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TECHNICAL REPORT ARBRL-TR-02528

AD-A134 738

THE OVERALL REACTION CONCEPT IN PREMIXED,
LAMINAR, STEADY-STATE FLAMES.
I.   STOICHIOMETRIES

Terence P. Coffee
Anthony J. Kotlar
Martin S. Miller

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October 1983

US ARMY ARMAMENT RESEARCH AND DEVELOPMENT CENTER
BALLISTIC RESEARCH LABORATORY
ABERDEEN PROVING GROUND, MARYLAND

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REPORT DOCUMENTATION PAGE		READ INSTRUCTIONS BEFORE COMPLETING FORM
1. REPORT NUMBER TECHNICAL REPORT ARBRL-TR-02528	2. GOVT ACCESSION NO. *AD-A134 738*	3. RECIPIENT'S CATALOG NUMBER
4. TITLE *(and Subtitle)* THE OVERALL REACTION CONCEPT IN PREMIXED, LAMINAR, STEADY-STATE FLAMES. I. STOICHIOMETRIES		5. TYPE OF REPORT & PERIOD COVERED Final
		6. PERFORMING ORG. REPORT NUMBER
7. AUTHOR*(s)* Terence P. Coffee Anthony J. Kotlar Martin S. Miller		8. CONTRACT OR GRANT NUMBER*(s)*
9. PERFORMING ORGANIZATION NAME AND ADDRESS US Army Ballistic Research Laboratory, ARDC ATTN: DRSMC-BLI(A) Aberdeen Proving Ground, MD 21005		10. PROGRAM ELEMENT, PROJECT, TASK AREA & WORK UNIT NUMBERS 1L161102AH43
11. CONTROLLING OFFICE NAME AND ADDRESS US Army AMCCOM, ARDC Ballistic Research Laboratory, ATTN:DRSMC-BLA-S(A) Aberdeen Proving Ground, MD 21005		12. REPORT DATE October 1983
		13. NUMBER OF PAGES 43
14. MONITORING AGENCY NAME & ADDRESS*(if different from Controlling Office)*		15. SECURITY CLASS. *(of this report)* Unclassified
		15a. DECLASSIFICATION/DOWNGRADING SCHEDULE

16. DISTRIBUTION STATEMENT *(of this Report)*

Approved for public release; distribution unlimited.

17. DISTRIBUTION STATEMENT *(of the abstract entered in Block 20, if different from Report)*

18. SUPPLEMENTARY NOTES

A version of this report will be published in Combustion and Flame.

19. KEY WORDS *(Continue on reverse side if necessary and identify by block number)*

Laminar Flames	Overall Reaction	Methane/Air Flames
Premixed Flames	Global Reaction	
Steady-State Flames	Ozone Flames	
One-Dimensional Flames	Hydrogen/Air Flames	

20. ABSTRACT *(Continue on reverse side if necessary and identify by block number)* meg

Combustion processes normally involve a large number of chemical species, related through a complicated reaction network and strongly interacting with the fluid flow and molecular transport. A common approach is to simplify the system by assuming a single overall or "global" reaction.

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20. Abstract (Cont'd):

In this paper, we will examine the adequacy of the overall reaction model for premixed, laminar, one-dimensional, steady-state flames. Our procedure is to first solve the equations governing the detailed chemistry model. The overall reaction rate parameters are then found from a least squares fit of the heat release profile. The overall reaction model equation can then be solved and the solution compared with the detailed model solution. This is done for three different flames over a range of stoichiometries.

The single reaction model gives quite accurate results for flame speed. The temperature and heat release profiles are also generally accurate. The accuracy of the major species profiles varies from fair to good. However, the optimal overall kinetic parameters do vary with stoichiometry.

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I. INTRODUCTION

Combustion processes normally involve many chemical species, related by complex kinetics and often strongly influenced by molecular transport and fluid flow. The difficult problem of combining the chemistry and transport is commonly made tractable by idealizing the complex kinetic network as a single overall or "global" reaction. Such a strategy is potentially useful when the detailed chemical steps are unknown or when the difficulty of the flow problem necessitates simplified chemistry. Relatively little work has been done, however, to assess the fidelity with which a global reaction can represent the net effects of the complex reaction network. This question is addressed here for the particular case of premixed, laminar, one-dimensional, steady-state flames.

Previous work in this vein was reported by Levy and Weinberg,[1] who obtained temperature profiles through very lean (and very slow) ethylene-air flames by the ray deflection method. Using a form of the energy conservation equation, they transformed the temperature profile into a profile of the volumetric rate of heat release through the flame front. The authors associated this net rate of heat release with that resulting from a hypothetical global reaction. A flame speed was then calculated from the "measured" reaction rate profile by means of the single-reaction flame theory of Spalding.[2] Close agreement was noted between this calculated result and the directly measured flame speed for a (rather narrow) range of stoichiometries and initial temperatures. Such a finding gave encouragement to the notion that the flame propagation formalism based on a single reaction might indeed have some utility.

In a subsequent paper Levy and Weinberg[3] probed the overall kinetics concept directly. By examining the heat release rates at the same temperature for a number of different flames, they determined that the effective reaction orders (with respect to fuel and oxidizer concentrations) vary greatly through the flame. Using the heat release profiles, they also found that the effective activation energy typically increases with temperature through the flame front then decreases near the maximum temperature. The conclusion was that no single reaction (of an Arrhenius form) could account for the thermal structure of the flame. However, they did note that the values of apparent activation energy and total order near the maximum heat release rate were

[1] A. Levy and E.J. Weinberg, "Optical Flame Structure Studies: Some Conclusions Concerning the Propagation of Flat Flames," 7th Intern. Symp. Combustion, pp. 296-303, 1959.

[2] D.B. Spalding, "I. Predicting the Laminar Flame Speed in Gases with Temperature-Explicit Reaction Rates," Combustion and Flame, Vol. 1, pp. 287-295, 1957. "II. One-Dimensional Laminar Flame Theory for Temperature-Explicit Reaction Rates," Combustion and Flame, Vol. 1, pp. 296-307, 1957.

[3] A. Levy and E.J. Weinberg, "Optical Flame Structure Studies: Examination of Reaction Rate Laws in Lean Ethylene-Air Flames," Combustion and Flame, Vol. 3, pp. 229-253, 1959.

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close to those obtained at blowout in a stirred reactor experiment. This last observation seemed to justify use of the overall reaction concept for those phenomena strongly dependent on the maximum energy release rate.

Our objective in this paper is similar to that of Levy and Weinberg; however, here we make use of a laminar flame model which includes multispecies and multireaction chemical kinetics. This approach offers the advantage of complete information about the system as well as access to a wide range of flames and stoichiometries. The only potential drawback lies in our uncertain knowledge of the many reaction steps and rates for some flames. Because our aim is heuristic, this trait is not considered a serious limitation. Our procedure is to solve the flame equations with the complex kinetics, obtain an overall rate for the flame from the heat release profile, solve the flame equations for this single reaction, and then make detailed comparisons between the two solutions. This is done for a wide range of stoichiometries of several flames.

Our results suggest that a single reaction formalism does a credible job of representing the thermal structure (and even the reactant profiles) of complex flames. This conclusion is not as contradictory to the Levy and Weinberg study[3] as it may seem. Their conclusion was based on a rather restrictive diagnosis of the heat release profile. A comparable analysis of our results leads to similar findings, i.e., the activation energy varies through the flame front. Our conclusion follows from the relative insensitivity of thermal structure to the reaction rate details. This can only be seen by actually solving the flame equations using an appropriate overall reaction.

