Turbulent Mixing of Passive Scalars at High Schmidt Number

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Turbulent Mixing of Passive Scalars at High Schmidt Number

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To my beloved parents

who brought me into this world against all odds
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SUMMARY

A numerical study of fundamental aspects of turbulent mixing has been performed, with emphasis on the behavior of passive scalars of low molecular diffusivity (high Schmidt number $Sc$). Direct Numerical Simulation (DNS) is used to simulate incompressible, stationary and isotropic turbulence carried out at high grid resolution. Data analyses are carried out by separate parallel codes using up to $1024^3$ grid points for Taylor-scale Reynolds number ($R_\lambda$) up to 390 and $Sc$ up to 1024. Schmidt number of order 1000 is simulated using a double-precision parallel code in a turbulent flow at a low Reynolds number of $R_\lambda \approx 8$ to reduce computational cost to achievable level.

The results on the scalar spectrum at high Schmidt numbers appear to have a $k^{-1}$ scaling range and agree very well with Kraichnan’s (1968) model in the diffusive range as well. In the presence of a uniform mean scalar gradient, statistics of scalar gradients are observed to deviate substantially from Kolmogorov’s hypothesis of local isotropy, with a skewness factor remaining at order unity as the Reynolds number increases. However, this skewness decreases with Schmidt number suggesting that local isotropy for scalars at high Schmidt number is a better approximation. Small scale intermittency seen in the flatness factor of scalar gradients and scalar dissipation tends to an asymptotic level at high Schmidt numbers. Intermittency exponents manifested by three types of two-point statistics of energy and scalar dissipation, i.e., the two-point correlator $\langle \chi(x)\chi(x+r) \rangle$, the second-order moment of local scalar dissipation $\langle \chi_i^2 \rangle$ and the variance of the logarithmic local scalar dissipation $\sigma_{in}^2 \chi_i$ are discussed. These intermittency exponents are indicators of scalar intermittency in inertial-convective or viscous-convective ranges. Several basic issues in differential diffusion between two scalars of different molecular diffusivities transported by the same turbulent flow, the physical process of scalar spectral transfer and subgrid-scale transfer are also briefly addressed.
CHAPTER I

INTRODUCTION

1.1 Background

Turbulent flows are more important than laminar flows in the sense that turbulence commonly exist in nature and engineering applications. Turbulent motion can be found from astrophysical flow including interstellar cloud movement, plasma motion in the sun, to the Earth’s atmospheric motion and atmospheric boundary layers, and to common observations such as the smoke stack motion from a chimney, the wake of a ship, the ocean current, flow over an aerodynamic surface, flow in a gasoline pipe as well as in chemically reacting flows in industrial processes. One of the most important characteristics of turbulent flows is irregularity, or randomness, which makes the deterministic approach of studying laminar flows inapplicable. In spite of the unpredictability and intractability of the instantaneous turbulent flow field, certain empirical laws can be extracted for the statistical properties of the turbulent fluctuation. The monograph *Statistical Fluid Mechanics* by Monin and Yaglom (Vol. II 1975) provides mathematical foundation for the statistical approach in turbulence research. Among the vast literature on turbulence, the seminal work of Kolmogorov (1941) on the similarity in small scales of turbulence has been greatly influential even 60 years later today.

It is well known that turbulent flows provide much more efficient mixing than laminar flows due to the fluctuations and randomness of velocity field. One of the important and desirable applications of turbulent mixing in industry is gaseous combustion, where the gas flow is often turbulent and the coupling between mixing and chemical reaction is a major challenge in combustion research (Turns 2000). The rate of chemical reaction of gaseous reactants is often controlled by the rate of turbulent mixing at the small scales. This thesis primarily focuses on the turbulent mixing of passive scalars, which are defined as diffusive contaminants that are chemically inert and present in such low concentrations that they
do not have dynamical effects on the turbulent flow (Warhaft 2000). Common examples of passive scalars are the concentration of certain substance in a turbulent flow or the temperature field in a weakly heated turbulent air jet. Passive scalars are distinguished by a non-dimensional parameter, i.e., Schmidt number ($Sc$) or Prandtl number ($Pr$). $Sc$ is defined as the ratio between the kinematic viscosity ($\nu$) and the molecular diffusivity when the scalar under investigation is a chemical species concentration. Similarly, $Pr$ is the ratio between the kinematic viscosity and thermal diffusivity when temperature fluctuations are the object of study. In this work, $Sc$ is used for the general purpose with no distinction between $Sc$ and $Pr$.

Scalars at high Schmidt number are weakly diffusive with small molecular diffusivity. A fluorescent dye in flow visualization experiment is a common example of a weakly diffusive scalar where the color dye is expected to follow the fluid flow closely. For different color dyes, the degree of accuracy of the flow imaging result depends on the Schmidt number. In applications, $Sc$ can vary widely from much less than unity in liquid metals with large molecular conductivities, to order one for most gaseous flows, and to the order of 1000 for color dyes and in some biological applications. Antonia and Orlandi (2003) give a thorough review on Schmidt number effects on the small-scale passive scalars of $Sc \gg 1$. For $Sc > 1$, scalar fluctuations arise at smaller scales than the velocity field. Batchelor (1959) and Kraichnan (1968) provide theoretical background for scalar mixing at $Sc > 1$, which is a major motivation for the work. For $Sc \leq 1$, scaling for scalar spectrum in inertial-convective range was proposed by Obukhov (1949) and Corrsin (1951). The present research emphasizes the high $Sc$ regime of the scalar mixing, for which many important issues are still not well understood.

In this work, Direct Numerical Simulation (DNS) is used to study the properties of passive scalars. In the approach of DNS, the full range of scales in turbulent flows is resolved by solving the exact conservation equations of mass, momentum and passive scalars. The DNS approach to studying turbulent flows, despite its restriction to flows with simple geometries and low Reynolds number, can provide very detailed physical information about the small-scale structure which, in some cases, is very difficult to measure in experiments.
For instance, energy dissipation rate defined as \( \epsilon \equiv 2\nu s_{ij}s_{ij} \), where the strain rate \( s_{ij} \) can be computed in DNS strictly according to the definition, whereas in experiments, it usually must be replaced by the one dimensional surrogate \( 15\nu(\partial u_1/\partial x_1)^2 \). DNS also allows greater freedom in the choice of parameters and helps avoid the practical difficulties in handling some substances and fluids (e.g., mercury which has \( Sc \ll 1 \)) in experiments. For \( Sc \gg 1 \), the smallest scales, the Batchelor scale \( (\eta_B \equiv \eta Sc^{-1/2}) \), that need to be resolved are much smaller than the smallest turbulence scale, namely, the Kolmogorov scale \( \eta = (\nu^3/\langle \epsilon \rangle)^{1/4} \), where \( \langle \epsilon \rangle \) is averaged energy dissipation rate. High resolution is therefore required, especially at high Reynolds number where \( \eta \) is very small. Batchelor’s theory on weakly diffusive scalars only requires a large enough separation between \( \eta \) and \( \eta_B \) without requirement of high Reynolds number. This makes DNS a feasible approach to capture the fine scales of weakly diffusive scalars by keeping the Reynolds number relatively low (Bogucki et al. 1997, Brethouwer et al. 2003, Yeung et al. 2002, 2004).

