Numerical simulation of low Prandtl number turbulent mixing

By C. Gibson¹, M. Rogers², J. Chasnov³ AND J. Petresky¹

Numerical simulations of turbulent mixing of strongly diffusive scalar fields were carried out with and without subgrid-scale modeling of the small-scale strain field. For low-Reynolds-number flows, when the rate-of-strain field (determined primarily by the small scales) is fully resolved, the scalar microstructure was found to collapse under Batchelor (1959) rate-of-strain scaling even for small Prandtl numbers, in agreement with Kerr (1990). For high-Reynolds-number flows, when small-scale straining is modeled with a subgrid-scale model, the scalar microstructure follows the Batchelor, Howells and Townsend (1959) prediction that the small-scale rate-of-strain is irrelevant.

1. Introduction

An important problem of turbulent mixing is to determine the mechanisms of small-scale mixing for the case of strongly diffusive scalar properties; that is, properties like temperature with Prandtl number \( Pr = \nu/D < 1 \), where \( D \) is the molecular diffusivity of the scalar \( \theta \) and \( \nu \) is the kinematic viscosity of the fluid. Recent contributions that review the theoretical and experimental issues can be found in Gibson, Ashurst and Kerstein (1988) and Kerr (1990).

Oboukhov (1949) and Corrsin (1951) independently inferred an inertial subrange for the scalar spectrum

\[
\Gamma = \beta_{si} \chi e^{-1/3} k^{-5/3}; \quad L_{c}^{-1} < k < L_{c}^{-1}; \quad L_{c} = (D^3/\epsilon)^{1/4}
\]

(1)

which terminates at the Oboukhov-Corrsin length scale \( L_{c} \). Here \( \beta_{si} \) is a universal constant, \( \chi \) is the dissipation rate of scalar variance, \( \epsilon \) is the dissipation rate of turbulent kinetic energy, \( k \) is the wavenumber and \( L_{O} \) is the energy, or Oboukhov, length scale of the turbulence. The spectral form in (1) was inferred by dimensional analysis without reference to any specific physical mechanisms or mathematical models, and is therefore analogous to the velocity inertial subrange

\[
\Phi = \alpha \epsilon^{2/3} k^{-5/3}; \quad L_{O}^{-1} < k < L_{K}^{-1}; \quad L_{K} = (\nu^3/\epsilon)^{1/4}
\]

(2)

that follows by dimensional analysis from the Kolmogorov (1941) universal similarity hypotheses (which also does not assume a particular mechanism or model for

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the flow field) where $\Phi$ is the energy spectrum, $\alpha$ is a universal constant, and $L_K$ is the Kolmogorov length scale.

The first specific physical model for scalar mixing by turbulence was the wave crest compression mechanism of Batchelor (1959) for the case of weakly diffusive scalars $\theta$ like salt concentration in water, with $Pr \gg 1$. The model is illustrated in figure 1.

Batchelor showed that Fourier elements of the scalar field with wavenumbers $k > L_K^{-1}$ would align with the compressive axis of the rate-of-strain tensor $e_{ij} = \frac{1}{2} (\partial u_i / \partial x_j + \partial u_j / \partial x_i)$ and would be rapidly convected by strain-mixing, not turbulent mixing, to the Batchelor length scale $L_B \equiv (D/\gamma)^{1/2}$, where $\gamma$ is the rate of strain $\gamma = (e/\nu)^{1/2}$. The velocity field acting on scales smaller than $L_K$ consists of locally uniform staining so wave crests would simply be convected together, as shown in figure 1. By this very plausible physical model a viscous-convective subrange was derived for the range of scales smaller than the viscous cutoff Kolmogorov scale but larger than the diffusive cutoff Batchelor scale,

$$\Gamma = \beta_{vc} \chi \gamma^{-1} k^{-1}; \quad L_B^{-1} < k < L_K^{-1}, \quad (3)$$

where $\beta_{vc}$ is another universal constant. Equation (3) can also be derived by dimensional analysis, but the Batchelor (1959) mathematical analysis permits a bound to be placed on the value of the universal constant

$$\sqrt{3} < \beta_{vc} < 2\sqrt{3} \quad (4)$$

as shown by Gibson (1968b), where the form of the spectrum derived by Batchelor (1959) is

$$\Gamma = \beta_{vc} \chi \gamma^{-1} k^{-1} \exp(-\beta_{vc} k^2 D/\gamma); \quad k > L_K^{-1} \quad (5)$$

