Variable Density Effects in Premixed Turbulent Flames

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Earlier calculations of planar, oblique, and normal combustion waves based on the Bray-Moss model of premixed turbulent flows have been improved and the theory exploited further. Variable density effects on the Prandtl-Kolmogoroff model for the eddy transport coefficient and on the scalar dissipation are shown to bring the predictions of the theory in more satisfactory agreement with experimental results for the orientation of the combustion wave in the case of strong interaction, the case most amenable to comparison. The theory is used to compare the distributions through the reaction zone of several statistical quantities as given by conventional and Favre averaging; large differences are found in some quantities with the implication that different modeling to achieve closure may be required for the two means of averaging when the heat release, and therefore variable density effects, are significant. In particular it is found that the triple correlation terms, which enter the momentum and scalar fluxes according to conventional averaging, are the principal source of the differences in the fluxes as given by the two means of averaging.

Nomenclature

a	= constant in Prandtl-Kolmogoroff model for the eddy transport coefficient, cf., Eq. (3)
c	= normalized product mass fraction
c_m	= mean product concentration weighted by reaction rate, cf., Eq. (19) of Ref. 1
C	= constant in scalar dissipation model
ℓ_1, ℓ_2	= characteristic turbulence length scales, cf., Eqs. (3) and (4)
p,k,m	= exponents of density ratio
$P(c,r)$, $P(u,c;r)$	= probability density functions, cf., Eqs. (11) and (28)
$\tilde{q}$	= turbulent kinetic energy
Q	= ratio of turbulent kinetic energies, $\tilde{q}/\tilde{q}_0$
$\tilde{Q}$	= kinetic energy function, cf., Eq. (5)
Q_∞	= ratio of turbulent kinetic energies, $\tilde{q}_\infty/\tilde{q}_0$
T	= static temperature
u	= velocity component in x direction
v	= velocity component in y direction
α,β,γ	= strengths of three modes of product concentration, cf., Fig. 2a
$\beta,\hat{\beta}$	= turbulent flame speed parameters
ϵ	= $\overline{\rho u''^2}/\bar{\rho}\tilde{q}$, fraction of turbulent kinetic energy due to x-wise velocity fluctuations
θ	= orientation of the reaction zone
ν_T	= eddy transport coefficient
ξ	= nondimensional normal coordinate, cf., Eq. (5)
ρ	= mixture mass density
τ	= heat release parameter
Φ	= turbulence parameter
Subscripts	
0	= conditions upstream of reaction zone, $x,\xi \to -\infty$
∞	= conditions downstream of reaction zone, x, $\xi \to -\infty$

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I. Introduction

BRAY and Libby[1] present the results of the application of the Bray-Moss[2] model for premixed turbulent reactions to planar, oblique combustion waves. The flow situation considered is shown schematically in Fig. 1; it represents an idealization of various laboratory experiments, e.g., those of Wright and Zukoski,[3] in which turbulent flames are stabilized in a two-dimensional duct flow by means of a rod. Figure 2 is a shadowgraph taken from Ref. 3 and shows such flames. A plane, oblique reaction zone is inclined at an angle θ to an oncoming turbulent flow of cold reactants with a turbulent kinetic energy $\tilde{q}_0 = \frac{1}{2}(\overline{\rho u_k'' u_k''}/\bar{\rho})_0$. As a result of the competition between the dilatation associated with the heat release and the turbulence production due to shear within the reaction zone, the turbulent kinetic energy downstream of the flame is altered, i.e., $\tilde{q}_\infty = \tilde{q}_0 Q_\infty$, $Q_\infty \neq 1$ in general.

According to the Bray-Moss model, one or more oscillating flame surfaces traverse the reaction zone; at these surfaces reactants are destroyed and product formed. The instantaneous state of the gas is referred to a progress variable c, which may be considered the mass fraction of product normalized to be unity when the reaction is complete. We shall term c the "product concentration." For times when all flame surfaces are downstream of a particular point within the reaction zone, or when a packet of unburned gas is at such a point, the instantaneous state of the gas corresponds to $c = 0$, i.e., to a cold mixture of reactants. Alternatively, when all of the flame surfaces are upstream of the same point, or a packet of completely burned gas is at that point, the state of the gas corresponds to $c = 1$, i.e., to hot products of reaction with one or both reactants totally consumed. Finally, when the flame surfaces themselves cross the point in question, their structure leads to values of c interior to the 0-1 range.

The probability density function for the product concentration at a point located by the vector r associated with this physical picture is shown schematically in Fig. 3a; involved are delta functions corresponding to the precise values $c = 0$, 1, and distributed values associated with the passage of the flame surfaces through the point r. The strengths of these three modes are identified with the values $\alpha(r)$, $\beta(r)$, and $\gamma(r)$. Central to the Bray-Moss model is the assumption that the flow conditions and chemical system are such that the chemistry is "fast" and thus that the intermediate values of c associated with the strength $\gamma(r)$ are relatively rare.

These physical ideas are supplemented by several additional assumptions; some pertain to the aerothermochemistry of the flow and are standard in combustion theory. One important assumption in Ref. 1 requires the mean streamline to be undeflected through the reaction zone, and permits the mean velocity field to be determined without further approximation; in fact, we obtain an explicit equation for the Reynolds stress free of a gradient approximation. The implication of this result is that the fluid is accelerated through the reaction zone by the force associated with the normal gradient of the Reynolds stress and not by the pressure gradient.

The equations for the mean product concentration, for the fluctuations of the product concentration, and for the turbulent kinetic energy are closed by appropriate gradient assumptions and by modeling the dissipation of product fluctuations. The final formulation results in two ordinary differential equations for the mean turbulent kinetic energy $\tilde{q}$ and the mean product concentration $\tilde{c}$. As suggested by our notation, the analysis is carried out in Favre variables.[4] Finally, the characteristics of the turbulence are embodied in two parameters; one denoted Φ involves several empirical constants and a second denoted ϵ is the fraction of the turbulent kinetic energy represented by the fluctuations of the x-wise velocity component. In Ref. 1, Φ is based on data obtained from constant density turbulent flows.

An important conclusion drawn from the nature of the describing equations is that dissipation of turbulent kinetic energy within the reaction zone is negligible. The physical basis for this conclusion resides in the rapid distortion of the mean flow due to heat release. In the balance of turbulent kinetic energy in oblique combustion waves, it is found that convection and production due to shear are dominant and nearly balancing. Thus, according to the present theory, assumptions of equilibrium or near-equilibrium turbulence are inappropriate for combustion waves of the sort considered.

There are two quantities that appear within the describing equations which must be determined as part of the solution. These are the turbulent flame speed $\tilde{u}_0$ in the form of the ratio $\tilde{u}_0/\tilde{q}_0{}^{1/2}$; and the ratio Q_∞, of turbulent kinetic energy far downstream of the reaction zone to that in the oncoming stream.

