

## 11 PREDICTING THE SCALAR MIXING PROCESS

The types of scalar mixing processes (and reaction) that we are concerned with here are completely described by the conservation equations of overall mass continuity, momentum transport, and chemical species conservation. Unfortunately, the wide range of length and time scales place impossible computational resource demands for numerical solutions of these equations. The computer time and memory requirements for full simulations will be beyond feasibility for the foreseeable future. On the other hand, analytic solutions to these equations exist for only a few simplified cases due to the inherent nonlinearity of the multi-dimensional coupled equations. As a result the researcher or engineer must resort to the use of models to provide predictions of the mixing and reaction process. Although essentially all models resort to use of empirical correlations at some level, it is hoped that the models are constructed so that they mimic as much of the known physical behavior of turbulent mixing as possible.

### 11.1 Moment methods applied to scalar mixing.

For engineering purposes, it is rarely, if ever, necessary to have the complete description of the flow field and scalar field, as is in theory possible from a full numerical simulation of the governing equations. In fact, knowledge of the mean values and a few of the higher order moments is usually sufficient for design purposes. Unfortunately, this information too is difficult to obtain in practice.

Among the most common approaches used to study scalar mixing in realistic configurations are methods based upon a decomposition of the fluctuating quantities into a mean component and a component which is the variation about the mean.

To obtain an equation for the mean values of the dependent variables, we first decompose the variables into their mean and fluctuating components, e.g.:

$$\begin{aligned} u_i &= \bar{u}_i + u'_i \\ \phi &= \bar{\phi} + \phi' \end{aligned} \tag{11.1}$$

Decomposing the variables into their mean and fluctuating components and averaging the equation gives the transport for the mean value of  $\phi$ .

$$\frac{\partial \bar{\phi}}{\partial t} + \frac{\partial \bar{u}_j \bar{\phi}}{\partial x_j} = - \frac{\partial \overline{\phi' u'_j}}{\partial x_j} + D \frac{\partial^2 \bar{\phi}}{\partial x_j \partial x_j} \tag{11.2}$$

or

$$\frac{\partial \bar{\phi}}{\partial t} + \frac{\partial \bar{u}_j \bar{\phi}}{\partial x_j} = \frac{\partial}{\partial x_j} \left( D \frac{\partial \bar{\phi}}{\partial x_j} - \overline{\phi' u'_j} \right) \tag{11.3}$$

This equation is very similar in appearance to the exact scalar transport equation. However, note the appearance of the term  $\overline{\phi' u'_j}$ . This term describes the effects of turbulence on the development of the mean scalar field.

If a simple chemical reaction of the form  $r_\alpha = [\phi_\alpha][\phi_\beta]$  is included in the species conservation equation, the equation for the mean scalar transport takes the following form:

$$\frac{\partial \bar{\phi}}{\partial t} + \frac{\partial \bar{u}_j \bar{\phi}}{\partial x_j} = \frac{\partial}{\partial x_j} \left( D \frac{\partial \bar{\phi}}{\partial x_j} - \overline{\phi' u'_j} \right) - \overline{\phi_\alpha \phi_\beta} - \overline{\phi'_\alpha \phi'_\beta} \quad (11.4)$$

In this case an additional correlation between the two reacting species shows up which represents the effects of scalar fluctuations on the mean reaction rate. For more realistic situations in which the reaction has an explicit temperature dependence, the expression for the mean reaction rate can become extremely complicated.

Another point of importance with respect to scalar mixing is that mean values are often not the primary quantity of interest. In many mixing applications it is the variance that is the main indicator of the amount of mixing that has occurred. You derived an equation for this in class and have discussed its importance. The proper characterization of scalar fluctuations is often most important.

