

The Probability Approach to the Modelling of Turbulent Reacting Flows

S. B. POPE

*Imperial College of Science and Technology, Department of
Mechanical Engineering, Exhibition Road, London SW7 2BX, U.K.*

The formulation of a closed set of averaged equations to describe a turbulent reacting flow is hindered by highly nonlinear relations between instantaneous quantities. This problem is overcome by considering the joint probability distribution of the scalars characterising the reaction. The transport equations for the single and joint probability distributions are derived and the unknown terms in the single probability distribution equation are modelled. Solutions of the modelled equation are obtained and the results are compared with previous models. The ability of the modelled equation to account for the influence of both turbulent mixing and finite chemical reaction rates is demonstrated.

1. Introduction

This paper describes a preliminary investigation into the use of the probability approach to model turbulent reacting flows with a view to developing a more accurate and general combustion model than those available at present. While the author is primarily interested in flames occurring in engineering situations, the analysis presented here is general, encompassing many problems encountered in chemical and environmental processes.

The difference between a turbulent reacting flow and an inert isothermal flow may be attributed to two agencies; the effect of the reaction on the turbulence and the effect of the turbulence on the reaction. The former is due to changes in the viscosity and more especially in the density due to the reaction: this aspect of the problem has been discussed extensively by Bray [1]. The second effect, that of the turbulence on the reaction, is of prime concern here and presents the most serious obstacle to formulating a closed set of averaged equations which describe the flow. The problem becomes evident when the set of instantaneous equations governing the flow is considered. These equations are:

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_i} (\rho U_i) = 0, \quad (1)$$

$$\frac{\partial}{\partial t} (\rho U_j) + \frac{\partial}{\partial x_i} (\rho U_i U_j) = \frac{\partial}{\partial x_i} \left(\frac{\mu \partial U_j}{\partial x_i} \right) - \frac{\partial P}{\partial x_j}, \quad (2)$$

$$\frac{\partial \rho \phi_\alpha}{\partial t} + \frac{\partial}{\partial x_i} (\rho U_i \phi_\alpha) = \frac{\partial}{\partial x_i} \left(\frac{\Gamma^\alpha \phi_\alpha}{\partial x_i} \right) + S_\alpha(\phi), \quad (3)$$

$$\rho = \rho(P, \phi). \quad (4)$$

where the Greek suffixes do not denote tensors but indicate a particular scalar of the set ϕ which is chosen to be sufficient to render Eqs. (1) to (4) closed. When Eqs. (3) and (4) are averaged $\langle S_\alpha(\phi) \rangle$ and $\langle \rho(P, \phi) \rangle$ occur and must be modelled. It is the modelling of terms of this form that pose the problem considered here. One possibility, and that employed by, for example, Patankar and Spalding [2] is to assume

$$\langle S_\alpha(\phi) \rangle = S_\alpha(\langle \phi \rangle). \quad (5)$$

The validity of Eq. (5) is guaranteed only when S_α is a linear function of ϕ or when ϕ' is zero. Bearing in mind that chemical reaction rates may be proportional to the exponential of temperature, this linearity may certainly not be generally assumed. Further, in the context of turbulent flames, not only is Eq. (5) unlikely to be correct but it may also be conceptually misleading since it is known that the averaged reaction rate becomes independent of S_α as S_α becomes large compared with the characteristic frequency of turbulence. In order to overcome this defect Spalding [3] proposed the "eddy-break-up model" which makes the averaged reaction rate independent of the instantaneous reaction rate. While this approach is certainly an improvement over Eq. (5) it is only valid for homogeneously premixed flames in which the instantaneous reaction rate is large.

In the case of an idealised diffusion flame in which the reaction rate is large, the instantaneous equations may be manipulated, with certain assumptions, to give an equation for the mixture fraction, f , which has no source term. The instantaneous values of the fuel and oxidant mass fractions, the density and the temperature may then be related to f . However, as these relations are nonlinear, the averaged values of these quantities may not be deduced from the averaged value of f . That is, for example

$$\langle \rho(f) \rangle \neq \rho(\langle f \rangle). \quad (6)$$

Toor [4] noted that, with a knowledge of the averaged probability distribution of f , $\langle p(\tilde{f}) \rangle$, all averaged quantities may be deduced. $p(\tilde{f})$ is defined such that the probability of f being in the range $\tilde{f} < f < \tilde{f} + d\tilde{f}$ is $p(\tilde{f}) d\tilde{f}$. Thus,

$$\rho(f) = \int_{-\infty}^{\infty} \rho(\tilde{f}) p(\tilde{f}) d\tilde{f}, \quad (7)$$

and consequently

$$\langle \rho(f) \rangle = \int_{-\infty}^{\infty} \rho(\tilde{f}) \langle p(\tilde{f}) \rangle d\tilde{f}, \quad (8)$$

and similarly for all other quantities. Elgobashi and Pun [5] solved a closed set of equations for this situation which comprised, as well as mean momentum and turbulence equations, equations for $\langle f \rangle$ and $\langle (f - \langle f \rangle)^2 \rangle$ and an assumed probability distribution based on the values of these quantities. The density, temperature and mass fractions were then deduced from relations of the form of Eq. (8).

An idealised premixed system may also be characterised by a single scalar. Bray and Moss [6] considered this situation and showed that all averaged thermodynamic and chemical properties of the flow may be related to the probability distribution of the mass fraction of reaction products and, further, proposed a closure based on an assumed probability distribution.

For both premixed and diffusion flames, characterised by a single scalar, closures based on an assumed probability distribution have been proposed which overcome the problems associated with nonlinear relations between instantaneous quantities. The approach advocated here may be regarded as a twofold extension of previous proposals. First, for a system characterised by only one scalar, a transport equation for the probability distribution is proposed, thus obviating the need for an assumed relation between the probability distribution and averaged quantities. This measure may be expected to result in greater precision since the transport of $\langle p(\tilde{\phi}) \rangle$ is accounted for in both position and probability spaces. Secondly, in order to allow the use of this approach in general systems, where more than one scalar characterises the flow, the possibility of solving a transport equation for the joint probability of all the scalar quantities is considered. The advantage of this approach is evident when it is realised that, for an arbitrary flow situation neither premixed nor diffusion and with any number of reactants, quantities such as the averaged source terms in Eq. (3) are given by

$$\langle S_\alpha(\phi) \rangle = \int_{-\infty}^{\infty} S_\alpha(\tilde{\phi}) \langle p(\tilde{\phi}) \rangle d\tilde{\phi}. \quad (9)$$

In the next section the exact probability distribution and joint probability distribution equations are derived from Eq. (3). This is done in the same manner employed by Lundgren [7] who derived the joint probability distribution equation for the velocity field. Physical interpretations of the terms appearing in these equations are given and the unknown terms in the averaged probability distribution equation are modelled. The term relating to molecular mixing is particularly important and the present modelling is compared with that of Dopazo and O'Brien [8]. In Sect. 3, where the modelled probability distribution equation is applied to homogeneous flows, exact and numerical solutions are presented. The inclusion of joint probability equations in a numerical solution scheme poses certain problems which are also considered in the Discussion. The paper closes with a summary of the more important conclusions.

