A Coalescence/Dispersion Model for Turbulent Flame Stability

Krishnan Radhakrishnan*
The University of Michigan, Ann Arbor, Michigan
and
David T. Pratt†
University of Washington, Seattle, Washington

A coalescence/dispersion model that couples finite rate fluid mechanic mixing with finite rate combustion chemistry has been developed for premixed turbulent flame stability studies. The kinetics of the fuel oxidation process is described by a two-step reaction mechanism. The model predictions of the lean ignition limits of premixed turbulent propane/air flames are verified by comparisons with data in the literature. The variations of the lean limits compare favorably with experimental magnitudes and trends.

Nomenclature

c_β = constant in Eq. (2)
F = fuel mass fraction
L = length of recirculation zone, length of reactor
m = mass
$\dot{m}$ = mass flow rate
n = number of elements ignited at $t = 0^+$
N = number of elements used to describe reactor composition
$\dot{N}$ = element feed rate
P = pressure
P_j = power input into reactor [see Eq. (2)]
t = time
T = temperature
U = velocity
$\bar{v}$ = ensemble mean specific volume
V = reactor volume
β = mixing frequency
Δt = time increment
σ = mole number
τ, τ_r = residence time
ϕ = fuel/air equivalence ratio

Subscripts

b = fully burnt
e = out
i = in
m = mixing
r = residence
u = unburnt

I. Introduction

In any practical continuous-flow combustion device, two types of mixing processes can be identified. If the fuel and air are not premixed, fuel/air mixing is required to achieve local zones of combustible mixture. In addition, a self-sustaining flame requires that unburned gas mix with partially or completely burned gas. The latter mixing is accomplished by means of a strong recirculating or "back-mixing" flow. The recirculation of chemically and thermally hot combustion products is usually obtained by means of bluff bodies placed in the flow, or swirl vanes (aerodynamic stabilization), as in gas turbine combustion chambers. Of practical importance to gas turbine combustor designers is a knowledge of the ignition and blowout velocities since they determine the maximum mass flow (i.e., reactant throughput) rates at which the mixture can be ignited, or at which stable combustion is achieved, respectively.

In the present study, we employ a stochastic mixing model that couples finite rate mixing with finite rate combustion chemistry to examine the effects of combustor inlet conditions on the ignition limits of lean premixed turbulent flames. The motivation of this work is the increasing emphasis on lean, premixed, prevaporized combustion for aircraft gas turbine engine applications, e.g., Mularz.[1] However, it is difficult to achieve perfect premixing (i.e., uniformity on the small turbulence scales) in practical combustion devices.[2] Also, future gas turbine combustors may be required to operate with fuels of much lower hydrogen-to-carbon ratio.[3,4] The eventual goal of the present work is to examine the effects of local fuel/air ratio nonuniformities and alternate fuels on flame stability. The present problem was chosen to assess the predictive capabilities of the model. This work will also serve as a test problem for a new algorithm being developed by Pratt and Radhakrishnan[5] for the efficient numerical integration of chemical kinetic rate equations.

The present model is based on and extends the work of Radhakrishnan et al.,[6-8] who have recently developed a stochastic mixing model for studies of ignition and blowout in a combustor primary zone. In their model, the primary zone downstream of the flameholder (a perforated plate) was treated as a partially segregated stirred reactor. The composition of the reactor at any time was described by a scalar ensemble of N equal-mass fluid elements, which have possibly different thermodynamic states. The major inputs into the model were the volume of the reactor, reference velocity, blockage ratio of the flame stabilizer, and mean residence time for the reactor. These inputs defined a mixing frequency at which the N elements interact, and a feed and removal rate of elements into and out of the reactor, determined by the residence time. The model also provided a methodology for describing the degree of segregation due to incomplete premixing in the combustor primary zone. To describe the chemical kinetics of the fuel oxidation process, a single-step

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*Assistant Professor, Mechanical Engineering and Applied Mechanics. Member AIAA.

†Professor and Chairman, Mechanical Engineering. Member AIAA.

overall rate expression due to Dryer and Glassman[9] for methane oxidation was used. The model assumed that the products of combustion were solely carbon dioxide, water, nitrogen, and possibly oxygen.