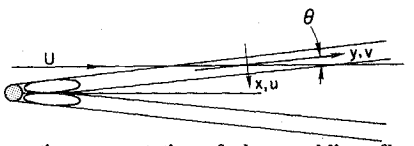


Fig. 1 Schematic representation of planar, oblique flames stabilized on a rod showing the coordinate system.

The extent of the heat release, which can be considered an indication of the degree of dilution of the reactants or of their proximity to a stoichiometric mixture, is related to a parameter τ; typical values of applied interest correspond to $4 \lesssim \tau \lesssim 9$. Associated with various specified values of θ and τ are various values of Q_∞; thus, e.g., for nearly normal reaction zones, the dilatation due to heat release decreases the turbulence and $Q_\infty < 1$. For highly oblique reaction zones with large amounts of heat release, the turbulence generated by shear overwhelms the dilatation effect, and $Q_\infty > 1$.

In Bray and Libby,[1] considerable attention is devoted to comparison between the predictions of the theory and results from a variety of experiments on premixed reactants. Generally no more than qualitative agreement can be expected because, for various reasons, the available experimental results in most cases do not permit direct quantitative comparison. In some cases the flow conditions preclude comparison; in others the experimental data provided are either insufficient or inappropriate. Nevertheless, in those cases wherein comparison can reasonably be carried out, the agreement is generally satisfactory.

With respect to comparison of prediction with experiment, a special case, that of so-called "strong interaction," is of particular interest. If the turbulence generated by shear within the reaction zone overwhelms that in the oncoming stream, the equations are altered so that the turbulent flame speed in the form $\tilde{u}_0/\tilde{q}_\infty{}^{1/2}$ and the orientation of the reaction zone, i.e., θ, are determined as part of the solution. In experiments such as those of Wright and Zukoski,[3] the angle θ is obtained from visual observation, and direct comparison between prediction and experiment can be made. The comparison in Ref. 1 with respect to θ is not satisfactory; typically values of θ of 20°-30° are predicted in contrast to measured values of 3°-6°. The discrepancy in part is attributed to the use in the parameter Φ of empirical constants based on constant density turbulence in a situation where the mean density varies with the heat-release parameter τ, and can therefore change by an order of magnitude.

The analysis of Refs. 1 and 2, on the one hand, has sufficient physical and chemical content, and on the other is sufficiently simple so that it provides a useful vehicle for studying a variety of effects that are present in more complex turbulent flows. Here we exploit this property of the analysis to examine the influence of variations in density arising from heat release. An examination of the available literature (cf., e.g., Ref. 5 and 6) on predictive methods for turbulent reacting flows indicates that many analyses apply to the case of highly dilute reactants, and thus to flows in which the heat release does not alter the turbulence; in those few analyses including significant heat release, the influence of density variations generally is assumed to be restricted to variations in

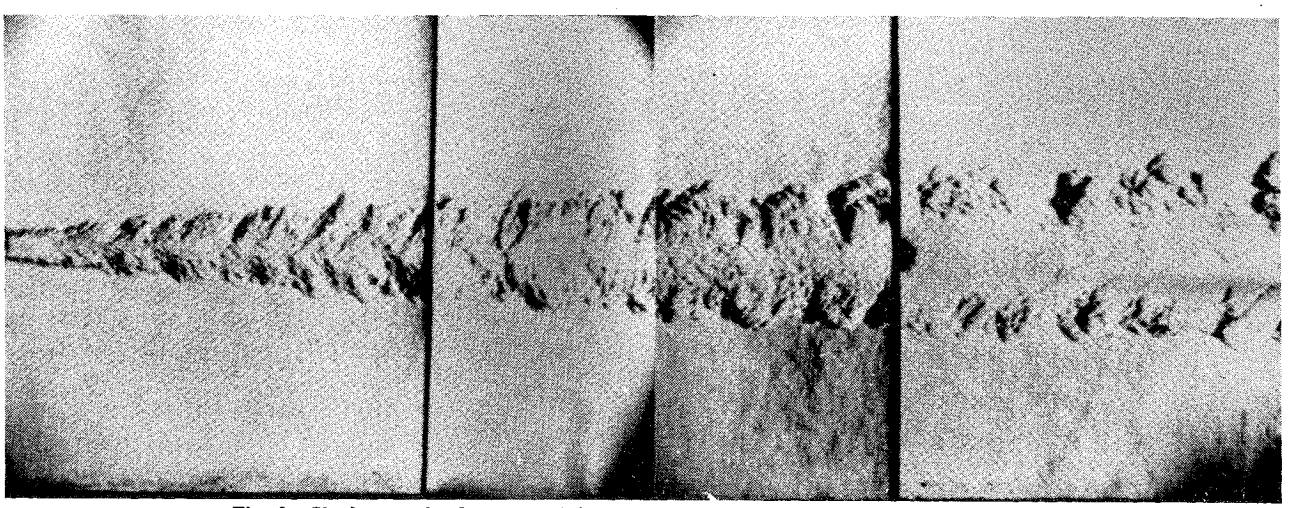


Fig. 2 Shadowgraph of planar, oblique flames stabilized on a rod (from Ref. 3).

the mean density while all density fluctuations are ignored, presumably not out of conviction as to their unimportance, but rather out of ignorance as to their proper treatment.

Accordingly, we first reconsider the modeling employed in Ref. 1, and incorporate variable density effects. Then we use the comparison between prediction and experiment for the orientation of the reaction zone in the case of strong interaction to guide the selection of a crucial exponent of the density ratio. We find that satisfactory agreement thereby is possible.

One means of incorporating variable density effects in the description of turbulent reacting flows is to employ Favre averaging; in this case density fluctuations do not appear explicitly, but their effects are contained implicitly in the various correlations of instantaneous density with velocity, concentration, etc. For example, the mean momentum flux term of interest in shear flows is exactly and completely given by $\overline{\rho u'' v''}$, where the double prime denotes the fluctuating difference between an instantaneous value and the mass averaged value. Comparison of corresponding statistical quantities are given by conventional and Favre averaging suggests that the modeling employed to effect closure may be different in the two cases. However, there has been little serious consideration of the modeling for turbulent flows with variable density, so that the modeling appropriate for either means of averaging is largely speculative.

