12 LINEAR EDDY MODEL OF TURBULENT MIXING

Of all the different mixing models that have been used in conserved scalar mixing, reacting flow, or microphysical applications, none have been successful in providing accurate and reliable predictions for a wide range of applications. Models are very often *tuned*, and therefore applicable to limited configurations and applications. This is particularly true of finite rate chemical reactions in turbulent environments. Unfortunately, many of the slower, secondary reactions that occur in hydrocarbon combustion are critical to the generation of unwanted byproducts (pollutants). In many other cases the physics are parameterized down to such an extent that little of the real physical processes that are occuring in a turbulent mixing environment are realistically treated.

Because the underlying physics of the mixing process is rarely realistically represented, and because interesting processes are occurring over a wide range of length scales, models cannot predict the wide range of physical processes that occur. In this section we will discuss a relatively new approach that has been used with success to model the mixing and reaction of a scalar quantity (like a chemical species) in a turbulent flow field. This technique is the *Linear Eddy Model* and was developed by Kerstein[1, 2]. It is not a self contained model of turbulence in general, but provides a very useful and insightful way to look at the turbulent mixing of passive or reacting scalars. The model as discussed here is strictly a mixing model, in that the statistics of the velocity field are inputs into the linear eddy model. In the following we will first discuss basic philosophy of the linear eddy model and the formulation of the model. We will follow this up with specific applications of the model and discuss how the model can be set up and implemented to discuss specific issues of technological relevance. This model, of course, has its own set of limitations which restrict its use in complex engineering simulations.

12.1 Linear Eddy Modeling Philosophy

The transport of a scalar in a turbulent flow field is governed by the equation:

$$\frac{\partial \phi}{\partial t} + \frac{\partial u_i \phi}{\partial x_i} = \frac{\partial^2 \phi}{\partial x_i \partial x_i} \tag{12.1}$$

In the formulation of the linear eddy model it is recognized that convection and diffusion which act on the scalar field are two distinctly different physical processes. As such, they should be modeled separately, with an approach that realistically represents the physics. These two processes (the third physical process we wish to consider, chemical reaction, will be discussed soon) are acting and interacting at all scales of the flow. Fluctuations in the velocity field cover a range from the integral scale to the Kolmogorov scale, while the scalar fluctuations span the integral scale to the Batchelor scale (or Corrsin scale for Sc<1). The relationship between the Kolmogorov scale and the Batchelor (Corrsin) scale is determined by the Schmidt number of the flow as described earlier. To account for the effects of both stirring and diffusion (and reaction) in a rigorous manner, their effects at all scales of the flow must be realistically represented. This can be achieved only by resolving all important scales of the flow. In traditional solution and modeling approaches, this is of course computationally prohibitive as the computer resources are severely inadequate to treat the full physics in multiple spatial dimensions.

Now, among the unique features of the linear eddy model is that it's description of the scalar field is a high-resolution, one-dimensional representation. Using a one-dimensional representation then allows for the full range of length and time scales to be resolved, even for flows with relatively high Reynolds and Schmidt numbers. The challenge, then, is to develop a model which provides a statistical description of the scalar field in one-spatial dimension, but is representative of the scalar statistics in a real three-dimensional flow. This is achieved by developing the model based on scaling laws representative of high-Reynolds number, three-dimensional flows. This formulation is discussed next.

12.2 Linear Eddy Model Formulation

As discussed above, the basic idea of the linear eddy approach is to treat separately the two different mechanisms acting to describe the evolution of a scalar (chemical species) over a linear domain. The first mechanism we discuss here is molecular diffusion (the last term in Eq. 12.1). Given a scalar field described on a one-dimensional space, diffusion can be implemented explicitly and essentially exactly the numerical time integration of the diffusion equation along the linear domain.

$$\frac{\partial \phi}{\partial t} = D\frac{\partial^2 \phi}{\partial x^2} \tag{12.2}$$

When chemical reactions are considered, treatment of their source term effect can be implemented explicitly with the diffusion equation:

$$\frac{\partial \phi}{\partial t} = D\frac{\partial^2 \phi}{\partial x^2} + \dot{w}_\phi \tag{12.3}$$

where the functional dependence of the reaction rate, $\dot{w}$, on the various chemical species is assumed known.