Radhakrishnan et al.[6-8] used their model to study the effects of inlet conditions—pressure, temperature, reference velocity, and mixture uniformity—on the flame stability of lean mixtures. The variations of the predicted lean ignition and blowout limits of premixed turbulent flames with mixture temperature, pressure, and velocity compared favorably with experimental magnitudes and trends. The effect of incomplete premixing of the fuel and air on the lean ignition limit was explored using an assumed (Gaussian) distribution in fuel fraction F (fuel mass divided by total mass) in the inlet stream. The model predicted a significant reduction in the lean ignition limit with increased mixture nonuniformity; a trend confirmed by experimental data.

In the present work, better approximations are made for describing the chemical kinetics of the fuel oxidation process and for simulating the transport of unburnt fuel/air mixture into the primary zone and of the reactor contents out of this zone. More specifically, the one-step overall reaction rate for methane oxidation due to Dryer and Glassman[9] is replaced by a two-step reaction mechanism recently developed by Westbrook and Dryer.[10] The use of a characteristic residence time for the primary zone is replaced by two feed rates: an input feed rate determined by the mass flow rate of fuel/air mixture and a feed rate out of the reactor governed by the change in the ensemble mean specific volume. The model is demonstrated by application to the prediction of lean ignition limits of premixed turbulent flames.

II. A Coalescence/Dispersion Model for Flame Stability

In the primary zone of any continuous flow combustor, a recirculating flow accomplishes the back mixing (or age mixing) needed to avoid flame blowout, irrespective of the premixing quality (or mixture uniformity) at the combustor inlet. Depending on the extent to which fuel and air have mixed upstream of the primary zone, the inlet stream will have some distribution of fuel/air ratio about the mean value. For incompletely premixed systems, this distribution will change with time due to mixing, through the action of turbulence and molecular diffusion, within the primary zone. To model the phenomena of ignition and blowout, this finite rate mixing within the primary zone must be coupled with finite rate combustion chemistry.

One technique that provides the coupling between finite rate fluid mechanic mixing and finite rate combustion chemistry is the stochastic or Monte Carlo "coalescence and dispersion" model. We briefly discuss this model: Pratt[11,12] gives a detailed description of Monte Carlo models for representing turbulent mixing. In this approach, originally proposed by Curl[13] (see also Corrsin[14]) and adapted by Spielman and Levenspiel,[15] Evangelista et al.,[16] and Flagan and Appleton,[17] the fluid composition at any time is described by a scalar ensemble of N equal mass fluid elements. These elements have a distribution of thermodynamic states which represent the temporal fluctuations in turbulent flows. Each element is assumed to be sufficiently small so that its properties may be assumed uniform throughout its volume, allowing its thermodynamic state to be well defined. At any point in time each such element has its own local fuel fraction.

The ensemble of fluid elements experiences mixing interactions which represent the turbulent and molecular mixing or micromixing process. Each mixing interaction is computed by randomly selecting two different fluid elements which are allowed to mix completely (properties are mass averaged) and then separate. For flows with chemical reactions, the chemical reactions proceed within each element at a rate that depends on its new enthalpy and chemical composition. Either a global rate equation or a complex reaction mechanism may be used to describe the chemical reactions of interest.

Mean values of concentration, temperature, and other properties, as well as variance or higher moments, can be obtained from instantaneous ensemble averaging over the combustor population. Thus, given an initial distribution function for scalar properties, the development with time of the distribution function can be followed.

We now discuss the application of the coalescence/dispersion model to studies of premixed flame stability. In particular, we study the variations with inlet conditions of the lean ignition limits of premixed turbulent propane/air flames stabilized behind perforated plates. This geometry was chosen for the following reason. In several recent experimental investigations perforated plates were used; hence, published data on the effects of high temperature and pressure on flame stability are available for comparison with model predictions. In the present work, as in the preceding work, the region immediately downstream of the perforated plate is characterized as a partially segregated stirred reactor. The composition of the reactor is described by a statistical ensemble of N equal mass fluid elements of uniform composition, where N must be large enough to adequately represent the distribution of thermodynamic states within the reactor. (The number was 1000 for the calculations presented herein.)