In this work, the scalar field at \( Sc \) up to 1024 (Yeung et al. 2004) is simulated and analyzed on IBM SP parallel computers at San Diego supercomputing center. In addition to basic statistics such as the scalar spectrum, structure functions, statistics of scalar gradient, which were given in Yeung et al. (2002), statistics of scalar and energy dissipation taken at two different points in space are also computed at various Reynolds number and Schmidt number combinations. One of the more challenging tasks in this work lies in the calculation of the moments of local scalar dissipation \( \chi_r \), where \( \chi_r \) is the averaged dissipation over a cube of linear size \( r \) as defined in Kolmogorov (1962). Averaging is taken over three-dimensional cubes of different size \( r \) strictly according to the definition, whereas in many numerical and experimental works, averaging is taken over a one-dimensional line of size \( r \). Difficulties arise in parallel programming when data points belonging to a given sub-domain of a cube with linear size \( r \) are stored on different processors. In order to see the sensitivity of the results to the averaging methods, local dissipation averaged over one-dimensional, two-dimensional and three-dimensional spaces is all computed and compared. The DNS results show that intermittency exponent (see Sec.1.2) in intermediate range increases with averaging dimensions, but the values of the moments of local dissipation at fixed \( r \) in the
middle range decreases with averaging dimensions. The statistics mentioned above help to address the issues of local isotropy and intermittency and the Schmidt number effects. The issue of local isotropy at small scales in the context of Kolmogorov's (1941) hypothesis is of special interest for passive scalars when a mean scalar gradient is present. Reviews on this subject (Sreenivasan 1991, Warhaft 2000) have emphasized that passive scalars show first-order deviation from local isotropy for $Sc \sim O(1)$ even at very high Reynolds number. It is reasonable to speculate that, when $Sc \gg 1$, the separation between $\eta$ and $\eta_B$ plays an important role, and that the scalar fluctuations may be more nearly isotropic at higher $Sc$. Intermittency, as an important property in turbulence, refers to short-lived or localized bursts of intense fluctuations often associated with the small scales. Many studies based on experimental and numerical work (e.g., Sreenivasan and Antonia 1997, Overholt and Pope 1996) have shown that the passive scalar field is more intermittent than the velocity. An important issue is the nature of this behavior for $Sc \gg 1$. Some experimental data (Sreenivasan and Prasad 1989) have suggested a lack of intermittency in the Batchelor range between $\eta$ and $\eta_B$.

In including more than one scalar in the simulations, it is possible to study differential diffusion at high $Sc$ when two scalars with different $Sc$ evolve differently (Bilger and Dibble 1982, Yeung 1996, 1998). In turbulent flames, Lewis number ($\equiv Sc/Pr$) is not unity. Differential diffusion is important because unequal mixing leads to non-uniformities in local stoichiometric conditions, which can cause inefficient combustion and increased formation of undesirable by-products (such as pollutants in the atmosphere). But in many models of turbulent combustion, multiple chemical species in reactions are assumed to have equal molecular diffusivity so that the Shvab-Zeldovich conserved-scalar approach can be used where a certain linear combination of the species concentration is conserved. The importance of accounting for differential diffusion effect in combustion models has been well recognized (Pope 1990).

The mechanisms of nonlinear interaction between different scales are essential in turbulence research. For passive scalars, triadic interactions between velocity and scalar modes are the key in the scalar transfer which affects the evolution of the scalar spectrum. Scalar
transfer is the net rate at which scalar fluctuations are transferred at one scale to another. Earlier work (Yeung 1996) has shown a local forward scalar transfer where the triadic interactions occur at about the same scales and scalar fluctuations are transferred from large to small scales. At high Sc, more contributions from high wave number interaction are expected. A detailed knowledge of spectral transfer is also important in subgrid scale modeling where a cut-off wavenumber is introduced to divide the flow into resolved scales \((k < k_c)\) and subgrid scales \((k > k_c)\). The work of Yeung and Zhou (1996) is extended to the high Sc regime. In Large Eddy Simulations, only the large scales of the turbulent motion are simulated and the small scales, or the subgrid scales are modeled. Subgrid-scale turbulent diffusivity and Schmidt number, which are directly related to subgrid scalar transfer provide pivotal information for scalar subgrid modeling (Moin \textit{et al.} 1991). It would be useful to see the dependence of subgrid-scale turbulent diffusivity and Schmidt number on the molecular Sc. Further literature review is given in the following Sec. 1.2.

\textbf{1.2 Literature Review}

Because of the essential role in turbulent mixing, combustion and pollutant dispersion, passive scalar provides part of the motivation for the study of turbulence itself. The major impetus for study scalars in the high Schmidt number regime comes from the theoretical hypothesis of Batchelor (1959) and Kraichnan (1968), in which a \(\kappa^{-1}\) scaling for scalar spectrum in viscous-convective range \(\eta^{-1} \ll \kappa \ll \eta_B^{-1}\) is proposed, where \(\kappa\) is the wave number. Review by Warhaft (2000) shows that the experimental support for the \(\kappa^{-1}\) range has been elusive. Miller and Dimotakis (1996) in their turbulent jet experiment for \(Sc \sim 2000\) found no \(\kappa^{-1}\) range. Williams \textit{et al.} (1997) found the scalar spectrum fell well below \(\kappa^{-1}\) in magnetically forced two-dimensional turbulence for \(Sc \sim 2000\). On the other hand, there also exists experimental evidence supporting the \(\kappa^{-1}\) range from color dye concentration spectrum (Nye and Brodkey 1967) to temperature spectrum in the ocean (Dillon and Caldwell 1980). Gibson and Schwarz (1963) and Prasad and Sreenivasan (1990) also support the existence of \(\kappa^{-1}\) scaling. Numerical results based on two-dimensional synthetic velocity field (Holzer and Sigga 1994) appear to support Batchelor scaling of the
scalar spectrum.

In turbulence research on scalar mixing, much attention has been given to scalars with $Sc \sim O(1)$, e.g., heat transport in the air with $Pr \sim 0.7$ (Sreenivasan 1991, Warhaft 2000). For $Sc \approx 1$, a well-known result on scalar spectra is the $\kappa^{-5/3}$ scaling in the inertial-convective range between the large turbulence scale $L$ and the Obukhov-Corrsin scale $\eta_{OC} = \eta_S c^{-3/4}$ at high Reynolds number proposed by Obukhov (1949) and Corrsin (1951) as a direct extension of Kolmogorov (1941) scaling for energy spectra in the inertial range. The Obukhov-Corrsin $\kappa^{-5/3}$ scaling is generally supported in the literature (Sreenivasan 1996). But there are relatively few results on weakly diffusive scalars of $Sc \gg 1$, partly due to the high resolution requirement for both experiments and numerical simulations. Antonia and Orlandi (2003) give a detailed review on the Schmidt number effects with emphasis on the scalar spectrum and the related second-order scalar structure functions $\langle (\Delta r \phi)^2 \rangle$, where $\phi$ is the scalar fluctuation and $r$ is the separation distance between two locations. They suggest the $\kappa^{-1}$ scaling in viscous-convective range is ambiguous.

Since the major requirement for Batchelor scaling is a relatively wide range of separation between $\eta_B$ and $\eta$ without the requirement for high Reynolds number, DNS study of weakly diffusive scalars is made possible by keeping the Reynolds number relatively low in order to reduce the computational cost. This approach has been used by several authors (Bogucki et al. 1997, Yeung et al. 2000, 2002, Orlandi and Antonia 2002, Brethouwer et al. 2003) in simulations of scalars of $Sc > 1$ in isotropic turbulence at relatively low Reynolds number. In particular, Brethouwer et al. (2003) reported data for $Sc = 144$ at Taylor Reynolds number $R_\lambda \approx 20$. Gotoh et al. (2000) studied two-dimensional turbulence for $Sc = 1000$ at $R_\lambda \approx 3$. The main results for the work presented in this thesis are for $Sc$ up to 64 at $R_\lambda \approx 38$ and $Sc$ up to 1024 at $R_\lambda \approx 8$.

Unlike the velocity field, the scalar field shows strong evidence for departure from local isotropy predicted by Kolmogorov (1941) similarity hypothesis (Sreenivasan 1991, Warhaft 2000, Lumley and Yaglom 2001). The $\kappa^{-5/3}$ Kolmogorov and Obukhov-Corrsin scalings for velocities and scalars are based on the assumption that in the limit of infinite Reynolds number, scalars and velocities are isotropic at small scales. Local isotropy requires that
the odd order moments of scalar gradients vanish due to symmetry of scalar gradient fluctuations. Evidence for \( Sc \sim O(1) \) (Shen and Warhaft 2000, Schumacher 2001) strongly suggests local anisotropy in the presence of mean scalar gradient at the level of third order moments up to seventh order. The deviation from local isotropy is believed to stem from the ramp-cliff structure of the scalar fluctuations (Gibson 1977, Sreenivasan and Antonia 1977). Considering the statistical uncertainty of higher order moments, the normalized third order moment, i.e., the skewness of scalar gradient is among the most important indicators of local anisotropy. It is reasonable to speculate that the scalar field may be more locally isotropic at high \( Sc \) because Batchelor scale \( \eta_B \) is less than than \( \eta \) and is further removed from the large scales, i.e., scalars at high \( Sc \) has wider range of scales than those at low \( Sc \) in the same turbulent flows. Schumacher et al. (2003) provides upper bound for derivative moments of scalar based on the approach of Batchelor (1959), in which the upper bounds for derivative moments of order \( n \) are shown to grow as \( Sc^{n/2} \) for high \( Sc \). Furthermore, combination of analytical and numerical results from his paper suggests that the normalized moments decrease with \( Sc \), at least for odd orders.

