

10 TURBULENT SCALAR MIXING PROCESSES

Consider a configuration that is initially composed of two distinct and segregated scalar constituents. These scalar constituents may be differentiated by different chemical composition, different temperatures, contain different trace elements, or any other scalar marker. The description and ideas of scalar mixing to be discussed in the next few sections are concerned with the process by which these different constituents mix at the *molecular* level to produce a homogeneous mixture and how we attempt to describe the statistical state of the scalar field throughout its development.

Accurately predicting the amount of mixing that will occur at the molecular level in a turbulent flow is important in many applications. For example, in combustion applications, chemical reactions can only take place when the fluid is mixed at the molecular level. In waste processing, constituents must interact at a molecular level. In atmospheric applications, the forces that drive the turbulence can be dramatically affected as cool and warm air mix at the molecular level. The mechanisms by which this mixing takes place, and approaches to modeling this process are the subject of this section. Unfortunately, accurately predicting the amount of molecular mixing that occurs in turbulent flows is a difficult task. Most models currently being used simply do not adequately treat this process. As a result, the reliability of predictions of turbulent flow that require a description of the molecular mixing process must be assessed on an individual basis. In the following we will discuss some of the physical mechanisms of turbulent mixing to illustrate the difficulties in accurately modeling this process.

10.1 Physical Mechanisms of Turbulent Mixing

As mentioned above, by turbulent mixing, we are referring to the process by which two separate constituents of the flow (different chemical species or scalar constituents with different values, i.e. temperature, etc.) eventually are brought together and interact at the molecular level. The governing equation that describes this process is the convection diffusion equation

$$\frac{\partial \phi_\alpha}{\partial t} + \frac{\partial u_j \phi_\alpha}{\partial x_j} = \frac{\partial}{\partial x_j} \left(D_\alpha \frac{\partial \phi_\alpha}{\partial x_j} \right) \quad (10.1)$$

In Eq. 10.1, ϕ_α represents scalar constituent α and D_α is the molecular diffusion coefficient of constituent α . In this equation, there is no summation over α (only j). Equation 10.1 describes the two distinctly different physical processes involved in

turbulent mixing: turbulent stirring (convection), and molecular diffusion. If chemical conversions are involved, a third process, the chemical reaction rate, involving yet another physical process must be accounted for. Chemical reaction, of course, can occur only when molecules interact at the molecular level. Below, we discuss these different processes.

10.1.1 Turbulent Convection

Consider a turbulent flow field containing two different constituents, initially unmixed. The action of this flow field on the scalar field is to distort and increase the surface area of the interface between the two constituents. As a result, the gradients of the scalar constituents will be increased and the scalar length scale will be decreased. As a result of this “stirring” process a complex structure of the scalar field evolves. Stirring has the effect of redistributing the scalar field throughout the flow field.

10.1.2 Molecular Diffusion

Mixing at the molecular level is a diffusion process. The turbulent stirring process described above acts only to redistribute or convect the scalar throughout the flow domain. Without molecular diffusion intermixing of separate constituents will not occur. Communication at the molecular level can only occur through the action of molecular diffusion. Our macroscopic view of molecular diffusion is a result of the random motion (Brownian motion) of fluid particles at the molecular level. This process is most effective in regions of high gradients and acts most effectively at the smallest scales of the flow. The enhanced mixing properties of turbulence are thus due to the action of turbulent stirring, which increases the effectiveness of molecular diffusion by increasing the scalar gradient and increasing the surface area over which the separate constituents can diffuse.

A little time spent thinking about these two processes will reveal the difficulties in modeling the mixing process. Namely, the actual diffusion is a small-scale process which depends critically on the small-scale structure of the scalar field. It cannot be parametrized easily in terms of the large scale features of the flow. As a result, a detailed description of the scalar field at the smallest length scales of the flow is, in principle, necessary if a reliable prediction of turbulent mixing is to be achieved.

10.2 Spectrum of the Scalar Field

Previously we discussed some properties of the turbulence energy spectrum. In particular, the energy spectrum can be roughly looked at consisting of a wave number regime characterizing the energy containing eddies, a universal equilibrium regime (the inertial range) described by the $k^{-5/3}$ law, and a dissipation range, below the Kolmogorov wave number. In discussing the spectrum of the scalar field, let us first define the scalar analogy to the Kolmogorov scale. Recall that the Kolmogorov scale is the smallest velocity length scale in the flow. Below this scale, viscosity effectively

damps out inhomogenieties in the flow. Analogously, there is a smallest scalar length of the flow which can be larger, smaller, or of the same scale as the Kolmogorov scale, depending on the relative magnitude of the kinematic viscosity to molecular diffusivity. This is parametrized by the Schmidt number, Sc , defined as $Sc \equiv \frac{\nu}{D}$, where ν is the kinematic viscosity of the fluid, and D is its molecular diffusivity. Below are some comments regarding the size of the scalar length scale.