As discussed earlier, the ensemble of fluid elements experiences mixing interactions which simulate the mixing process. These interactions, computed sequentially, occur at time intervals Δt_m given by

$$\Delta t_m = 1/(\beta N)^{1/3} \tag{1}$$

where β is an empirically determined frequency. Following Radhakrishnan et al.,[6-8] the following relation for the mixing frequency in the primary zone is used.

$$\beta = c_\beta (P_j/mL^2)^{1/3} \tag{2}$$

where P_j is the flux of kinetic energy through the perforated plate into the mixing region, m the mass within the reactor, and L the length of the reactor. The constant c_β, of order unity, represents the efficiency of transfer of kinetic energy to turbulent flow. In this study β is assumed constant within the reactor and the length L is assumed equal to the length of the recirculation zone downstream of the flameholder. We also note that Eq. (2) was used to calculate β only at $t=0$; for later times it was calculated from the residence time as discussed in Sec. II.A.

For a continuous-flow combustor, the transport of unburnt fuel/air mixture into the primary zone, and of the reactor contents out of this zone, must be modeled. These transport processes are simulated by element additions and removals. These "flux events" occur at time intervals Δt_r, given by

$$\Delta t_r = \tau_r/N \tag{3}$$

where τ_r is the average residence time for the reactor

$$\tau_r = V/(\dot{m}\bar{v}) \tag{4}$$

V the volume of the reactor, $\dot{m}$ the mass flow rate into the reactor, and $\bar{v}$ the mean specific volume within the reactor. Equation (4) is valid for steady-state operation of the combustor. During the (unsteady) phenomena of ignition and blowout, $\bar{v}$ fluctuates and therefore τ_r of Eq. (4) is ambiguous. In their model, Radhakrishnan et al.[8] therefore assumed, following Beer and Chigier,[18] an alternative measure for τ_r, using the estimate

$$\tau_r = L/U \tag{5}$$

where L is the length of the recirculation zone and U the approach flow velocity. We note that τ_r, given by Eq. (5), is inversely proportional to the mass loading of the primary zone.

In the present study, however, the unsteady nature of the problem is incorporated, in a conceptually simple manner, as follows. The use of one residence time is replaced by two feed rates; one into and one out of the reactor. The mass flow rate into the reactor is constant, but that out of the zone is time dependent, reflecting the transience of the ignition and blowout phenomena. If, at any time t, the mass of the reactor contents is $m(t)$, and the number of elements characterizing the composition of the reactor contents is $N(t)$, then the feed rates $\dot{N}_i(t)$ into and $\dot{N}_e(t)$ out of the reactor are, respectively,

$$\dot{N}_i(t) = \dot{m}_i N(t)/m(t) \tag{6}$$

$$\dot{N}_e(t) = \dot{m}_e N(t)/m(t) \tag{7}$$

where $\dot{m}_i$ and $\dot{m}_e$ are, respectively, the mass flow rates into and out of the reactor. The flow rate $\dot{m}_i$ is specified by the boundary conditions, and the flow rate $\dot{m}_e$ is given by the equation of continuity

$$\dot{m}_e = \dot{m}_i - \frac{\mathrm{d}m(t)}{\mathrm{d}t} \tag{8}$$

where $\mathrm{d}m(t)/\mathrm{d}t$, the time rate of change of mass within the reactor, is estimated using a conventional backward difference.

$$\frac{\mathrm{d}m(t)}{\mathrm{d}t} = \frac{m(t) - m(t-\Delta t)}{\Delta t} \tag{9}$$

and where $m(t)$ is given by

$$m(t) = V/\bar{v}(t) \tag{10}$$

Here V is the volume of the reactor and $\bar{v}(t)$ the mean specific volume within the reactor.

The computational procedure therefore involves updating the state of each element at time intervals Δt. The mean value of the specific volume is then obtained by ensemble averaging over the $N(t)$ fluid elements. Equations (6-10) are then used to estimate the element feed rates into and out of the reactor.

To simulate the inflow of unburnt fuel/air mixture, an unburnt element at inlet conditions is added at time intervals Δt_i given by

$$\Delta t_i = 1/\dot{N}_i \tag{11}$$

To simulate both the flow out of the reactor and the random nature of the flow within it, an element is randomly chosen from the reactor and removed from it at time intervals Δt_e

$$\Delta t_e = 1/\dot{N}_e \tag{12}$$

We note that the use of two feed rates allows the definition of an unambiguous average residence time τ for the reactor as follows:

$$\tau(t) = V/(\dot{m}_e(t)\bar{v}(t)) \tag{13}$$

To describe the chemical kinetics of the fuel oxidation process, Radhakrishnan et al.[8] used a single-step overall rate expression for methane oxidation due to Dryer and Glassman.[9] Methane was chosen as the fuel because of uncertainties in available overall reaction rates for higher hydrocarbons. Their model assumed that the products of combustion were carbon dioxide, water, nitrogen, and oxygen. The use of a single-step reaction mechanism is adequate for fuel lean mixtures, since the levels of carbon monoxide and hydrogen are quite low relative to those of carbon dioxide and water, respectively. However, one of the features of non-premixed systems is the presence of locally fuel-rich and high-temperature zones in the primary zone. For rich mixtures, significant amounts of CO (and H_2 for very rich mixtures) exist in equilibrium in the combustion products with CO_2 and H_2O. In the present study we have therefore used a two-step reaction mechanism as a compromise between accuracy and the large computer time requirements for more detailed kinetic mechanisms. Following Dryer and Glassman[9] and Westbrook and Dryer,[10] who have recently examined simplified reaction mechanisms for the oxidation of hydrocarbon fuels, we use a single finite rate reaction of fuel and oxygen to form CO and H_2O, followed by an oxidation rate for CO.

$$C_3H_8 + 3.5\,O_2 \xrightarrow{k_{ov}} 3\,CO + 4\,H_2O \tag{14a}$$

$$k_{ov} = 10^{12}\exp(-30/RT)[C_3H_8]^{0.1}[O_2]^{1.65}\ \text{mole/cm}^3\ \text{s} \tag{14b}$$

$$CO + 0.5\,O_2 \underset{k_b}{\overset{k_f}{\rightleftharpoons}} CO_2 \tag{15a}$$

$$k_f = 10^{14.6}\exp(-40/RT)[CO]^1[H_2O]^{0.5}[O_2]^{0.25}\ \text{mole/cm}^3\ \text{s} \tag{15b}$$

$$k_b = 5\times 10^8\exp(-40/RT)[CO_2]^1\ \text{mole/cm}^3\ \text{s} \tag{15c}$$

where all rate constants have been taken from Refs. 9 and 10. However, the pre-exponential constants had to be adjusted, as will be discussed later.

At any time, the mean composition and other mean properties are evaluated by first integrating the chemical rate equations (14) and (15) up to the time of interest for each element and by taking an average over all fluid elements.

Computational Procedures

The computational procedures used for predicting the lean ignition limit are essentially those given by Radhakrishnan et al.[7,8] and are as follows:

1) For given values of the combustor inlet conditions (pressure P, unburnt temperature T_u, and fuel/air equivalence ratio ϕ) the unburned gas thermodynamic properties are computed according to the procedure outlined by Pratt and Wormeck.[19]

2) The fully burnt mixture thermodynamic properties and composition are calculated using the method described by Pratt and Wormeck together with Eqs. (14) and (15), assuming an adiabatic constant pressure combustion process from the unburnt mixture state.

3) The ensemble of elements is initialized at time $t=0$ with all elements unburnt; i.e., for each element B (=burnt fraction) $=0$, T (=temperature) $=T_u$. In this work, the burnt fraction B was defined as $B=\sigma_{CO_2}/\sigma_{CO_2,b}$ where σ_{CO_2} is the mole number (mole/g mixture) of CO_2 and the subscript b denotes the fully burnt state. B therefore varies from 0 (unburnt state) to 1 (fully burnt state).

4) The specific volume for the burnt mixture is computed and the mass is given by Eq. (10). At $t=0$, the mixing frequency β and residence time τ are computed using Eqs. (2) and (4), respectively. Following Radhakrishnan et al.,[8] β was calculated using a value $c_\beta = 1$.

For later times, β was calculated as follows. The product $\beta\tau$ was held constant at its initial (unburnt) value and β was computed from the residence time τ. This was necessary in order to predict the correct variation of the burned fraction with equivalence ratio, i.e., that richer mixtures burn faster than leaner ones. This approach is in agreement with the practice adopted either explicitly[15,16,20-22] or implicitly[7,23] by other researchers using coalescence/dispersion models.

5) To model the spark process, at time $t=0^+$, n (with $n/N \ll 1$) of these elements are assumed fully burnt so that their properties become $B=1$, $T=T_b$ (=fully burnt tem-

perature), and $\sigma_i = \sigma_{i,b}$ for all i. The ensemble burnt fraction B is therefore n/N at $t=0$. Results from previous investigations[8] indicate that the lean ignition limit is relatively insensitive to values of n and n/N. These two were therefore not varied in this study; values of $n=10$ and $N=1000$ were used for all of the calculations presented here.

