0$ (the cold boundary) at the flame holder.

The comprehensive theory of Hirschfelder et al. is important for the understanding of laminar flame propagation, but at present it is extremely difficult to predict the burning velocities of hydrocarbon-air flames without making further simplifying assumptions. The comprehensive equations have been solved by approximate methods for only a few of the simplest flames e.g., ethylene oxide, hydrazine, and ozone decomposition flames.

## REFERENCES

1. G. Dixon-Lewis and M.J.G. Wilson, *Trans. Farady Soc.*, 1951, **47**: 1106.
2. R. Friedman and E. Burke, *J. Chem. Phys.*, 1954, **22**: 824.
3. R.M. Fristrom, C. Grunfelder and S. Favin, *J. Phys. Chem.*, 1960, **64**: 1386.
4. A.A. Westenberg and R.M. Fristrom, *Tenth Symposium (International) on Combustion*, The Combustion Institute, Pennsylvania, 1965, p. 473.
5. W. Michelson, *Ann. Physik.*, 1889, **37**: 1.
6. G. Gouy, *Ann. Chem. Phys.*, 1879, **18**: 27.
7. H.F. Coward and F.J. Hartwell, *J. Chem. Soc.*, 1932, 1996 and 2676.
8. D.A. Frank Kamenetsky, *Compt. Rend. Acad. Sci. (URSS)*, 1945, **46**: 232.
9. G.A. Ball, *Combustion Project Report*, Harvard University, July 1951.
10. E. Mallard and H.L. Le Chatelier, *Ann. Mines*, 1883, **4**: 379.
11. M.W. Evans, *Chem. Rev.*, 1952, 51 (3): 363-429.
12. Y.B. Zeldovich and D.A. Frank-Kamenetsky, *G.R. Acad. Sci. (URSS)*, 1938, **19**: 693-697.
13. N. Semenov, *Adv. Phys. Sci.*, Moscow, 1940, **24**: 438-486. English Translation, NACA, *Technical Memorandum 1026*, 1942.
14. S.F. Boys and J. Corner, *Proc. Roy Soc.*, 1949, **197**: 90-106.