**Figure 1.** Batchelor (1959) wave crest compression model for $Pr \gg 1$. A scalar Fourier element $\theta$ smaller than $L_K$ is compressed to the Batchelor scale $L_B$, without decay, in time $\ln(D/\nu)^{1/2}/\gamma$, by uniform straining $\gamma$. At $L_B$ its amplitude begins to decrease by molecular diffusion. This model fails for $Pr \ll 1$. 
For $Pr \gg 1$. The spectral form given by (5) has been tested experimentally many times, starting with Gibson and Schwarz (1963), and has generally been verified with respect to the form in (5) and the constant in (4). Gargett (1985) finds a large departure from (4), by a factor of 4, in a Fjord, but Gibson (1986) shows the departure may be the result of averaging together fossil turbulence and active turbulence patches without accounting for the extreme intermittency of viscous and scalar dissipation rates usually observed in such stratified flows.

For the case of $Pr \ll 1$, however, the Batchelor wave crest compression mechanism fails because the separation of wave crests for the smallest Fourier elements used to represent the scalar field will be larger than the size of the regions of uniform strain, which should be of order $L_K$. Consequently, Batchelor, Howells and Townsend (1959) proposed that the rate-of-strain should become irrelevant for turbulent mixing of such strongly diffusive scalars. Based on this hypothesis, they derive an inertial-diffusive cutoff spectrum for $Pr \ll 1$ beginning at the Oboukhov-Corrsin scale $L_C \equiv (D^3/\varepsilon)^{1/4}$

$$\Gamma = \frac{\alpha}{3} \chi D^{-3} \epsilon^{2/3} k^{-17/3}; \quad k > L_C^{-1}$$

where $\alpha$ is the inertial subrange constant of the turbulent velocity spectrum in (2).

From an analysis of the velocities of isoscalar surfaces and zero-gradient points, Gibson (1968a) suggested that other physical mechanisms besides the wave crest compression mechanism of figure 1 exist by which the smallest scalar fluctuations for $Pr \ll 1$, or indeed arbitrary $Pr$, could be mixed to smaller scale by the rate-of-strain tensor $e_{ij}$, and proposed that probability laws describing the smallest scale features of scalar fields with arbitrary $Pr$ should become universally similar under "Batchelor" coordinate normalization with length $L_B$, time $T_B \equiv \gamma^{-1}$ and scalar $S_B \equiv (\chi/\gamma)^{1/2}$ scaling of space, time and scalar, respectively. For $Pr \ll 1$, this shifts the beginning of the inertial-diffusive cutoff of (6) to $L_B$ rather than $L_C$, and results in an intermediate strain-rate-diffusive $k^{-3}$ subrange

$$\Gamma = \beta_{sr} \chi D^{-1} k^{-3}; \quad L_B^{-1} < k < L_C^{-1}$$

prior to the final inertial-diffusive cutoff, presumably with the form of (6), but with a different constant, an explicit Prandtl number dependence

$$\Gamma = \beta_{id} Pr^{-2/3} \chi D^{-3} \epsilon^{2/3} k^{-17/3}; \quad L_K^{-1} < k < L_B^{-1},$$

and an exponential cutoff at the Kolmogorov scale $L_K$. Gibson (1968a) suggested that turbulence produces extremum points, hot spots and cold spots for temperature, by distorting isothermal surfaces until they become diffusively unstable and split up, at scales no smaller than $L_C$, to form multiply connected surfaces. The extremum points diffuse to positions of symmetry and then tend to be convected as fluid particles so they can be compressed and stretched as fluid particles by the local strain field, with a stretching-diffusion equilibrium length scale $L_B$ for all $Pr$. Other topological features of the scalar field exhibit similar sensitivity to the
FIGURE 2. Interaction and alignment of the local rate-of-strain tensor $\bar{e}$ with topological features of scalar fields mixed by turbulence that have minimal or zero gradient, according to the Gibson (1968a) strain-mixing model. Extrema and saddle points have zero gradient, and are connected by the checkered minimal gradient line, which tends to be aligned with the stretching axes of the local $\bar{e}$, independent of the Prandtl number of the scalar field.