The real key to the model is the manner in which turbulent convection is treated. This constitutes another of the unique features of the model. Convection, or stirring is modeled in a stochastic manner by randomly occurring (subject to certain rules, of course) *rearrangement events* of the scalar field along the linear domain at intervals dependent upon the flow field conditions. The size of the rearranged region is also randomly chosen based on the eddy size distribution within the flow. The determination of these parameters will be discussed in detail.

To help achieve a qualitative and conceptual feel for the rearrangement process it is instructive to make an analogy of the rearrangement process with the action of individual eddies acting on the scalar field. The rearrangement events are formulated so that they reproduce the same effects of eddies acting on the flow. These effects include a spatial redistribution of the scalar field, an increase in scalar gradients, and an increase in the surface area differentiating scalar values. The size of the rearranged domain represents the eddy size, and the distribution of the eddy sizes and frequency of the events are obtained by using Kolmogorov scaling laws for high Reynolds number turbulent flows.

The rearrangement events involve the following: 1) the location x is chosen within the domain and is dependent on the turbulence intensity distribution in the domain. For a homogeneous turbulence, the location is randomly chosen. 2) the "eddy" size l, is selected (according to scaling laws, which will be discussed in detail shortly) over which the rearrangement will occur. 3) A time is selected for the next "event." 4) The species distribution in the chosen domain is rearranged.

The particular mapping used is termed the "triplet" map. The details of this will be described in lecture. Note that this choice of a rearrangement map is not unique. See class handouts for details. As a side note, it should be recognized that the functions that are derived below which parameterize the mixing process in the model must be consistent with whatever mapping process is selected (if something other than the triplet map may be desired).

In brief summary then, the two steps in the process for the evolution and evaluation of the species field are diffusion, which is implemented explicitly:

$$\frac{\partial \phi}{\partial t} = \frac{\partial^2 \phi}{\partial x^2} \tag{12.4}$$

and the rearrangement events, as described above.

To carry out the complete model, the frequency of the inversion events must be specified, along with the distribution of the eddy sizes. The frequency of the rearrangement events is accomplished by realizing that the random rearrangement events produce a random walk of a marker particle on a line. It can be shown that the diffusivity associated with a random walk is

$$D_T = \frac{1}{2} N \langle x^2 \rangle \tag{12.5}$$

where N is the frequency of the events and x^2 is the mean-square displacement associated with each event. For a classical discussion of the statistics of random walks see Chandrasekar[3]. In its association with turbulent transport, D_T can be interpreted as the turbulent diffusivity. The rearrangement frequency must thus be chosen so that the diffusivity associated with the random rearrangement process (the triplet map in the case considered here) is equal to the physical turbulent diffusivity.

Consider the motion of a particular particle. If an eddy of size l is to displace this particle, the "center" of the rearrangement event must lie within a distance $l/2$ of that particle. The frequency of such a rearrangement event is simply $N = \lambda l$, where λ is a rate parameter. The displacement of any particle by the triplet map will depend on the location of the particle within the eddy. The mean square displacement of all particles within the rearranged domain can be shown to be equal to

$$\langle x^2 \rangle = \frac{4}{27} l^2 \tag{12.6}$$

Plugging expression 12.6 into 12.5 and using $N = \lambda l$, we arrive at

$$D_t = \frac{2}{27} \lambda l^3 \tag{12.7}$$

In a general turbulent flow there will not be just one length scale, but a wide range of scales (eddies) ranging from the integral scale , L, down to the Kolmogorov scale, η. If $f(l)dl$ is the fraction of blocks (eddies) in the range $(l,\, l + dl)$ then the total diffusivity associated with an eddy of size l is

$$D_t = \frac{2}{27} \lambda l^3 f(l) dl \tag{12.8}$$

The total diffusivity associated with all eddies up to size l will then be given by