2. Probability Distribution Equations

In this section the probability distribution equation is derived and modelled and the joint probability distribution equation, for an arbitrary number of scalars is derived. First, probability is mathematically defined and some useful consequences of the definition are shown. The probability distribution of ϕ , $p(\phi)$, is de-

finied such that the probability of ϕ being in the range

$$\bar{\phi} < \phi < \bar{\phi} + d\bar{\phi} \text{ is } p(\bar{\phi}) d\bar{\phi}.$$

Clearly, the instantaneous value of $p(\bar{\phi})d\bar{\phi}$ is either zero or unity and so $p(\bar{\phi})$ may be identified as the Dirac delta function:

$$p(\bar{\phi}) \equiv \delta(\bar{\phi} - \phi), \tag{10}$$

where $\bar{\phi}$ is the new independent variable representing probability space. From this definition it follows that for any good function, h ,

$$\int_{-\infty}^{\infty} h(\bar{\phi}) p(\bar{\phi}) d\bar{\phi} = h(\phi), \tag{11}$$

and consequently,

$$\langle h(\phi) \rangle = \int_{-\infty}^{\infty} h(\bar{\phi}) \langle p(\bar{\phi}) \rangle d\bar{\phi}. \tag{12}$$

These relations confirm the validity of Eqs. (7) to (9).

A further result which will be used extensively below is

$$\int_{-\infty}^{\infty} \bar{\phi}^m \frac{\partial^n}{\partial \phi^n} [p(\bar{\phi}) h(\bar{\phi})] d\bar{\phi} = \begin{cases} 0, m < n \\ (-1)^n m! / (m-n)! \int_{-\infty}^{\infty} \bar{\phi}^{(m-n)} p(\bar{\phi}) h(\bar{\phi}) d\bar{\phi}, n \leq m. \end{cases} \tag{13}$$

2.1 Single Probability Distribution Equation

Differentiating $p(\bar{\phi})$ with respect to time gives

$$\begin{aligned} \frac{\partial p(\bar{\phi})}{\partial t} &= \frac{\partial}{\partial t} \delta(\bar{\phi} - \phi) \\ &= \frac{\partial \phi}{\partial t} \frac{\partial}{\partial \phi} \delta(\bar{\phi} - \phi) = - \frac{\partial \phi}{\partial t} \frac{\partial \delta(\bar{\phi} - \phi)}{\partial \bar{\phi}} \\ &= - \frac{\partial \phi}{\partial t} \frac{\partial p(\bar{\phi})}{\partial \bar{\phi}}, \end{aligned} \tag{14}$$

and similarly for the derivative with respect to x . Multiplying Eq. (3) (in terms of ϕ) by $-\delta p(\bar{\phi})/\delta \bar{\phi}$ and making use of Eq. (1) yields

$$\begin{aligned} \frac{\partial}{\partial t} \rho p(\bar{\phi}) + \frac{\partial}{\partial x_i} \rho U_i p(\bar{\phi}) \\ = - \frac{\partial p(\bar{\phi})}{\partial \bar{\phi}} \left[\frac{\partial}{\partial x_i} \Gamma \frac{\partial \phi}{\partial x_i} + S(\phi) \right]. \end{aligned} \tag{15}$$

It has been implicitly assumed that S is an

algebraic function of ϕ (that is, not a function of $\partial U_i/\partial x_j$ or P). Thus

$$S(\phi) \frac{\partial p(\tilde{\phi})}{\partial \tilde{\phi}} = \frac{\partial}{\partial \tilde{\phi}} [p(\tilde{\phi}) S(\phi)]$$

$$= \frac{\partial}{\partial \tilde{\phi}} [p(\tilde{\phi}) S(\tilde{\phi})]. \quad (16)$$

If the further assumption of low Mach number is made, then the density will not be significantly affected by pressure fluctuations, i.e.,

$$\rho(P, \phi) = \rho(\langle P \rangle, \phi) = \rho(\phi). \quad (17)$$

With the further relation

$$\frac{\partial p(\tilde{\phi})}{\partial \tilde{\phi}} \frac{\partial}{\partial x_i} \Gamma \frac{\partial \phi}{\partial x_i} =$$

$$\frac{\partial^2 p(\tilde{\phi})}{\partial \tilde{\phi}^2} \Gamma \left(\frac{\partial \phi}{\partial x_i} \right)^2 - \frac{\partial}{\partial x_i} \Gamma \frac{\partial p(\tilde{\phi})}{\partial x_i}, \quad (18)$$

Eq. (15) may be averaged to give

$$\rho(\tilde{\phi}) \frac{D}{Dt} \langle p(\tilde{\phi}) \rangle =$$

$$\left\{ \begin{array}{l} \text{change in } \langle p \rangle \text{ along} \\ \text{averaged streamline} \end{array} \right\} =$$

$$\frac{\partial}{\partial x_i} \left[\Gamma \frac{\partial}{\partial x_i} \langle p(\tilde{\phi}) \rangle - \rho(\tilde{\phi}) \langle p(\tilde{\phi}) u_i \rangle \right],$$

$$\left\{ \begin{array}{l} \text{transport in} \\ \text{x - space} \end{array} \left[\begin{array}{l} \text{molecular} \\ \text{diffusion} \end{array} \right] + \left[\begin{array}{l} \text{turbulent} \\ \text{convection} \end{array} \right] \right\}$$

$$- \frac{\partial}{\partial \tilde{\phi}} \left[\langle p(\tilde{\phi}) \rangle S(\tilde{\phi}) + \left\{ \begin{array}{l} \text{transport in} \\ \phi - \text{space} \end{array} \left[\begin{array}{l} \text{source} \\ \text{term} \end{array} \right] \right\} \right]$$

$$+ \frac{\partial}{\partial \tilde{\phi}} \left[\langle p(\tilde{\phi}) \rangle \Gamma \left(\frac{\partial \phi}{\partial x_i} \right)^2 \right]$$

$$+ \left. \left[\begin{array}{l} \text{molecular} \\ \text{action} \end{array} \right] \right\}. \quad (19)$$

The most notable feature of Eq. (19) is that the term in S does not contain any unknown correlations, and so there are no problems of modelling as was the case with $\langle S(\phi) \rangle$. The term $\langle p(\tilde{\phi}) \rangle S(\tilde{\phi})$ represents a flux of $\langle p \rangle$ through probability space due to the source. The molecular diffusion term, which is negligible at high Reynolds Number, is again known. The turbulent convection term, which, at high Reynolds number, accounts for almost all the transport in \mathbf{x} - space, contains the unknown correlation $\langle p(\tilde{\phi}) u_i \rangle$. It is expected that the modelling of this term, through a mixing length hypothesis, as

$$\langle p(\tilde{\phi}) u_i \rangle = -C_1 u' l \frac{\partial \langle p(\tilde{\phi}) \rangle}{\partial x_i}, \quad (20)$$

will be as satisfactory as the analogous modelling of more familiar terms, such as $\langle u_i \phi \rangle$.