strain-field history. For example, the lines of minimal gradient that must connect a set of extrema and saddle points (resulting from secondary splitting of an original extremum produced by turbulence) tend to be stretched out as material lines. This is illustrated schematically in figure 2. The steepest scalar gradients occur in the vicinity of the extremum points and the minimal gradient lines are aligned with the compression axes of the strain-rate tensor. Using numerical simulations of two-dimensional turbulence, Gibson, Ashurst and Kerstein (1988) confirmed that this was the case, and suggested a positive feedback mechanism based on the expression

$$\vec{v}_\theta = \vec{v} - \vec{v}_D = \vec{v} - D \left( \frac{\nabla^2 \theta}{|\nabla \theta|} \right) \vec{g}; \quad \vec{g} = \frac{\nabla \theta}{|\nabla \theta|}$$

for the velocity of isoscalar surfaces $\vec{v}_\theta$ in terms of the fluid velocity $\vec{v}$ and the diffusive velocity $\vec{v}_D$ derived in Gibson (1968a). As shown in (9), the convective velocity of the fluid will dominate the motion of $\theta$ surfaces when the diffusive velocity is small, i.e. when gradient magnitudes $|\nabla \theta|$ are large and $\nabla^2 \theta$ values are small. But gradient magnitudes $|\nabla \theta|$ will be increased by such convection of isoscalar surfaces and this results in a positive feedback mechanism of mixing.

Based on the rate-of-strain mixing mechanisms of figure 2, Gibson (1968b) proposed the universal similarity hypotheses in table 1. According to these hypotheses, the $n$-joint probability laws $F_{\theta n}$ describing turbulent mixing of scalars $\theta$ at $n$ points separated by vectors $\vec{y}_k$, where $k = 1, \ldots, n$, will become universally similar in normalized Batchelor, Corrsin and Kolmogorov spaces (see table 2), depending on the Prandtl number and length scale $\gamma_k$ ranges of the $k^{th}$ separation vector. The
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Table 1. Universal similarity hypotheses of turbulent mixing

<table>
<thead>
<tr>
<th>Hypothesis</th>
<th>Length range</th>
<th>Prandtl number, ( Pr )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1a. ( F_{\theta n}(\chi, \gamma, D, y_k) )</td>
<td>( y_k &lt; L_B ) ( y_k &lt; L_K ) ( y_k &lt; L_C )</td>
<td>all values ( \gg 1 ) ( \ll 1 )</td>
</tr>
<tr>
<td>1b. ( F_{\theta n}(\chi, \epsilon, y_k) )</td>
<td>( L_K &lt; y_k &lt; L_O )</td>
<td>( \gg 1 )</td>
</tr>
<tr>
<td>2a. ( F_{\theta n}(\chi, \epsilon, D, y_k) )</td>
<td>( L_B &lt; y_k &lt; L_O )</td>
<td>( \ll 1 )</td>
</tr>
<tr>
<td>2b. ( F_{\theta n}(\chi, \epsilon, y_k) )</td>
<td>( L_B &lt; y_k &lt; L_C )</td>
<td>( \ll 1 )</td>
</tr>
<tr>
<td>3a. ( F_{\theta n}(\chi, \epsilon, \nu, y_k) )</td>
<td>( L_B &lt; y_k &lt; L_O )</td>
<td>( \gg 1 )</td>
</tr>
<tr>
<td>3b. ( F_{\theta n}(\chi, \gamma, y_k) )</td>
<td>( L_B &lt; y_k &lt; L_K )</td>
<td>( \gg 1 )</td>
</tr>
</tbody>
</table>

Evidence supporting the Gibson (1968a,b) theory has been gradually accumulating from low \( Pr \) mixing experiments such as Clay (1973), and numerical mixing experiments of Kerr (1985) and Kerr (1990). However, numerical mixing experiments of Chasnov, Canuto and Rogallo (1988) and Chasnov (1990), using a subgrid-scale model for the small scales of the velocity field, give strong support to the Batchelor, Howells and Townsend (1959) theory and expression (6) in the far-inertial-diffusive subrange, \( k \gg L_C^{-1} \). The purpose of this paper is to attempt to clarify possible reasons for the discrepancies between these apparently contradictory results.
2. Numerical experiments

Numerical simulations of turbulent mixing are constrained to relatively small Reynolds numbers by computer speed and memory limitations. The larger the number of mesh points in the grid, the larger the Reynolds number of the simulation but the higher the cost of the calculation in time and money. Clearly it would be advantageous if approximations could be made for the smaller-scale features of turbulence and mixing by means of subgrid-scale modeling, so that the larger-scale features characteristic of high-Reynolds-number turbulence could be explored. The results shown below indicate that if turbulent mixing at low Prandtl number is dominated by direct interactions of the velocity strain rate and scalar fields, then the subgrid-scale model does not capture this effect, at least over a wide range of Pr.