In this connection it is of interest to note that, when conventional averaging is employed and the correlations involving density fluctuations are neglected, the consequence is a mixed, inconsistent calculation, implicitly involving Favre averaging for some terms and conventional averaging for others, a consequence without appeal (cf., e.g., Borghi, in Ref. 5, Spalding,[7] and Bellan and Sirignano[8]).‡

The analysis of Refs. 1 and 2 permits comparison to be made of the distribution of statistical quantities within planar, oblique reaction zones as given by conventional and Favre averaging. Part of this comparison will involve calculation of the density fluctuation terms, e.g., $\overline{\rho' u'}$, which, as we have noted, generally are neglected in methods employing conventional averaging. We find that the triple correlation terms, e.g., $\overline{\rho' u' v'}$, are significant and that in general there are relatively large differences between conventional and Favre averaged quantities when the heat release corresponds to values of practical interest.

II. Revised Modeling for Variable Density Effects

In the interests of brevity, the starting point for the reconsideration of the modeling will be two differential equations that are obtained readily from Eqs. (44) and (47) of Bray and Libby[1] §; they are

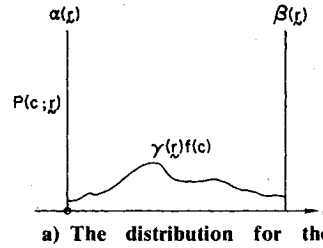
$$\frac{dQ}{dx} - \frac{d}{dx}\left(\frac{\tilde{\rho}}{\rho_0}\frac{\nu_T}{\tilde{u}_0}\frac{dQ}{dx}\right) = \left(\frac{\tilde{u}_0^2}{\tilde{q}_0}\frac{\tau^2\tilde{c}}{\tan^2\theta} - \frac{\epsilon Q\tau}{1+\tau\tilde{c}}\right)\frac{d\tilde{c}}{dx} \quad (1)$$

$$\frac{d\tilde{c}}{dx} - \frac{d}{dx}\left(\frac{\tilde{\rho}\nu_T}{\rho_0\tilde{u}_0}\frac{d\tilde{c}}{dx}\right) = \left(\frac{C}{2c_m - 1}\right)\frac{\tilde{q}_0^{1/2}}{\tilde{u}_0}\frac{1}{\ell_2}\frac{Q^{1/2}\tilde{c}(1-\tilde{c})}{1+\tau\tilde{c}} \quad (2)$$

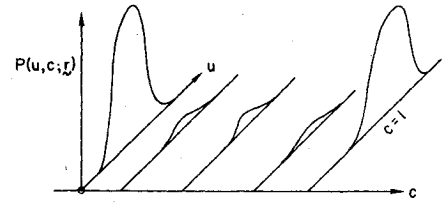
These forms of the describing equations are convenient because they expose the means for altering readily the modeling to account for variable density effects.

‡An anonymous reviewer has accused us of "using double standards," in that we criticize those who neglect density fluctuations while retaining the ill-founded notion of eddy diffusion. We note that a satisfactory theory for turbulent reacting flows would include *both* variable density effects and closure models without gradient approximations. Developments on both aspects should go forward, but we may at present be remote from such a theory.

§Reference 1 should be consulted for details.



a) The distribution for the product concentration $P(c;r)$



b) The joint distribution for the u-velocity component and the product concentration $P(u,c;r)$

Fig. 3 The probability density functions.

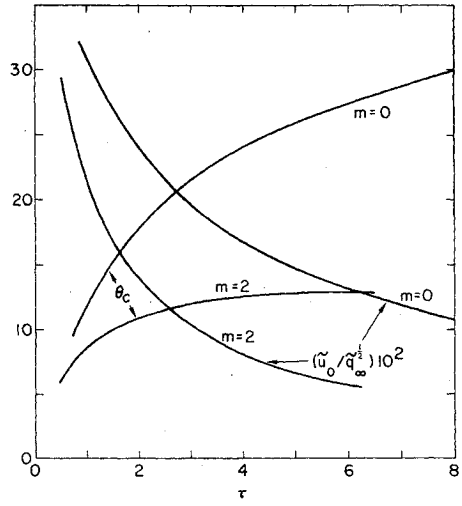


Fig. 4 Strong interaction solutions—variation of flame angle and flame speed parameter with heat release parameter and exponent m: $\tilde{c}_0 = 0.02$.

The two terms to be considered are the eddy transport coefficient ν_T and the scalar dissipation function on the right side of Eq. (2). Dimensional considerations suggest that the modeling of these functions should include a dependence on $\tilde{\rho}/\rho_0$. Therefore, we modify the usual Prandtl-Kolmogoroff form and let

$$\nu_T = a\tilde{q}^{1/2}\ell_1(\tilde{\rho}/\rho_0)^p \quad (3)$$

where p is an exponent as yet undetermined. In addition, let

$$C\ell_1/\ell_2 = (\tilde{\rho}/\rho_0)^k (C\ell_1/\ell_2)_0 \quad (4)$$

where again k is an undetermined exponent. The constant a and the ratio $(C\ell_1/\ell_2)_0$ apply to constant density flows,¶ so that for such flows we recover, with Eqs. (3) and (4), the assumptions used in Ref. 1 and in related studies.

Now we can introduce a new variable related to the turbulent kinetic energy; and a nondimensional, transformed normal coordinate, closely related to that used in Ref. 1; let

$$\xi = \int_0^x \left(\frac{\rho_0\tilde{u}_0}{\tilde{\rho}\nu_T}\right)dx' \quad \tilde{Q} = (Q - Q_\infty)/(1 - Q_\infty) \quad (5)$$

¶In Ref. 1, a is taken equal to 0.09 and C equal to 1.79, $\ell_1/\ell_2 = 1$; we retain these values.

Then Eqs. (1) and (2) become

$$\frac{d^2\tilde{Q}}{d\xi^2}-\frac{d\tilde{Q}}{d\xi}+\left[\frac{\Phi\tau^2\tilde{c}}{\beta(1-Q_\infty)\tan^2\theta}-\frac{\epsilon\tau}{1+\tau\tilde{c}}\left(\frac{Q_\infty}{1-Q_\infty}+\tilde{Q}\right)\right]\frac{d\tilde{c}}{d\xi}=0 \tag{6}$$

$$\frac{d^2\tilde{c}}{d\xi^2}-\frac{d\tilde{c}}{d\xi}+\beta\frac{(Q_\infty+(1-Q_\infty)\tilde{Q})\tilde{c}(1-\tilde{c})}{(1+\tau\tilde{c})^{2+m}}=0 \tag{7}$$

where $m=(p+k)$, $\beta=a(C\ell_1/\ell_2)_0(\tilde{q}_0/\tilde{u}_0^2)/(2c_m-1)=\Phi(\tilde{q}_0/\tilde{u}_0^2)$. As in Ref. 1, all of the empiricism relative to the turbulence is contained in Φ and ϵ; we assume here the same values as used in Ref. 1; namely, $\Phi=0.40$, $\epsilon=0.3$.