Westbrook and Dryer[4] have developed a procedure for determining global kinetics parameters from the experimental flammability limits and stoichiometric flame speed at atmospheric conditions. A single-reaction flame model using these parameters can be expected to predict reasonable flame speeds over a wide range of equivalence ratios from very lean to very rich. The procedure may prove useful to those applications in which flame speed is of decisive importance. However, an application of interest to us is propellant combustion where two-phase flame holder effects give importance to temperature gradients near the flame front. Calibration of the global parameters by flame speeds alone does not guarantee accurate temperature profiles, but both the flame speed and temperature profile can be computed from an accurate heat release profile. The thrust of this paper is that one can find a global reaction which mimics the original heat release profile sufficiently well that accurate flame speeds and temperature profiles (at least through the flame front) can be computed from the global description. The significance of this conclusion is not necessarily diminished by the finding that the optimum global kinetics values vary with stoichiometry. In

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[4]C.K. Westbrook and F.L. Dryer, "Simplified Reaction Mechanisms for the Oxidation of Hydrocarbon Fuels in Flames," Comb. Sci. Tech., Vol. 27, pp. 31-43, 1981.

application work, generality might be achieved simply by parameterizing the kinetics values in terms of stoichiometry, pressure, etc., as suggested by Dryer and Westbrook.[5]

Our interest in the global reaction concept springs from two potential application schemes. The first assumes that the detailed multireaction kinetics are known, but so complex as to preclude their use in practical flow problems. One might then determine the appropriate global parameters in a manner similar to that used in this paper. The alternative scheme assumes that little is known of the detailed kinetics of a flame. It is for this case that Westbrook and Dryer[4] developed their method of predicting flame speeds vs. equivalence ratio from only a few selected measurements. To realize the thermal structure as well as the flame speed, more extensive measurements are required to calibrate the global reaction. The procedure would involve measuring temperature profiles in the subject flame using fine thermocouples or laser Raman techniques and then computing heat release profiles via the energy conservation equation.[1,6,7] Determination of the global parameters would then proceed as described in this paper. Prerequisite to either of these two approaches is the assurance that global reactions can reproduce the thermal structure of real flames with reasonable fidelity. This paper provides both this assurance and a systematic procedure for determining appropriate global reaction parameters from a heat release profile, which is either calculated from known detailed kinetics or deduced from a measured temperature profile.

II. DETAILED CHEMISTRY MODEL

In a previous paper,[8] the equations describing a one-dimensional, laminar, premixed, steady-state flame were derived for different approximations to the multicomponent transport coefficients. We will use the simplest approximation (Method V), which still gives accurate results. The corresponding equations are the following.

Conservation of energy is expressed by

$$- c_p \, m_o \, \frac{dT}{dx} + \frac{d}{dx} \left(\lambda \, \frac{dT}{dx} \right) - \Sigma \, R_i \, M_i \, h_i = 0 \qquad (1)$$

[5] F.L. Dryer and C.K. Westbrook, NATO AGARD Conference Proceedings No. 275, pp. 14-1 to 14-17, 1979.

[6] R. Friedman and E. Burke, "Measurement of Temperature Distribution in a Low-Pressure Flat Flame," J. Chem. Phys., Vol. 22, pp. 824-830, 1954.

[7] J.A. Hicks, "The Low-Pressure Decomposition Flame of Ethyl Nitrate," 8th Symposium (International) on Combustion, The Combustion Institute, 1962, pp. 487-496.

[8] T.P. Coffee and J.M. Heimerl, "Transport Algorithms for Premixed, Laminar Steady-State Flames," Combustion and Flame, Vol. 43, pp. 273-289, 1981.

where T is the temperature of the mixture, c_p is the specific heat of the mixture, m_o is the mass flux through the flame, λ is the thermal conductivity of the mixture, R_i is the rate at which species i is produced (or consumed) by chemistry, M_i is the molecular weight of species i and h_i is the specific enthalpy of species i.

The species continuity equations are given by

$$- m_o \frac{dY_i}{dx} + \frac{d}{dx} (\rho \, D_{im} \frac{dY_i}{dx}) + R_i \, M_i = 0, \tag{2}$$

where Y_i is the mass fraction of species i, ρ is the density of the mixture, and D_{im} is the diffusion coefficient of species i into the mixture. The boundary conditions are

$$T = T_u \text{ and } Y_i = Y_{iu}, \quad i = 1, 2, \ldots N \tag{3}$$

at $x = -\infty$ and

$$\frac{dT}{dx} = \frac{dY_i}{dx} = 0, \quad i = 1, 2, \ldots N \tag{4}$$

at $x = \infty$.

In the above equations, the effects of radiation, viscosity, and body forces are ignored. Since the burning velocity is small compared with the local speed of sound, the pressure is taken to be constant. Besides these standard assumptions, we have also assumed (see Ref. 8 for discussion) that thermal diffusion is negligibly small, that Fick's law holds for the diffusion velocities, and that the quantities $\rho^2 D_{im}$, $\rho\lambda$, and c_p are constant. The constants are chosen a priori.

The equations above are for the steady state solution. The numerical procedure actually uses the time dependent equations and a transformed space coordinate. Starting with arbitrary profiles, the equations are integrated in time until the steady state solution is obtained.[9,10] The burning velocity, S, of the flame is defined as the velocity of the flame relative to the fluid at rest, i.e., at $x = -\infty$. Since in our coordinate system the flame is at rest, $S = v(-\infty) = m_o/\rho_u$, where ρ_u is the density of the unburned mixture.

The production rate functions, $R_i(T)$, are defined by

$$R_i = \sum_{r=1}^{NR} (\nu''_{i,r} - \nu'_{i,r}) \, [k_{fr} \prod_{j=1}^{N} (C_j)^{\nu'_{j,r}} - k_{br} \prod_{j=1}^{N} (C_j)^{\nu''_{j,r}}] \tag{5}$$

[9] T.P. Coffee and J.M. Heimerl, "A Method for Computing the Flame Speed for a Laminar, Premixed, One Dimensional Flame," BRL Technical Report, ARBRL-TR-02212, January 1980 (AD A082803).

[10] T.P. Coffee, "A Computer Code for the Solution of the Equations Governing a Laminar, Premixed, One-Dimensional Flame," BRL Memorandum Report, ARBRL-MR-03165, April 1982 (AD A114041).

where $\ddot{\nu}_{i,r}$ and $\dot{\nu}_{i,r}$ are the number of molecules of species i entering into reaction r as product and reactant, respectively. NR is the number of reactions, C_j is the concentration of species j ($\rho Y_j/M_j$), and k_{fr} and k_{br} are the forward and reverse rate coefficients, respectively. The rate coefficients depend on the temperature through the generalized Arrhenius relations

$$k_{fr} = A_{fr} \; T^{B_{fr}} \exp(- E_{fr}/RT) \tag{6}$$

and

$$k_{br} = A_{br} \; T^{B_{br}} \exp (- E_{br}/RT), \tag{7}$$

where R is the gas constant, E is the activation energy and A is the frequency factor for the reaction.

The net rate of heat release per unit volume is defined by

$$q = - \Sigma \; R_i M_i h_i. \tag{8}$$

It is through this term (Eq. 1) that the chemical kinetics influences the temperature profile.

III. ONE REACTION MODEL

We will now assume a single irreversible overall reaction of the form fuel plus oxidizer goes to product, that is,

$$\nu_F \; F + \nu_o \; O \rightarrow \nu_p \; P, \tag{9}$$

where ν_F, ν_o, and ν_p are the stoichiometric coefficients. The governing Eqs. (1) through (4) remain the same. Equation (5) can be simplified. We obtain

$$R_F = - \nu_F \; k \; (C_F)^{\nu_F} (C_o)^{\nu_o}, \tag{10}$$

$$R_o = - \nu_o \; k \; (C_F)^{\nu_F} (C_o)^{\nu_o}, \tag{11}$$

and

$$R_p = \nu_p \; k \; (C_F)^{\nu_F} (C_o)^{\nu_o} . \tag{12}$$

The heat release is then

$$q = M_F \nu_F k \; (C_F)^{\nu_F} (C_o)^{\nu_o} \; [h_F + \frac{M_o \nu_o}{M_F \nu_F} \; h_o - \frac{M_p \nu_p}{M_F \nu_F} \; h_p \;]. \tag{13}$$

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We define

$$Q = h_F + \frac{M_o \nu_o}{M_F \nu_F} h_o - \frac{M_p \nu_p}{M_F \nu_F} h_p \tag{14}$$

where Q is the heat of reaction per unit mass of fuel.