All simulations examined here are of three-dimensional incompressible homogeneous isotropic turbulence. Several low-Prandtl-number passive scalar quantities were mixed simultaneously by each of the velocity fields simulated. The cases considered here fall into three classes. The first employs both forcing of the large scales and a subgrid-scale model to obtain as wide an inertial subrange as possible and statistically stationary turbulence. The second type uses only a subgrid-scale model, thereby permitting the simulation of high-Reynolds-number decaying turbulence. The third class maintains the forcing of the large scales to obtain a statistically stationary flow but fully resolves the small-scale motions, thereby significantly reducing the flow Reynolds number. Scalar fields both with and without mean scalar gradients were considered. Because of the low Prandtl numbers considered, the scalar fields were well-resolved on the computational mesh (i.e. no subgrid-scale model was required for the scalar fields in any of the simulations). The simulation results were evaluated in terms of the form of the velocity and scalar variance spectra, mixed skewness statistics, and direct visual inspection of the three-dimensional computed fields. Spectra were normalized with the length, time and scalar scales listed in table 2.

Energy spectra $(k^{5/3} \Phi)_K$ versus $(k)_K$ for the three types of numerical simulations are shown in figure 3, where $K$ subscripts indicate normalization with Kolmogorov length $L_K$ and time $T_K$ from table 2. All have the same 1.5 decades of wavenumber range corresponding to the $64^3$ mesh used in the calculations. The direct numerical simulation has only a short inertial subrange (part of the flat portion being associated with the forced modes) but agrees well with the universal spectral form of laboratory and field experiments. The forced subgrid-scale simulation is reasonably flat over all wavenumbers (i.e. contains only inertial subrange) whereas the unforced subgrid-scale simulation becomes flat only at the largest wavenumbers.

3. Direct numerical simulations

The direct numerical simulations (no subgrid-scale model) were made for a flow with viscosity $\nu = 0.01$ on a $64^3$ mesh with $\Delta x = 2\pi/64 = 0.0982$ (note all dimensional quantities given in this paper are in arbitrary but consistent units). The scalar fields all evolved in the presence of a mean scalar gradient of magnitude
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Figure 3. Kolmogorov normalized energy spectra for numerical simulations, multiplied by $k^{5/3}$. —— forced subgrid-scale model, - - - - unforced subgrid-scale model, ——— direct numerical simulation.

$\partial \overline{T}/\partial z = 1.0$. The field examined here has evolved for about 1.5 eddy turnover times and has $\epsilon = 0.0595$ and $L_K = 0.0640$. Four scalars were simultaneously mixed, with $Pr$ values of 0.769, 0.434, 0.172, and 0.118. Spectra multiplied by $k^2$ and normalized by Batchelor scales of table 2 are shown in figure 4 for the various $Pr$ values. Such spectra must have integrals equal to $1/2$ from the Batchelor normalization, as shown by Gibson (1968b). It is readily apparent that the spectra collapse under this scaling.

The longitudinal mixed skewness parameter $\Sigma$, with components

$$\Sigma_u \equiv \frac{\frac{\partial u}{\partial x} (\frac{\partial \theta}{\partial x})^2}{\left(\frac{\partial u}{\partial x}\right)^2 \left(\frac{\partial \theta}{\partial x}\right)^2} , \quad \Sigma_v \equiv \frac{\frac{\partial v}{\partial y} (\frac{\partial \theta}{\partial y})^2}{\left(\frac{\partial v}{\partial y}\right)^2 \left(\frac{\partial \theta}{\partial y}\right)^2} , \quad \Sigma_w \equiv \frac{\frac{\partial w}{\partial z} (\frac{\partial \theta}{\partial z})^2}{\left(\frac{\partial w}{\partial z}\right)^2 \left(\frac{\partial \theta}{\partial z}\right)^2}$$