The last term in Eq. (19) contains the unknown correlation

$$G(\tilde{\phi}) \equiv \langle p(\tilde{\phi}) \rangle \Gamma \left(\frac{\partial \phi}{\partial x_i} \right)^2, \quad (21)$$

which, by definition, is nonnegative. The rôle of this term may be demonstrated by integrating its moments to form a source term in equations for $\langle \phi \rangle$ and $\langle \phi'^2 \rangle$ respectively,

$$- \int_{-\infty}^{\infty} \tilde{\phi} \frac{\partial^2 G}{\partial \tilde{\phi}^2} d\tilde{\phi} = 0, \quad (22)$$

$$- \int_{-\infty}^{\infty} \tilde{\phi}^2 \frac{\partial^2 G}{\partial \tilde{\phi}^2} d\tilde{\phi} = -2 \int_{-\infty}^{\infty} G d\tilde{\phi} \leq 0. \quad (23)$$

Thus, the effect of molecular action is to reduce the standard deviation of the probability distribution while leaving the mean value unchanged. The term is the correlation of two quantities; $\Gamma(\partial\phi/\partial x_i)^2$ pertains to small fluctuations on the microscale while $p(\tilde{\phi})$ is dominated by large fluctuations associated with the macroscale. It appears, therefore, that the two quantities are uncorrelated. Thus,

$$G(\tilde{\phi}) = \langle p(\tilde{\phi}) \rangle \langle \Gamma \left(\frac{\partial\phi}{\partial x_i} \right)^2 \rangle. \quad (24)$$

And, following the conventional modelling of $\langle \Gamma(\partial\phi/\partial x_i)^2 \rangle$,

$$G(\tilde{\phi}) = C_2 \frac{u'}{1} \langle p(\tilde{\phi}) \rangle \langle \phi'^2 \rangle \langle \rho \rangle. \quad (25)$$

The modelled form of Eq. (19) then becomes

$$\begin{aligned} \rho(\tilde{\phi}) \frac{D}{Dt} \langle p(\tilde{\phi}) \rangle = & \frac{\partial}{\partial x_i} \left\{ C_1 \rho(\tilde{\phi}) u' \frac{\partial}{\partial x_i} \langle p(\tilde{\phi}) \rangle \right\} \\ & - \frac{\partial}{\partial \tilde{\phi}} \left\{ \langle p(\tilde{\phi}) \rangle S(\tilde{\phi}) + C_2 \langle \rho \rangle \frac{u'}{1} \langle \phi'^2 \rangle \frac{\partial}{\partial \tilde{\phi}} \langle p(\tilde{\phi}) \rangle \right\}. \end{aligned} \quad (26)$$

This equation will be examined for inert ($S(\phi) = 0$), constant density ($\rho = 1$) flows. Integrating the equation to form equations for $\langle \phi \rangle$ and $\langle \phi'^2 \rangle$ produces

$$\frac{D}{Dt} \langle \phi \rangle = \frac{\partial}{\partial x_i} C_1 u' \frac{\partial \langle \phi \rangle}{\partial x_i} \quad (27)$$

$$\begin{aligned} \frac{D}{Dt} \langle \phi'^2 \rangle = & \frac{\partial}{\partial x_i} C_1 u' \frac{\partial \langle \phi'^2 \rangle}{\partial x_i} + \\ & 2C_1 u' \left(\frac{\partial \langle \phi \rangle}{\partial x_i} \right)^2 - 2C_2 \frac{u'}{1} \langle \phi'^2 \rangle \end{aligned} \quad (28)$$

These equations are seen to be identical to those used by, for example, Lockwood and Naguib [9] and, for consistency with these authors, the constants C_1 and C_2 take values of 0.127 and 0.925, respectively. While the consistency of Eq. (28) with previous models is encouraging, it provides no check on the behaviour of the equation in probability space and hence the modelling of G in particular is not validated. To this end, the decay of the probability distribution in a stagnant, homogenous flow is considered. Equation (26) reduces to

$$\begin{aligned} \frac{\partial}{\partial t} \langle p(\tilde{\phi}) \rangle = \\ - C_2 \frac{u'}{1} \langle \phi'^2 \rangle \frac{\partial^2}{\partial \tilde{\phi}^2} \langle p(\tilde{\phi}) \rangle, \end{aligned} \quad (29)$$

which has a solution

$$\begin{aligned} \langle p(\tilde{\phi}, t) \rangle = \\ (\phi' \sqrt{2\pi})^{-1} \exp \left\{ -\frac{1}{2} \left(\frac{\tilde{\phi} - \langle \phi \rangle}{\phi'} \right)^2 \right\}, \end{aligned} \quad (30)$$

where

$$\begin{aligned} \phi'(t) = & \langle \phi'^2 \rangle^{1/2} \\ = & \phi_0 \exp \left\{ -C_2 \frac{u'}{1} (t - t_0) \right\}. \end{aligned} \quad (31)$$

That is, for this situation, an initially Gaussian probability distribution remains Gaussian while its standard deviation decreases exponentially at a rate proportional to the turbulent time scale. Similarly, a steady, stagnant flow in which $\langle \phi \rangle$ varies linearly with \mathbf{x} yields the following solution

$$\langle p(\tilde{\phi}, \mathbf{x}) \rangle = (\phi' \sqrt{2\pi})^{-1} \exp$$

$$\left\{ -\frac{1}{2} \left(\frac{\tilde{\phi} - \langle \phi \rangle}{\phi'} \right)^2 \right\}, \quad (32)$$

where

$$\phi' = \left(\frac{C_2}{C_1} \frac{\partial \langle \phi \rangle}{\partial x_i} \frac{\partial \langle \phi \rangle}{\partial x_i} \right)^{1/2}. \quad (33)$$

Again, the probability distribution is Gaussian with a standard deviation proportional to the gradient of $\langle \phi \rangle$ multiplied by the turbulent length scale. These solutions of the modelled probability distribution equation are in accord with intuition and thus support the modelling assumptions. In addition, for these situations the modelled equations of Dopazo and O'Brien [8] produce the same results. However, in spite of the good performance of these models for the situations considered above, it will be shown that they are not appropriate to more general situations.