6) The ensemble mean specific volume $\bar{v}$ is computed and the mass $m(t)$ is given by Eq. (10). The element feed rate $\dot{N}_i$ into the reactor an the feed time Δt_i are calculated using Eqs. (6) and (11), respectively. To initialize the calculation procedure (i.e., at time $t=0$), $\dot{N}_e$ and Δt_e are set equal to $\dot{N}_i$ and Δt_i, respectively. Thereafter they are calculated using Eqs. (7-9) and (12). The residence time τ is computed from Eq. (13) and the mixing frequency β is calculated from τ, as discussed above.

7) The mixing process and material flow through the primary zone are simulated as described previously.

8) At any time t, the mean properties of the ensemble are evaluated by numerically integrating the rate equations (14) and (15) for each element (provided its burnt fraction is greater than 0) up to that time and by taking an average over the N fluid elements.

The use of the rate equations (14) and (15) resulted in predicted lean ignition limits much leaner than measured values. The pre-exponential constants were adjusted (by a factor 0.6) to give agreement between the measured and predicted lean ignition limits at one operating condition ($T_u = 500$ K, $U=10$ m/s, $P=1$ atm). We note that since this multiplying factor of 0.6 was applied to all three rate equations the burned gas temperature and composition are not affected. Such an adjustment is consistent with the philosophy behind these global rate equations.[10]

The state of the ensemble is updated at time intervals of Δt and steps 4 and 5 are repeated until the phenomenon of ignition is identified, as discussed below. We note here that the accuracy of the approximation given by Eq. (9) improves with a reduction in the value of Δt; however, the computation time increases with a reduction in Δt. An optimal value of Δt was chosen as follows. A nondimensional time increment $(\Delta t)^*$ was defined as $\Delta t/\Delta t_i$ (note that Δt is now a function of time) and values of $(\Delta t)^*$ of 10, 50, and 100 ($N=1000$) were tested. The lean ignition limit was found to be relatively insensitive to these values of $(\Delta t)^*$. Hence, a value of $(\Delta t)^* = 50$ was used in all of the results presented here.

The lean ignition limit was determined as decribed by Radhakrishnan et al.[7,8]; the calculation procedure for this limit is briefly discussed below. To determine the lean ignition limit for a given set of inlet conditions (ϕ, T_u, and mixture reference velocity U), the ensemble of fluid elements is initialized as described above. The ensemble properties are then allowed to evolve with time for various fuel/air equivalence ratios ϕ. For values of ϕ less than some value, the ensemble burnt fraction, B, decreases with time (see Fig. 1 for example), thereby denoting nonignition. In Fig. 1, the nondimensional t^* was defined to be $t^* = t/\tau_r$ where τ_r ($=L/U$) is the residence time given by Eq. (5). The leanest mixture that shows an increase in $\bar{B}$ is defined to be the lean ignition limit. For the example given in Fig. 1 ($T_u = 500$ K, $P=1$ atm, $U=10$ m/s) the model has predicted a lean ignition equivalence ratio limit of 0.63. The computation was restricted to one residence time after Radhakrishnan et al.,[7,8] who found that computations carried out for much longer times showed essentially no change in the lean ignition limit of uniform mixtures. Also, computations carried out for much longer times confirmed this. It is, however, recognized that ignition should be a probabilistic phenomenon in that, at incipient ignition, a given value of fuel/air ratio may or may not lead to ignition on successive trials. The oscillations in the ensemble burnt fraction vs time curves (Fig. 1) for values of ϕ close to the ignition limit suggest this behavior. Preliminary results from previous investigations indicate that this behavior is more pronounced for non-premixed fuel/air