$$D_t(l) = \int_\eta^l \frac{2}{27} \lambda l^3 f(l) dl \tag{12.9}$$

To complete the description of the model it is necessary to determine the eddy size distribution, $f(l)$, and the rate parameter, λ under these more general conditions. This is accomplished by making use of some additional scalings for the diffusivity. Dimensional analysis yields

$$D_t(L) \sim \frac{L^2}{T_t} \tag{12.10}$$

T_t is a characteristic time scale. This time scale of the turbulence is

$$T_t \sim \frac{L}{u'} \tag{12.11}$$

giving

$$D_t \sim u' L = \nu Re_L \tag{12.12}$$

The l dependence of $D_t(l)$ in Eq. 12.9 is assumed to scale as the Reynolds number based on l:

$$\int_\eta^l l^3 f(l) dl \propto Re_l \sim \left(\frac{l}{\eta}\right)^{4/3} \tag{12.13}$$

or

$$\int l^3 f(l) dl \propto l^{4/3} \qquad \Rightarrow f(l) = cl^{-8/3} \tag{12.14}$$

Using the fact that the fraction of block sizes (eddies) between L and η is one, i.e,

$$\int_\eta^L f(l) dl = 1 \tag{12.15}$$

allows the determination of c in Eq. 12.14. Substituting Eq. 12.14 into 12.15 and solving for c gives

$$c = \frac{5}{3} \frac{1}{\eta^{-5/3} - L^{-5/3}} \tag{12.16}$$

or

$$f(l) = \frac{5}{3} \frac{l^{-8/3}}{\eta^{-5/3} - L^{-5/3}} \tag{12.17}$$

Eq. 12.17 specifies $f(l)$. The value of λ can now be determined by equating Eq. refdtint with 12.12:

$$\begin{aligned} \nu Re_L &= \int_\eta^L \frac{2}{27} \lambda l^3 \frac{l^{-8/3}}{\eta^{-5/3} - L^{-5/3}} dl \\ &= \frac{\lambda 5}{54} \frac{\text{Ł}^{4/3} - \eta^{4/3}}{\eta^{-5/3} - L^{-5/3}} \end{aligned} \tag{12.18}$$

Solving for λ:

$$\lambda = \frac{54}{5} \frac{\nu Re_L}{L^3} \frac{(L/\eta)^{5/3} - 1}{1 - (\eta/L)^{4/3}} \tag{12.19}$$

For high Reynolds number flow, $L \gg \eta$. The leading order approximation to Eq. 12.19 is

$$\lambda = \frac{54}{5} \frac{\nu Re_L}{L^3} \left(\frac{L}{\eta} \right)^{5/3} \tag{12.20}$$

Note that all order one constants that appear in the previous scaling relations are set equal to one. This completes the basic description of the model.

The model applications to date have strictly been as a one-dimensional description of the mixing process. This allows one to resolve *all* relevant length and time scales for flows of practical interest. The model was originally developed to investigate the qualitative mixing properties of turbulent flows. Some important qualities of this model stem from the fact that the basic physics of turbulent mixing are explicitly incorporated. Molecular diffusion is treated exactly, and turbulent convection is modeled in a physically reasonable way by the rearrangement event, or eddy turn-over events. The distinction between molecular diffusion and turbulent convection, even at the subgrid scales is crucial to the accurate description of the species field, especially when chemical reactions or nonlinear microphysics are involved. This distinction is not made in most turbulent mixing models. This model shares a property with some other commonly used mixing models such as coalescence-dispersion models, in that the hydrodynamic field is assumed to be specified in advance. In other words, the flow field structure is an input to the model, rather than a result of prediction. Even with this specification, the prediction concerning the mixing of a scalar variable transported in the turbulent flow field have been difficult to achieve with existing methods. However, the linear eddy model has the distinction in that the effects of molecular diffusion and turbulent transport are treated separately and explicitly.

Another important aspect of the linear eddy model is that in its implementation as described below, it contains no adjustable parameters. All order unity factors in the scaling relations have been set to one. (Although these can be adjusted to give the best quantitative fit to data.)