Equations (6) and (7) differ from the final equations in Ref. 1 only in the exponent in the denominator of Eq. (7); i.e., if $m=0$, the two sets of equations are identical. The most appropriate means for selecting m so as to achieve agreement with experiment is to treat the strong interaction case, since comparison on the basis of the angle of the reaction zone is direct. Accordingly, we let Q_∞ increase indefinitely, and obtain the alternate equations

$$\frac{d^2\tilde{Q}}{d\xi^2}-\frac{d\tilde{Q}}{d\xi}-\left(\frac{\Phi\tau^2\tilde{c}}{\hat{\beta}\tan^2\theta}-\frac{\epsilon\tau}{1+\tau\tilde{c}}(1-\tilde{Q})\right)\frac{d\tilde{c}}{d\xi}=0 \tag{8}$$

$$\frac{d^2\tilde{c}}{d\xi^2}-\frac{d\tilde{c}}{d\xi}+\frac{\hat{\beta}(1-\tilde{Q})\tilde{c}(1-\tilde{c})}{(1+\tau\tilde{c})^{2+m}}=0 \tag{9}$$

Again, these differ from those in Ref. 1 only in the exponent m. The parameter $\hat{\beta}=\beta Q_\infty=\Phi\tilde{q}_\infty/u_0^2$ relates the turbulent flame speed to the turbulent kinetic energy downstream of the reaction zone; $\hat{\beta}$ and the angle θ are determined as part of the solution.

The boundary conditions for both sets of equations are as follows:

$$\begin{aligned}&\text{at } \xi\to-\infty \quad \tilde{Q}=1 \quad \tilde{c}=0\\ &\text{at } \xi=0 \quad \tilde{c}=\tilde{c}_0\\ &\text{at } \xi\to\infty \quad \tilde{Q}=0 \quad \tilde{c}=1\end{aligned} \tag{10}$$

We remark that the theory encounters the usual problem of the "cold boundary condition," so that the last term on the left side of Eqs. (7) and (9) is set equal to zero for $\xi<0$, and $\tilde{c}_0$ is a parameter of the solutions along with the value of the heat release parameter τ. For highly oblique reaction zones, the results are insensitive to the value of $\tilde{c}_0$.

We have used the same numerical techniques discussed in Ref. 1 to solve Eqs. (8) and (9) and to obtain the results shown in Fig. 4. Briefly, the integration is carried out with $\tilde{c}$ as the independent variable and with asymptotic approximations applied at $\tilde{c}\sim 0, 1$. The method of quasilinearization is used to handle the three point boundary conditions.

In Fig. 3, we see that for $m=2$ the predicted angle of the reaction zone is considerably reduced over that obtained in Ref. 1, i.e., for $m=0$. In addition to predicted values of θ in closer agreement with experiment, the revised modeling indicates that in the range of τ of practical interest, θ is insensitive to τ; this result is in agreement with the experimental finding of Wright and Zukoski.[3]

It would be expected that somewhat larger values of m might reduce the predicted angles further, but in view of the idealizations involved in the theory, it appears inappropriate to push excessively the comparison of prediction and experiment. In fact, if a further reduction of two is desired in the predicted values of θ, it might be preferable to reduce the value of Φ. This can be rationalized by reducing the two constants, a and $(C\ell_1/\ell_2)$, and by increasing the parameter c_m, e.g., to unity. Note that, in Eq. (8), $\Phi/\tan^2\theta$ may be considered to be a new parameter, so that if $\Phi\simeq 0.1$, a value that can be rationalized readily, $\theta\simeq 6°$ for $\tau=6$.

We are unable to divide the effect associated with $m=2$ between the two exponents p and k, i.e., between a turbulence Reynolds number effect and a scalar dissipation effect. Also it is not possible to establish whether the alteration of the scalar dissipation by variations in density is due to changes in the empirical constant C or in the length scale ratio (ℓ_1/ℓ_2).

It will be interesting to apply Eqs. (3) and (4) to other variable density turbulent flows and to seek other comparisons with experiment. Nevertheless, the clear suggestion from this study is that variable density effects should be considered in the modeling invoked to obtain closure in predictive methods for turbulent reacting flows.

III. Distributions of Statistical Quantities Within Reaction Zone

Now we turn to the determination of the distributions within a reaction zone of various statistical quantities. It is a feature of predictive methods based on consideration of the relevant probability density functions that, once certain quantities have been calculated, additional information can be determined readily from the *pdf* model employed. In the present context, it is convenient to consider distributions in terms of $\tilde{c}$; the actual spatial distributions, in terms of the physical coordinate x, are of little interest in the absence of comparable experimental data, but in most instances can be obtained from Ref. 1 if required.

Our exposition is facilitated if we review briefly the basic notions of the Bray-Moss model. The probability density function for the product concentration at a spatial location identified by the position vector r is denoted $P(c;r)$, and is shown schematically in Fig. 3a. We have

$$P(c;r)=\alpha(r)\delta(c)+\beta(r)\delta(c-1)+\gamma(r)f(c)\cdot[H(c)-H(c-1)] \tag{11}$$

where δ and H denote the usual delta and Heaviside functions, respectively. According to the assumption of "fast chemistry," $\gamma(r)\ll 1$, i.e., the probability density function is dominated by the two delta functions.

The aerothermochemistry of the system is such that the instantaneous density and temperature are related to the product concentration c according to

$$\rho/\rho_0=(1+\tau c)^{-1} \qquad T/T_0=(1+\tau c) \tag{12}$$

If Eqs. (11) and (12) are used to calculate the mean product concentration $\tilde{c}$, we can estimate $\alpha(r)$ and $\beta(r)$ in terms of $\tilde{c}$ with corrections of order $\gamma(r)$ neglected, so that

$$\alpha(r)=1-\beta(r)-\gamma(r)\simeq\frac{1-\tilde{c}(r)}{1+\tau\tilde{c}(r)}+O(\gamma)$$

$$\beta(r)\cong\left(\frac{1+\tau}{1+\tau\tilde{c}(r)}\right)\tilde{c}(r)+O(\gamma) \tag{13}$$

Statistical Quantities Dependent on State Variables Alone

Equations (11-13) permit all statistical quantities exclusively dependent on state variables to be determined. We shall see that these quantities depend solely on $\tilde{c}$ and the heat release parameter, and are independent of the orientation of the reaction zone. For simplicity we drop, whenever clarity is not compromised, the position vector as a functional argument.