From the thermodynamics[8] the relation

$$c_p (T_b - T_u) = \Sigma_i h_i (Y_{iu} - Y_{ib}) \tag{15}$$

can be obtained, where T_b is the temperature of the completely burned mixture and the Y_{ib} are the mass fractions. Since there is only a single reaction, however, any change in the fuel must be matched by a change in the oxidizer and product; that is,

$$Y_{ou} - Y_{ob} = \frac{M_o \nu_o}{M_F \nu_F} (Y_{Fu} - Y_{Fb}) \tag{16}$$

and

$$Y_{pu} - Y_{pb} = -\frac{M_p \nu_p}{M_F \nu_F} (Y_{pu} - Y_{pb}). \tag{17}$$

Substituting into (15) and solving for Q,

$$Q = c_p (T_b - T_u) / (Y_{Fu} - Y_{Fb}) . \tag{18}$$

The reaction rate k is expressed as an unmodified Arrhenius rate

$$k = A_r \exp (-E/RT). \tag{19}$$

For convenience, the constants in Eq. (13) will be absorbed into a new constant A, giving

$$q = Q (\rho Y_F)^{\nu_F} (\rho Y_o)^{\nu_o} A \exp (-E/RT). \tag{20}$$

Equation (20) indicates that, given a solution of the detailed chemistry model (q), a set of constants Q, A, and E may be found for which the one reaction model most closely follows the detailed model.

IV. DERIVING THE ONE REACTION MODEL PARAMETERS

In this section we derive expressions for the one reaction model such that Eq. (20) can be used for finding the kinetic parameters, given a heat release profile q from the detailed chemistry model.

Equation (20) expresses q as a function of T, Y_F, Y_o, and Y_p, since

$$\rho = \frac{p}{R_a T \, (Y_F/M_F + Y_o/M_o + Y_p/M_p)}. \tag{21}$$

However, it is inconsistent to use the values of Y_F, Y_o, and Y_p from the detailed chemistry model. In the detailed model, there are other species, so that $Y_F + Y_o + Y_p \neq 1$. In the simplified model, by assumption there are no other species.

Consequently, we make an additional assumption that all the Lewis numbers are one; that is,

$$L_e = \frac{\rho \, D_{im} c_p}{\lambda} = 1 \tag{22}$$

for fuel, oxidizer, and product. For all except the light species, this is a good approximation. Eqs. (1) and (2) can be written

$$\frac{d}{dx} \left(\lambda \, \frac{dT}{dx} \right) - c_p \, m_o \, \frac{dT}{dx} = Q \, R_F M_F = - q \tag{23}$$

and

$$\frac{d}{dx} \left(\frac{\lambda}{c_p} \, \frac{dY_F}{dx} \right) - m_o \, \frac{dY_F}{dx} = - R_F M_F . \tag{24}$$

The equation in terms of $(-c_p T/Q)$ and Y_F are formally identical. Also matching boundary conditions, we obtain

$$Y_F - Y_{Fb} = c_p \, (T_b - T)/Q. \tag{25}$$

So given T, Y_F can be computed, and also Y_o and Y_p since the stoichiometric coefficients are known for the overall reaction, Eq. (9).

The heat release can now be viewed as a function only of T. Moreover, the one reaction model simplifies to the single Eq. (23).

The heat of reaction Q can be computed from Eq. (14), since the enthalpies are known quantities.[11,12] Q may also be computed from Eq. (18). The adiabatic or burned temperature and the mixture specific heat c_p can be computed from thermodynamic considerations. Since the one reaction in the simplified model is assumed irreversible, Y_{Fb} can be computed knowing Y_{Fu} and Y_{ou}. So all the quantities on the right side of Eq. (18) are known.

However, Eqs. (14) and (18) are inconsistent. This occurs because the two models have different adiabatic species concentrations. In particular, some intermediates and radicals will still exist at the burned conditions. And, since the reactions are reversible, combustion may be incomplete. In order to preserve the proper adiabatic temperature, Eq. (18) will be used to compute Q.

What remains is to find "best fit" values of A and E in

$$q/Q[(\rho Y_F)^{\nu_F} (\rho Y_o)^{\nu_o}] = A \exp(-E/RT). \tag{26}$$

There can be a difficulty here. The expression on the right will be monotonically increasing for positive A and E. For the cases considered, the expression on the left normally reaches a peak somewhere past the q peak and then decreases. We then only fit the expression up to the peak. This means the post flame region will not be well resolved. However, this region probably will not be well resolved by any one reaction model. The important reactions in this region are radical recombinations, and radicals are ignored by the simplified model. The fit is made using an absolute error criterion with proper transformation of weights.[13]

In using the fitted values of A and E to solve Eq. (23), we must be concerned with the cold boundary difficulty. That is, from Eq. (20), heat is generated at any temperature, including the temperature of the unburned mixture T_u. Given enough time, the mixture will spontaneously combust. This contradicts our idealization of an infinite unreacting column of gas with the flame front propagating through the mixture. In practice, we will numerically integrate over a finite interval. As long as the heat release at T_u is small, the heat generated before the gas encounters the flame front will be negligible. This is true for most of the cases studied in this paper. However, for a few cases the heat release is too large at T_u, and the cold boundary conditions will be distorted.

[11]D.R. Stull and H. Prophet, *JANNAF Thermochemical Tables*, 2nd Edition, NSRDS-NBS-37, June 1971.

[12]S. Gordon and B.J. McBride, "Computer Program for the Calculation of Complex Chemical Equilibrium Compositions, Rocket Performance, Incident and Reflected Shocks and Chapman-Jouguet Detonations," NASA-SP-273, 1971 (1976 program version).

[13]R.J. Cvetanovic and D.L. Singleton, Internat. J. Chem. Kinet., Vol. 9, pp. 481-488, 1977; R.J. Cvetanovic and D.L. Singleton, Internat. J. Chem. Kinet., Vol. 9, pp. 1007-1009, 1977.

To avoid this, we utilize the concept of an ignition temperature.[14] For $T < T_u + 10$ K, the heat release q is set to zero. For $T > T_u + 10$ K, Eq. (20) is used. That is, the gas cannot ignite until it reaches the ignition temperature $T_u + 10$. This circumvents the cold boundary difficulty, while having little effect on the rest of the flame.

So far we have assumed that ν_F and ν_O are known. It is also possible to make a 3 parameter fit, where ν_F is a new parameter to be chosen and the relation between ν_F and ν_O is determined by the overall stoichiometry. Then the quantity $\nu_F + \nu_O$ is the overall order of the reaction. We will also discuss this type of fit.

There are several differences between the above procedure and that recommended by Westbrook and Dryer.[4] The primary distinction is that Westbrook and Dryer fit flames speeds, while we fit the heat release. Correctly fitting the thermal structure will lead to the proper flame speed; the converse is not true. Also, the Westbrook and Dryer model leads to an incorrect adiabatic temperature; since we are interested in the thermal structure, our procedure has been developed so as to reproduce the proper adiabatic temperature. Since we assume unit Lewis numbers, our global model reduces to only the temperature equation, while the Westbrook and Dryer model includes equations for the reactants and products. Also, in the Westbook and Dryer model, a single set of parameters is selected which fit a range of stoichiometries. As we shall see, our parameters will vary with stoichiometry, reflecting the changes in thermal structure due to different initial conditions.

V. FLAMES TO BE CONSIDERED

To increase the generality of our conclusions, we will consider three different types of flames.

The simplest flame mechanism is that of an ozone decomposition flame.[15] There are three reactions, only two of which are important in the pre-flame and flame region:

$$O_3 + M \rightleftarrows O + O_2 + M$$

$$O + O_3 \rightleftarrows O_2 + O_2.$$
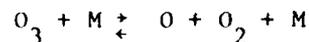
In the post flame region the radical recombination reaction

$$O + O + M \rightleftarrows O_2 + O_2.$$
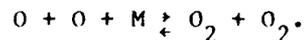
becomes important.

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[14] F.A. Williams, *Combustion Theory*, Addison-Wesley, Reading, MA, 1965.

[15] J.M. Heimerl and T.P. Coffee, "The Detailed Modeling of Premixed, Laminar Steady-State Flames. I. Ozone," *Combustion and Flame*, Vol. 39, pp. 301-315, 1980.

A more complicated case is hydrogen/air flames. The mechanism used is due to Dixon-Lewis,[16] and consists of 8 species and 17 reversible reactions.

Last, we consider methane/air flames. The mechanism used is obtained from Dixon-Lewis,[17] and consists of 14 species and 34 reactions. The hydrogen/air scheme is a subset of this mechanism. While the mechanism is intended for lean and slightly rich flames, we will also use it for rich flames in order to obtain our comparisons.