The linear eddy model has recently been generalized to treat a variety of flow configurations. Below we discuss how the model is implemented and illustrate its application in studying mixing in various flow configurations.

12.3 Implementation of Linear Eddy

The total number of computational elements along a line must be chosen to resolve the largest and smallest scales in the flow. We will assume that the domain under consideration is on the order of the integral scale, L. From Kolmogorov scaling the ratio of the largest to smallest length scales in the flow is approximately $L/\eta = (Re)^{3/4}$. If the Reynolds number is 10^4, then this ratio is 1000. By taking six computational elements to resolve the eddies at the Kolmogorov scale (by use of the triplet map), then at least 6000 elements are needed to resolve the scalar distribution. Let us chose an initial scalar field that is equal to 1 in half of the domain, and 0 in the other half of the domain. The rate of inversion events is given by λL where L is the domain size. For this example we will also assume periodic boundary conditions in this linear domain. With time discretized according to the fastest time scales of the flow (remember we want to explicitly account for turbulent convection by the rearrangement process for all scales), diffusion is implemented by regularly advancing Eq. 12.4 numerically.

To implement the triplet map, a location for inversion is randomly selected within the domain. The block size is also randomly chosen, but in such a way as to satisfy the probability distribution given by $f(l)$. Inversion takes place at intervals determined by λL. This process is repeated until a desired time has elapsed.

To satisfy the given distribution for l, the block size is chosen as follows: First we form the cumulative of l. The cumulative, denoted by $F(l)$, is the probability that a given block size (eddy) will have a linear dimension less than l. Obviously, $F(\eta) = 0$ since η is the smallest length scale in the flow, and $F(L) = 1$ since all eddies have

$l \leq L$. The cumulative is given by

$$F(l) = \int_\eta^l f(l)dl = \frac{5}{3}\frac{1}{\eta^{-5/3} - L^{-5/3}}\int_\eta^l l^{-8/3}dl$$
$$= \frac{1}{L^{-5/3} - \eta^{-5/3}}\left(l^{-5/3} - \eta^{-5/3}\right) \quad (12.21)$$

Solving for l:

$$l = \left[F(l)\left(L^{-5/3} - \eta^{-5/3}\right) + \eta^{-5/3}\right]^{-3/5} \quad (12.22)$$

Numerically this is implemented by selecting a random number uniformly distributed in $x \in [0, 1]$ and using this as a value for $F(l)$. l is then computed from Eq. 12.22. Choosing a large quantity of random numbers for $F(l)$ and using them to determine l will give the proper distribution for l.

The complete model is implemented as a Monte-Carlo simulation of many individual flow field realizations. The statistics are then computed by averaging over the different realizations. The accuracy of the statistics will of course increase as the number of realizations is increased.

12.4 Applications of Linear Eddy

The model has been successfully implemented in a number of different configurations including grid turbulence, planar mixing layers, and axisymmetric jets. By varying the spatial domain over which the inversion events occur and changing the model inputs (Reynolds number and diffusion coefficient) the mechanisms of mixing in the various configurations can be studied.

The first application of linear eddy was to study mixing in grid turbulence. The laboratory equivalent of this simulation has been provided by Warhaft [4] who used a single heated wire to provide a heat source. The downstream turbulent mixing and measurement of the temperature statistics were the objective of his experiments. In the linear eddy simulations, the initial conditions were arranged by setting the value of the scalar at one grid point to 100 (the point source), and zero else where. Many of the features of the downstream distribution were predicted well. An interesting observation of this experiment (and simulation) is that the peak rms scalar fluctuation did not appear along the centerline of the flow (with respect to the heat source). The lower fluctuations along the centerline where shown by Kerstein to be due to the enhanced mixing due to "eddy-diffusion" which is accounted for in the linear eddy model.