Another important phenomenon that generally exist in turbulent flows is the concept of intermittency, which refers to sporadic large fluctuations that are localized in space. An intermittent signal is not self-similar. For example, a typical self-similar Gaussian random process displays a similar image for any portion of the signal. However, an intermittent process may have very strong signals in some portions whereas stay inactive for other portions. Intermittency implies that there are occasional large deviations from the mean value of the turbulent fluctuations. Such extremal events in statistics can be captured by normalized high-order moments, e.g., the flatness factor \( F_4 = \langle v^4 \rangle / \langle v^2 \rangle^2 \) of a turbulent quantity \( v \). For self-similar and Gaussian signals, the flatness factor is usually small. In fact, \( F_4 = 3 \) for Gaussian process has been used as a benchmark for detecting intermittency. Intermittent turbulent quantities have a higher value of flatness factor due to the contribution from the “spikes” in the signal. For instance, flatness factor of turbulent dissipation rate is usually of order 10. Small-scale intermittency can be captured by the distribution and normalized even-order moments of such small-scale quantities as gradients, time derivative and
dissipation rate etc.

Kolmogorov’s (1941) theory implies that turbulence is self-similar in inertial range, which is appreciably different from observation (Frisch 1995). The observed discrepancies between K41 theory and experiments have led to the development of Refined Similarity Hypothesis (Kolmogorov 1962). The discrepancies account for the intermittency effects in inertial range. For example, K41 theory predicts that the velocity structure function of order $p$ over a separation distance $l$ in inertial range grows as a power law of $l$ with an exponent $p/3$, and more generally, it can be written as

$$\langle (\Delta v_l(l)^p \rangle \propto l^{3p}. \quad (1.1)$$

Many experimental results show discrepancy of intermittency exponent $\zeta_p$ from $p/3$ predicted by K41 (Van Atta and Chen 1970, Anselmet et al. 1984). Other indicators of inertial range intermittency are based on statistics of the energy dissipation rate. In particular, local energy dissipation averaged over a sphere of size $l$ follows the scaling

$$\langle \epsilon_l^p \rangle \propto l^{\tau_p}. \quad (1.2)$$

Under Obukhov’s hypothesis (Obukhov 1962 or Frisch 1995), the two intermittency exponents $\zeta_p$ and $\tau_p$ based on velocity and energy dissipation, respectively, are related by

$$\zeta_p = p/3 + \tau_p/3. \quad (1.3)$$

Consequently, given measurement of either $\zeta_p$ or $\tau_p$, the other can be deduced. The prediction of the intermittency exponents have been much investigated and many models are developed such as Kolmogorov’s (1962) lognormal model, the $\beta$ model (Frisch et al. 1978) and bi-fractal model, the multifractal model (Meneveau and Sreenivasan 1987,1991), and the mapping closure model (She and Orszag 1991). Borgas (1992) suggests that the multifractal model gives the most satisfactory predictions.

Experimental and numerical studies (Sreenivasan and Antonia 1997, Overholt and Pope 1996, Vedula et al. 2001) generally show that scalar field is more intermittent than velocity field. Moreover, even for a strictly Gaussian velocity field without intermittency, the scalar field is still intermittent (Kraichnan 1994). In this work, attempt is made to investigate
scalar intermittency as a function of $Sc$ and the size of the scales. For scalars at high $Sc$, intermittency scaling in the viscous-convective range may exist. In particular, the scaling of local scalar dissipation $\chi_r$ over a cube of size $r$ and the possible intermittency exponents in viscous-convective range are also studied. In the literature, two-point correlator $\langle \epsilon(x)\epsilon(x + r) \rangle$, which has equivalent scaling as $\langle \chi_r^2 \rangle$ (Sreenivasan and Kailasnath 1993), is often studied for intermittency exponents. In this work, the two-point correlator of energy and scalar dissipation are also calculated for comparison.

Energy transfer is an important physical process influencing the evolution of energy spectrum. In the transport equation for energy spectrum, the non-linear energy transfer causes the closure problem and is usually modeled as a function of energy spectrum through various hypothesis (Monin and Yaglom 1975). Domaradzki and Rogallo (1990) studied the energy transfer through local and non-local interactions using DNS and showed excellent agreement with the prediction based on eddy-damped quasinormal Markovian theory (EDQNM). However, the process of scalar transfer that appears in the equation of scalar spectrum is less investigated. Yeh and Van Atta (1973) provided some one-dimensional measurements. Yeung (1996) studied the triadic interactions of scalar transfer by extending the technique of computing energy transfer used by Domaradzki and Rogallo (1990) to scalar transfer. In this work, the work of Yeung and Zhou (1996) is extended to high Schmidt numbers.

Scalar subgrid transfer used in LES for solving the scalar transport equation has been modeled based on different approaches (Moin et al. 1991, Zhou and Vahala 1993, Pullion 2000). Lesieur and Rogallo (1989) performed LES using a subgrid viscosity proposed by Kraichnan (1976) and subgrid diffusivity from EDQNM theory. Detailed process of subgrid transfer has also been studied using numerical simulation by various authors (Domaradzki et al. 1987, 1993, Yeung and Zhou 1996). In this work, scalar subgrid transfer at high $Sc$ based on Yeung and Zhou (1996) are studied by DNS.

The importance of differential diffusion has been well acknowledged (Bilger and Dibble 1982, Pope 1990). Saylor and Sreenivasan (1998) performed experiments using color dyes and showed significant differential diffusion effects even at scales much larger than the Batchelor scale. Smith et al. (1995) studied differential diffusion in turbulent jets of

1.3 Outline

The remaining thesis is organized as follows: Chapter 2 gives the numerical method of DNS, simulation parameters and data analysis. Basic statistics including scalar spectrum, structure functions and scalar gradient are discussed in Chapter 3, where local isotropy and its dependence on $Sc$ are evaluated. In Chapter 4, discussions of scalar intermittency through various indicators such as the kurtosis and probability density function of scalar gradient, dissipation, structure functions are presented. Two-point statistics of energy and scalar dissipation as a function of $Re$, $Sc$ and separation distance $r$ are also discussed. In particular, the two-point correlator $\langle \chi(x)\chi(x+r) \rangle$, the second order moment of local dissipation $\langle \chi_r^2 \rangle$ and the variance of logarithmic local dissipation $Var(\ln \chi_r)$ are analyzed and compared, their corresponding intermittency exponents are computed and discussed. Chapter 5 present results on differential diffusion between two scalars, scalar transfer and sub-grid transfer at various $Sc$. Finally, conclusions and future work on weakly diffusive scalars are discussed in Chapter 6.

In the appendices, abstracts from relevant journal papers and conference meeting are attached. Appendices A and B are are based on the DNS data for high Schmidt numbers at $R_\lambda \approx 38$ and 8, respectively, where most of the results are included in Chapter III. The conference paper in appendix C is on the Lagrangian statistics of three-particle dispersion. The conference presentation in appendix D studies the dispersion problem of molecules (scalars) by Lagrangian approach, where the velocities of molecules are modeled as the combination of the velocities of the fluid particles and 3-D Brownian motions. The work in appendices C and D is not included in this thesis.
CHAPTER II

NUMERICAL METHOD OVERVIEW

In this work, Direct Numerical Simulation is used to provide instantaneous velocity and scalar fields on a three-dimensional computational domain. Data from DNS are then analyzed by separate post-processing code. Section 2.1 reviews the techniques used in the DNS code. In Sec. 2.2, the methods of data analysis and simulation parameters are described.

2.1 Direct Numerical Simulation

In this thesis, stationary isotropic turbulence is simulated using a parallelized version of Rogallo’s (1981) pseudo-spectral algorithm. Periodic boundary conditions are applied to turbulent fluctuations over a cube of length $2\pi$ units on each side. Turbulent velocity and scalar fields are both maintained statistically stationary in time, which allows multiple realizations of the flow field at different times to be treated as different samples for the purpose of ensemble averaging. In the absence of energy input, homogeneous, isotropic turbulence will decay due to viscous dissipation. An artificial forcing at the large scales is used to obtain stationarity. Various forcing schemes based on deterministic or stochastic approaches have been developed for DNS and no general consensus on what is the best scheme has been reached (Overholt and Pope 1998). On the other hand, details of forcing schemes do not alter the statistics of the small scales significantly (Sreenivasan 1998). Eswaran and Pope’s (1988) stochastic forcing scheme is used in this work, which has been used by various authors.