All flames are computed for atmospheric pressure. For the ozone flames, the initial temperature of the gas is 300K. For the other flames, the initial temperature is 298K. The overall reactions for these mechanisms are taken to be

$$O_3 \rightarrow 1.5 \, O_2,$$

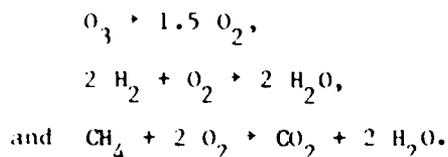$$2 \, H_2 + O_2 \rightarrow 2 \, H_2O,$$

and $CH_4 + 2 \, O_2 \rightarrow CO_2 + 2 \, H_2O.$

First, we consider the feasibility of the overall reaction fit. To do this, consider taking the logarithm of Eq. (26); that is,

$$\ln \left[q/Q \, (\rho Y_F)^{\nu_F} (\rho Y_O)^{\nu_O} \right] = \ln(A) - E/RT, \tag{27}$$

and graphing both sides as a function of $1/T$. The right side is the equation of a straight line. The shape of the left side, where q is the heat release for the detailed chemistry model, gives a quick impression of the adequacy of a single Arrhenius type reaction.

Figure 1 gives these graphs for a 50% Ozone flame (oxygen diluent), a rich H_2/air flame (40% H_2), and a stoichiometric CH_4/air flame (9.5 % CH_4). The activation energies of the least square fits to q are, respectively, 7.9 kcal, 6.4 kcal, and 29.1 kcal.

All three graphs display a high activation energy (that is, a steep slope) near the cold boundary. The Arrhenius fits cannot resolve this, necessitating the concept of an ignition temperature.

Next, there is a long region where the slope gradually increases. For the O_3 and H_2 flames, this increase is very gradual, and the Arrhenius fit is

[16] G. Dixon-Lewis, "Kinetic Mechanism Structure and Properties of Premixed Flames in Hydrogen-Oxygen-Nitrogen Mixtures," Proc. R. Soc. Lond. A, Vol. 292, pp. 45-99, 1979.

[17] G. Dixon-Lewis, "Aspects of the Kinetic Modeling of Methane Oxidation in Flames," First Specialists Meeting (International) of the Combustion Institute, Vol. 1, pp. 284-289, 1981.
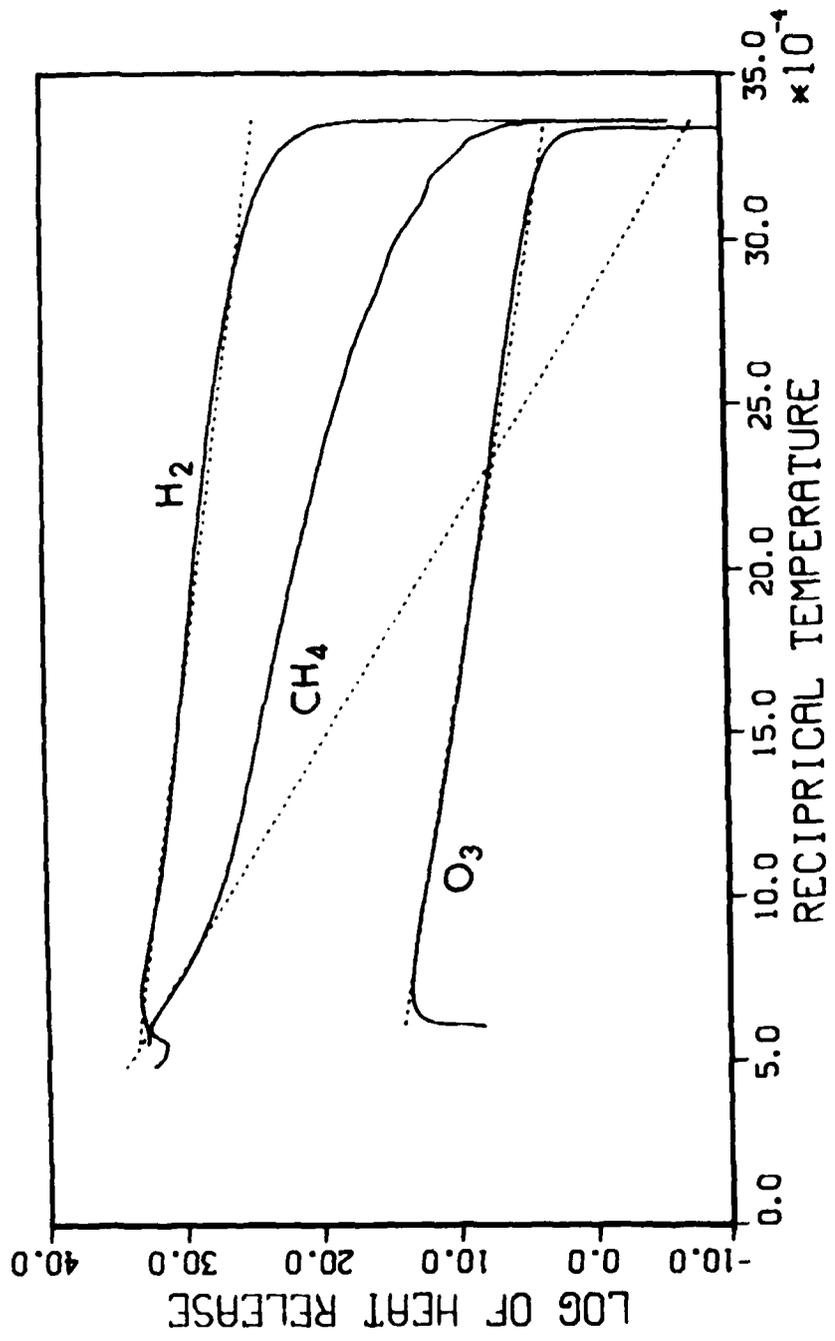
Figure 1. Logarithm of the Heat Release Divided by the Concentrations (Line) Versus the Logarithm of the Overall Arrhenius Fit (Dot)

quite good over most of the temperature range. The CH_4 flame exhibits a more complicated structure, but there is still a fairly large region near the peak heat release where the Arrhenius fit is quite good.

Finally, there is a post-flame region, where the slope changes sign. An Arrhenius fit cannot resolve this.

The results for the methane/air heat release profile agree qualitatively with those of Levy and Weinberg for an ethylene/air flame. The activation energy (or slope) increases with increasing temperature. Since our single reaction parameters are generated by a least squares fit with an absolute error criterion,[13] the fit is most accurate in the region of maximum heat release, which Levy and Weinberg found most influential to the burning rate. It is of interest to learn how accurately these same parameters reproduce the thermal structure as well.

VI. TEMPERATURE AND SPECIES PROFILES

In this section we will compare the profiles generated by the detailed chemistry model with those generated by the single reaction model. The same three examples considered in the last section will be used.

Figures 2, 3, and 4 show the heat release and temperature profiles for our three examples. The heat release profiles from the overall reaction are reasonable. However, the CH_4/air profile is especially inaccurate for the early part of the flame, as expected from considering Figure 1. Nevertheless, all three temperature profiles are quite accurate through the flame front. In the post-flame region, the detailed model shows a slow temperature rise, due to the recombination of radicals. The overall reaction model, which ignores radicals, rapidly approaches the adiabatic temperature. Consequently, the single reaction model is somewhat inaccurate in the post-flame region.

Since we have assummed unit Lewis number in the overall reaction model, species profiles can also be derived. Figure 5 shows the comparisons for the ozone flame. The agreement is quite good. The errors are primarily due to the neglect of the O profile, rather than the unit Lewis number assumption. The agreement becomes better for slower flames (less O), and not quite as good for faster flames (more O). For the hydrogen/air flame, the mole fractions, as shown in Figure 6, are not in good agreement. In the detailed model, there are large radical concentrations in the flame front. These lead to rapid consumption of the H_2 and O_2 through the chain branching reactions. The one reaction model, which has a low activation energy, cannot match this. For a slower flame (either richer or leaner), the agreement is much better.

Figure 7 shows the major species profiles for the CH_4/air flame. The main errors in the species profiles for a CH_4/air flame are due not to radicals, which have small concentrations in all cases, but to intermediates. The overall reaction model assumes that the only species are CH_4, O_2, CO_2, and H_2O. There are several intermediate species, of which H_2 and CO are the most important, and except for lean flames, the equilibrium products include substantial amounts of H_2 and CO. This causes the CO_2 and H_2O profiles from the one reaction model to approach incorrect values. The profile agreement is better for lean flames and not quite as good for rich flames.