Consider the probability distribution shown on Fig. 1. The main features of this distribution may be realised in turbulent reacting flows; the distribution is bounded at $\tilde{\phi}_1$ and $\tilde{\phi}_4$ where there is a delta function. For $\tilde{\phi}_1 < \tilde{\phi} < \tilde{\phi}_4$, $\langle p(\tilde{\phi}) \rangle$ may not be zero because this would imply infinite gradients of ϕ ; however, a region $\tilde{\phi}_2 < \tilde{\phi} < \tilde{\phi}_3$ may occur in which $\langle p(\tilde{\phi}) \rangle$ is arbitrarily small. From consideration of the definition of G , for the general probability distribution outlined above, the following properties of G may be deduced:

(i) $G \geq 0$.

G is, by definition, nonnegative reflecting the fact that molecular action increases rather than decreases disorder on the microscale.

(ii) $G = 0$, for $\tilde{\phi} < \tilde{\phi}_1$ and $\tilde{\phi} > \tilde{\phi}_4$.

This condition, which again follows from the definition, guarantees that molecular action does not increase the bounds of a bounded distribution.

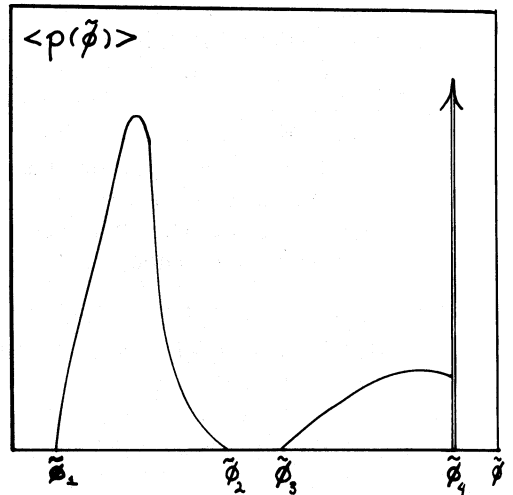


Fig. 1. General single probability distribution: $\langle p(\tilde{\phi}) \rangle$ against $\tilde{\phi}$.

(iii) as $\langle p(\tilde{\phi}) \rangle \rightarrow 0$, $\frac{\partial^2 G}{\partial \tilde{\phi}^2} \leq 0$ ($\langle p(\tilde{\phi}) \rangle / \tau$),

where τ is a characteristic time scale of distribution. It is readily shown that this condition is both necessary and sufficient for $\langle p(\tilde{\phi}) \rangle$ to be nonnegative.

(iv) G is finite and continuous.

This property is deduced from the other terms in Eq. (19) by taking its definite integral together with the knowledge that the conditional expectation of ϕ is continuous in x and t (although not necessarily in $\tilde{\phi}$).

It is apparent that, for the probability distribution of Fig. 1, the model for G given by Eq. (25) and that of Dopazo and O'Brien [8] violate all the conditions except for the first. These four conditions are sufficient to suggest a modelled form of G : condition (iv) requires that G be an integral function of the potentially discontinuous and infinite $\langle p(\tilde{\phi}) \rangle$ while condition (ii) suggests the form

$$G(\tilde{\phi}) = C_2 \frac{u'}{1} \phi' H(\tilde{\phi}) \rho(\tilde{\phi}), \quad (34)$$

where

$$H(\tilde{\phi}) = \int_{-\infty}^{\tilde{\phi}} g\left(\frac{\tilde{\phi} - \phi^*}{\phi'}\right) \langle p(\phi^*) \rangle d\phi^* + \int_{\tilde{\phi}}^{\infty} g\left(\frac{\phi^* - \tilde{\phi}}{\phi'}\right) \langle p(\phi^*) \rangle d\phi^*, \quad (35)$$

and g is any continuous function with $g(0) = 0$. Conditions (i) and (iii) require that g be non-negative and that its second derivative be non-positive. Thus, Eq. (34) and (35) form a model for G which is consistent with the four conditions imposed by the exact expression. However, a function g cannot be chosen that results in the desired Gaussian behaviour for the idealised flows considered above. It must be concluded, therefore, that the modelling of G is not completely satisfactory, although predictions based on it can be expected to be qualitatively correct. In the absence of experimental data, the choice of

$$g(y) = \ln(1 + y), \tag{36}$$

used in subsequent calculations was based on an intuitive appraisal of the shape of $\langle p(\tilde{\phi}) \rangle$ for various functions of g . The more obvious choice of $g(y) = y$ results in unrealistic multimodal distributions.

The equation for $\langle \phi'^2 \rangle$ which results from integrating this equation is no longer consistent with that employed by Lockwood and Naguib and so C_2 may not be evaluated directly. The value 4.5 used in subsequent calculations does, however, predict approximately the same values of $\langle \phi'^2 \rangle$.

The multiplier $u'/l \phi'$ in Eq. (34) replaces $\Gamma \frac{\partial}{\partial x_i^2}$ of Eq. (19) reflecting the assumption that the microscale adjusts itself to the macroscale as is the case with the dissipation of turbulent kinetic energy. With the revised closure approximation for G the modelled equation becomes

$$\begin{aligned} \rho(\tilde{\phi}) \frac{D}{Dt} \langle p(\tilde{\phi}) \rangle = & \\ \frac{\partial}{\partial x_i} \left[C_1 u' l \rho(\tilde{\phi}) \frac{\partial \langle p(\tilde{\phi}) \rangle}{\partial x_i} \right] & \\ - \frac{\partial}{\partial \tilde{\phi}} \left\{ S(\tilde{\phi}) \langle p(\tilde{\phi}) \rangle + \right. & \end{aligned}$$

$$\left. \frac{\partial}{\partial \tilde{\phi}} \left[C_2 \frac{u'}{l} \phi' \rho(\tilde{\phi}) H(\tilde{\phi}) \right] \right\}. \tag{37}$$

2.2 Joint Probability Distribution Equation

While a system characterised by a single scalar is fully described by the probability of that scalar, for more complex systems the joint probability of all scalars must be considered. The joint probability of a set of n scalars, ϕ ($\phi_1, \phi_2 \dots \phi_n$), is defined as the product of the individual probabilities of each scalar.

$$p(\tilde{\phi}) \equiv \prod_{\alpha=1}^n p(\tilde{\phi}_\alpha) = \prod_{\alpha=1}^n \delta(\tilde{\phi}_\alpha - \phi_\alpha). \tag{38}$$