The governing equations for incompressible turbulent flow are the continuity equation, momentum or Navier Stokes equations and the transport equation for passive scalars written as follows:

\[
\frac{\partial u_i}{\partial t} + u_j \frac{\partial u_i}{\partial x_j} = -\frac{1}{\rho} \frac{\partial p}{\partial x_i} + \nu \frac{\partial^2 u_i}{\partial x_j \partial x_j} = 0
\]  

(2.1)

\[
\frac{\partial u_i}{\partial x_i} = 0
\]  

(2.2)
\[
\frac{\partial \phi}{\partial t} + u_j \frac{\partial \phi}{\partial x_j} = -u_j \frac{\partial \Phi}{\partial x_j} + D \frac{\partial^2 \phi}{\partial x_j \partial x_j}
\]

where \( u_i \ (i = 1, 2, 3) \) denotes the velocity component along \( x_i \) direction, \( \rho \) is the pressure fluctuation and \( \phi \) is the scalar fluctuation. The constant coefficients \( \nu \) and \( D \) are the kinematic viscosity and molecular diffusivity, respectively, and \( \Phi \) is the mean scalar field.

In this work, scalar field is also maintained stationary by velocity fluctuations acting upon the mean scalar gradient. The evolution of the scalar variance follows

\[
\frac{\partial \langle \phi^2 \rangle}{\partial t} = -2 \langle u_j \phi \rangle \frac{\partial \Phi}{\partial x_j} - \langle \chi \rangle,
\]

where \( \langle \chi \rangle = 2D\langle (\partial \phi / \partial x_i)^2 \rangle \). In stationary state, the production term caused by the correlation of velocity and scalar fluctuations acting on the mean scalar gradient and the scalar dissipation term on the RHS are in balance with each other. For a homogeneous scalar field, the terms in Eq. 2.4 should be independent of spatial coordinates, which implies that the mean scalar gradient should be constant. In this work, a uniform mean scalar gradient \( \nabla \Phi = (1, 0, 0) \) is used for all cases, where different choices of the magnitude of the mean scalar gradient will not alter the normalized statistics, neither does the direction of the mean scalar gradient affect the statistics due to isotropy. The introduction of a uniform mean scalar gradient in DNS helps maintain a stationary scalar field for the ease of ensemble averaging over multiple times. However, I realize that in experiments, the mechanisms of maintaining such a uniform mean scalar gradient can hardly be realistic. In the simulations, scalars are introduced into the flow after the velocity field has attained stationarity, starting with zero scalar fluctuations. After the scalar field reaches stationary state, the simulation is continued for of order 10 eddy turnover times in order to obtain multiple realizations of data field at appropriate time intervals. Data are extracted and analyzed at time interval of about one eddy turnover time, and processed as independent samples in ensemble averaging of multiple realizations (e.g. Yeung 1998).

Direct numerical simulation using spectral methods gives greater accuracy in the evaluation of the spatial derivatives in the Navier-Stokes equations compared to finite-difference methods. The conservation equations are solved in Fourier spectral space. After taking Fourier transforms of Eq. 2.1 – 2.3, the obtained the continuity equation, the momentum
equations and the scalar equation in Fourier space can be written as

\[ k_j \hat{u}_j (k, t) = 0, \]  
\[ \frac{d\hat{u}_j (k, t)}{dt} = -\nu k^2 \hat{u}_j (k, t) - i k_i P_{jm} (k) \sum_{k'} \hat{u}_m (k', t) \hat{u}_i (k - k', t), \]  
\[ \frac{d\hat{\phi} (k, t)}{dt} = -D k^2 \hat{\phi} (k, t) - \frac{\partial \Phi}{\partial x_j} \hat{u}_j - i k_j \sum_{k'} \hat{u}_j (k', t) \hat{\phi} (k - k', t), \]

where \( k \) and \( k' \) are wavenumber vectors, \( i = \sqrt{-1} \), and \( P_{jm} (k) = \delta_{jm} - k_j k_m / k^2 \) is the projection tensor in wavenumber space.

In applying forcing, an additional term is added to Eq. 2.6 in the form

\[ \frac{\partial \hat{u} (k, t)}{\partial t} = \hat{a} (k, t) + \hat{a}^F (k, t), \]

where \( \hat{a} (k, t) \) represents the RHS of Eq. 2.6 and \( \hat{a}^F (k, t) \) is the forcing term. Following Eswaran and Pope (1988), \( \hat{a}^F (k, t) \) is non-zero only at large scales for all modes with a sphere of radius \( k_F \) centered at the origin (excluding the node at the origin), i.e., for all modes with magnitude of wavenumber satisfying \( 0 < k < k_F \). The \( k_F \) is normally chosen to be \( \sqrt{2}, 2 \) or \( 2\sqrt{2} \). The specification of the forcing term is based on Uhlenbeck-Ornstein (UO) random processes. A complex vector-valued stochastic process is formed based on combination of 6 independent UO processes with the same specified variance and timescale. Projection of this vector process onto the plane normal to \( k \) gives the forcing term \( \hat{a}^F \). Mathematical details can be found in Eswaran and Pope (1988).

A fully-spectral method for evaluating the convolution terms in Eq. 2.6 and Eq. 2.7 would require of order \( N^6 \) operations (each wavenumber mode involves \( N^3 \) multiplications, hence the total number of operations for all grid points \( N^6 \)). To avoid this large cost, in pseudo-spectral method, the nonlinear terms in the Navier-Stokes equations are evaluated by first transforming the velocity field to physical space where the nonlinear terms \( u_i u_j \) are formed and then transformed back to Fourier space. The computational cost for this procedure by multiplication is of order \( N^3 \log N \) in operations. However, this procedure causes aliasing errors and the aliased terms with high wavenumbers are added to the low wavenumber terms in Fast Fourier Transform (FFT) algorithm which is used in the DNS code. In Rogallo’s
scheme, aliasing errors are minimized by a combination of truncation and phase shifting methods.

The task is to solve Eqs. 2.6 and 2.7 as ordinary differential equations in time. A second-order Runge-Kutta method is used in predictor-corrector form. In the predictor step, a predictor velocity \( \hat{\mathbf{u}}^* \) is estimated by

\[
\hat{\mathbf{u}}^* = \hat{\mathbf{u}}(t_n) + \Delta t \hat{\mathbf{a}}(\hat{\mathbf{u}}(t_n)) \tag{2.9}
\]

In the corrector step, an improved approximation is obtained by

\[
\hat{\mathbf{u}}(t_{n+1}) = \hat{\mathbf{u}}(t_n) + \frac{\Delta t}{2} [\hat{\mathbf{a}}(\hat{\mathbf{u}}(t_n)) + \hat{\mathbf{a}}(\hat{\mathbf{u}}^*)] \tag{2.10}
\]

For each time step, the predictor-corrector method requires four sets of Fourier transforms per flow variable, which are carried out by using machine optimized FFT software library. Fourier transforms are the most CPU expensive operations in the DNS code. In parallel computing as described further below, the communication time among all the processors also becomes a bottleneck, especially when the number of processors is large.

In an explicit time-advancement scheme, the size of time step is subject to a Courant number restriction necessary for numerical stability. In three-dimensions, the Courant number is defined as

\[
C \equiv \frac{1}{\max \left[ \frac{|u|}{\Delta x}, \frac{|v|}{\Delta y}, \frac{|w|}{\Delta z} \right]} \Delta t \tag{2.11}
\]

where the maximum is taken over all grid points in physical space, \( u, v, \) and \( w \) are Cartesian velocity components and \( \Delta x, \Delta y \) and \( \Delta z \) are grid spacing in corresponding directions. In finite difference methods, explicit scheme usually requires Courant number less than unity in order to maintain numerical stability. Although no theoretical constraints of numerical stability in spectral method is known, Eswaran and Pope (1988) suggested that \( C \leq 1 \) is a necessary condition. In the simulation, Courant numbers at 0.6 or less is used to ensure stability. The tests also show that smaller Courant number should be used in simulating high-\( Sc \) scalars to avoid errors.