(10)

are sensitive indicators of the role of rate-of-strain in turbulent mixing ($u$, $v$ and $w$ are velocity components in the $x$, $y$ and $z$ directions, respectively). Note that $\Sigma_w$ may be different from $\Sigma_u$ and $\Sigma_v$ because of the presence of the mean scalar gradient in this direction. Clearly $\Sigma$ should approach zero as $Pr$ approaches zero if the rate-of-strain becomes irrelevant to the mixing, but if Hypothesis 1a is correct, $\Sigma$ should be approximately independent of $Pr$ and negative because compressive negative straining should enhance scalar gradient magnitudes. Values of $\Sigma$ for the
Figure 4. Batchelor-scaled scalar dissipation spectra from direct numerical simulation of low Pr mixing. —— Pr = 0.769, ---- Pr = 0.434, ------ Pr = 0.172, ---- Pr = 0.118. Convergence of spectra for low Pr values is consistent with Hypothesis 1a of Table 1.

Table 3. Σ values for the direct numerical turbulence simulation

<table>
<thead>
<tr>
<th>Pr</th>
<th>Σu</th>
<th>Σv</th>
<th>Σw</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.769</td>
<td>-0.473</td>
<td>-0.329</td>
<td>-0.518</td>
</tr>
<tr>
<td>0.434</td>
<td>-0.426</td>
<td>-0.309</td>
<td>-0.505</td>
</tr>
<tr>
<td>0.172</td>
<td>-0.333</td>
<td>-0.262</td>
<td>-0.493</td>
</tr>
<tr>
<td>0.118</td>
<td>-0.277</td>
<td>-0.246</td>
<td>-0.478</td>
</tr>
</tbody>
</table>

All the values of Σ in Table 3 are negative and significantly nonzero. Differences in magnitude and the tendency to decrease somewhat as Pr decreases may be the result of the small mesh size. Kerr (1985) used a larger mesh of 128³, and reports no such trend when the Peclet number Peλ (here based on the Taylor-microscale Reynolds number) is greater than about 10. For Peλ < 10 he observes a decrease in Σ. The value of −Σ is proportional to the integral of \((k^4\Gamma)_B\),

\[
Σ = -\frac{4\sqrt{15}}{5} \int_0^\infty (k^4\Gamma)_B d(k)_B ,
\] (11)
as shown by Wyngaard (1971). Thus the collapse shown in figure 4 implies that $\Sigma$ should be nearly the same for all four Prandtl numbers. However, for the spectra in figure 4, the value of $\Sigma$ is primarily determined by the behavior of $(k^4 \bar{\Gamma})_B$ over the wavenumber range $0.5 < (k)_B < 1.5$ with $(k^4 \bar{\Gamma})_B$ peaking at about $(k)_B = 0.8$. The value of $\Sigma$ is thus very sensitive to the details of the spectra for these wavenumbers. The smaller values of $\Sigma$ for the lower $Pr$ cases in table 3 are a result of the slight drop in the spectra (figure 4) for these cases near $(k)_B = 0.8$.

4. Simulations employing a subgrid-scale model

The subgrid-scale model of Chasnov (1990) was used to generate high-Reynolds-number flow fields with an inertial subrange. Use of such a model, however, implies that the actual small-scale behavior (including that of the strain field) is not resolved. The subgrid-scale model seeks to simulate the case where $\nu = 0$. In reality the large scales feel an “effective” viscosity which is fairly constant away from the cutoff wavenumber. Here this effective viscosity is used to estimate the Prandtl number. Simulations were run with and without forcing of the large-scale motions and with and without a mean scalar gradient (again $\bar{\partial \bar{T}}/\bar{\partial z} = 1$ for mean gradient cases). The energy spectra for both the forced and unforced cases are shown in figure 3. 

**FIGURE 5.** Batchelor-normalized scalar dissipation spectra of unforced subgrid-scale modeled simulations. Estimated Prandtl numbers are $Pr = 0.045$, $Pr = 0.019$, $Pr = 0.007$, $Pr = 0.003$. The upper and lower straight solid lines represent $k^{-3}$ and $k^{-17/3}$ behavior of $\Gamma$, respectively.
Table 4. Σ values for the unforced subgrid-scale turbulence simulation

<table>
<thead>
<tr>
<th>Estimated Pr</th>
<th>Σ_u</th>
<th>Σ_v</th>
<th>Σ_w</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.045</td>
<td>-0.428</td>
<td>-0.383</td>
<td>-0.448</td>
</tr>
<tr>
<td>0.019</td>
<td>-0.279</td>
<td>-0.271</td>
<td>-0.247</td>
</tr>
<tr>
<td>0.007</td>
<td>-0.121</td>
<td>-0.107</td>
<td>-0.116</td>
</tr>
<tr>
<td>0.003</td>
<td>-0.046</td>
<td>-0.052</td>
<td>-0.046</td>
</tr>
</tbody>
</table>