The exact equation for $p(\tilde{\phi})$ appropriate to Eq. (3) may be formed by multiplying Eq. (15), written for ϕ_α , by $\prod_{\substack{\alpha=1 \\ \alpha \neq \gamma}}^n p(\tilde{\phi}_\gamma)$ and summing

for all α . This gives

$$\begin{aligned} \frac{\partial}{\partial t} [\rho p(\tilde{\phi})] + \frac{\partial}{\partial x_i} \rho U_i p(\tilde{\phi}) = & \\ - \sum_{\alpha=1}^n \frac{\partial}{\partial \tilde{\phi}_\alpha} p(\tilde{\phi}) \left[\frac{\partial}{\partial x_i} \Gamma \frac{\partial \phi_\alpha}{\partial x_i} + S_\alpha(\phi) \right]. & \end{aligned} \tag{39}$$

Again, making the assumption of low Mach number, Eq. (39) may be averaged to give the exact joint probability equation

$$\begin{aligned} \rho(\tilde{\phi}) \frac{D}{Dt} \langle p(\tilde{\phi}) \rangle = & \\ \frac{\partial}{\partial x_i} \left[\Gamma \frac{\partial \langle p(\tilde{\phi}) \rangle}{\partial x_i} - \rho(\tilde{\phi}) \langle p(\tilde{\phi}) u_i \rangle \right] & \\ - \sum_{\alpha=1}^n \frac{\partial}{\partial \tilde{\phi}_\alpha} \left[\langle p(\tilde{\phi}) \rangle S_\alpha(\tilde{\phi}) + \right. & \\ \left. \sum_{\beta=1}^n \frac{\partial}{\partial \tilde{\phi}_\beta} \langle p(\tilde{\phi}) \Gamma \frac{\partial \phi_\alpha}{\partial x_i} \frac{\partial \phi_\beta}{\partial x_i} \rangle \right]. & \end{aligned} \tag{40}$$

This equation is similar to that for the single probability distribution, Eq. (19), and the physical interpretation of each term is the same. Again, the term involving the source is known. While the turbulent convection may be modelled in the same way as before, the final term poses a much more serious problem; one which will not be considered here. While the modelling of this term is essential to the closure of Eq. (40), its complex nature requires greater consideration than is appropriate to this preliminary investigation.

3. Discussion

The behaviour of the modelled probability distribution equation, Eq. (37), was examined first for ϕ representing a passive contaminant or the mixture fraction in a diffusion flame and then for ϕ representing the mass fraction of products in a simplified premixed system.

3.1 Modelled Equation: Diffusion Flame

The equation for a passive contaminant or the mixture fraction in an idealised diffusion flame contains no source term. For simplicity, assuming the density to be constant, the modelled equation appropriate to this situation may be written as

$$\frac{D \langle p(\tilde{\phi}) \rangle}{Dt} = \frac{\partial}{\partial x_i} \left[C_1 u' \frac{\partial \langle p(\tilde{\phi}) \rangle}{\partial x_i} - \frac{\partial^2 G(\tilde{\phi})}{\partial \tilde{\phi}^2} \right]. \quad (41)$$

In order to study the probability distributions predicted by the modelled equation, a steady, homogeneous, isotropic flow was considered in which equal quantities of fluid with values of $\tilde{\phi}_1$ and $\tilde{\phi}_2$ were homogeneously introduced and an equal amount of the resulting mixture was withdrawn, the residence time being τ_R . The form of Eq. (37) appropriate to the situation is

$$\begin{aligned} & \frac{1}{2} [\delta(\tilde{\phi} - \tilde{\phi}_1) + \delta(\tilde{\phi} - \tilde{\phi}_2)] - \langle p(\tilde{\phi}) \rangle \\ & = \frac{\tau_R}{\tau_T} \phi' C_2 \frac{\partial^2 H(\tilde{\phi})}{\partial \tilde{\phi}^2}. \end{aligned} \quad (42)$$

The time scale ratio, τ_R/τ_T , ($\tau_T \equiv 1/u'$) is of great physical significance for it determines the degree of mixing. Equation (42) was solved numerically for various values of the time scale ratio and the resulting distributions of $\langle p(\tilde{\phi}) \rangle$ are shown on Fig. 2. It is seen that two limiting cases exist.

$$\begin{aligned} \text{as } \tau_R / \tau_T & \longrightarrow 0, \\ \langle p(\tilde{\phi}) \rangle & \longrightarrow \frac{1}{2} [\delta(\tilde{\phi} - \tilde{\phi}_1) + \delta(\tilde{\phi} - \tilde{\phi}_2)], \end{aligned} \quad (43)$$

$$\begin{aligned} \text{as } \tau_R / \tau_T & \longrightarrow \infty, \\ \langle p(\tilde{\phi}) \rangle & \longrightarrow \delta(\tilde{\phi} - \langle \phi \rangle). \end{aligned} \quad (44)$$

These two results, which are certainly correct, are an inevitable consequence of the restrictions imposed on the modelling of G . The real test of the modelling is the predicted values of $\langle p(\tilde{\phi}) \rangle$ for intermediate values of the time scale ratio. In the absence of experimental data, the predictions can only be appraised intuitively: there is no feature that is contrary to expectations.

3.2 Modelled Equation: Premixed Flame

In order to study the behaviour of the modelled equation with a finite source term, a similar situation to that described above is considered. In this case, a one step reaction takes place between homogeneously premixed fuel and oxidant to form a single product. ϕ represents the mass fraction of product which lies in the range $\tilde{\phi}_1 \leq \phi \leq \tilde{\phi}_2$. The reactants are added to the system at $\tilde{\phi} = \tilde{\phi}_1$ and the resultant mixture is withdrawn. The application of the probability approach to the situation clearly demonstrates the influence of the time scales of the system. Again, setting the density constant (and equal to unity), the modelled equation for this situation is

$$\frac{1}{\tau_R} [\delta(\tilde{\phi} - \tilde{\phi}_1) - \langle p(\tilde{\phi}) \rangle]$$