It is well-known that DNS approach is computationally intensive, especially at high Reynolds numbers. This is because the range of scales grows fast with increasing Reynolds
number, which means for the fixed largest scale, flows with higher Reynolds number have smaller dissipation scales, hence requires higher grid resolution. The required number of grid points increases as a power law of Reynolds number, i.e., \( N^3 \sim R_\lambda^{9/2} \), where \( R_\lambda \) is the Reynolds number based on Taylor scale. DNS has to resolve all scales of turbulent flow, and hence resolution of the smallest scales is critical. An empirical criterion used in the simulations is \( k_{max} \eta \geq 1.5 \) for velocity field, where \( k_{max} = \sqrt{2}N/3 \) is the highest wavenumber resolved on an \( N^3 \) grid. For scalars of high \( Sc \), the smallest scale \( \eta_B \) that needs to be resolved is smaller than \( \eta \) and resolution requirements for \( Sc > 1 \) are more demanding than those for velocity field. In other words, resolution requirement increases with both Reynolds number and Schmidt number for scalar field. One possible approach in simulating scalars at high \( Sc \) is to keep Reynolds number relatively low. In this work, the results include \( Sc = 64 \) at \( R_\lambda \approx 38 \) and \( Sc = 1024 \) at \( R_\lambda \approx 8 \), both with \( 512^3 \) grid points.

High-resolution DNS requires both longer CPU time and larger memory storage. The work in this thesis has been performed on IBM SP parallel computers at San Diego Supercomputer Center with resolution up to \( 512^3 \). The parallel algorithms are based on a single-program multiple data (SPMD) approach suitable for distributed-memory parallel computers. Every processor runs the same code but operates on different sub-domain stored in its own memory. Distributed-memory computers are in contrast to shared-memory computers, in which all processors share the same memory but different processor may run different codes. Because of the large memory requirement in high-resolution DNS, distributed-memory computers are chosen. In the parallel DNS code, the three-dimensional cubic domain is evenly divided into a number of slabs in \( x - y \) or \( x - z \) plane, with the number of slabs equal to the number of processors. Data on each slab are stored in a different processor. Communication between processors is required when it is necessary for each processor to have access to the data stored on other processors. Such necessity arises when Fourier transforms are taken in \( y \) direction for data divided into \( x - z \) slabs, because for data on \( x - z \) slabs, Fourier transforms can only be taken in \( x \) and \( z \) directions. Each slab has only part of the data in \( y \) direction which is insufficient for Fourier transforms. In the DNS algorithm (see Yeung and Moseley 1995 for details), data are transposed between
\(x - y\) and \(x - z\) slabs in order to take Fourier transform in the third direction perpendicular to the original slab. This is accomplished by packing the data on each slab into "pencils" of data with the number of "pencils" equal to the number of processors, and each processor exchanges a "pencil" of data with another. This task of data exchanges is implemented using a portable standard Message Passing Interface (MPI). The tests show that the percentage of communication time spent on data transposition increases with the number of processors, and communication becomes the most time-consuming operation in high-resolution simulations. In the parallel DNS code, data are divided evenly among processors which execute the same operations and participate equally in communications, except that the output is usually written by just one of the processors. This way of even distribution of workload improves parallel efficiency.

The number of processors used in the DNS runs is based on considerations for the total CPU time and memory usage. The number of processors must be large enough so that the memory usage on each processor does not exceed the memory limit, since usage close to the limit can greatly reduce performance efficiency due to paging in the computer memory. Fixed arrays of large size and dynamic memory allocations are efficiently used to minimized the memory usage. On the other hand, using too many processors leads to a reduction in parallel efficiency (ratio between speedup and the number of processors) because of increased time spent in communication calls, especially for larger grid-resolutions.

### 2.2 Data Analysis and Simulation Parameters

In this sub-section, the data analysis of the turbulent flow fields produced from DNS are discussed, with emphasis on the methods used to calculate the statistics of locally averaged dissipation rate on parallel computers. Descriptions of the simulation parameters are also presented.

In this work, the velocity and scalar fields are statistically stationary in time, although substantial temporal variations of space-averaged statistics such as turbulence kinetic energy can occur (e.g., Overholt and Pope 1996). Stationarity allows data taken at different times to be used as multiple realizations for the purpose of ensemble averaging. In the DNS,
the three-dimensional velocity and scalar fields are saved at time intervals of about one
eddy-turnover time (the ratio of longitudinal integral length scale to r.m.s. velocity) for the
purpose of post-processing. One eddy-turnover time is chosen such that data at different
times are statistically independent. The data from DNS are analyzed by separate post-
processing codes.

The computation and sampling of local averages, such as the average local energy dissipation in a cube of linear size $r$, i.e., $\epsilon$, is a non-trivial task that warrants some discussion. From a theoretical point of view (Kolmogorov 1962), in locally isotropic turbulence, or at least for scale sizes $r$ much smaller than the integral length scales, it is best to average over a sphere of radius $r$, which in practice for Cartesian geometries is replaced by a cube of length $r$ on each side. In experiments such 3-D box averages are generally not available and are routinely replaced by 1-D averages along a line of length $r$. However, most previous results from DNS (e.g. Chen et al. 1993, Wang et al. 1996) were also based on line averaging even though full three-dimensional fields are available in the simulations. Although some arguments can be made for the physics of using line averages of $\epsilon$ taken along the separation vector in the scaling of velocity structure functions (Wang et al. 1996), the main consideration has been CPU expense.

The CPU expense can be traced to the fact that in distributed-memory parallel codes the solution domain is divided among the processors as slabs of equal size. Each cubic box involved in a local average contains a number of grid planes, which in general may be spread over more than one slab. Partial sums are calculated on each processor that contains the data and final result is obtained by a communication call, which is time-consuming especially if a large number of processors must be used to accommodate the overall memory requirements for a given grid resolution. Since one communication call is required for every sample of the box average, the CPU cost is especially high for small boxes (i.e. small $r$) for which numerous samples exist in the solution domain. However, for large data sets (such as $1024^3$) a great improvement is possible if memory constraints can be circumvented in order to allow the data analysis to be carried out using only a small number of processors (say 32 for $1024^3$ versus 512 needed by the DNS code). This is achieved by first writing 3-D fields
of flow variables of interest (e.g. $\epsilon$) onto external files and then running a stand-alone code which needs to hold only one variable at a time for the sole purpose of obtaining box-average statistics.

In order to save CPU time and simplify the algorithm, only non-overlapping boxes are considered where $r$ is an integer multiple of the grid spacing and is varied in powers of 2: i.e. $r = 2^n \Delta x$, where $n = 0, 1, \ldots, \ln_2(N)$. While statistics for large boxes (which are relatively few in number) may be subject to sampling limitations, inclusion of overlapping boxes would not result in much improvement because the overlap would reduce the degree of statistical independence among different samples for the same box size. On the other hand, because intermittency exponents are inferred from the slopes of linear regimes in log-log plots, the restriction to logarithmically spaced values of $r$ does not have a great effect on the data quality.

The calculation of one- and two-dimensional averages and two-point correlators is much simpler, requiring communication calls only in collecting global statistics but not in forming individual samples. Comparisons are made for local averages computed in one dimension along a line, in two dimensions over a square, and in three dimensions over a box, all with the same linear dimension $r$. For the two-point correlator $\langle \epsilon(x)\epsilon(x+r) \rangle$ there is no difficulty in varying the distance $r$ linearly (instead of logarithmically) along each coordinate axis. In isotropic turbulence, average is taken over three components and the result can be written in simpler notation as $\langle \epsilon(x)\epsilon(x+r) \rangle$, where $r$ is taken to be $\Delta x$, $2\Delta x$, $3\Delta x\ldots$, etc. However, because homogeneity and periodic boundary conditions imply that two-point correlators are even functions of $r$, results are presented only for $r$ up to half of the length of each side of the solution domain.