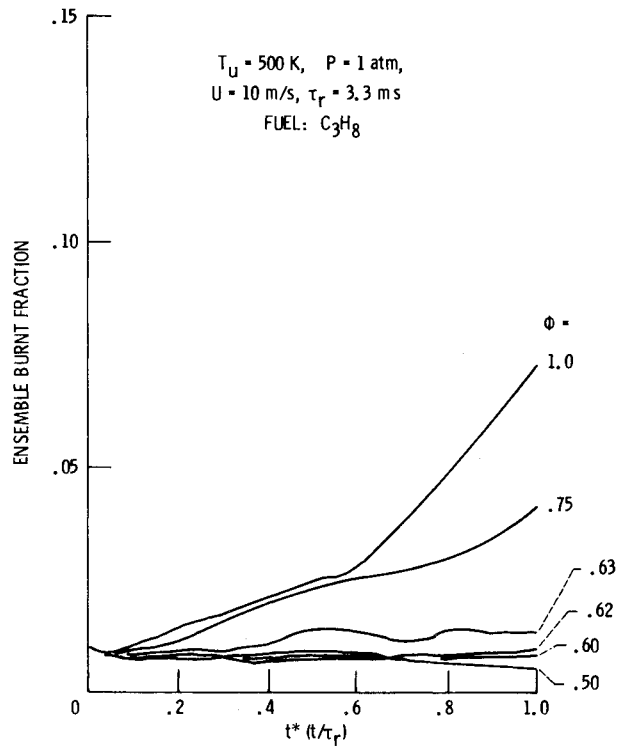

Fig. 1 Example of lean ignition limit calculation.

mixtures. A systematic investigation of this phenomenon was therefore not attempted in this study where we deal with premixed systems only. The present ignition limits may, therefore, be interpreted as those that lead to near-certain ignition.

III. Results and Discussion

The procedure outlined in the previous section was used to generate lean ignition limits for various operating conditions. The length L ($=33$ mm in isothermal flow) of the recirculation zone (and hence, of the reactor) was taken from Radhakrishnan.[24] The parameters used in this study and their effects on the lean ignition limit are discussed below, and, where possible, quantitative comparisons are made with experimental data.

A. Reference Velocity

The effect of the reference velocity U on the lean ignition limit was studied by generating lean ignition limits for $U=5$, 10, and 25 m/s, all at 500 K, 1 atm. With increased velocity the lean ignition limit is richer. This is due to the faster mixing rates and lower residence times associated with increasing U. The requirement of richer mixtures for successful ignition at higher velocities has been observed also by Bolt and Harrington[25] and Ballal and Lefebvre.[26] The lean blowoff limit also exhibits a similar behavior (see Ref. 7 for details). Figure 2 compares the prediction from the present work with the results of Radhakrishnan et al.[6-8] Their results include experimental data for propane and model predictions generated with a single-step mechanism for methane. The predictons from the present model compare well with the experimental data.

B. Inlet Temperature

The effects of inlet temperature T_u on the lean ignition limit were studied at constant reference velocity (10 m/s) and pressure (1 atm). Ignition limits were generated for $T_u = 300$, 500, and 700 K and are shown in Fig. 3. Also shown for comparison are the experimental data (for propane) and model predictions (for methane) of Radhakrishnan et al.[8] The

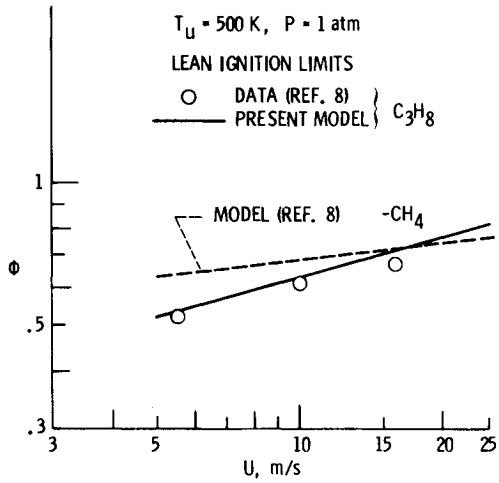

Fig. 2 Variation with reference velocity of the predicted (solid line) lean ignition limit compared with the exprimental data (o) and model predictions (dashed line) of Radhakrishnan et al.[8] Modeled kinetic parameter was adjusted for agreement at 500 K.