The Batchelor-scaled scalar dissipation spectra for scalars of four different molecular diffusivities are shown in figure 5 for the unforced case in the absence of a mean scalar gradient. It is clear that they do not collapse. Spectra for the smaller Pr values in figure 5 approach the \(-17/3\) subrange of (6), both in slope and absolute value. The largest Pr value approaches the \(-3\) subrange of (7), and as will be shown below, it approaches the universal Batchelor diffusive cutoff form of figure 4.

The behavior of the lower Pr cases in figure 5 is limited by the computational box size. Visual examination of the Pr = 0.003 scalar field shows that essentially only one large structure is in the computational domain and the results are therefore clearly affected by the imposed periodicity. The spectra have significant contributions from a few low wavenumbers, then drop very rapidly (faster than \(k^{-17/3}\)) before finally decaying at the expected \(k^{-17/3}\) rate. Effectively, the computation is setting up a large structure which provides a mean scalar gradient. A limited range of wavenumbers (about half those in the computation) can then respond to this gradient. Because it is not feasible to dramatically increase the computational domain size, another means of increasing the range of useful wavenumbers is needed. By explicitly imposing a uniform mean scalar gradient the computation does not have to form its own large-scale structures and the entire range of computational wavenumbers becomes useful for the study of the problem considered here.

Table 4 lists Σ values for this flow. As the Pr values of the scalars approach zero in table 4, the correlations Σ_{u,v,w} between compressive strain and the scalar gradient also approach zero. However, close examination of the microstructure of the scalar fields revealed that only the field with the largest Pr value of 0.045 possessed significant numbers of zero-gradient points. The conditions for the strain-mixing mechanism of figure 2 were thus not met. The effective Peclet number (product of Reynolds and Prandtl numbers) of the simulated turbulence for smaller Pr values was too small for any extrema to be produced. For the spectra of the lower Pr cases in figure 5 the dominant contribution to Σ comes from \((k)_B = 0.3\) with virtually no contribution from wavenumbers \((k)_B > 0.6\). The value of Σ for the Pr = 0.045 case is similar to the values in the direct numerical simulations given in table 3 and the \((k)_B\) wavenumber range which contributes to Σ is also similar to that observed in the direct numerical simulations.

Figure 6 shows the Corrsin/Batchelor-scaled spectra (same scaling for the quantity \(k^3\)) plotted against the Corrsin-scaled wavenumber for several forced cases
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FIGURE 6. Corrsin/Batchelor-normalized $k^3 \Gamma$ spectra for forced turbulence with a subgrid-scale model. Estimated Prandtl numbers —— $Pr = 0.069$, --- $Pr = 0.039$, —— $Pr = 0.015$, —— $Pr = 0.011$. curves are results from a 128$^3$ simulation for $Pr = 0.043$ and $Pr = 0.0251$. The left and right straight solid lines represent $k^{-5/3}$ and $k^{-17/3}$ behavior of $\Gamma$, respectively.

with an explicitly imposed mean scalar gradient. Time-averaged spectra (permitted by statistical stationarity and done to smooth the curves) from a 64$^3$ simulation with four passive scalars are shown along with results for two scalars from a single time of a (different velocity field) 128$^3$ simulation. All the curves exhibit a good collapse onto an apparently "universal" spectrum when the mean scalar gradient is included in the scalar dissipation used for the normalization (note that for the high Peclet number fields the dissipation due to the mean is insignificant compared to that of the fluctuating field). This collapse is in agreement with the predictions of Batchelor, Howells & Townsend (1959) but may be an artifact of the subgrid-scale model. There is a fairly wide transition region between the $k^{-5/3}$ and $k^{-17/3}$ subranges, the latter occurring for $(k)_C > 2.5$.