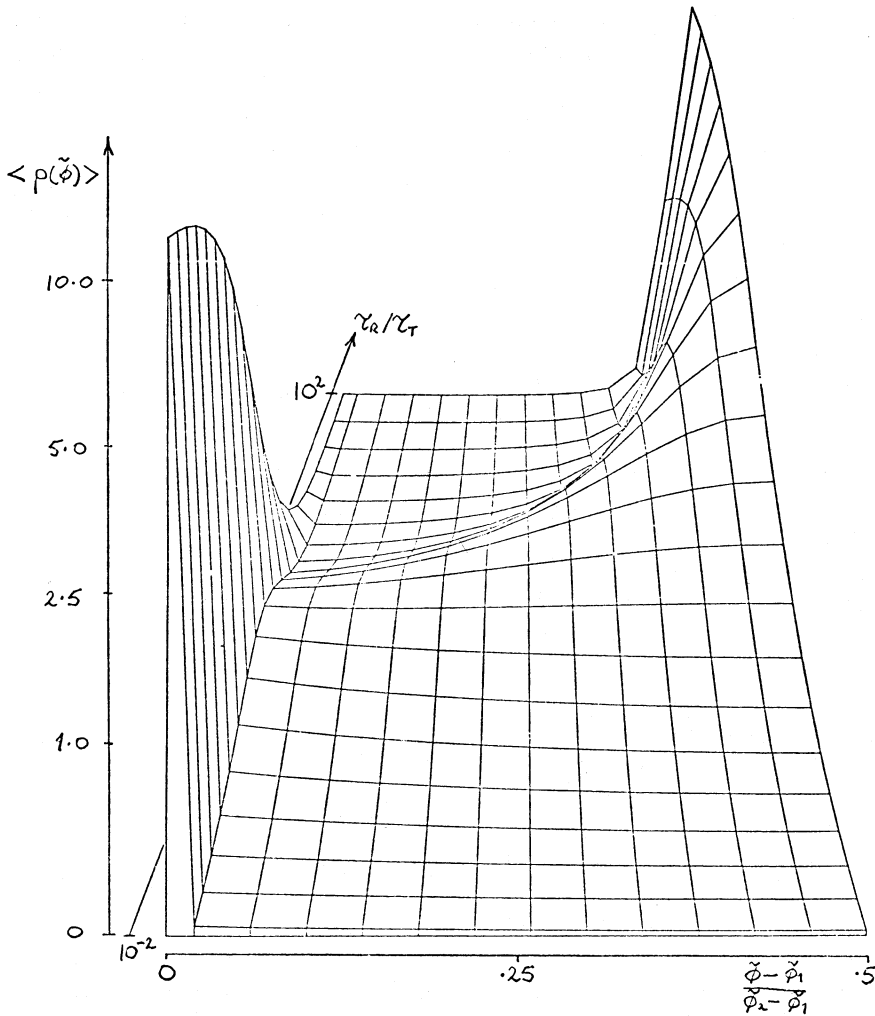


Fig. 2. Inert, homogeneous, flow: $\langle p(\tilde{\phi}) \rangle$ against $\tilde{\phi}$ and τ_R/τ_T .

$$= \frac{\partial}{\partial \tilde{\phi}} \left[\langle p(\tilde{\phi}) \rangle S(\tilde{\phi}) + \frac{C_2 \phi'}{\tau_T} \frac{\partial H(\tilde{\phi})}{\partial \tilde{\phi}} \right]. \quad (45)$$

The specific form of the reaction rate will not be defined at this point except to set it to zero for $\tilde{\phi} = \tilde{\phi}_1$ and $\tilde{\phi} = \tilde{\phi}_2$ and positive for $\tilde{\phi}_1 < \tilde{\phi} < \tilde{\phi}_2$. $\tilde{\phi} = \tilde{\phi}_2$ corresponds to a situation where all the reactants have reacted, hence $S(\tilde{\phi}_2) = 0$; at $\tilde{\phi} = \tilde{\phi}_1$ where there are pure reactants, in a typical premixed flame, the temperature is too low for reaction to take place, thus $S(\tilde{\phi}_1) = 0$. The time scale of the reaction, τ_K , is taken as the inverse of the maximum value of $S(\tilde{\phi})$, and the normalised reaction rate, $S^*(\tilde{\phi})$, is given by

$$S^*(\tilde{\phi}) = \tau_K S(\tilde{\phi}). \quad (46)$$

Equation 45 may now be written in the form

$$\delta(\tilde{\phi} - \tilde{\phi}_1) - \langle p(\tilde{\phi}) \rangle =$$

$$\frac{\partial}{\partial \tilde{\phi}} \left[\frac{\tau_R}{\tau_K} \langle p(\tilde{\phi}) \rangle S^*(\tilde{\phi}) + C_2 \phi' \frac{\tau_R}{\tau_T} \frac{\partial H(\tilde{\phi})}{\partial \tilde{\phi}} \right] \quad (47)$$

The averaged reaction rate may be obtained from Eq. (45) by multiplying by $\tilde{\phi}$ and integrating

$$\langle S(\phi) \rangle = (\langle \phi \rangle - \tilde{\phi}_1) / \tau_R. \quad (48)$$

The form of the solution of Eq. (47) is demonstrated for the nine situations characterised by each of the time scale ratios being either zero, finite or infinite. These solutions are more clearly demonstrated by taking the definite integral of Eq. (47).

$$\int_{-\infty}^{\tilde{\phi}} \delta(\tilde{\phi} - \tilde{\phi}_1) - \langle p(\tilde{\phi}) \rangle d\tilde{\phi} \\ = \frac{\tau_R}{\tau_K} \langle p(\tilde{\phi}) \rangle S^*(\tilde{\phi}) + \frac{\tau_R}{\tau_T} C_2 \phi' \frac{\partial H(\tilde{\phi})}{\partial \tilde{\phi}}. \quad (49)$$

A cursory inspection of Eq. (49) reveals two important conclusions. First, a trivial solution given by

$$\langle p(\tilde{\phi}) \rangle = \delta(\tilde{\phi} - \tilde{\phi}_1); \quad \langle \phi \rangle = \tilde{\phi}_1; \\ \langle S(\phi) \rangle = 0, \quad (50)$$

exists regardless of the values of the time scale ratios. (For this solution, each term in Eq. (49) is zero.) Secondly, a necessary condition for another solution to exist is that both time scale ratios be nonzero. If τ_R/τ_K is zero, $\langle S(\phi) \rangle$ is zero and hence Eq. (48) becomes the trivial solution. Physically, fluid at $\tilde{\phi} = \tilde{\phi}_1$ is introduced tending to decrease $\langle \phi \rangle$. As the mixing term cannot alter the value of $\langle \phi \rangle$, the result is a tendency toward the trivial solution. If τ_R/τ_T is zero, the fluid introduced at $\tilde{\phi} = \tilde{\phi}_1$ has no way to pass to higher mass fractions since $\langle p(\tilde{\phi}) \rangle S^*(\tilde{\phi})$ at $\tilde{\phi} = \tilde{\phi}_1$ is zero. This observation highlights the importance of the process referred to as back-mixing, whereby hot combustion products mix with cold reactants raising their temperature until reaction is possible. Thus, the five situations characterised by combinations of time scale ratios in which one or

both is zero result in the trivial solution only.