The prediction of the linear eddy model in the early stages of development were less successful. This was partly attributed to the discontinuous nature of the fluid motion, necessitated by the one-dimensional model. Never the less, the linear eddy formulation provides a physically sound description of turbulent mixing. Namely, molecular diffusion is accounted for explicitly, turbulent mixing is treated by rearrangements (triplet map), and by limiting application to one dimension, all relevant length and time scales can be resolved. Furthermore, the model contains no adjustable parameters. Order one coefficients that appear in the scaling relations are set equal to one. The purpose of this is at present to study the qualitative features of turbulent mixing and to provide a mechanistically sound description of turbulent mixing. In future applications, linear eddy type models will likely find application as a closure to Navier-Stokes based equations used in predicting turbulent mixing and reaction in engineering application. In such uses, adjustments of constants may be necessary to give correct quantitative description.

A second application of the linear eddy model was in studying shear layer mixing. Experimental observations show the thickness of a planar mixing layer (δ) grows linearly in the stream wise direction. The growth of the mixing layer is commonly characterized by a spreading angle, α, such that $\alpha = \tan^{-1}\delta/x$. The linear eddy calculation is performed along a transverse line who's spatial extent then grows linearly with time. (This spatial growth is an input to the model, not a prediction from the model - it is determined from the development of the hydrodynamic field.) Another important observations about shear layer mixing is that the entrainment ratio, E, is not equal to one. That is, the amount of fluid entrained into the shear layer from each of the two streams depends on the velocity difference between them. Within the linear eddy model, the boundaries of the flow in the transverse direction are specified such that $Y_1 + Y_2 = \delta$ and $Y_1/Y_2 = E$.

A distinctive character of mixing in shear layers is the development of a preferred mixed fluid concentration that is independent of the spatial location within the mixing layer (we have discussed this in lecture previously). The mechanisms of mixing by which this peak occurs was explained in the previous section. The linear eddy model has been successful in reproducing this character, and in providing a means of understanding the differences in the pdf concentrations that develop for different flows and similar flows with different transport coefficients.

The linear eddy model can also be extended in a straight forward manner to account for chemical reactions. In this case a number of scalar values corresponding to the different reacting species and their reaction products must be specified. For the reaction $A + B \rightarrow C$, the evolution of the scalars A, B, and, if desired, C. Within each linear eddy cell the species A will evolve governed by:

$$\frac{\partial A}{\partial t} = -kAB + \frac{\partial^2 A}{\partial x^2} \tag{11.23}$$

k is a reaction rate coefficient with units $(\frac{1}{t})$. Turbulent mixing is again accounted for by random rearrangements. An additional input in the reacting case is the Damköhler number, Da, a nondimensional number characterizing the ratio of the reaction frequency to the mixing frequency. The mixing frequency based on the large scale t_L is U/L, so $Da = kL/U$.

Subsequent to these first two applications, the model has been applied in a wide variety of applications including radial and axial descriptions of reacting and non-reacting jets [5, 6, 7], and homogeneous turbulence with and without mean scalar gradient [2, 8, 9]. The model has reproduced most of the known spectral scaling properties of the scalar field as well as reproduced statistical properties of the flow as measured from both experiments and direct numerical simulation.

Although the model has been mainly used as a tool to study physics of turbulent mixing,[1] it is now being used in works to make predictions and provide design guidelines for real engineering problems [7]. Projects include atmospheric mixing with application to droplet formation, emission production from combustion processes, in particular NO production in hydrogen-air combustion, and pollutant formation in turbulent plumes (smoke stacks). It is interesting to note that these applications all involve microphysics or chemical reactions where the rate of mixing is crucial to the determine the physics of chemistry of the process. Also in these applications, many of the unwanted byproducts (pollution) involve chemical reactions that are slower than the energy releasing reactions, and don't participate much in the overall energetics of the process. In cases where the details of the chemical rates are important, all existing mixing models fail to provide accurate predictions. This is one area in which the linear eddy model is expected to make some significant contributions.

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[1] This statement reveals a feature that sets the linear eddy model apart from all other mixing models. The fact that the model incorporates enough of the appropriate physics of the flow to be used as a tool to *study* physics, as opposed to give predictions is a unique feature and tremendous asset of this model.

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