### 11.1.1 The closure problem

The equations for the mean scalar field derived above are exact as no approximations have been made. We have used these equations to conceptualize how the turbulence affects the mean flow and to identify some of the mechanisms of turbulent transport. However, a fundamental problem associated with the statistical treatment of turbulent mixing (and the statistical treatment of turbulent flows in general) is revealed in the equations for the mean properties derived above. Just as in the equations for the mean momentum transport, through the process of decomposing the flow into its mean and fluctuating components and averaging the governing equations, we have ended up with equations that contain more unknowns than before the averaging procedure was applied. No additional equations have been added so the equations no longer constitute a closed set. This “closure” problem is the central stumbling block in most all predictive methods for turbulent flow. These additional unknowns take the form of correlations between the fluctuating quantities. In order to close the equations above, it is necessary to introduce empirical models to describe the behavior and effects of the turbulent transport terms.

One potential solution to the problem is to derive a set of transport equations that describe the time evolution of these unknown terms. This can be done (we will derive some of these equations later, in particular, equations for  $\overline{\phi'_a \phi'_b}$ ), but higher order moments appear in the equations for the lower order moments. A hierarchy of equations can be derived for the unclosed terms, but closure is never achieved. Equations for the second order moments contain third order moments; equations for the third order moments contain fourth order moments, and so on. At some level in

this hierarchy, approximations must be introduced to close the equations. Providing a realistic closure has been a dominant motivation in turbulence research.

Therefore, to solve Eq. 11.4, the unknown scalar-scalar and scalar-velocity correlations must be modeled. In practice, this is usually accomplished by making gradient-diffusion assumptions and handling the effects of turbulence on the transport by using an *enhanced*, or *eddy diffusivity*. In such a formulation, the turbulent scalar flux can be modeled as

$$\overline{\phi' u_j'} = \frac{\mu_t}{\sigma_t} \frac{\partial \overline{\phi}}{\partial x_j} \quad (11.5)$$

where  $\mu_t$  is the eddy viscosity and  $\sigma_t$  is a constant to be determined.

Although we will see that there are problems with this modeling approach, even more severe difficulties arise when one is concerned with modeling the reaction rate term. In addition, modeling the eddy viscosity itself remains a challenging problem as already described in §??.

## 11.2 Modeling the Mean Reaction Rate

Although this course is not directed at reacting flows, taking a look at issues with modeling reaction rates illustrates some exceptionally challenging issues in turbulent flows. Below, some of this will be discussed.

### 11.2.1 Modeling Difficulties

Appearing in the transport equation for the average species concentration is the mean reaction rate. For a binary reaction, say



a realistic form of the reaction rate is

$$\dot{w} = k Y_1 Y_2 \quad (11.7)$$

Using Favre averaging, the mean reaction term can be written as

$$\tilde{w} = \tilde{k}(\tilde{Y}_1 \tilde{Y}_2 + \widetilde{Y_1'' Y_2''}) + \widetilde{k'' Y_2'' Y_1} + \widetilde{k'' Y_1'' Y_2} + \widetilde{k'' Y_2'' Y_1''} \quad (11.8)$$

where  $Y_1$  and  $Y_2$  are the concentrations of the two reacting species, and  $k$  is a reaction rate coefficient. If the reaction rate coefficient remains constant the reaction rate term reduces to

$$\tilde{w} = \tilde{k}(\tilde{Y}_1 \tilde{Y}_2 + \widetilde{Y_1'' Y_2''}) \quad (11.9)$$

A closure problem is evident, because the correlation between the fluctuating scalar fields must be supplied. Even more complexity arises owing to the fact that

the reaction rate coefficients cannot, in most applications, be treated as constant. For a rate coefficient of the form

$$k = k_o \exp(-T_a/T), \quad (11.10)$$

$k$  clearly strongly depends on temperature. Decomposing the temperature,  $T$  into its Favre averaged mean and fluctuating components and then expanding the exponential gives

$$k = k_o \exp[-T_a/\tilde{T}] \left[ 1 + \frac{T_a}{\tilde{T}^2} T'' + \left( \frac{T_a^2}{2\tilde{T}^4} - \frac{T_a}{\tilde{T}^3} \right) T''^2 + \dots \right] \quad (11.11)$$