The first situation of practical interest is that in which $\tau_R/\tau_T \rightarrow \infty$ while τ_R/τ_K remains finite. In order that the mixing term in Eq. (45) remains finite, ϕ' must tend to zero. Thus, the probability distribution will tend to a single delta function which, clearly, is centred on $\langle \phi \rangle$, i.e.,

$$\langle p(\tilde{\phi}) \rangle = \delta(\tilde{\phi} - \langle \phi \rangle). \quad (51)$$

The averaged reaction rate is given by

$$\langle S(\phi) \rangle = \int_{-\infty}^{\infty} S(\tilde{\phi}) \langle p(\tilde{\phi}) \rangle d\tilde{\phi} = S(\langle \phi \rangle), \quad (52)$$

and hence, from Eq. (48)

$$\langle \phi \rangle = \tilde{\phi}_1 + S^*(\langle \phi \rangle) \tau_R/\tau_K. \quad (53)$$

It is seen that in this situation, which corresponds to a perfectly stirred reactor, Eq. (5) is valid, i.e.,

$$\langle S(\phi) \rangle = S(\langle \phi \rangle).$$

It should also be noted that Eq. (53) may have one or more than one solution; one being the trivial solution. As an extension of this situation it is seen that as τ_R/τ_K tends to infinity also, in order to satisfy Eq. (53), $\langle \phi \rangle$ must take a value such that $S^*(\langle \phi \rangle)$ is close to zero. Thus, in the case where both time scale ratios are infinite a solution is given by

$$\langle p(\tilde{\phi}) \rangle = \delta(\tilde{\phi}_2 - \tilde{\phi}), \quad (54)$$

i.e., all the reactants are converted into products.

The final case for which an analytic solution is presented is that in which τ_R/τ_K tends to infinity while τ_R/τ_T remains finite. It is for this situation that the eddy-break-up model is intended. The form of the solution is again found by examining Eq. (49) and noting that the reaction

rate term can remain finite only by $\langle p(\tilde{\phi}) \rangle$ tending to delta functions at $\tilde{\phi}_1$ and $\tilde{\phi}_2$

$$\langle p(\tilde{\phi}) \rangle = a \delta(\tilde{\phi} - \tilde{\phi}_1) + (1 - a) \delta(\tilde{\phi} - \tilde{\phi}_2). \quad (55)$$

Substituting $\langle \phi \rangle$ given by Eq. 55 into Eq. (48) gives

$$\langle S(\phi) \rangle = (1 - a) (\tilde{\phi}_2 - \tilde{\phi}_1) / \tau_R. \quad (56)$$

Now, if Eq. (49), with $\langle p(\tilde{\phi}) \rangle$ given by Eq. (55), is evaluated at the limit as $\tilde{\phi}$ tends to $\tilde{\phi}_1 +$ there results

$$(1 - a) = \frac{\tau_R}{\tau_K} \lim_{\tilde{\phi} \rightarrow \tilde{\phi}_1 +} \langle p(\tilde{\phi}) \rangle S^*(\tilde{\phi}) + C_2 \frac{\tau_R}{\tau_T} \phi' \lim_{\tilde{\phi} \rightarrow \tilde{\phi}_1 +} \frac{\partial H(\tilde{\phi})}{\partial \tilde{\phi}}. \quad (57)$$

As the limit of the first term is zero, Eq. (56) and (57) may be combined to give

$$\langle S(\phi) \rangle = 2 C_2 / \tau_T \phi' \phi'_{\max} \frac{\partial H(\tilde{\phi})}{\partial \tilde{\phi}}, \quad (58)$$

where

$$\phi'_{\max} = \frac{1}{2} (\tilde{\phi}_2 - \tilde{\phi}_1), \quad (59)$$

is the maximum value that ϕ' may obtain. The notable result is that, as τ_R/τ_K tends to infinity, the averaged reaction rate remains finite and is independent of both τ_R/τ_K and $S^*(\tilde{\phi})$. As is implied by the name of the eddy-break-up model, the reaction rate is directly proportional to the rate of back-mixing. Evaluating the limit of the differential, the averaged reaction rate is given by

$$\langle S(\phi) \rangle = \frac{1}{2} C_2 / \tau_T \frac{\langle \phi'^2 \rangle}{\phi'_{\max}} \ln \left(1 + \frac{2\phi'_{\max}}{\phi'} \right). \quad (60)$$

Comparing this result with the eddy-break-up model

$$\langle S(\phi) \rangle = C_{\text{EBU}} \phi' / \tau_T, \quad (61)$$

a relation for the eddy-break-up ‘‘constant’’ is obtained.

$$C_{\text{EBU}} = \frac{1}{2} C_2 \frac{\phi'}{\phi'_{\max}} \ln \left(1 + \frac{2\phi'_{\max}}{\phi'} \right). \quad (62)$$

The variation of C_{EBU} with ϕ' / ϕ'_{\max} is shown on Fig. 3 and should be compared with the values of .53 and 1.0 used by Mason and Spalding [10] and Khalil et al. [11], respectively. It appears that C_{EBU} given by Eq. (62), is too large; however, the assumption of very fast chemistry in the flow situations of the above authors may not be completely valid. It may certainly be expected that near complete combustion the reaction rate will be very rapid but, at the cold end of the probability distribution, the reaction rate will still be small. Thus, in this situation a delta function may be expected at $\tilde{\phi} = \tilde{\phi}_2$, but not at $\tilde{\phi} = \tilde{\phi}_1$. The effect of finite rate chemistry over a region of probability space is to decrease the averaged reaction rate and hence to make the effective eddy-break-up constant smaller than that predicted by Eq. (62).

In each of the above cases, in which one or

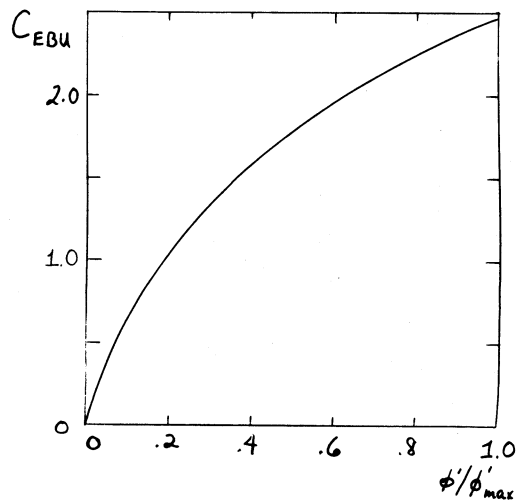


Fig. 3. Reacting homogeneous flow: C_{EBU} against ϕ'/ϕ'_{\max} .

both of the time scale ratios tend either to zero or infinity, it has been shown that the probability distribution is known a priori. The solution of the probability distribution equation is, therefore, unnecessary. However, these situations are idealised and in practice both time scales are finite; it is for situations of this type that the probability approach is intended. Equation (47) was solved numerically for various values of one time scale ratio while the other was held at unity. Figure 4 shows the predicted reaction rate against τ_R/τ_K for $\tau_R/\tau_T = 1$ and Fig. 5 shows the reaction rate against τ_R/τ_T for $\tau_R/\tau_K = 1$. The normalised reaction rate was given by

$$S^*(\tilde{\phi}) = 4(\tilde{\phi}_2 - \tilde{\phi})(\tilde{\phi} - \tilde{\phi}_1)(\tilde{\phi}_2 - \tilde{\phi}_1)^{-2}. \quad (63)$$

In both cases the predictions follow the expected trends, but there is no basis for a quantitative assessment of the model's performance.