Major simulation parameters are summarized in Tables I-III. The simulations can be divided into three groups. In the first, the Schmidt number is varied from 1 to 64 while the Taylor-scale Reynolds number $R_\lambda$ is kept approximately constant at 38. Table II gives the simulation parameters at $R_\lambda \approx 8$ with $Sc$ varied from 1 to 1024. Part of the interest in scalar mixing at $Sc = 1024$ is that $Sc \sim 1000$ corresponds to the regime of color dyes used in fluid visualization experiments. Questions may arise as to whether turbulence at such
low Reynolds number may have proper scalings, at least for Kolmogorov's first hypothesis. It is known that several authors have reported simulation results at \( R_\lambda \) below 20. For instance, Brethouwer et al. (2003) presented limited data at \( Sc = 144 \) and \( R_\lambda \approx 20 \). Chen et al. (1993) studied far-dissipation range where \( k\eta \gg 1 \) at \( R_\lambda \approx 15 \). Gotoh et al. (2000) reported results at \( Sc = 1000 \) and \( R_\lambda \approx 3 \) in two-dimensional turbulence. Simulations in this work show (FIG. 2.1) that there is a good collapse of the energy spectrum in Kolmogorov scaling for \( R_\lambda \) at 8 and 38. This result suggests that the high-\( Sc \) scalar field driven by the dissipation-range motions in this flow is still physically realistic. However, it should be pointed out that the forcing at large scales at such a low Reynolds number may have some effects on the DNS results and it will be useful to compare with the cases without forcing for a decaying turbulence. Since the main objective of studying high-\( Sc \) scalars is to understand the behavior in viscous-convective range, which does not require a high Reynolds number, simulations at \( R_\lambda \approx 8 \) still provide insightful results for scalars. Caution is taken in simulating turbulence at such a low \( R_\lambda \), where energy spectrum at very high wavenumbers falls to values so small that round-off errors become significant. To alleviate this problem, a double precision version of the DNS code is used, although at the cost of more memory requirements and somewhat larger CPU time per time step. In the third series of simulations, Reynolds number effects are addressed for \( Sc \leq 1 \). Simulation parameters at \( R_\lambda \approx 140, 240 \) and 390 are given in Table III. Energy spectra at \( R_\lambda \approx 240 \) and 390 appears to have a well-defined inertial range. The resolution criterion for \( Sc > 1 \) is that parameter \( k_{\max} \eta_B \) should be at least 1.5, where \( k_{\max} = \sqrt{2}N/3 \) is the highest wavenumber resolved on an \( N^3 \) grid, Tables I and II show that this criterion is met for all \( Sc \geq 1 \). For simulations at \( R_\lambda 140, 240 \) and 390, the corresponding criterion is that \( k_{\max} \eta \) should be no less than 1.5, although Table III shows \( k_{\max} \eta \) is slightly less than 1.5 in the high-\( re \) runs.

It can be seen from Tables I and II that, for fixed velocity parameters, scalar variance \( \langle \phi^2 \rangle \) increases with \( Sc \), while the scalar dissipation rate \( \langle \chi \rangle \) remains nearly constant. When the scalar field is statistically stationary, balance between production of scalar variance due to the mean gradient and dissipation by molecular action requires that

\[
-2\rho u_\phi u' \phi' G = \langle \chi \rangle,
\]  

(2.12)
where the primes denote root-mean-square fluctuations, and \( \rho_{u\phi} \) is the velocity-scalar correlation coefficient. Tables I and II show that the magnitude of \( \rho_{u\phi} \) decreases as \( Sc \) increases. Tables I-III also give the ratio of the mechanical time scale to the scalar time scale, \( r_\phi = (K/\langle \epsilon \rangle)/(\langle \phi^2 \rangle/\langle \chi \rangle) \), where \( K \) is the turbulent kinetic energy. The ratio \( r_\phi \) is an important parameter in many studies of turbulent mixing (e.g., Warhaft and Lumley 1978, Eswaran and Pope 1988). In simplified mixing models, \( r_\phi \) is often set to be 2 (Pope 2000). This ratio \( r_\phi \) is also related to the time ratio between scalar Taylor time scale and Kolmogorov time scale (see Yeung and Sawford 2002 for details). Table III for high-\( R_\lambda \) simulations at \( Sc \leq 1 \), \( r_\phi \) is between 2 and 3, which has very weak dependence on \( R_\lambda \), but for high-\( Sc \) scalars at \( R_\lambda \approx 38 \) and 8, Tables I and II clearly show that \( r_\phi \) decreases with \( Sc \). For \( R_\lambda \approx 8 \), \( r_\phi \) decreases from 0.96 at \( Sc = 1 \) to 0.17 at \( Sc = 1024 \), and it becomes systematically lower at high \( Sc \). Thus, Schmidt number effects should be incorporated in modeling.
Table 2.1: Simulation parameters at $R_\lambda \approx 38$

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Table 2.2: Simulation parameters at $R_\lambda \approx 8$

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Table 2.3: Simulation parameters at higher Reynolds numbers

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FIGURE 2.1. Comparison of Kolmogorov-scaled energy spectrum at $R_\lambda \approx 38$ (△) and $R_\lambda \approx 8$ (○), using double precision code.
CHAPTER III

SCALING PROPERTIES AND SMALL-SCALE CHARACTERISTICS

In this chapter, results based on scalar spectrum and structure functions are presented. In the latter part, discussions are made on the issues of local isotropy and intermittency and their Schmidt number dependence.

3.1 Scalar spectrum and structure functions

A. Moderately diffusive scalars

For scalars with $Sc \leq 1$, effects of molecular diffusion are dominant for scales smaller than the Obukhov-Corrsin scale, $\eta_O = \eta Sc^{-3/4}$. Under similar high Reynolds number arguments as those of Kolmogorov (1941), Obukhov (1949) and Corrsin (1951) predicted the scalar spectrum in inertial convective range of wavenumbers $1/L \ll k \ll 1/\eta_O \leq 1/\eta$ has the form

$$E_\phi(k) = C_\phi^* \langle \chi \rangle \langle \epsilon \rangle^{-1/3} k^{-5/3},$$

(3.1)

where $C_\phi^*$ is the Obukhov-Corrsin constant in three-dimensional spectrum. To compare the DNS data with Eq. 3.1, Fig. 3.1 shows the “compensated” three-dimensional spectrum corresponding to the suggested scaling, for scalars at $Sc = 1/8$ and 1 for four different Reynolds numbers. A narrow flat region around $k\eta \approx 0.04$ begins to emerge at $R_\lambda \approx 140$ for scalar with $Sc = 1/8$. At the highest $R_\lambda \approx 390$, a pronounced inertial-convective range of about a decade wide appears beginning from $k\eta \approx 0.008$. For $Sc = 1$ a spectral “bump” following the inertial-convective range can also be observed, which is most pronounced at around $k\eta \approx 0.2$, independent of the Reynolds number. The existence of a spectral bump has not been fully understood. Falkovich (1994) pointed out that viscous suppression of small-scale modes makes non-linear energy transfer less efficient and leads to a pile-up of
energy around the inertial scales. It is possible that a combination of viscous and diffusive effects causes the scalar spectral bump. Reynolds number similarity is also reflected by the “collapse” at high wavenumbers for different $R_A$ but fixed $Sc$. On the other hand, a similar collapse occurs at low wavenumbers for different $Sc$ but fixed $R_A$. The latter feature is consistent with previous studies of differential diffusion, in which scalars with different molecular diffusivities differ primarily in small scales (Yeung and Pope 1993, Yeung 1996, Saylor and Sreenivasan 1998).

Although it is straightforward to compute the spectrum in Eq. 3.1 as a function of wavenumber magnitude in three-dimensional space, in experiments usually only the one-dimensional version $E_{1\phi}(k)$ is available. However, if isotropy is assumed to hold, there is the spectral relation (Monin and Yaglom 1975)

$$E_{\phi}(k) = -k \frac{dE_{1\phi}(k)}{dk}. \quad (3.2)$$

This relation implies that $C_{\phi}^*$ should be $5/3$ of the one-dimensional constant $C_{\phi}$. It follows that the experimental value (Sreenivasan 1996) of $C_{\phi} \approx 0.4$ corresponds to $C_{\phi}^* = 0.4(5/3) = 0.67$. Eq. 3.2 can also be used to test the isotropy of the spectrum and it holds well except in the two lowest wavenumber shells, which correspond to the largest scales for which only a limited number of samples exist in the computational domain.