Assuming that  $T_a/\tilde{T}$  is large, the Favre average of Eq. 11.11 can be written as

$$\tilde{k} = k_o \exp[-T_a/\tilde{T}] \left[ 1 + \left( \frac{T_a^2}{2\tilde{T}^4} \right) \frac{\overline{\rho T''^2}}{\bar{\rho}} + \dots \right] \quad (11.12)$$

Unfortunately, the higher order terms in the expansion above are not generally insignificant. This makes the above formulation impractical for computing mean reaction rates, because a large number of terms in the expansion must be retained to give meaningful results. Fortunately, approximations can be invoked to compute major species reactions rates in many applications.

The most significant simplification in modeling the reaction rate can be achieved if the chemical reactions are fast compared to fluid mixing rates. In this case, the assumption of chemical equilibrium can be applied, and the rate of reaction is determined from chemical equilibrium considerations, and not from detailed kinetics. In many hydrocarbon flames, this assumption works reasonably well for the major species. However, the formation of some pollutants, such as nitric oxide, proceeds relatively slowly. The formation of NO has little effect on the heat generation or major species concentrations, but it cannot be predicted from equilibrium considerations because its formation is kinetically limited. A method that can effectively be used in the limit of fast chemistry is discussed below.

### 11.2.2 The Mixture Fraction.

In many combustion applications, the fuel and oxidizer are introduced into the combustion chamber in separate feeds, 1 and 2. Under these conditions, it is convenient to define a conserved scalar,  $f$ , called the mixture fraction,

$$f = \frac{Y_1}{Y_1 + Y_2} \quad (11.13)$$

$f$  is the mass fraction of fluid that originated in stream 1. Since the mixture fraction is a conserved variable, it obeys the transport equation

$$\frac{\partial \rho f}{\partial t} + \frac{\partial}{\partial x_k} (\rho u_k f) = \frac{\partial}{\partial x_k} \left( \rho D \frac{\partial f}{\partial x_k} \right) \quad (11.14)$$

For high Reynolds number flows, the Favre averaged form of Eq. 11.14 is

$$\frac{\partial \bar{\rho} \tilde{f}}{\partial t} + \frac{\partial}{\partial x_k} (\bar{\rho} \tilde{u}_k \tilde{f}) = - \frac{\partial}{\partial x_k} (\bar{\rho} u_k'' \tilde{f}'') \quad (11.15)$$

The last term in Eq. 11.15 must be modeled. Within the  $k - \epsilon$  formulation, the model described in Eq. 11.5 is often used. If the fluids in the two feeds have the same diffusivities and their boundary conditions are the same, then the mixture fraction can be used to reduce reacting flow problems to nonreacting turbulent flow problems. Of particular significance is the fast chemistry limit. For a fast, single-step irreversible reaction, fuel and oxidizer cannot coexist. If a reaction of the form



is considered, the stoichiometric mixture fraction,  $f_s$ , is

$$f_s = \frac{Y_{o_2}}{rY_{f_1} - Y_{o_2}} \quad (11.17)$$

where the subscripts 1 and 2 refer to the mass fractions in the two feed streams. These assumptions allow  $Y_o$  and  $Y_f$  to be computed directly from the mixture fraction:

$$\begin{aligned} f \leq f_s \quad Y_f &= 0 \\ Y_o &= rY_b(f_s - f) \end{aligned} \quad (11.18)$$

$$\begin{aligned} f \geq f_s \quad Y_f &= Y_b(f - f_s) \\ Y_o &= 0 \end{aligned} \quad (11.19)$$

where  $Y_b = Y_{f_1}/(1 - f_s)$ . For a fast reaction of the form given in Eq. 11.16, it can be seen that if the mixture fraction is known, the complete mixture composition can be obtained. The chemistry problem has been reduced to one of solving for a nonreacting scalar in a turbulent flow.