When the "universal" subgrid-scale spectrum shown in figure 6 is fitted to a smooth curve (consisting of $k^{-5/3}$ and $k^{-17/3}$ subranges and the fitted transition between them) $\Sigma$ can be calculated from (11). The existence of a "universal" spectrum in these coordinates implies that $\Sigma$ decays like $Pr^{1/2}$ for small $Pr$. Use of the fitted curve yielded $\Sigma \approx -3Pr^{1/2}$ (the exact value of the coefficient being somewhat dependent on wavenumber cutoffs chosen for the different subranges), with the dominant contribution coming from the $k^{-17/3}$ subrange, closely followed by that from the transition region. Contribution to $\Sigma$ from the $k^{-5/3}$ range was
negligible. $\Sigma$ values calculated directly from the computed flowfields may not agree exactly with this formula due to the more limited range of wavenumbers captured by any one computation and departures from the fitted curve.

5. Comparison of direct and subgrid-scale modeled simulations

It is interesting to compare the largest $Pr$ value unforced subgrid-scale simulation (with $Pr = 0.045$) to the direct numerical simulations of §3, since this is still a factor of 2.6 smaller than the smallest direct numerical simulation $Pr$ value. Figure 7 shows a comparison of the scalar dissipation spectra. The Batchelor-normalized subgrid-scale spectrum is in excellent agreement with the results from the direct numerical simulations, collapsing onto a single “universal” curve for $(k)B > 0.3$. The larger effective Reynolds number of the subgrid-scale modeled flow seems to have led to the development of a small region of strain-rate-diffusive $k^{-3}$ subrange, as shown also in figure 5. The subgrid-scale simulation suggests that with still higher Reynolds number simulations, a strain-rate-diffusive $k^{-3}$ subrange might be found. The universal constant $\beta_{sr}(k)$ indicated by figures 5 and 7 is about 0.23 (note $(k^2 \Gamma)_B = \beta_{sr}(k)_B^{-1}$ in the $k^{-3}$ subrange and therefore $\beta_{sr}$ equals the value of the $k^{-3}$ line at $(k)B = 1$). It is also interesting to note the rather strong departures between the Batchelor (5) viscous-diffusive behavior for $Pr \gg 1$ and the numerically computed behavior for $Pr = 0.1-0.5$.

6. Conclusions

Scalar spectra resulting from turbulent mixing by a high-Reynolds-number velocity field generated with a subgrid-scale model collapse under Corrsin scaling as predicted by Batchelor, Howells & Townsend (1959). The “universal” spectrum in this case exhibits a wide transition (nearly a decade) between the $k^{-5/3}$ and $k^{-17/3}$ subranges. The corresponding spectra obtained in low-Reynolds-number direct numerical simulations collapse under the Batchelor scaling of Gibson (1968b). Two possible explanations for this discrepancy exist. The first is that virtually all the scales of the direct numerical simulation are affected by viscosity and are therefore not in the inertial-diffusive subrange but rather in a viscous-diffusive region. In this case the scaling put forth by Batchelor, Howells & Townsend (1959) would be expected to break down. The second is that the subgrid-scale model is not accurate enough to capture the physics of the interaction between the predominantly subgrid-scale strain-rate field and the scalar. It is interesting to note that for moderate Peclet numbers (as opposed to the usually smaller values generated by the extremely low Prandtl numbers considered here) the subgrid-scale simulations produce spectra that collapse with the direct numerical simulation results and show the beginnings of a strain-rate-diffusive $k^{-3}$ subrange in agreement with Gibson (1968b). This case is also the only one of those shown in figure 5 that contains a significant number of scalar extremum points required for the strain-mixing mechanism to be effective.

Future plans include extension to higher Reynolds/Peclet numbers by using 128$^3$ simulations and direct examination of the direct numerical simulation scalar fields.
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Figure 7. Comparison of scalar dissipation spectra from the subgrid-scale simulation with estimated $Pr = 0.045$ (also shown in figure 5), with direct numerical simulation results of figure 4. --- subgrid-scale model simulation with estimated $Pr = 0.045$, ........ direct numerical simulation results for four values of $Pr$. The straight solid line is an extended version of the same $k^{-3}$ line shown in figure 5. The curved solid line represents the Batchelor (1959) spectrum (valid for $Pr \gg 1$) given by (5) with $\beta_{vc} = 2.0$.

in an effort to observe the mechanisms suggested by Gibson (1968a). Collapse of scalar spectra from direct numerical simulations on a $128^3$ mesh with the $64^3$ results presented here would seem to indicate that the scaling proposed by Gibson (1968b) may be correct, whereas a tendency towards the “universal” spectrum of figure 6 would favor the Batchelor, Howells & Townsend (1959) theory.

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REFERENCES