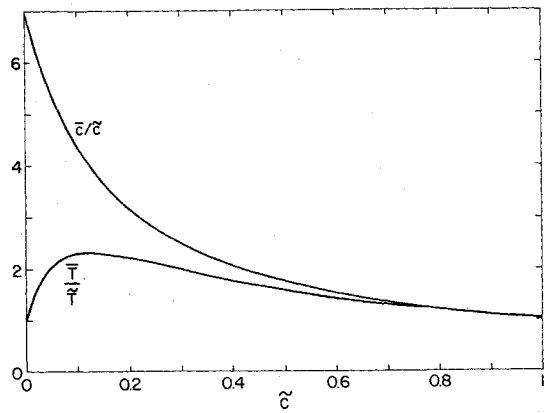


Fig. 5 Variation of the ratios of mean values obtained by the two means of averaging with the Favre averaged mean product concentration: $\tau = 6$.

Consider first the intensity

$$\overline{\rho c''^2} = \int_0^1 dc\, \rho (c-\tilde{c})^2 P(c) = \alpha \rho_0 \tilde{c}^2 + \beta \frac{\rho_0}{1+\tau} (1-\tilde{c})^2 + O(\gamma)$$

Thus,

$$\overline{\rho c''^2}/\bar{\rho} = \tilde{c}(1-\tilde{c}) + O(\gamma) \tag{14}$$

In a similar fashion we find

$$\overline{\rho c''^3}/\bar{\rho} = \tilde{c}(1-\tilde{c})(1-2\tilde{c}) + O(\gamma) \tag{15}$$

As an aside, we note that Eqs. (14) and (15) permit an estimate for the skewness of the Favre-averaged product fluctuations to be made, namely.

$$\frac{\overline{\rho c''^3}\,\bar{\rho}^{1/2}}{(\overline{\rho c''^2})^{3/2}} \cong \frac{1-2\tilde{c}}{[\tilde{c}(1-\tilde{c})]^{1/2}} + O(\gamma)$$

We see that highly skewed fluctuations of opposite sign are predicted at the two edges of the reaction zone.

Temperature statistics may be computed using Eq. (12); we find, for example,

$$\overline{\rho T''^2}/\bar{\rho}\tilde{T}^2 = \tau^2 \tilde{c}(1-\tilde{c})/(1+\tau\tilde{c})^2 + O(\gamma)$$

$$\overline{\rho T''^3}/\bar{\rho}\tilde{T}^3 = \tau^3 \tilde{c}(1-\tilde{c})(1-2\tilde{c})/(1+\tau\tilde{c}) = O(\gamma) \tag{16}$$

We are now in a position to compare conventional and Favre averaged quantities involving only state variables; in this comparison and throughout the following analysis we shall repeatedly use an equation for the density fluctuations readily obtained from Eq. (12), namely

$$\rho' = \tau(\bar{\rho}\tilde{c} - \rho c) \tag{17}$$

Suppose we wish to compare the conventional and Favre averaged values for the progress variable c. We have as a starting point the exact relation

$$\tilde{c} = \bar{c} - \overline{\rho' c'}/\bar{\rho} \tag{18}$$

If Eq. (17) is multiplied by c' and averaged, we find exactly

$$\frac{\overline{\rho' c'}}{\bar{\rho}} = -\frac{\tau}{1+\tau\tilde{c}} \frac{\overline{\rho c''^2}}{\bar{\rho}} \tag{19}$$

If the approximation for $\overline{\rho c''^2}/\bar{\rho}$ from Eq. (14) is substituted, we have the estimate

$$\bar{c} = [(1+\tau)(1+\tau\tilde{c})]\tilde{c} + O(\gamma) \tag{20}$$

Equation (20) shows that for $\tau\tilde{c} \ll 1$, $\bar{c} \simeq (1+\tau)\tilde{c}$, whereas for $\tilde{c} \simeq 1$, $\bar{c} \simeq \tilde{c} \simeq 1$; thus, in the upstream portion of the reaction zone, the conventional mean concentration is larger than is Favre-averaged counterpart by the factor $(1+\tau)$.

A closely related calculation yields for the two mean temperatures

$$\bar{T} = \frac{(1+2\tau\tilde{c}+\tau^2\tilde{c})}{(1+\tau\tilde{c})^2}\tilde{T} + O(\gamma) \tag{21}$$

In Fig. 5 we show the distribution with $\tilde{c}$ for the typical value $\tau = 6$ of the ratios $\bar{c}/\tilde{c}$ and $\bar{T}/\tilde{T}$. The remarkable difference between the two mean values of product concentration for small concentrations is noted.

Intensities of State Quantities

We treat next the various intensities involving only state variables as given by the two means of averaging. Consider first $\overline{c'^2}$; we have the exact relation

$$\overline{c'^2} = \frac{\overline{\rho c''^2}}{\bar{\rho}} - \frac{\overline{\rho' c'^2}}{\bar{\rho}} + \left(\frac{\overline{\rho' c'}}{\bar{\rho}}\right)^2 \tag{22}$$

Equations (14) and (19) provide estimates for the first and last terms; we must compute the second term on the right side by multiplying Eq. (17) by c'^2 and averaging. Thus,

$$\frac{\overline{\rho' c'^2}}{\bar{\rho}} = \tau\left[\tilde{c}\overline{c'^2} - \frac{\overline{\rho c''^2}}{\bar{\rho}}\left(\tilde{c} + 2\frac{\overline{\rho' c'}}{\bar{\rho}}\right) - \frac{\tilde{c}(\overline{\rho' c'})^2}{\bar{\rho}^2} - \frac{\overline{\rho c''^3}}{\bar{\rho}}\right] \tag{23}$$

From Eqs. (14, 15, and 19), some algebra gives

$$\overline{c'^2} = \frac{1+\tau}{(1+\tau\tilde{c})^2}\frac{\overline{\rho c''^2}}{\bar{\rho}} + O(\gamma) \tag{24}$$

Similar procedures applied to the relation

$$\overline{T'^2} = \frac{\overline{\rho T''^2}}{\bar{\rho}} - \frac{\overline{\rho' T'^2}}{\bar{\rho}} + \left(\frac{\overline{\rho' T'}}{\bar{\rho}}\right)^2 \tag{25}$$

which yields

$$\overline{T'^2} = \frac{1+\tau}{(1+\tau\tilde{c})^2}\frac{\overline{\rho T''^2}}{\bar{\rho}} + O(\gamma) \tag{26}$$

We see from Eqs. (24) and (26) that the ratio of the conventional and Favre averaged product concentration and

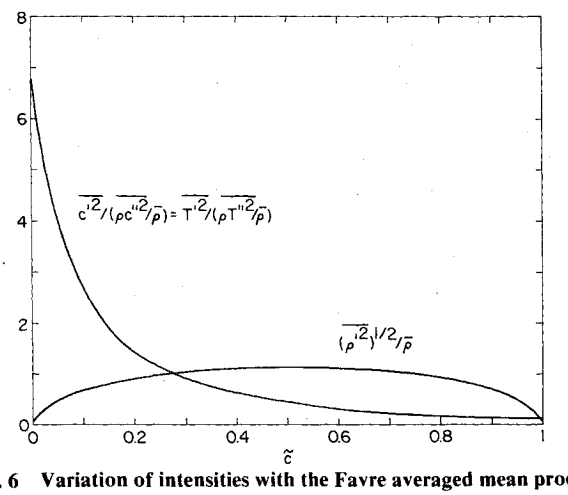


Fig. 6 Variation of intensities with the Favre averaged mean product concentration: $\tau = 6$.

temperature intensities are distributed across the reaction zone in identical fashion, and that they are approximately $(1+\tau)$ in the upstream portion of the zone and unity in the downstream portions.