If back reactions occur, the above formulation can still be applied with some modification. In this case, the fast chemistry assumption implies that the forward and backward reactions have shorter time scales than the turbulence. The complete composition is thus again obtainable from the mixture fraction  $f$ .

As stated earlier, the major heat-generating reactions in the combustion process of most hydrocarbon fuels occur rapidly with respect to fluid mixing times. An approach based on the above mixture fraction formulation is often used in these conditions. Finite rate kinetic models must be applied to compute slower reactions that are characteristic of other aspects of the combustion process, particularly pollutant formation. Modeling finite rate chemistry in turbulent flows becomes a much more difficult problem. Will discuss issues related to this more extensively later.

### 11.3 Probability Density Function Methods

In general, the most convenient way to treat the mean reaction rate is in terms of probability density functions (pdf's). The pdf methods have many advantages over mean flow and Reynolds stress closures when applied to reacting flows. Given the one point pdf, all single point statistics can be determined. Most important to reactive flow calculations, however, is the treatment of the mean reaction rate.

Since the mean reaction rate is a function of  $n$  scalars  $\psi_n$ , the joint pdf  $p(\psi_n; x)$  is needed, where  $\psi_n$  are the values that the scalar,  $\phi_n$  can take. If the kinetic mechanisms are known, the mean reaction rate can be expressed in terms of the joint pdf of the scalar variables as

$$\tilde{w}_\alpha = \int \int \int \dot{w}_\alpha \tilde{p}(\psi_n; x) d\psi_1 d\psi_2 \dots d\psi_n \quad (11.20)$$

where  $\tilde{p}$  is a density averaged pdf given by

$$\tilde{p}(\psi_n; x) = \frac{\rho(\psi)}{\bar{\rho}} p(\psi; x) \quad (11.21)$$

The task now is focused on specifying the pdf. One of two approaches is generally used to determine the pdf. One involves solving a transport equation for the pdf. This will be briefly discussed shortly.

The other method, called the assumed pdf technique, is to assume a form of the pdf based on information of the particular flow. For example, if a jet of fuel  $F$  is issuing into air, the pdf of  $F$  will consist of a delta function that represents the fluid in the jet, another delta function that represents the fluid outside the jet, and another function that represents the fluid mixture in the turbulent zone

$$p(Z) = c_1 \delta(Z) + c_2 \delta(1 - Z) + c_3 p_m(Z) \quad (11.22)$$

where  $c_1$ ,  $c_2$ , and  $c_3$  are constants, and  $p_m(Z)$  is the pdf in the turbulent region. Calculations of mixing and reaction have been made using a number of shapes for the pdf  $P_m(Z)$ . These include Gaussian, clipped Gaussian, and beta functions. Once the form of the pdf is assumed, it is generally characterized by its first and second moments. Most approaches that use this method solve modeled equations for the first two moments. The equation for the mean value is given by Eq. 11.15. A modeled form of the second moment equation is (the notation  $f'$  is used to the variance,  $\overline{f'^2}$ ) [1]

$$\frac{\partial \bar{\rho} f'}{\partial t} + \frac{\partial}{\partial x_j} \bar{\rho} \tilde{u}_j f' = \frac{\partial}{\partial x_j} \left[ \frac{\mu_t}{\sigma_t} \frac{\partial f'}{\partial x_j} \right] - c_1 \frac{\mu_t}{\sigma_t} \left[ \frac{\partial \tilde{f}}{\partial x_j} \frac{\partial \tilde{f}}{\partial x_j} \right] - c_2 \frac{\bar{\rho} f'}{k} \quad (11.23)$$

$\sigma_t$ ,  $c_1$ , and  $c_2$  are constants. This reflects standard modeling for turbulent transport, production, and dissipation - like the homework problem you were assigned.

As multiple species equations are encountered, the assumed pdf technique becomes limited by computational resources and uncertainties in modeling. This is due in part

to the large number of second moment equations that must be solved for  $(\overline{\phi'_\alpha \phi'_\beta})$  to specify the joint pdf of many species. Furthermore, numerical evaluation of the multi-variable integral for the reaction rate given by Eq. 11.20 for multiple species is not reliable [2]. More details on the implementation of this method can be found in Bilger[3].