For a given flow configuration (i.e., where the integral length and velocity scales, U and L , are specified), the size of the Kolmogorov scale will depend on the viscosity. (Recall that earlier we discussed that the viscosity does not determine the amount of dissipation in a flow, but the scale at which that dissipation occurs.) Similarly, the smallest scalar length scale will be determined by the molecular diffusivity, D . Intuitively, for $\nu \sim D$, it should be expected that the two scales (velocity and scalar) will be of the same order of magnitude. For $\nu > D$, velocity fluctuations will be damped out at scales larger than the scalar fluctuations so $\eta > l_s$ for $\nu > D$. Similarly for $\nu < D$ we can argue that $\eta < l_s$.

To arrive at an estimate for the scalar length scale consider the scalings implied by the diffusion equation, $l^2 \sim Dt$. First consider the case where $Sc > 1$ ($\nu > D$). Our region over which we are applying the scale analysis is the smallest scalar length scale, l_s . In this region, the scalar field is subject to the complete range of strain-rate fluctuations (since $l_s < \eta$) and the appropriate time scale is the Kolmogorov time scale, $\tau = (\nu/\epsilon)^{1/2}$. This gives $l_s^2 \sim D(\nu/\epsilon)^{1/2}$. In this regime of $Sc > 1$ the smallest scalar length scale is referred to as the Batchelor scale, l_B . Then using the expression for the Kolmogorov scale, $\eta = (\nu^3/\epsilon)^{1/4}$ gives

$$\frac{l_B}{\eta} \sim (D/\nu)^{1/2} = Sc^{-1/2} \quad (10.2)$$

Now for small $Sc < 1$, the above scaling will not be correct. In this case, the smallest scalar length scale will be greater than the Kolmogorov scale and may extend into the inertial subrange. The scalar length scale in this case is termed the Obukov-Corsin scale, l_C . Under this condition, the only parameters describing the scalar field will be the dissipation and the molecular diffusivity (recall that the viscosity does not play a role in the inertial subrange). The appropriate time scale in this case is $\tau = (D/\epsilon)^{1/2}$. Using this in our scale analysis results in $l_C \sim (D^3/\epsilon)^{1/4}$. Multiplying and dividing this equation by $\eta = (\nu^3/\epsilon)^{1/4}$ then gives:

$$\frac{l_C}{\eta} \sim (D/\nu)^{3/4} = Sc^{-3/4} \quad (10.3)$$

Besides providing extremely useful information on the structure of the scalar field (it has implications in numerical simulation, among many other things), this scale analysis illustrates the importance of carefully specifying the region over which the scale analysis is conducted and correctly defining the appropriate length, time, and velocity scales in that domain.

For most gases, the Schmidt number is approximately one, so the smallest scalar length scales are approximately equal to the Kolmogorov scale. For liquids, Sc can

be on the order of 10^3 or greater. In liquids then, the scales at which diffusion occurs is over an order of magnitude smaller than the smallest hydrodynamic scales. This illustrates an additional complication associated with predicting mixing and reaction in liquids. Namely, since the scales at which diffusion is occurring are so much smaller, the computational requirements to numerically resolve these scales, and thus accurately describe the mixing process are correspondingly increased.

10.2.1 Spectrum of the Scalar Field, $Sc > 1$

For Schmidt number greater than 1, the Batchelor scale will be smaller than the Kolmogorov scale. In the inertial subrange, the velocity and scalar spectrum will behave similarly. Beyond the Kolmogorov wave number cut-off, velocity fluctuations cease. Scalar fluctuations beyond this range will be reduced by the strain field, which below the Kolmogorov scale is $(\epsilon/\nu)^{1/2}$. This reduction occurs until the Batchelor scale is reached. This region of wavenumbers for $k_\eta > k > k_{l_B}$ is termed the *viscous-convective* subrange. (The velocity scales are in the viscous range, but the scalar scales are convective.)

For wave numbers $k > k_{l_B}$, the scalar fluctuations are effectively damped by molecular diffusion. In this region the scalar fluctuations are rapidly dissipated. This is called the *viscous-diffusive* subrange.

10.2.2 Spectrum of the Scalar Field, $Sc < 1$

For $Sc < 1$, we have $l_C > \eta$ or $k_{l_C} < k_\eta$. In this case, the diffusive cut-off for the scalar field will appear in the inertial subrange. This subrange is referred to as the *inertial-diffusive* subrange. (Velocity field inertial, scalar field diffusive.)