Next we consider the relative density intensity in the reaction zone; if Eq. (17) is multiplied by ρ' and the result averaged, we obtain by use of previous relations

$$\frac{\overline{(\rho'^2)}^{1/2}}{\bar{\rho}} = \tau \left[\frac{\tilde{c}(1-\tilde{c})}{1+\tau}\right]^{1/2} + O(\gamma) \tag{27}$$

The peak relative density intensities are predicted to occur where $\tilde{c} \cong 1/2$ and to have magnitudes equal to $1/2\tau/(1+\tau)^{1/2}$. The large values of this relative intensity are associated with the intermittent values of $\rho(t;r)$, and should indicate the need for caution in the neglect of density fluctuations in the descriptions of turbulent flows with significant heat release.

In Fig. 6 we show the variation with $\tilde{c}$ of the relative intensity and of the ratio of the two averages for the product concentration and temperature intensities. We note the significant differences in the two averages in the upstream portion of the reaction zone.

Similar comparisons of other statistical quantities, dependent only on the state variables, can be developed in the same fashion, but our point has been made. Now we turn to the statistical quantities dependent on the velocity components.

Joint Probability Density Function

In order to carry out calculations involving the velocity components, it is necessary to extend the Bray-Moss model. We show schematically in Fig. 3b a model for the joint probability density function for the u-velocity component and the product concentration, i.e., $P(u, c;r)$. It is considered to be dominated by the distributions associated with the precise values $c=0$, 1. Accordingly, we can write

$$P(u,c;r) = \alpha(r)P_0(u,0;r)\delta(c) + \beta(r)P_1(u,1;r)\delta(1-c) + \gamma(r)P_{uc}(u,c;r)[H(c)-H(c-1)] \tag{28}$$

The usual normalization of $P(u,c;r)$, i.e.,

$$\int_{-\infty}^{\infty} du \int_0^1 dc\, P(u,c;r) = 1$$

is consistent with the primary relation among the strengths of the three modes, i.e.,

$$\alpha(r) + \beta(r) + \gamma(r) = 1$$

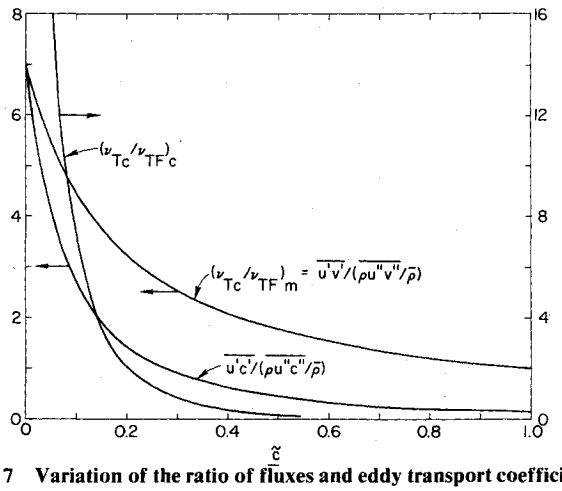


Fig. 7 Variation of the ratio of fluxes and eddy transport coefficients with the Favre averaged mean concentration: $\tau = 6$.

provided

$$\int_{-\infty}^{\infty} du\, P_0(u,0;r) = 1$$

$$\int_{-\infty}^{\infty} du\, P_1(u,1;r) = 1$$

$$\int_{-\infty}^{\infty} du \int_0^1 dc\, P_{uc}(u,c;r) = \int_{0+}^{1-} dc\, f(c;r) = 1$$

In order to utilize the model *pdf* given by Eq. (28), additional assumptions are needed; to show this, consider the calculation using Eq. (28) of the mean velocity $\tilde{u}$. We have

$$\bar{\rho}\tilde{u} = \overline{\rho u}(r) = \int_{-\infty}^{\infty} du\, u \int_0^1 dc\, \rho\, P(u,c;r)$$

$$= (1-\tilde{c})\bar{\rho}\int_{-\infty}^{\infty} du\, u\, P_0(u,0;r)$$

$$+ \tilde{c}\bar{\rho}\int_{-\infty}^{\infty} du\, u\, P_1(u,1;r) + O(\gamma)$$

$$= \bar{\rho}[(1-\tilde{c})U_0(r) + \tilde{c}U_1(r)] + O(\gamma) \tag{29}$$

where the definitions of $U_0(r)$ and $U_1(r)$ are obvious, and where we include the functional dependence as required for clarity. The physical significance of U_0 and U_1 relates to the mean values of the u-velocity component when packets of gas with the precise values $c=0$, 1 pass the spatial location identified with r. Thus, we deal with conditioned averaging. The determination of such conditioned quantities involves additional modeling, or perhaps application of the theory of conditioned turbulence after Libby.[9] For present purposes we carry out a self-consistent calculation based on Ref. 1.

To proceed, first we eliminate U_1; mass conservation requires $\overline{\rho u} = \rho_0 \tilde{u}_0$, so that from Eq. (29) we obtain

$$U_1 = U_0 + (\tilde{u} - U_0)/\tilde{c} + O(\gamma) \tag{30}$$

Equation (30) yields the intuitively correct results that, as $\tilde{c} \sim 0$, $U_0 = \tilde{u} = \tilde{u}_0$, and that, as $\tilde{c} \sim 1$, $U_1 = \tilde{u} = \tilde{u}_0(1+\tau)$.