### 11.3.1 Evolution Equation for the PDF

From Eq. 11.20 it is apparent that the joint pdf of the species mass fraction can be used to obtain the mean reaction rate. A more rigorous approach than outlined above involves solving a transport equation for the joint pdf. This equation can be derived in a relatively straightforward manner by algebraic manipulation of the governing equations and application of the properties of the pdf. For example, if the flow field is homogeneous the pdf evolution equation for a single random variable is [4],

$$\frac{\partial p(\psi, t)}{\partial t} = -\frac{\partial}{\partial \psi} \left[ p(\psi, t) \left( \langle D \nabla^2 \phi | \psi \rangle + \dot{w}(\psi) \right) \right] \quad (11.24)$$

In this equation, the reaction rate term appears in closed form. The molecular diffusion term appears as a conditional expectation and must be modeled. If the flow field were not statistically homogeneous, a term describing the convective transport of the pdf would appear. In the transport equation for the composition pdfs, this term is not closed and must also be modeled. In such cases, the information about the flow field is usually obtained by other means, such as the  $k - \epsilon$  model. The treatment of convective transport is eliminated if the joint velocity-composition pdf is considered.

In general, the velocity-scalar joint pdf,  $P(V_i, \psi_n; \mathbf{x}, t)$ , provides a complete statistical description of the flow (velocity and scalar fields). Once the joint pdf equation is known it can, in theory, be integrated in time to give the temporal development of the statistical behavior of the flow. However, a number of difficult realities must be dealt with.

The joint pdf transport equation for velocity and scalar fields can be expressed as [4]

$$\begin{aligned} \rho(\psi_n) \frac{\partial P}{\partial t} + \rho(\psi_n) V_j \frac{\partial P}{\partial x_j} + \left( \rho(\psi_n) g_j - \frac{\partial \langle p \rangle}{\partial x_j} \right) \frac{\partial P}{\partial V_j} + \frac{\partial}{\partial \psi_\alpha} [\rho(\psi_n) \dot{w}_\alpha(\psi_n) P] \\ = \frac{\partial}{\partial V_j} \left[ \left\langle -\frac{\partial \tau_{ij}}{\partial x_i} + \frac{\partial p'}{\partial x_j} \middle| V_i, \psi_n \right\rangle P \right] + \frac{\partial}{\partial \psi_\alpha} \left[ \left\langle -\frac{\partial J_i^\alpha}{\partial x_i} \middle| V_i, \psi_n \right\rangle P \right] \end{aligned} \quad (11.25)$$

All terms on the left hand side of Eq. 11.25 are in closed form. This includes effects of convective transport, density differences, and the chemical reaction term  $\dot{w}_\alpha$ . In this formulation it is seen that all the difficulties in other modeling techniques with the nonlinear reaction term simply do not exist. The conditional expectations that appear on the right-hand side of Eq. 11.25 are not known and must be modeled. These terms each represent diffusive processes. The first term includes the effects of viscous stresses and pressure gradients; the last term represents the molecular mixing.

Even considering that the closures for the diffusion term are far from satisfactory, it is remarkable that all other terms in the joint velocity-composition pdf appear in closed form.

Aside from the difficulties associated with modeling the unclosed term, another problem is readily apparent upon inspection. This is associated with the high dimensionality of the equation. For three-dimensional flows, the pdf equation is a  $7+n$  dimensional equation (three spatial coordinates, time, three velocity components, and  $n$  scalar variables). From an Eulerian standpoint, the computational costs of constructing a numerical solution are prohibitive. Fortunately, such a system is conveniently handled by Monte-Carlo techniques.