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Figure 2. 50% O_3, 50% O_2 Flame. Detailed Chemistry Model (Line). Overall Reaction Model (Dot)

Figure 3. 40% H_2, 60% Air Flame. Detailed Chemistry Model (Line). Overall Reaction Model (Dot)

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Figure 4. Stoichiometric CH_4/Air Flame. Detailed Chemistry Model (Line). Overall Reaction Model (Dot)
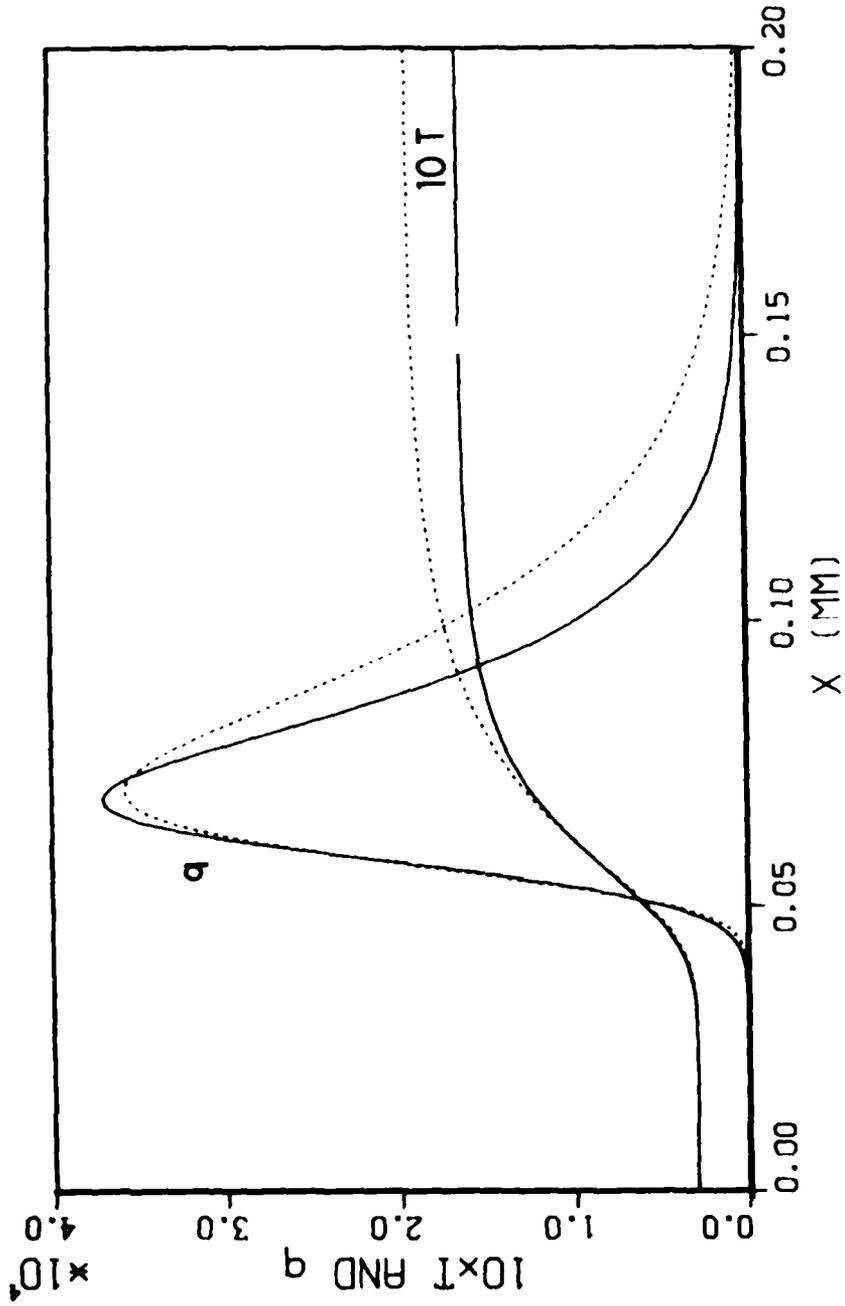
Figure 5. 50% O_3, 50% O_2 Flame. Detailed Chemistry Model (Line). Overall Reaction Model (Dot)