In order to determine U_0, consider the mean flux of product concentration; we have

$$\overline{\rho u'' c''} = \int_{-\infty}^{\infty} du(u-\tilde{u}) \int_0^1 dc\, \rho(c-\tilde{c})P(u,c)$$

$$= -\tilde{c}(1-\tilde{c})\bar{\rho}(U_0-\tilde{u}) + (1-\tilde{c})\tilde{c}\bar{\rho}(U_1-\tilde{u}) + O(\gamma)$$

$$= \bar{\rho}(1-\tilde{c})(\tilde{u}-U_0) + O(\gamma) \tag{31}$$

But in Ref. 1 a gradient assumption is employed, so that from Eq. (5)

$$\overline{\rho u'' c''} = -\nu_T \bar{\rho}\frac{d\tilde{c}}{dx} = -\rho_0 \tilde{u}_0 \frac{d\tilde{c}}{d\xi} \tag{32}$$

Thus, if the two calculations are to be self-consistent,

$$U_0 = \tilde{u}\left(1 + \frac{(d\tilde{c}/d\xi)}{1-\tilde{c}}\right) \tag{33}$$

where $(d\tilde{c}/d\xi)$ as a function of $\tilde{c}$ is obtained from the solution of either the equations in Ref. 1, or Eqs. (6) and (7), or Eqs. (8) and (9) of the present work.** Since $(d\tilde{c}/d\xi)$ will depend

**The behavior of $dc/d\xi$ as $\tilde{c} \sim 1$ is such that the quotient in Eq. (33) approaches a constant.

on the orientation of the reaction zone, we expect in general that the variation across the reaction zone of the various statistical quantities dependent on the velocity components will change with θ as well as with τ.

Two Mean Velocities

Now we are able to compare the two averages for the x-wise velocity component; we start with the exact relation

$$\tilde{u}=\tilde{u}-\overline{\rho' u'}/\bar{\rho}$$

and must calculate $\overline{\rho' u'}$; if Eq. (17) is multiplied by u' and averaged, we obtain, again, exactly,

$$\frac{\overline{\rho' u'}}{\bar{\rho}}=-\frac{\tau}{1+\tau\tilde{c}}\frac{\overline{\rho u'' c''}}{\bar{\rho}} \tag{34}$$

If Eq. (32) is substituted into Eq. (34), there results the estimate

$$\frac{\overline{\rho' u'}}{\bar{\rho}\tilde{u}}=\frac{\tau}{1+\tau\tilde{c}}\left(\frac{\mathrm{d}\tilde{c}}{\mathrm{d}\xi}\right)+O(\gamma) \tag{35}$$

so that

$$\frac{\tilde{u}}{\tilde{u}}=1-\frac{\tau}{1+\tau\tilde{c}}\left(\frac{\mathrm{d}\tilde{c}}{\mathrm{d}\xi}\right)+O(\gamma) \tag{36}$$

In order to evaluate the ratio of the mean velocities, we must select a solution for the reaction zone, i.e., a particular heat release and orientation. For this comparison we select one of those obtained in the present work, since it includes variable density effects. In particular, we chose the strong interaction solution with $\tau=6$, $\theta=13.0°$, $\tilde{u}_0^2/\tilde{q}_\infty=3.23$ (10^{-3}). The variation of $\tilde{u}/\tilde{u}$ with $\tilde{c}$ for this case is less than unity with a minimum value of about 0.82; since $(\mathrm{d}\tilde{c}/\mathrm{d}\xi)$ is generally small as compared to unity for all τ and θ, this behavior is typical for the ratio $\tilde{u}/\tilde{u}$.

The situation regarding the v-velocity component is somewhat different; if the gradient approximation is consistently applied, we find that $\overline{\rho' v'}=0$, and thus that $\tilde{v}=\bar{v}$. A consequence of this result is that, in terms of the conventionally averaged velocity components $\tilde{u}$ and $\bar{v}$, the mean streamline for the flow of Ref. 1 is not a straight line.

Momentum Fluxes

We turn now to a consideration of the mean momentum fluxes. As a preliminary point it is worth noting that, as a consequence of the assumption of an undeflected mean streamline, we have the following explicit equation for the Reynolds stress according to Favre averaging:

$$\frac{\overline{\rho u'' v''}}{\bar{\rho}\tilde{u}_0^2}=-\frac{\tau\tilde{c}(1+\tau\tilde{c})}{\tan\theta}$$

With Favre averaging the entire mean flux is $\overline{\rho u'' v''}$, whereas for conventional averaging the mean flux consists of the usual Reynolds stress $\overline{u'v'}$ plus two mass transfer terms in the terminology of Morkovin,[10] and a triple correlation $\overline{\rho' u' v'}$. In many predictive methods only the Reynolds stress term is retained, and it is therefore of interest to consider the ratio $\overline{u'v'}/(\overline{\rho u'' v''}/\bar{\rho})$, which is exactly given by

$$\frac{\overline{u'v'}}{\overline{\rho u'' v''}/\bar{\rho}}=1-\frac{\overline{\rho' u'}\;\overline{\rho' v'}}{\bar{\rho}\;\overline{\rho u'' v''}}+\frac{\tau}{1+\tau\tilde{c}}\frac{\overline{\rho u'' v'' c''}}{\overline{\rho u'' v''}} \tag{37}$$

The second term on the right side is zero according to our present calculations, and therefore we must consider only the third term, which arises from the triple correlation contribution to the momentum flux with conventional averaging.

To do so we must extend the considerations that lead to the joint probability density function given by Eq. (28), and model the *pdf* corresponding to $P(u,v,c;r)$. We make the additional assumption that the conditioned correlation $(\overline{u'v'})$, when $c=0$, within the reaction zone is zero; i.e., the u- and v-velocity components remain uncorrelated in parcels of unburned reactants within the reaction zone. The argument in support of this assumption is as follows: The u- and v-velocity components within parcels of unburned reactants in the reaction zone can become correlated only by shear stresses due to molecularity at the boundary of the parcels. However, in gases these stresses are accompanied closely by diffusion of product and temperature into the interior of the parcel; when $c=0$, this diffusion has not as yet been effective, and thus the shear stresses have not been effective. Employing this argument and the resultant assumption, we find

$$\frac{\overline{\rho u'' v'' c''}}{\overline{\rho u'' v''}}=(1-\tilde{c})+O(\gamma)$$

and thus that,

$$\frac{\overline{u'v'}}{\overline{\rho u'' v''}/\bar{\rho}}=1+\frac{\tau(1-\tilde{c})}{1+\tau\tilde{c}}+O(\gamma) \tag{38}$$

Therefore, we see that the ratio of the two correlations is dependent only on τ and $\tilde{c}$, and does not depend on the orientation of the reaction zone; we also see that the ratio varies as $(1+\tau)$ for $\tilde{c}\ll 1$ and approaches unity as $\tilde{c}\sim 1$.

We show in Fig. 7 for $\tau=6$ the variation of the two correlations given by Eq. (38); it is seen that in the upstream portions of the reaction zone the ratio of the correlations is considerably greater than unity. The implication from this result is that, at least in the reaction zones described here, the triple correlation term $\overline{\rho' u' v'}$ is significant.