Figure 3.2 shows the one-dimensional compensated spectrum, for scalars with $Sc = 1/8$ and 1 at $R_A \approx 390$. To infer $C_{\phi}$ accurately, a linear ordinate is used and a dashed line corresponding to the experimental value in Sreenivasan (1996) is included. Although the range is narrow, there is some evidence for scaling with Obukhov-Corrsin constant close to the dashed line 0.4. The spectral bump for $Sc = 1$ is quite conspicuous. The bump occurs within about the same range of normalized wavenumbers as observed in the higher-Reynolds number grid experiments of Mydlarski and Warhaft (1998) for temperature fluctuations in air with $Sc = 0.7$. Experimental data from Fig. 12 of Mydlarski & Warhaft (1998) is included in figure 2 for comparison. The authors considered the apparent Obukhov-Corrsin constant in their data to be in broad agreement with the estimates by Sreenivasan (1996).

In Yeung  et al.  (2002), a similar result is shown at $R_A \approx 240$. The simulation results in
Fig. 3.1 and Fig. 3.2 show that spectral bump occurs at $Sc = 1$ for $R_\lambda$ between 90 and 390 and it does not seem to depend on Reynolds number, whereas in Mydlarski & Warhaft scalar spectrum at higher Reynolds number show a more distinct bump. Instead, the DNS results show that the scalar spectral bump occurs at Schmidt number close to unity or higher. The Schmidt number effects are weaker, as will be seen in the later part of this section that spectral bump does not occur at relatively low Reynolds number even for high Schmidt numbers. The presence of spectral bump at $Sc = 1$ affects the $-5/3$ scaling range: Without the bump it is likely that one would see a more extensive stretch of the $-5/3$ scaling.

The bump effect is particularly striking in the second-order structure function, which is the spatial equivalent of the one-dimensional spectrum. The classical result for spatial separations in the inertial-convective range is given by

$$D_{\phi\phi}(r) \equiv \langle (\Delta_r \phi)^2 \rangle = C_2 \langle \chi \rangle \langle \epsilon \rangle^{-1/3} r^{-2/3},$$  \hspace{1cm} (3.3)

where, as shown in Monin and Yaglom (1975), $C_2 = 1.5 \Gamma(1/3) C_\phi \approx 4.02 C_\phi$. In this flow configuration, distinction should be made between two-point differences in directions parallel and perpendicular to the mean scalar gradient, as $\Delta_\parallel \phi(r)$ and $\Delta_\perp \phi(r)$. However, because isotropy at the intermediate scales is implied in Eq. 3.3, it is appropriate to make comparisons using DNS data averaged over $r$ taken in three different coordinate directions.

Figure 3.3 shows the component-averaged structure function $\langle (\Delta_r \phi)^2 \rangle$ normalized by the Obukhov-Corrsin variables as suggested in Eq. 3.3. It can be seen that, as the Reynolds number increases, results for $Sc = 1$ show a tendency towards a flat scaling region. The apparent scaling constant suggested by the data is higher than 1.61 (corresponding to $C_\phi = 0.4$) for $Sc = 1$ and lower for $Sc = 1/8$. In other words, in contrast to the behavior observed in the spectrum, the apparent scaling constant in structure functions shows a significant dependence on Schmidt number. This could be an artifact of the spectral bump which succeeds in masking the limited scaling region in the Fourier-transformed version. In support of this inference, it is noted that this apparent dependence on the Schmidt number weakens with increasing Reynolds number. It is also noted that the scaling region
at $R_\lambda \approx 390$ for $Sc = 1$ stretches over more than one decade with a power law exponent a little less than $2/3$ as suggested in Eq. 3.3. But the scaling trend with Reynolds number implies that as Reynolds number further increases, the scaling in inertial-convective range approaches a power law of $r^{2/3}$. On the other hand, since results at $Sc = 1/8$ behave as power law of $r^{2/3}$, it is possible that the scaling exponents at $Sc = 1$ may be affected by the presence of spectral bump.

The limiting behaviors in Fig. 3.3 for small and large scale separation are both amenable to theoretical analysis, and can therefore be used as checks on the quality of the simulation data. In the limit of small $r$ (i.e. $r \ll \eta_{OC}$), Taylor series arguments yields the result

$$\frac{\langle (\Delta r \phi)^2 \rangle}{\langle \chi \rangle \langle \epsilon \rangle^{-1/3} r^{2/3}} = \frac{1}{6} \left( \frac{r}{\eta_{OC}} \right)^{4/3},$$

which is indicated by a dotted line. Its perfect agreement with the data indicates that the small scales are adequately resolved. For large $r$, as values of $\phi$ at two points far apart in space become statistically independent, $\langle (\Delta r \phi)^2 \rangle$ is expected to approach a constant value equal to $2 \langle \phi^2 \rangle$. The inset shows the ratio $\langle (\Delta r \phi)^2 \rangle / \langle \phi^2 \rangle$, which approaches a value close to 2 at large $r$. The asymptotic behavior at large $r$ implies that the normalized form shown in the main body of Fig. 3.3 should decrease as $r^{-2/3}$. Indeed by using the time-scale ratio $(K/\langle \epsilon \rangle) / \tau_\eta \approx (3/2\sqrt{15}) R_\lambda$ the large-separation asymptote can be derived as

$$\frac{\langle (\Delta r \phi)^2 \rangle}{\langle \chi \rangle \langle \epsilon \rangle^{-1/3} r^{2/3}} \approx \frac{3 R_\lambda Sc^{1/2}}{\sqrt{15} r_\phi} \left( \frac{r}{\eta_{OC}} \right)^{-2/3},$$

where $r_\phi \equiv (K/\langle \epsilon \rangle)/(\langle \phi^2 \rangle / \langle \chi \rangle)$ is the mechanical-to-scalar time scale ratio (See Tables I-III). Because of the periodic boundary conditions used on the computational domain, it is meaningful to compute the structure functions only for $r$ up to half of the length $L_0$ of each side of the solution domain. However, because of finite domain size (with $L_0$ only about six times of the integral length scale of the scalar field, which is 40% longer in the direction of the mean scalar gradient), the rate of approach to the large $r$ asymptote is somewhat distorted.

The scaling in inertial-convective range based on the argument of Kolmogorov (1941),
Obukhov (1949) and Corrsin (1951) for any order structure function can be written as

\[ \langle (\Delta_r u)^m (\Delta_r \phi)^n \rangle \sim e^{m/3-n/6} \chi^{-n/2} (m+n)/3, \]  

(3.6)

where \( \Delta_r u \) is the velocity difference over a linear length of \( r \). In particular, the mixed third-order structure function, defined as \( D_L(\phi)(r) \equiv \langle \Delta_r u (\Delta_r \phi)^2 \rangle \) where \( \Delta_r u \) is a longitudinal velocity increment in space, has a more fundamental role in similarity scaling. An exact result for intermediate \( r \) in the inertial-convective range was given by Yaglom (1949), as

\[ \langle \Delta_r u (\Delta_r \phi)^2 \rangle = -(2/3) \langle \chi \rangle r. \]  

(3.7)

(Note that this relation was originally given by Yaglom with half the present scalar dissipation rate, and so the coefficient here was 4/3 instead of the present 2/3.) In the limit of small \( r \), the velocity and scalar difference can be related to their corresponding gradients as

\[ \langle \Delta_r u (\Delta_r \phi)^2 \rangle \approx S_{u\phi} \left( \frac{1}{2} \left( \frac{\partial u}{\partial x} \right)^2 \right)^{1/2} \left( \frac{1}{2} \left( \frac{\partial \phi}{\partial x} \right)^2 \right)^{1/2} r^3, \]  

(3.8)

where \( S_{u\phi} \) is the mixed gradient skewness defined by (see Kerr 1985)

\[ S_{u\phi} \equiv \frac{\left\langle \left( \frac{\partial u}{\partial x} \right) \left( \frac{\partial \phi}{\partial x} \right)^2 \right\rangle}{\left\langle \left( \frac{\partial \phi}{\partial x} \right)^2 \right\rangle} \left\langle \left( \frac{\partial u}{\partial x} \right) \right\rangle^{1/2}. \]  

(3.9)

Considerations of local isotropy for both velocity and scalar fields lead to the normalized form

\[ \frac{\langle \Delta_r u (\Delta_r \phi)^2 \rangle}{\langle \chi \rangle r} \approx \frac{S_{u\phi} \left( \frac{r}{\eta_B} \right)^2}{6 \sqrt{15}}. \]  

(3.10)

In the large \( r \) limit, isotropy of the velocity field implies that \( \langle \Delta_r u (\Delta_r \phi)^2 \rangle \) approaches zero.