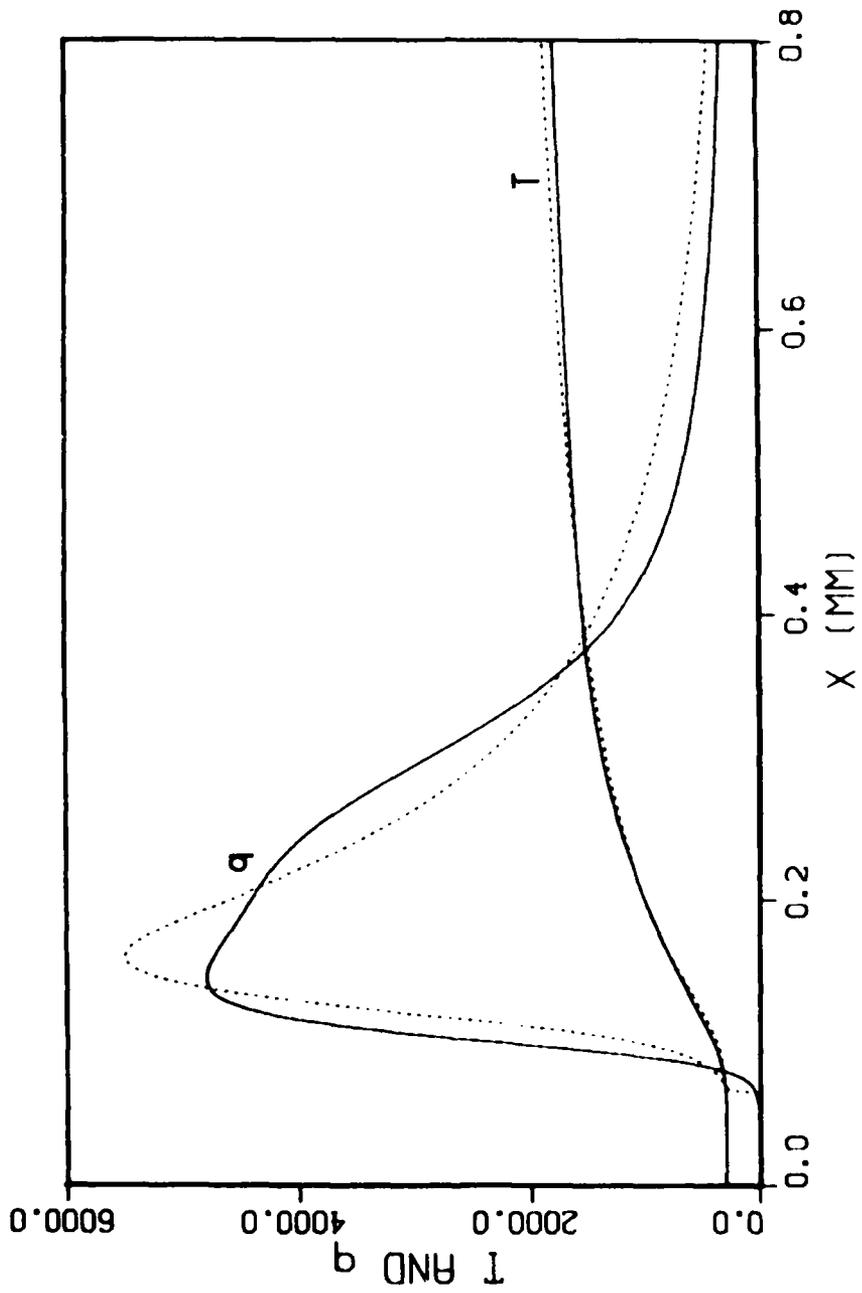
Figure 6. 40% H_2, 60% Air Flame. Detailed Chemistry Model (Line). Overall Reaction Model (Dot)
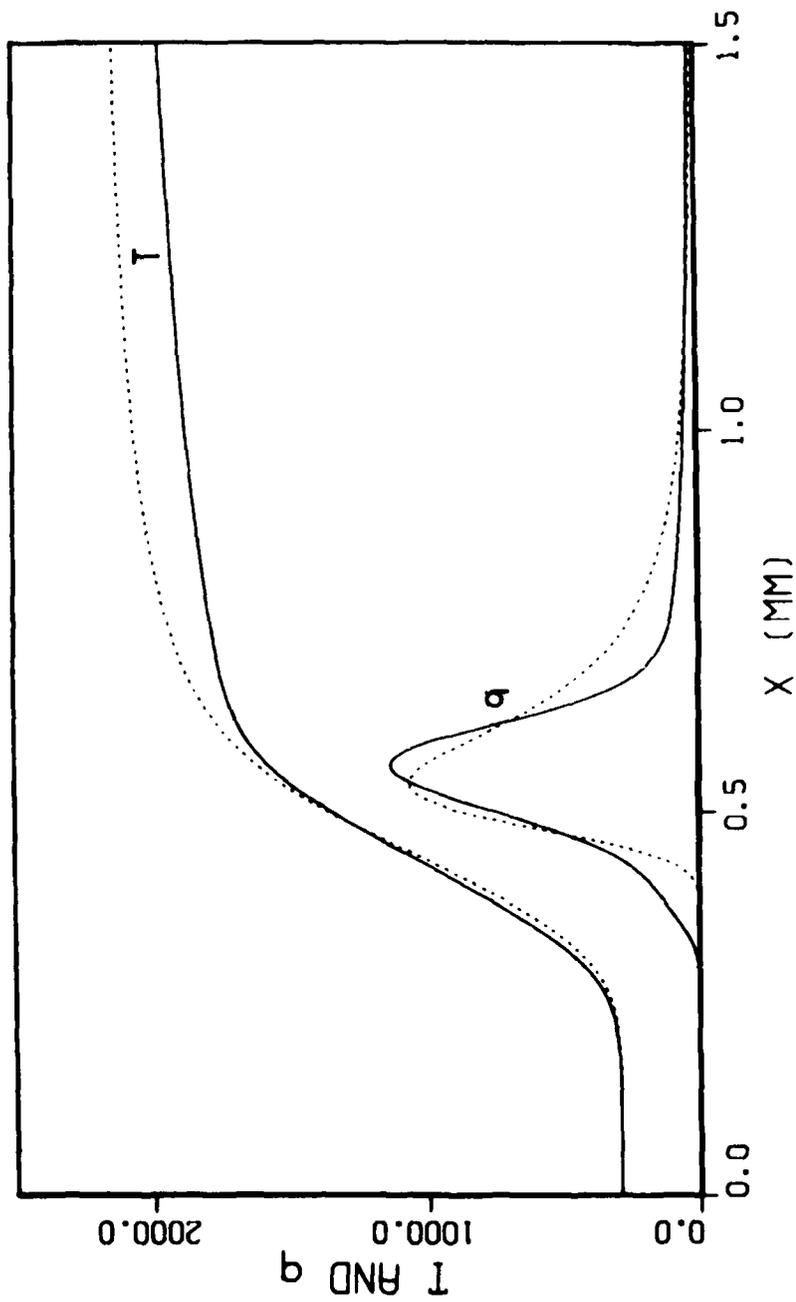
Figure 7. Stoichiometric CH_4/Air Flame. Detailed Chemistry Model (Line). Overall Reaction Model (Dot.)
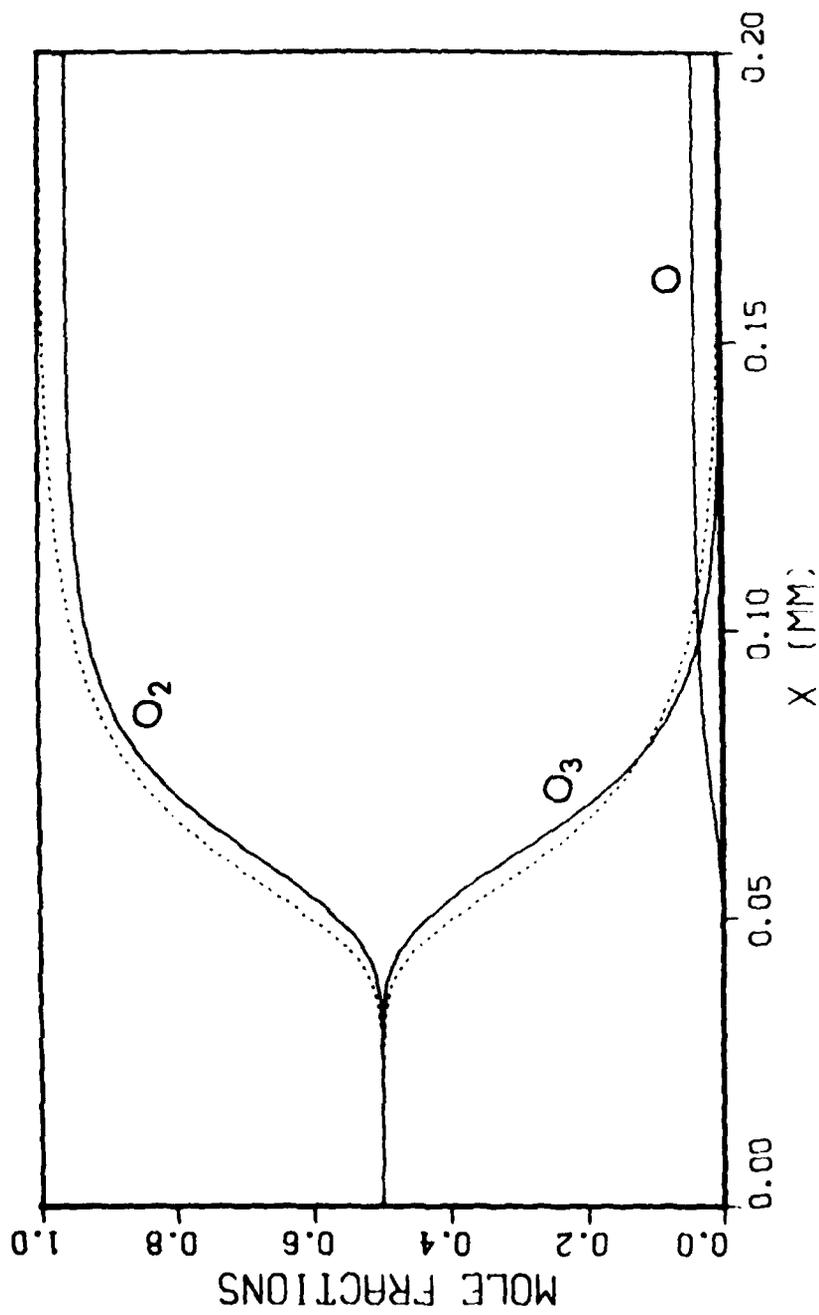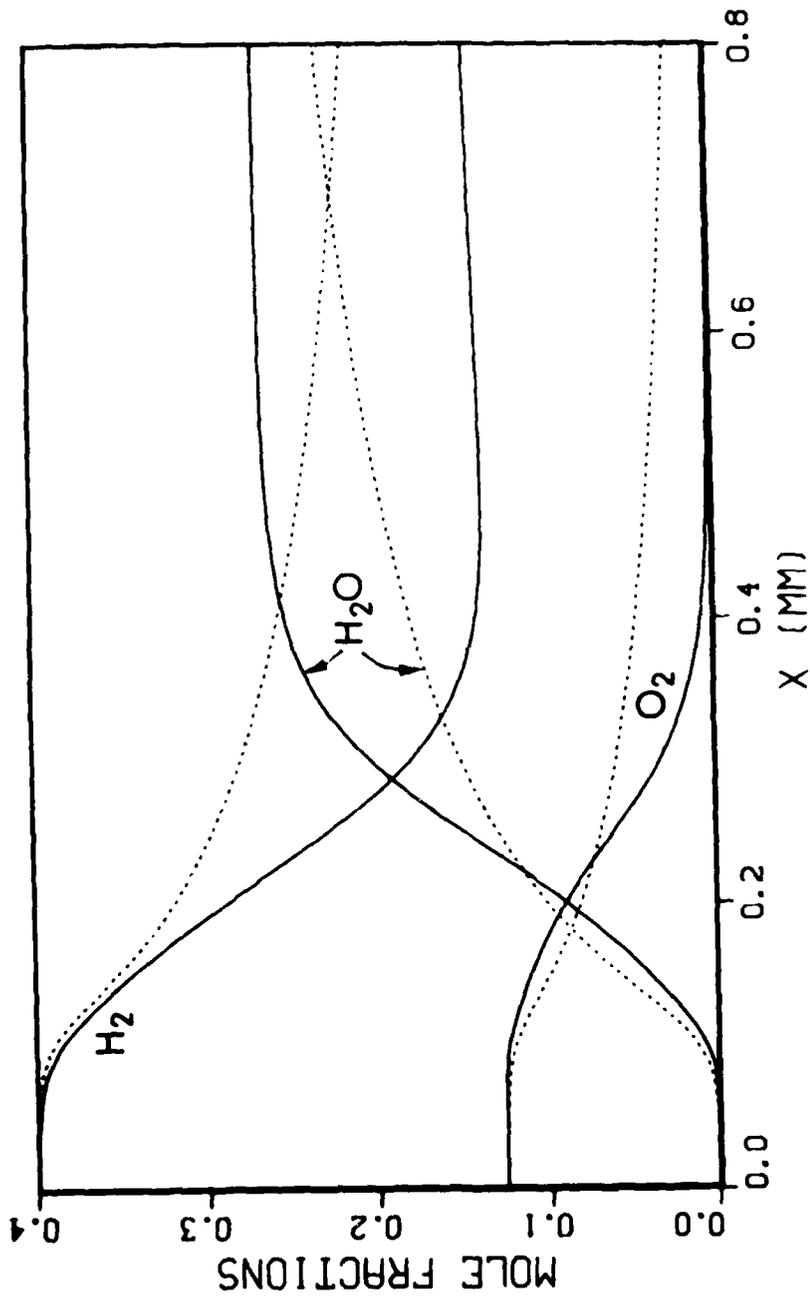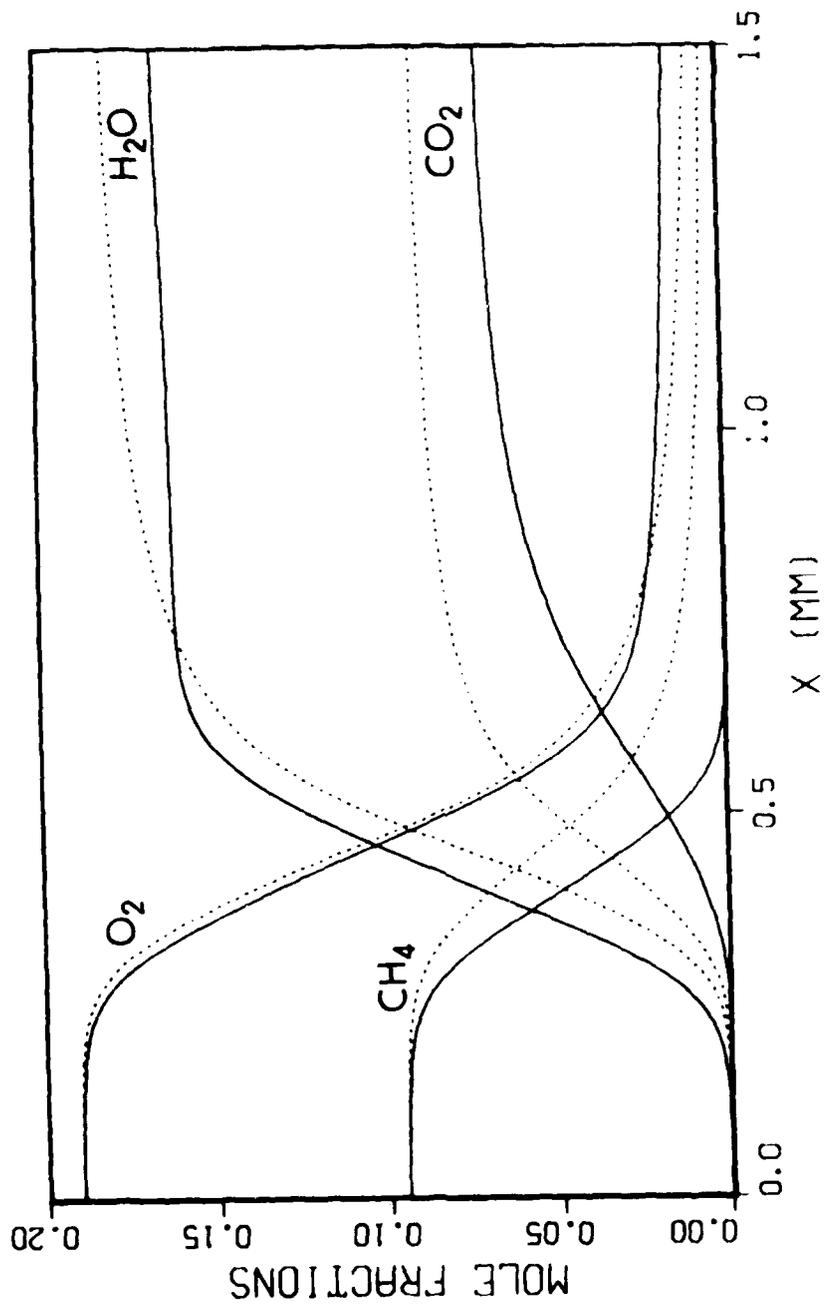
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Overall, the species profiles are reasonable, considering the simplification in the one reaction model.