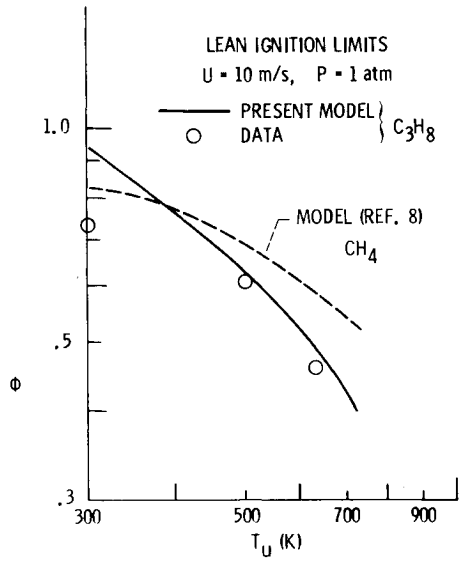

Fig. 3 Variation with inlet temperature of the predicted (solid line) lean ignition limit compared with the experimental data (o) and model predictions (dashed line) of Radhakrishnan et al.[8] Modeled kinetic parameter was adjusted for agreement at 500 K.

lean ignition limit is reduced with increasing inlet temperature. Increases in inlet temperature lead to higher temperature burned products and increased burning rates. Hence, at constant inlet velocity (i.e., constant mixing rate and residence time), this leads to a reduction in the fuel flow rate needed for successful ignition. For inlet temperatures above 500 K we notice good agreement between the experimental data and predictions from the present work. Again, the use of a two-step mechanism has resulted in improved predictions. However, for an inlet temperature of 300 K the predicted limit is significantly richer than the experimental data. This suggests that the reaction rates used in the present work do not predict the correct trend with the unburnt temperature. Westbrook and Dryer[10] estimated the rate constants by matching calculated laminar flame speeds with experimental observations. They state that these mechanisms reliably predict flame speeds over a range of equivalence ratios and pressures. However it is not clear from their discussion if the variation with unburnt temperature was examined. If not, suitable corrections may have to be made in order to provide better agreement with temperature.

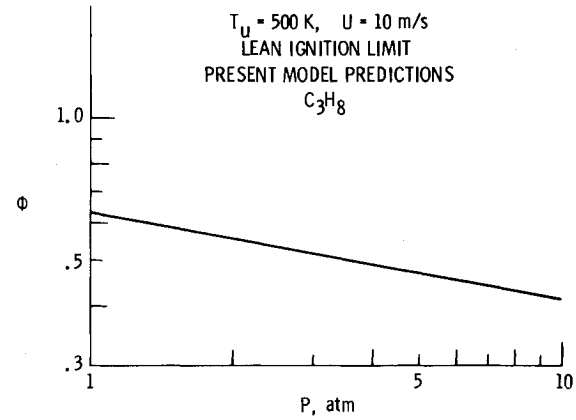

Fig. 4 Variation of the predicted lean ignition limit with pressure.

Another possible explanation for the discrepancy at low temperature is the use of a constant mixing parameter $\beta\tau$. The mixing parameter has been estimated from data generated under steady-state burning conditions, see, e.g., Ref. 27. In applying these correlations to the transient phenomena of ignition and blowout, modifications may have to be made.

C. Pressure

Lean ignition limits were generated for $P = 1$, 3, 5, 7.5, and 10 atm at a reference velocity of 10 m/s and inlet temperature of 500 K. The variation of the predicted lean ignition limit is shown in Fig. 4. We see that the lean ignition limit does not have a strong dependence on the pressure. Lack of experimental data at high pressures prevents quantitative comparisons. However, the predicted trends are consistent with the known fact that increasing pressures above 1 atm has a small effect on the lean flammability limit of methane air mixtures, see, e.g., Ref. 28. In addition, from experiments with propane/air mixtures in a constant volume bomb, Bolt and Harrington[25] concluded that inlet pressures between 1.7 and 12.2 atm had no noticeable effect on the lean ignition limit for either moving or stagnant mixtures.

IV. Conclusions

A coalescence/dispersion model has been developed for turbulent flame stability studies in a combustor primary zone. A two-step reaction mechanism was used to describe the fuel oxidation process.

The use of the model was demonstrated by generating lean ignition limits of premixed turbulent flames. The variations of the lean ignition limit with reference velocity, inlet temperature, and pressure have been studied. The predicted trends compared favorably with experimental observations. The variation of the predicted ignition limit with reference velocity compared well with experimental data. The agreement between the predicted limits and experimental data was good at high temperatures. However, at low temperatures the model predicted substantially richer limits. Further work needs to be done to resolve this discrepancy at low temperatures. Lack of high-pressure lean ignition limit data prevented a quantitative comparison in this regime.

Acknowledgements

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