10.3 Mixing Configurations

In this section we wish to put some of the discussion above into a clearer perspective by discussing the mixing process in two specific configurations: the planar mixing layer, and mixing in a homogeneous turbulent flow.

10.3.1 The Planar Mixing Layer

The planar mixing layer is generated when two parallel flow streams of different velocity come into contact. In the laboratory, this flow is generated by allowing two streams to come into contact at the end of a splitter plate. This configuration is approximated in practice when any stream of fluid is injected into another. As a result of the shear generated at the interface of the two fluids, the flow becomes characterized by large scale vortex structures that grow and interact with each other as the flow develops in the streamwise direction. This has been an intensely studied flow both because it is relatively easy to study in the laboratory, as well as being a generic configuration for mixing between two streams. We discuss this flow here as

it illustrates quite clearly the mechanisms involved in the overall mixing process as outlined above in section 10.1. For this configuration, the mixing process involves: 1) The entrainment of fluid from the two free streams into the mixing region, and 2), mixing of the fluids between the two streams as they come into contact at the molecular level.

In the laboratory, a useful measure of molecular mixing has been to measure the amount of chemical product formed when the fluids in the two feed streams consist of initially nonpremixed chemically reacting species. If the rate of chemical reaction is fast compared to the local fluid time scales, and since reaction can only occur at the molecular level, the amount of product formed will give a direct indication of the extent of molecular mixing.

A series of laboratory studies conducted at Caltech has had as their focus the mechanisms of mixing in this configuration. In our previous discussions on turbulent mixing, we have used order of magnitude scaling arguments and shown that for “high” Reynolds number flows (those commonly encountered in practice) that turbulent diffusion effects dominated over molecular viscosity. However, experiments directed at studying the mixing in fluids of different molecular diffusivities (D), or flows with different Schmidt numbers ($Sc = \frac{\nu}{D}$), have shown important differences.

Comparison of the results of two separate experiments illustrate the unexpected behavior. In the first of these experiments, Mungal and Dimotakis [1] measured the chemical product formed in a fast reaction between hydrogen and fluorine. The hydrogen and fluorine were carried separately in dilute concentrations in the two streams. Nitrogen was used as the carrier gas and the Reynolds number of the flow was approximately 10^5 . Chemical reaction between the two occurred as they mixed at the molecular level within the shear layer.

In a similar experiment at about the same Reynolds number, Koochesfahani and Dimotakis [2] measured the amount of product formed for a fast chemical reaction in water. (Here and in the above paragraph “fast” means that the reaction rate is essentially instantaneous once the fluids have mixed at the molecular level). The only substantial difference between these two experiments was that the Schmidt number of water is approximately a factor of 1000 times greater than that of the nitrogen. If turbulent diffusion is the dominant factor in the mixing process, this variation in Schmidt number would be expected to have little effect on the total amount of product formation. However, it was found that the amount of mixing in the gas experiments was about a factor of two greater than in the water experiments. Furthermore, the concentration of the mixed fluid in the water experiments was uniform across the layer, even though the average concentration of the fluids from the two streams varied across the mixing layer.

10.3.2 The Broadwell–Breidenthal model for shear layer mixing.

A model developed by Broadwell and Breidenthal [3] provides an interpretation of these observations. As mentioned above, the path to molecular mixedness can be

characterized by two processes. In the first stage of the mixing process, fluid is entrained into the layer by a process characterized by the large scale features of the flow: an integral length scale L (the thickness of the layer), and a time scale, T_L , given by $L/(U_1 - U_2)$. T_L is the “eddy turnover” time, taken to be the time to reduce length scales to the Kolmogorov scale, η . Once the length scales have been reduced to this scale, molecular diffusion (the second step in the process) occurs in a time scale negligible compared to T_L (i.e., the time to reduce the length scale from L to η). In this scenario, the time to mix the fluid depends only on T_L and is independent of Reynolds number or Schmidt number.

During the mixing process, however, diffusion layers will form between the fluid from the two streams. The thickness of these layers will scale with the diffusion coefficients, and the strain rate. Dimensional analysis gives $w = (D/s)^{1/2}$, where s is the strain rate. Assuming that the strain rate is characterized by $1/T_L$, we have

$$w = (DT_L)^{1/2} \quad (10.4)$$

This result is also obtained from a scaling analysis of the diffusion equation. The time scale for this process is a large eddy turnover time, T_L . The contribution of the diffusion layers to the total mixed fluid concentration will then be given by the surface area of the layer per unit volume multiplied by the layer thickness. If the surface layer/unit volume is assumed to scale as $1/L$, the contribution of the diffusion layer to the total mixing is proportional to

$$P \sim (DT_L/L^2)^{1/2} = Pe^{-1/2} = Re^{-1/2} Sc^{-1/2} \quad (10.5)$$

where Pe is the Peclet number.