It is interesting to make the following considerations relative to the two eddy transfer coefficients implied by Eq. (38): Suppose, as is frequently done, we assume that $\overline{u'v'}=-\nu_{T_c}\mathrm{d}\bar{v}/\mathrm{d}x$ and that $\overline{\rho u'' v''}=-\bar{\rho}\nu_{T_F}\mathrm{d}\bar{v}$.†† Then we find, as a consequence, that $\tilde{v}=\bar{v}$, and that the ratio of the two eddy transport coefficients equals the ratio of the two correlations, and is thus given by Eq. (38). This result suggests that the eddy transport coefficients for conventional and Favre averaging should be assumed to be different from each other if consistent predictions are to be obtained.

Flux of Product Concentration

Next we consider the two fluxes of product concentration. Again it is customary in predictive methods employing conventional averaging to consider the correlation $\overline{u'c'}$ to be dominant, whereas in Favre averaging, the entire flux is $\overline{\rho u'' c''}$. To compare the two correlations, we start with the exact relation

$$\frac{\overline{u'c'}}{\overline{\rho u'' c''}/\bar{\rho}}=1-\frac{\overline{\rho' u'}\;\overline{\rho' c'}}{\bar{\rho}\;\overline{\rho u'' c''}}+\frac{\tau}{1+\tau\tilde{c}}\frac{\overline{\rho u'' c''^2}}{\overline{\rho u'' c''}} \tag{39}$$

Since the second term on the right side of this equation will not disappear as in the case of the momentum flux, it is of interest to note that it is not possible to relate the second term directly to the mass transfer term, since the triple correlation $\overline{\rho' u' c'}$ contributes to both the second and third terms; however, as in Eq. (37), the third term is due solely to the triple correlation. Using Eqs. (32) and (33), we can, without

‡‡We add a subscript "F" to ν_T to distinguish it from the coefficient appropriate for conventional averaging. We recall that we have not in fact used a gradient assumption for the momentum exchange.

further approximation, find the estimate

$$\frac{\overline{u'c'}}{\overline{\rho u''c''}/\bar{\rho}} = 1 - \left(\frac{\tau}{1+\tau\tilde{c}}\right)^2 \tilde{c}(1-\tilde{c}) + \frac{\tau}{1+\tau\tilde{c}}(1-2\tilde{c}) + O(\gamma) \tag{40}$$

In the upstream portions of the reaction zone, the ratio of the two correlations again approaches $(1+\tau)$; in the downstream portions the ratio approaches $(1+\tau)^{-1}$. Clearly for large τ the two correlations differ considerably. Moreover, from the source of the second and third terms on the right side of Eq. (40), we can conclude that the triple correlation term is dominant at the two edges of the reaction zone, depending only on $\tilde{c}$ and τ.

In Fig. 7 we show the distribution of the ratio of fluxes with $\tilde{c}$; we see the considerable deviation from unity of the ratio throughout the reaction zone. In this case, if we compute the ratio of the two eddy transport coefficients, appropriate for $\overline{u'c'}$ and $\overline{\rho u''c''}/\bar{\rho}$, we find by using Eq. (20) that

$$\left(\frac{\nu_{Tc}}{\nu_{TF}}\right)_c = \frac{1+\tau}{(1+\tau\tilde{c})^2} \frac{\overline{u'c'}}{\overline{\rho u''c''}/\bar{\rho})} \tag{41}$$

We show the distribution of the ratio of the two coefficients in Fig. 7. It will be noted that the two ratios of eddy transport coefficients shown in Fig. 7 do not coincide. If it is assumed, following Ref. 1, that the turbulent Prandtl-Schmidt numbers for Favre averaged variables is a constant of order unity, then the corresponding quantity for conventionally averaged variables must be a strong function of $\tilde{c}$ and τ, if consistent predictions are to be obtained.

Mass Transfer Terms

By using the relations developed earlier, we can determine the distribution of the one operative mass transfer term in the momentum exchange in planar, oblique reaction zones. Consider the ratio $\bar{v}\,\overline{\rho' u'}/\bar{\rho}\,\overline{u'v'}$, which provides a measure of the mass transfer term relative to the Reynolds stress term according to conventional averaging. It is customary in predictive methods to assume this ratio is small as compared to unity. From our earlier results we find

$$\frac{\bar{v}\,\overline{\rho' u'}}{\bar{\rho}\,\overline{u'v'}} = -\frac{(\mathrm{d}\tilde{c}/\mathrm{d}\xi)}{\tilde{c}(1+\tau(1-\tilde{c})(1+\tau\tilde{c})^{-1})} \tag{42}$$

As $\tilde{c}\sim 0$, $\tilde{c}^{-1}$ $(\mathrm{d}\tilde{c}/\mathrm{d}\xi)\sim 1$, so that the ratio approaches $-(1+\tau)^{-1}$; as $\tilde{c}\sim 1$, the ratio goes to zero.

If the strong interaction solution given here is used to evaluate the right side of Eq. (42), we find that the ratio of the correlation is indeed small compared to unity throughout the reaction zone. We conclude therefrom that the significant differences between the correlations given by Eqs. (38) and (40) are associated with the triple correlation terms, i.e., the terms that are most likely to be neglected in the modeling for predictive methods based on conventional averaging.

IV. Conclusions

On the basis of the results presented here the following conclusions can be drawn:

1) Variable density effects are shown to play an important part in the modeling of premixed turbulent combustion.

2) The introduction of a density ratio dependence into the model expressions for the eddy transport coefficient and the scalar dissipation function improves agreement with experimental results for the flame angle θ in the strong interaction limit. A need to test the new modeling expressions in other variable density flows is identified.

3) The distributions of several statistical quantities within the flame zone are predicted in a manner consistent with the analysis of Ref. 1. In particular, Favre and conventional averages are compared. For scalar quantities, it is found that the two averaging procedures give results that may differ from one another by large factors. The conventional averaged velocity differs from the Favre averaged value by a smaller but still not negligible factor.

4) If these results are at all representative, they clearly demonstrate a need for consistent use of either Favre or conventional averaging in turbulent combustion modeling. Studies in which density-velocity correlations and other terms are neglected, so that the left-hand sides of the equations are effectively Favre averaged, whereas the treatment of source terms on the right-hand sides assumes that the same variables are conventionally averaged, must involve significant errors.

5) As order-of-magnitude differences are predicted, it is important to identify whether available experimental data refer to Favre or conventionally averaged variables, or to some other type of mean.

6) It appears that the application of normal modeling assumptions, such as neglect of third-order covariances and use of constant Prandtl-Schmidt numbers, in the conventionally averaged equations for the planar, oblique premixed turbulent flame, will lead to results that will be inconsistent with the Favre averaged predictions of Ref. 1. The normal modeling must be revised, for either the Favre or the conventional equations, or both, if consistent results are to be obtained.

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