In methods developed by Pope[5], the flow field (or, the pdf) at any time  $t$  is represented by  $N$  stochastic particles, which are intended to simulate fluid particles. Each of these particles is characterized by its spatial position, velocity, and composition, which are described by

$$\frac{\partial x_i^n}{\partial t} = U^n \quad (11.26)$$

$$\frac{\partial U_i^n}{\partial t} = \frac{1}{\rho} \frac{\partial \tau_{ij}}{\partial x_j} - \frac{1}{\rho} \frac{\partial p}{\partial x_i} + g_i \quad (11.27)$$

$$\frac{\partial \phi^n}{\partial t} = \frac{1}{\rho} \frac{\partial J_j^\alpha}{\partial x_j} + S_\alpha \quad (11.28)$$

where  $x^n$ ,  $U^n$ , and  $\phi^n$  are the individual particle position, velocity, and composition. Stochastic models are used to model the right hand side of Eqs. 11.27 and 11.28. An outline of the solution procedure and the stochastic models is given in a comprehensive review of the pdf method [4]. This review also provides a detailed account of the underlying theory and formulation of the pdf technique in reactive flow problems.

Although the equations above can be treated numerically, the question of modeling the molecular mixing term remains. Let us consider again the pdf transport equation in a homogeneous turbulent flow. Note that there is no convective term in this equation. This makes sense, because in probability space, convection acts to transport the probability spatially. Since the flow is assumed homogeneous, this term then plays no role (by definition, the statistics are space independent in a homogeneous flow.) To model the molecular mixing term, many models have been developed. Most of these are variants of Curl's [6] *coalescence-dispersion model*.

## 11.4 Coalescence-Dispersion Modeling

The Coalescence-Dispersion (C-D) model has been utilized extensively in many different forms for predicting mixing processes in turbulent flows. As such, it is worth taking some time to discuss some of the features and implementation of the process.

The model was originally introduced by Curl[6] to describe the mixing and reaction process that occurred in a mixed phase process involving interaction among droplets.



Mixing is assumed to take place randomly between individual droplets. Individual droplets also are allowed to redisperse into an identical pairs of droplets. The coalescence between two particles is assumed to result in instantaneous mixing between the two and the rates of coalescence and dispersion are determined by characteristic mixing frequencies and number of particles of and in the system. The model has been extended to treat gaseous phase mixing by considering the fluid to be composed of a large number of Lagrangian fluid elements which collectively describe the statistical state of the fluid. Many variants of this model have appeared, e.g. [7, 8].

Let us consider the case of a passive scalar in a homogeneous turbulence flow. Neglecting the reaction term is not a significant omission here since it appears in closed form in the pdf transport equation. The C-D model can be described within an evolution equation for the pdf. Pope[5] showed a general form of the C-D model could be expressed as

$$\begin{aligned} \frac{\partial p(\psi, t)}{\partial t} &= -2\beta\omega p(\psi, t) \\ &+ 2\beta\omega \int \int_{-\infty}^{\infty} p(\psi', t)p(\psi'', t)K(\psi, \psi', \psi'')d\psi' d\psi'' \end{aligned} \quad (11.29)$$

where a general form for  $K$  is

$$K(\psi, \psi', \psi'') = \int_0^1 A(\alpha)\delta\left[\psi - (1 - \psi)\psi' - \frac{1}{2}\alpha(\psi' - \psi'')\right] d\alpha \quad (11.30)$$

No convection term appears because of the assumption of spatial homogeneity.  $A(\alpha)$  is the pdf of  $\alpha$  where  $\alpha$  is a random variable and a measure of the mixing.  $A(\alpha)$  is zero outside the interval  $[0, 1]$  and is nonnegative and normalized to unity within  $[0, 1]$ .  $\beta$  is a parameter defined by Pope as

$$\beta = \frac{1}{a_1 - \frac{1}{2}a_2} \quad (11.31)$$

where

$$a_m = \int_0^1 \alpha^m A(\alpha)d\alpha \quad (11.32)$$

$\omega$  is the mixing frequency and must be supplied by an external source.