VII. FLAME SPEEDS

In this section we will consider more closely the parameters generated by the overall reaction fits, as well as comparing flame speeds. In order to discern possible patterns, many initial stoichiometries are considered for each of the three flames.

The parameters for a set of ozone flames are given in Table 1. The activation energies derived are between those of reaction 1 (22.2 kcal) and reaction 2 (4.6 kcal). The slower and cooler the flame (that is, the smaller the initial O_3 concentration), the higher the overall activation energy. This can be explained by studying the detailed model. For a slower flame, only small amounts of O are produced. The O that is created reacts almost immediately via reaction 2. So reaction 1 is close to a rate limiting step, and the overall reaction has a similar activation energy. For a fast flame, large amounts of O are produced, which diffuses ahead of the flame. The flame propagation is determined to a large extent by the low activation energy reaction 2. This is reflected in the fitted values of E. Table 2 compares the flame speeds from the detailed chemistry model (S_D) and the overall reaction model (S_O). The percentage error in the one reaction model is defined as $100 (S_O - S_D)/S_D$. The agreement in flame speeds is excellent.

Tables 3 and 4 show the corresponding results for a set of hydrogen/air flames. Here, the overall activation energies also decrease for hotter and faster flames, for reasons similar to those discussed for the ozone case. For a slow flame, only small amounts of the radical species (H, OH, O, HO_2) are produced. The chain branching reactions ($H + O_2 \rightarrow OH + O$ and $O + H_2 \rightarrow OH + H$), which have relatively high activation energies, tend to be rate limiting. For a fast, hot flame, large amounts of radicals are created. The flame propagation is to a large extent determined by low activation energy reactions ($OH + H_2 \rightarrow H_2O + H$).

Results for methane/air flames are given in Tables 5 and 6. As before, the overall activation energies increase for slower flames. All of these activation energies are relatively high, higher than for any of the reactions in the detailed mechanism. The detailed model assumes a sequence of reactions ($CH_4 \rightarrow CH_3 \rightarrow CH_2O \rightarrow CHO \rightarrow CO \rightarrow CO_2$). In fitting this by a one reaction model, a high activation energy seems to best fit the overall rate of the sequence.

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TABLE 1. ONE REACTION MODEL PARAMETERS FOR OZONE/OXYGEN FLAMES.[*]

% O_3	c_p	T_b	Q	$\rho\lambda$	A	E
20	.244	1094	710	7.32E-8[**]	1.44E8	15.3
25	.248	1256	710	7.20E-8	5.10E7	12.8
50	.259	1943	709	6.86E-8	1.39E7	7.9
75	.265	2425	689	6.71E-8	1.33E7	6.5
100	.269	2702	646	6.63E-8	1.59E7	6.0

* Units are in list of symbols
** 7.32E-8 is read as 7.32×10^{-8}

TABLE 2. A COMPARISON OF FLAME SPEEDS FOR THE DETAILED
CHEMISTRY MODEL AND THE ONE REACTION MODEL FOR
OZONE/OXYGEN FLAMES.

% O_3	S_D	S_o	% Error
20	33.1	34.1	3
25	61.5	64.1	4
50	241.6	253.7	5
75	391.1	409.2	5
100	496.8	517.5	4

TABLE 3. ONE REACTION MODEL PARAMETERS FOR HYDROGEN/AIR FLAMES.