3.3 Joint Probability Approach

It has been shown that, for a system characterised by only one scalar, with the knowledge of the probability distribution of that scalar, all averaged quantities may be evaluated through Eq. (12). Similarly for a general system, the relation

$$\langle h(\phi) \rangle = \int_{-\infty}^{\infty} h(\tilde{\phi}) \langle p(\tilde{\phi}) \rangle d\phi, \quad (64)$$

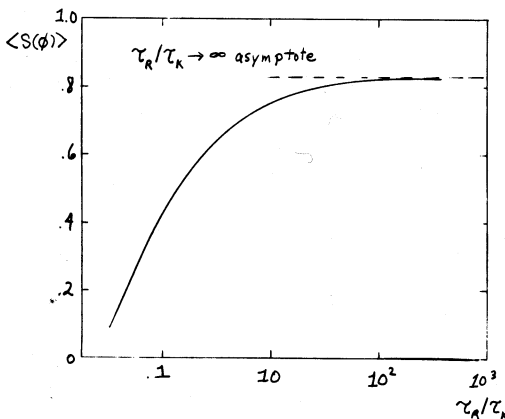


Fig. 4. Reacting homogeneous flow: $\langle S \rangle$ against τ_R/τ_K , $\tau_R/\tau_T=1$.

allows averaged quantities to be evaluated from the averaged joint probability distribution. Thus, the solution of a modelled form of the joint probability distribution equation, Eq. (30), would lead to a knowledge of all averaged quantities. However, before such an approach may be advocated it is necessary to establish that a modelled joint probability distribution equation is soluble by numerical means.

In a general reacting flow with n species, the joint probability of temperature and $n-1$ species must be considered, thus increasing the number of independent variables by n . For example, in a steady, two-dimensional flow there will be $n+2$ independent variables. The ability of present day digital computers to solve differential equations is limited; to solve the joint probability equation in more than, say, four independent variables would be a formidable task. With two independent spatial variables and two independent probability variables, the most general flow for which a solution could be obtained would be one with a one-step global reaction and favourable boundary conditions on temperature. While the limitation of the single probability approach to premixed or diffusion flames would be removed, the degree of generality would still be small.

Two simplifications are proposed which will increase the generality of the flow situations that may be considered. First, only those reactions which are not well approximated by one

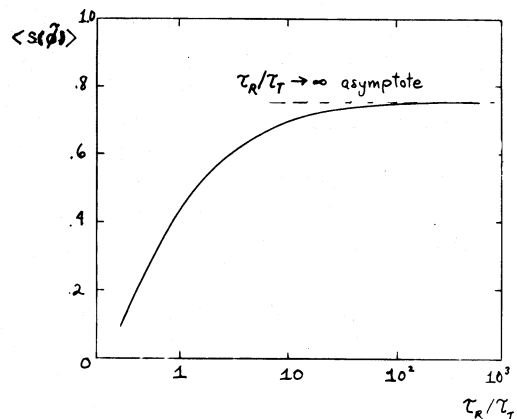


Fig. 5. Reacting homogeneous flow: $\langle S \rangle$ against τ_R/τ_T , $\tau_R/\tau_K=1$.

or other of the time scale ratios tending to infinity and which cause a significant chemical or thermodynamic change should be considered by the probability approach. Secondly, by approximating the transport in x space through the gradients of the averaged value of the scalars, the independent variables in x space may be eliminated. While these measures would undoubtedly introduce errors, the resultant scheme could take account of turbulence and finite rate chemistry for the four dominant species.

3.4 Suggestions for Further Work

As the work described here is essentially a preliminary investigation, many assumptions have been made without direct experimental support. It would, therefore, be valuable to check the modelled equation against experimental data for both isothermal and reacting systems. The available data for this purpose is in short supply; Odidi [12] presents some measurements of the temperature probability distribution in a methane diffusion flame. Ribeiro and Whitelaw [13] who developed the sampling technique used by Odidi, measured joint velocity probability distributions and concluded that probability distributions may be measured with good accuracy.

The molecular mixing term in the joint probability distribution equation must be modelled before the full potential of this approach may be exploited.

4. Conclusions

The main conclusions that can be extracted from the text are as follows:

(i) The averaged joint probability distribution of all independent scalars characterising a flow is sufficient to determine all averaged functions of these scalars. In a combustion system, the averaged mass fraction and reaction rate of each species and the averaged density and temperature may be determined from the averaged joint probability distribution of temperature and the species.

(ii) Exact transport equations have been derived for the probability and joint probability distributions. The term in the probability dis-

tribution equation representing turbulent convection has been modelled by a mixing length hypothesis while the modelling of the molecular mixing term has been shown to be subject to four constraints. A model, in accord with these constraints, has been proposed which, although not entirely satisfactory, can be expected to be qualitatively correct.

(iii) Solutions of the modelled probability distribution equation have been obtained for homogeneous isotropic flow situations corresponding to diffusion and premixed flames. The equation offers a clear mathematical description of the processes involved in premixed flames and, for the appropriate conditions, an expression for the averaged reaction rate is obtained which is similar to Spalding's [3] eddy-break-up model. The empirical constant in this model is predicted.

(iv) The numerical solution of a modelled equation for the joint probability of up to four scalars is feasible.

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Nomenclature

C_1, C_2	constants in modelled equation
C_D, C_{g1}, C_{g2}	constants in equations of Ref. [9]
C_{EBU}	eddy-break-up constant
f	mixture fraction
G	molecular mixing correlation defined by Eq. 21
g	function, defined by Eq. 26
H	function, defined by Eq. 24
k	kinetic energy of turbulence, $\frac{1}{2} \langle u_i u_i \rangle$
l	turbulent length scale
P	pressure
P	probability distribution
S	source term in scalar equation
t	time
U	instantaneous velocity
u	fluctuating velocity
u'	turbulent velocity scale
x	position vector

Γ	scalar exchange coefficient
δ	Dirac's delta function
ϵ	dissipation rate of turbulent kinetic energy
μ	viscosity
ρ	density
σ_f, σ_g	constants in equations of Ref. [7]
τ_K	characteristic time scale of reaction
τ_R	residence time
τ_T	turbulent time scale
ϕ	scalar variable
ϕ'	averaged fluctuation $\langle (\phi - \langle \phi \rangle)^2 \rangle^{1/2}$
ϕ'_{\max}	maximum possible value of ϕ'

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