The various choices of  $A(\alpha)$  define the difference variants of the C-D models. For example, Curls original model is recovered by setting  $A(\alpha) = \delta(\alpha - 1)$ . The closure used by Janicka et al.[7] is obtained by setting  $A(\alpha) = 1$ , while Kosaly[9] showed that the Dopazo-O'Brien[8] model of mixing can be recovered from this formulation by setting  $A(\alpha) = \delta(\alpha - \epsilon)$  in the limit as  $\epsilon \rightarrow 0$ . During the class lecture we will provide a more physical based interpretation of this and discuss the relation between the stochastic Lagrangian implementation of the CD model to its pdf representation.

In practice, the pdf equation is solved in the stochastic Monte-Carlo approach mentioned above. The mixing by the C-D model involves randomly selecting pairs of elements for mixing. In the original version of Curl's model, the two elements

are assumed to mix completely, and redisperse into two identical particles with the same concentration. The choice of the different models (different  $A(\alpha)$ 's) simply determine the extent of mixing between the two particles before they redisperse. For example, in the model of Janicka et al., the extent of mixing between the two particles is determined by sampling the pdf(uniform)  $A(\alpha)$ . So as can be seen, there are basically an infinite number of variant of the C-D model, depending on how the mixing between the chosen particles is handled.

C-D modeling has been used by several researchers to predict experimental data. A discussion of some of this can be found in the paper by Kosaly and Givi[10]. A comparison of the C-D results for scalar mixing in a homogeneous turbulent flow with results of DNS has revealed some of the shortcomings of the C-D modeling approach. In particular none of the variants of the model tested correctly predict the evolution of the higher moments of the scalar field. Inspection of the model reveals the source of some of its difficulties. There is not a lot of physical justification for choosing one form of  $A(\alpha)$  over any other, except that one may give a better representation of the evolution of the scalar field. In particular there is no small-scale structural information regarding behavior of the scalar field. Fluid elements, once selected for mixing, mix instantaneously. The combined physics of turbulent convection and molecular diffusion is not accounted for. In cases where this is important, the C-D models will not perform well.

## 11.5 Other Mixing Models

There are, of course, many other mixing models being used in turbulent flow situations. Most of them suffer from similar difficulties which stem from their failure to realistically represent the physics of the small scales. Here we briefly discuss a few others that are regularly used.

### 11.5.1 Interaction By Exchange With the Mean (IEM)

The IEM model is also a Lagrangian model where the scalar field is described by eddies or fluid elements with particular scalar values. However, the fluid elements do not interact directly with each other. They instead interact, or exchange information only with the mean. Consider a flow consisting of a single scalar constituent that takes on values between 0 and 1 (a mixture fraction, for example). The complete scalar field is described by a number of fluid elements with concentration  $c_i$ . The mean scalar concentration is given by  $\bar{c}=1/N \sum_{i=1}^N c_i$ , where  $N$  is the number of elements. In the most general case a different weighting can be given to the different eddies. The governing equation for the concentration of each fluid element in this model formulation is

$$\frac{dc_i}{dt} = h(\bar{c} - c_i) \tag{11.33}$$

$h$  is a frequency describing the rate of mixing between different constituents.

To apply the model, consider a homogeneous, statistically steady turbulent flow consisting of an initial scalar distribution described by a double delta distribution at two extreme values of the scalar (say, -1 and 1; i.e., half the fluid is at a concentration of -1 and half has a concentration of 1). The turbulent mixing process will eventually result in a mixed fluid concentration of 0. The mean remains at  $c = 0$  throughout the mixing process. The scalar field can be initialized with two eddies at the different scalar concentrations. Given a particular mixing frequency,  $h = 1/\tau_m$ , Each fluid element evolves according to Eq. 11.33:

$$\frac{dc}{dt} = -\frac{1}{\tau_m}c \quad (11.34)$$

or

$$c = c_o \exp[-t\tau_m] \quad (11.35)$$

This example serves to show a deficiency of this model. Note that the pdf of the scalar field will evolve as two marching delta functions, approaching each other to the final mixed fluid concentration. This is clearly an unphysical situation. There is no variation of the scalar field in the domain as described by this version of the model. In more general, inhomogeneous flow situations, the flow will be described by a large number of particles. Each element will evolve according to Eq. 11.33 where the local mixing frequency is obtained from the fluid mechanical calculation