%H_2	c_p	T_b	Q	$\rho\lambda$	A	E
15	.297	1473	28890	6.63E-8	1.58E17	15.2
20	.319	1835	28803	6.60E-8	1.48E16	9.6
30	.367	2398	27264	6.72E-8	5.51E15	7.2
40	.416	2214	28604	7.32E-8	2.06E15	6.4
50	.479	1939	28827	7.65E-8	9.61E14	6.3
60	.567	1642	28890	7.66E-8	4.84E14	6.6
70	.703	1329	28898	7.32E-8	3.47E14	8.3
75	.803	1166	28890	7.01E-8	7.60E14	11.6

TABLE 4. A COMPARISON OF FLAME SPEEDS FOR THE DETAILED CHEMISTRY
MODEL AND THE ONE REACTION MODEL FOR HYDROGEN/AIR FLAMES.

% H_2	S_D	S_o	% ERROR
15	33.6	32.9	-2
20	100.5	89.1	-11
30	217.9	203.8	-7
40	280.6	270.5	-4
50	251.9	251.9	-0
60	178.0	182.4	3
70	82.4	84.6	3
75	35.5	36.3	2

TABLE 5. ONE REACTION MODEL PARAMETERS FOR METHANE/AIR FLAMES.

% CH_4	c_p	T_b	Q	$\rho\lambda$	A	E
6.5	.300	1778	11960	5.72E-8	3.37E18	35.1
7.5	.308	1960	11908	5.66E-8	8.15E17	30.1
8.5	.316	2121	11768	5.62E-8	5.36E17	28.1
9.5	.323	2231	11355	5.61E-8	1.01E18	29.1
10.5	.327	2202	11396	5.68E-8	9.15E17	29.0
11.5	.330	2107	10002	5.80E-8	1.86E18	31.1
12.5	.334	2009	10582	5.94E-8	3.62E18	33.8
13.5	.337	1914	10164	6.10E-8	4.10E18	35.6

TABLE 6. A COMPARISON OF FLAME SPEEDS FOR THE DETAILED CHEMISTRY
MODEL AND THE ONE REACTION MODEL FOR METHANE/AIR FLAMES

% CH_4	S_D	S_o	% ERROR
6.5	16.0	18.4	15
7.5	25.3	27.7	9
8.5	33.8	34.6	2
9.5	39.8	38.4	-4
10.5	43.9	40.8	-7
11.5	42.6	38.2	-10
12.5	34.2	30.1	-12
13.5	23.5	20.6	-12

In summary, an overall reaction model appears to be a quite accurate representation of a wide variety of flames and stoichiometries. The activation energies generated are relatively low compared to the range often assumed for overall reactions. The overall reaction normally does not correlate with any single reaction in the detailed model, and is a function of stoichiometry as well as the detailed kinetics.

Up to this point we have arbitrarily chosen the order $\nu_F + \nu_O$ (1 for ozone, 3 for hydrogen/air and methane/air), based on the assumed overall reactions. Some results were computed with different choices for the order but with the ratio ν_F/ν_O constant. The consistent result was that as the order increases, the fitting parameters A and E also increased. However, the accuracy of the fit was almost independent of the order assumed.

Also, a number of three parameter fits were made, where ν_F, A, and E were all determined by a least squares fit. The order so determined varied substantially with stoichiometry. The accuracy of the three parameter fit was only a slight improvement over the two parameter fit, and for a few cases it was less accurate.

Thus, over a large interval, the order can be arbitrarily chosen without affecting the accuracy of the overall reaction fit. An increase in the order also increases the parameters A and E. Preliminary work, however, indicates that the reaction order is not arbitrary if the same kinetics are applied to different pressures.

VIII. CONCLUSIONS

The aim of this work has been to explore the applicability of the overall reaction rate concept to premixed laminar flames with complex chemistry. The results demonstrate the ability of a single reaction formalism, having a rate constant of simple Arrhenius form, to track the temperature, heat release, and to some extent, species profiles obtained from multireaction network calculations. A straightforward method using a least squares fitting procedure is presented which extracts the kinetic parameters directly from the heat release profile as a function of temperature. These global kinetic parameters are then tested for their ability to reproduce the overall features of the complex reaction network, thereby allowing a quantitative assessment to be made of their utilization as a contracted representation for the thermochemistry of a multicomponent flame. We believe our approach is the first attempt to derive overall reaction rates systematically by using the "complete" information obtainable from a detailed laminar flame model. This differs significantly from previous methods which were tailored to extract kinetic parameters from a very limited amount of experimental data. Consequently, the results obtained from this study indicate the exact extent to which our global reaction model is capable of condensing a complex reaction network to a single overall reaction.

One can organize the findings into several echelons of detail. The first, and most detailed, involves how well a single formal reaction can mimic the net rate of heat release (due to the multireaction network) as a function of position in the flame. A related issue is the determination of the overall reaction parameters which best represent this heat release profile. At an intermediate level of detail a comparison can be made between the temperature

and reactant profiles as computed by the multireaction code and those predicted by the overall reaction. Finally, one can compare the flame speed predicted by the overall reaction model with the multireaction code value.

The levels of decreasing detail correspond to increasing degrees of integration over the underlying reaction processes. One might expect, therefore, that the flame speed would be less sensitive than the temperature profile to imperfect fidelity in the overall reaction rate profile. This expectation is generally borne out by the results. Calculation of flame speed with the overall reaction is accurate for all flames to about 15% at worst and frequently in the 5% range. Accuracy of the temperature profiles computed using the overall reaction is generally good and is limited primarily by our requiring that the proper adiabatic temperature be achieved. Attainment of this complete heat release is often considerably delayed due to slow radical recombination in the late stages of the flame. The fidelity with which the net heat release rate can be approximated by a single reaction varies somewhat with the flame identity. The ozone and H_2/air representation is quite credible over a very wide temperature range, whereas for the CH_4/air the range is rather narrow.

Another finding of this study is that the kinetic parameters of the overall reaction do not correlate with any single reaction step of the complex kinetics. Furthermore, the values of these parameters change with stoichiometry. The use of a single set of kinetic parameters to represent a number of different stoichiometries will lead to further compromises in the thermal structure description. We have not examined this trade-off exhaustively, but our feeling is that one would be better advised to treat the overall reaction parameters as functions of stoichiometry.

Preliminary work suggests that the overall reaction concept retains accuracy over a wide range of pressures and initial temperatures. The effective values of the kinetics constants vary only slightly with changes in the initial temperature; variation with pressure is slight for some flames and large for others. These considerations will be addressed in a subsequent paper.

We have shown that an overall reaction model can quite accurately reproduce many of the features of a detailed chemistry model for laminar flames, despite the vast simplification involved. The extent to which the overall reaction parameters determined from this problem can be applied to other flow conditions remains an important question for future study.

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LIST OF SYMBOLS

A = lumped parameter, centimeter-gram-second units.

C_j = concentration of species j, mole-cm^{-3}.

c_p = specific heat of the mixture, cal-g^{-1}-K^{-1}.

D_{im} = diffussion coefficient of species i in the mixture, cm^2-s^{-1}.

E = activation energy, kcal-mole^{-1}.

h_i = specific enthalpy of species i, cal-g^{-1}.

k = rate coefficient in centimeter-mole-second units.

m_o = mass flux, g-cm^{-2}-s^{-1}.

M_i = molecular weight of species i, g-mole^{-1}.

p = pressure, atm.

q = heat release per unit volume, cal-cm^{-3}-s^{-1}.

Q = heat of reaction per unit mass of fuel, cal-g^{-1}.

R = gas constant = 1.9872E-3 kcal-mole^{-1}-K^{-1}.

R_a = gas constant = 82.05 cm^3-atm-mole^{-1}-K^{-1}.

R_i = rate of production of species i, mole-cm^{-3}-s^{-1}.

S = velocity of the flame relative to the unburned mixture, cm-s^{-1}.

T = temperature, K.

v = fluid velocity, cm-s^{-1}.

x = spatial coordinate, cm.

Y_i = mass fraction of species i.

λ = thermal conductivity of the mixture, cal-cm^{-1}-s^{-1}-K^{-1}.

ρ = density of the mixture, g-cm^{-3}.

ν = stoichiometric coefficient.

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