After a time $t + T_L$, all fluid that was entrained into the layer prior to t will have been reduced to the Kolmogorov scale. However, a certain amount of fluid entrained between t and $t + T_L$ may attain molecular mixing based on Eq. 10.5. The Broadwell-Breidenthal model can then be expressed as

$$\delta_p = \phi_d Re^{-1/2} Sc^{-1/2} + \phi_m \quad (10.6)$$

where δ_p is a normalized measure of the mixed fluid concentration, ϕ_m is a constant that describes the mixed fluid at the Kolmogorov scale, and $\phi_d Re^{-1/2} Sc^{-1/2}$ represents the contribution from the diffusion sheets.

A Reynolds number and Schmidt number dependency is apparent in Eq. 10.6 and explains the difference between the mixing experiments in water and air. In the experiments in air, the Schmidt number is about 1000 times smaller than that in water, resulting in the higher amounts of mixing observed. In the experiments of Koochesfahani and Dimotakis the condition $ReSc \rightarrow \infty$ is apparently met, and mixing is delayed until the entrained fluid reaches the Kolmogorov scale and is then subject to uniform straining.

The lack of lateral variation in the pdfs of the experiments of Koochesfahani (see notes from lecture) can also be explained by the arguments given above. For a fluid

with a high Schmidt number, the amount of mixing in the diffusion sheets will be negligible ($ScRe \rightarrow \infty$). Under these conditions, significant mixing only takes place at beyond the Kolmogorov scale. Because there is a delay of $t = T_L$ in mixing once the fluid is entrained into the layer, it has a chance to become distributed, which can account for the more uniform peak concentration across the layer. Under conditions of low Schmidt number, measurable diffusion may take place in the diffusion layers, allowing for lateral variation in the pdf's.

The type of behavior we have described here is not consistent with simple gradient transport, and therefore will not be reproduced by turbulence models based on gradient diffusion. Mixing layer type configurations appear in many applications. Any time turbulent mixing takes place between two initially segregated fluids, or heat (or any other scalar) mixes with the surrounding environment, mechanisms as discussed here can influence the rate of molecular mixing. As we have seen earlier, even boundary layers show regimes where entrainment and mixing occur as described above. Later we will discuss a new model that has been developed to try to describe and provide explanations for the various anomalous features observed in mixing experiments. The key feature of this model is to make an explicit distinction between the effects of molecular diffusion and turbulent transport.

10.3.3 Mixing in Statistically Steady Homogeneous Turbulence

Another configuration in which the mixing process has been extensively studied is the decay of scalar fluctuations in a statistically steady, homogeneous turbulent flow. The initial scalar field consists of initially segregated “marked” and “unmarked” fluid. As mixing proceeds, the scalar concentration throughout the domain evolves to a constant value at the mixed fluid concentration. Of interest here are the statistical details of the scalar field during its evolution from the unmixed to mixed state.

This configuration of a stationary homogeneous turbulent flow is not easy to set up in the laboratory. As a result most of the data available for mixing in this configuration has been obtained from DNS [4, 5]. In interpreting these data, it is important to keep in mind that the DNS data is limited to flows with relatively low Reynolds numbers and Schmidt numbers of order unity. This is a constraint resulting from finite computational resources. None-the-less, the results have proven very useful in helping understand the mixing process and in stimulating further studies. Extrapolation of these results to high high Reynolds number flows must be made with caution however. Some implications will be discussed later.

Results of these simulations have provided interesting information for both theoreticians and modelers. Details of the evolution are, of course, important as it is the goal of model development efforts to incorporate as much of the known physics and behavior as possible into models that are intended to describe the mixing.

The simulations of Eswaran and Pope focused on two main issues: the effects of the initial scalar length scale on the evolution of the scalar statistics, and the functional form of the single-point scalar pdf of the scalar field during its evolution.

As discussed earlier, the single point pdf provides a complete statistical description of the one-point scalar statistics. It was observed that the scalar field evolved from an initially bimodal distribution (representing the two initial unmixed concentration) to a form approximating a Gaussian distribution centered on the mean mixture fraction. The asymptotic form of the pdf is important from a modeling point of view as this behavior should be reproduced by models expecting to provide accurate predictions of this process.

Although a large amount of data has been produced for this specific configuration, there is some evidence that the results may not be easily extendable to mixing in high-Reynolds number flows. [6, 7]. Discussion of this issue is deferred until later.

References

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