Some randomness can be added to the process to produce a more physically realistic evolution of the scalar pdf. For the homogeneous mixing problem described above, now consider initializing the scalar field with a large number of fluid elements, half at a concentration of -1, the other half at a concentration of 1. Fluid elements will interact with the mean, but randomness can be added by randomly selecting the time for exchange based on the mixing frequency, and also selecting the mixing frequency to randomly distributed about the mean mixing frequency. That is, let each element evolve according to

$$\frac{dc}{dt} = -r c \quad (11.36)$$

where  $r$  is sampled from a pdf  $g(r)$ . The standard IEM model is obtained by taking  $g(r) = \delta(r - 1/\tau_m)$ .

Although this *randomized exchange with the mean* (REM) produces a more realistic scalar distribution during the time evolution, there are still problems with this approach. An analysis of the evolution of the higher order moments reveals that the moments diverge in the long time limit, at least for the forms of  $g(r)$  that have been studied so far. This is a similar behavior to many of the C-D type models in use. This is an indication of a more fundamental shortcoming of these modeling approaches. Namely, the inability of the models to realistically describe and distinguish between the effects of the important physical processes in the mixing evolution.

### 11.5.2 Three and four environment models

Of the many different types of mixing models, here we mention two others. The two models mentioned here were basically developed for reactors with two separate, nonpremixed feed stream. In the three environment model the flow is assumed to be described by three different parcels of fluids: the two entering parcels (environments), and the leaving environment. The transfer (or mixing) from the entering environments to the leaving environments is given by a transfer function that depends of the *age* of the material. For a pure mixing problems with no chemical reaction the pdf of the scalar field will be represented initially by a double delta distribution. As time evolves, another delta distribution will develop at the mixed fluid concentration (the concentration of the exiting environment), and the delta distributions representing the entering environments will decrease in magnitude. So at any time only three concentration values exist. Although a calculation using this technique will be much more affordable than a monte-carlo simulation involving many parcels, there are clearly more unphysical aspects of this model.

An extension of this model is the four environment model, which is represented by two leaving environments. In this case each of the entering parcels exchanges mass with only one of the leaving environments. An addition transfer between leaving environments results is the pdf described by a quadruple delta distribution throughout its mixing time: The double delta representing the two incoming feed streams, and two other delta distributions. These are rich in one of the feed stream concentrations, but march in towards the mixed fluid concentration as time progresses.

#### A Final Comment

To repeat again, although the models that we have mentioned briefly above mimic some features of the real turbulent mixing process, there are clearly deficiencies associated with them. Mainly, the real physics of the mixing process becomes lost. This is not to say that these models are not useful. Many of them, in particular the variants of coalescence-dispersion are established components of predictive numerical codes. However, it is clear that all of the models suffer from deficiencies that make the search for a better mixing model a high priority in turbulent combustion research. Many of the details of the models briefly discussed above can be found in throughout the literature. Other useful references in addition to those already mentioned include: Brodkey, Mehta, and Tarbell[11] [12] [13].

Many variants of these mixing models, as well as different models have been proposed and used. The discussion in this section is by no means complete. It is meant as an introduction and background for further study.

In the next section we will discuss in detail a different model that is currently being used to model the mixing process. This model, the *linear eddy model* has some unique features that have proven to have made it a rather remarkable model of the mixing process. Although the model is not without flaws and drawbacks, it treats the mixing from a most physical viewpoint, and is therefore also a good tool not only to provide predictions of the mixing, but as means to actually study and try to

understand the fundamental behavior of the turbulent mixing process.

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