Figure 3.4 shows DNS results for the mixed structure function, in normalized forms suggested by Eqs. 3.7, where an average is taken over three coordinate components. With \( S_{u\phi} \) taken to be of order -0.5 (see Table 3.1), the behavior at small \( r \) is indeed seen to follow Eq. 3.10 for all Reynolds and Schmidt numbers in the data. It can be seen that as Reynolds number increases, the scaling range of the mixed structure function becomes wider and the normalized mixed structure function increases toward a plateau of height 2/3 (centered around \( r/\eta_B \approx 50 \) at \( R_\lambda 390 \) and \( Sc = 1 \)). At larger values of \( r \) the curves become more
widely spaced among each other as the range of scales become wider with increasing $R_\lambda$ and $Sc$. A rapid drop is seen in the limit as $\langle \Delta_r u (\Delta_r \phi)^2 \rangle$ approaches zero.

The assumptions used to derive Eq. 3.7 are that the scalar field is stationary and isotropic. Yaglom’s (1949) transport equation for scalar structure function, which is based on Kármán & Howarth (1938)’s equation for two-point correlations, has the form

$$D_{L\phi\phi}(r) - 2D \frac{dD_{\phi\phi}(r)}{dr} = -\frac{2}{3} \langle \chi \rangle r.$$  (3.11)

Eq. 3.7 is thus derived under the assumption that the diffusive term on the left-hand-side of Eq. 3.11 can be neglected in the inertial-convective range. In fact, both the DNS simulations and recent studies by Orlandi and Antonia (2002) for decaying turbulence suggest that the diffusive term is indeed small compared to the other terms in Eq. 3.11 in intermediate scale ranges. In the simulations, nonstationarity contributions vanish when averaged over a sufficiently long period of time. Deviations from Eq. 3.7 and Eq.3.11 must be caused mainly by departures from local isotropy. Significant anisotropy is indeed seen in Fig. 3.5, which shows a comparison between normalized structure functions taken in different coordinate directions for $Sc = 1$ at $R_\lambda \approx 390$. In particular, the structure function is systematically larger for $r$ taken parallel to the mean gradient direction. Since in experiments structure functions are often measured in only one direction, this result suggests caution for inferences on Yaglom’s relation.

The scaling behavior of structure functions in inertial-convective range is a major issue in Kolmogorov’s (1941) theory. In this work, velocity and scalar structure functions from order 2 up to order 8 at $R_\lambda$ up to 390 are also obtained. Figure 3.6 shows compensated even-order scalar structure functions normalized based on Eq. 3.6, where average is taken over separation along the three coordinate directions. The compensation power law $r^{\xi_{m,n}}$ is chosen based on trial and error such that the structure functions show a flat scaling region. The odd-order scalar structure functions should vanish under the assumption of local isotropy in homogeneous turbulence. However, the simulation results in Fig. 3.7 for odd-order scalar structure functions with separation taken in the direction parallel to the mean scalar gradient show an unambiguous scaling range and the scaling exponents are
in sequence with those of even-order structure functions. This is consistent with the fact that odd-order moments of scalar gradient in the direction parallel to the mean gradient have magnitude of order 1 even at very high Reynolds number (Sreenivasan 1991, Warhaft 2000), e.g., the presence of mean scalar gradient causes anisotropy to some extent. Similar findings for the odd-order scalar structure functions have also been reported by Antonia and Van Atta (1978) and Mydlarski and Warhaft (1998).

It is also shown in figure 3.8 and 3.9 the compensated longitudinal velocity structure functions. The deviation of $\zeta_{m,n}$ from the KOC prediction of $n/3$ in Eq. 3.6 for any structure function of order $n$ accounts for the intermittency in inertial or inertial-convective range, except for the third-order longitudinal velocity structure function where the scaling is exact according to the Kolmogorov’s four-fifth law

$$\langle (\Delta_r u)^3 \rangle = -\frac{4}{5}\langle \epsilon \rangle r,$$  \hspace{1cm} (3.12)

with which the DNS simulation result agrees. The scaling power law exponent $\zeta_{m,n}$ for both velocity and scalar structure functions are shown in Fig. 3.10 at the highest $R_\lambda \approx 390$ with $Sc = 1$ for scalar. Fig. 3.10 also includes Mydlarski and Warhaft (1998)’s results for scalar structure functions at $R_\lambda \approx 461$ and $Sc \approx 0.7$ for grid turbulence, Dasi (2004)’s result for scalars in turbulent boundary layer at $Sc \approx 1000$ and results for velocity structure functions at $R_\lambda \approx 536$ for a jet from Anselmet et al. (1984). The KOC prediction of $n/3$ is plotted as a dashed line for comparison. Figure 3.10 suggests that scaling behaviors of both velocity and scalar structure functions deviate from KOC theory. But the behavior of scalar field deviates far more than that of velocity field. The power law exponents obtained in the simulations are smaller than those of Mydlarski and Warhaft (1998) and Anselmet et al. (1984). Especially for the exponents of scalar structure functions, there is considerable difference between the DNS results and those of Mydlarski & Warhaft, which can be partly explained by the difference of $R_\lambda$ and $Sc$. The DNS results for scalars are close to those of Dasi’s (2004) for up to the fourth-order, however, Dasi’s data for higher order scalar structure functions are well above the DNS results. Figure 3.10 supports the general perception that scalar field is more intermittent than velocity field in inertial-convective
range.

B. Weakly diffusive scalars

For $Sc \gg 1$ Batchelor’s result for the scalar spectrum is

$$E_\phi(k) = q\langle \chi \rangle (\nu / \langle \epsilon \rangle)^{1/2} k^{-1} \exp(-q(\kappa \eta_B)^2),$$  \hspace{1cm} (3.13)

where the non-dimensional coefficient $q$ was assumed to be universal. Batchelor’s theory was based on an assumption of persistent straining of the scalar field by the small scale motions of the characteristic time $\tau_\eta = (\nu / \langle \epsilon \rangle)^{1/2}$. The essential fact underlying Batchelor’s analysis is that the strain rate is approximately uniform over the viscous-convective range. Later Kraichnan (1968) proposed a more refined treatment which accounted for fluctuations of the strain rate and arrived at the form

$$E_\phi(k) = q\langle \chi \rangle (\nu / \langle \epsilon \rangle)^{1/2} k^{-1} (1 + (6q)^{1/2} \kappa \eta_B) \exp(-(6q)^{1/2} (\kappa \eta_B)).$$  \hspace{1cm} (3.14)

The main difference between the two expressions is in the viscous-diffusive range, $k \eta_B > 1$. In the viscous-convective range $1/\eta < k < 1/\eta_B$ both expressions give

$$E_\phi(k) = q\langle \chi \rangle (\nu / \langle \epsilon \rangle)^{1/2} k^{-1}$$  \hspace{1cm} (3.15)

which is commonly referred to as $k^{-1}$ scaling. A substantial scale separation between $\eta$ and $\eta_B$ is required to observe this feature: this requires a high Schmidt number, but not necessarily a high Reynolds number. The value of $q$ is generally estimated by reference to either measurements or closure theories, but without general agreement. For example, Batchelor (1959) took $q = 2$, whereas Qian (1995) suggested $q = 2\sqrt{5}$. The latter was used for comparisons with DNS by Bogucki etal. (1997).

Figure 3.11(a) and (b) show un-normalized scalar spectra for $Sc$ from 1/4 to 64 at $R_\lambda \approx 38$ and $Sc$ from 64 to 1024 at $R_\lambda \approx 8$, respectively. As $Sc$ increases, weaker molecular diffusivity reduces the length scales at which scalar dissipation occurs and more scalar fluctuations arise at high wavenumbers. At both $R_\lambda$, a clear $k^{-1}$ scaling range appears and becomes well-defined with increasing $Sc$. The spectrum progressively spreads out toward wavenumbers higher than $1/\eta$ with increasing $Sc$. At low wavenumbers, the spectrum is
almost independent of $Sc$, which confirms the Reynolds number similarity at large scales, similar as in Fig. 3.1. The spectra for $Sc = 256$ computed from $256^3$ and $512^3$ simulations in Fig. 3.11(b) appear to virtually coincide, which suggests $k_{max} \eta_B = 1.5$ gives sufficient resolution, at least for second-order statistics.

In order to compare the scaling behavior at high $Sc$ with the KOC scaling, it is shown in Fig. 3.12(a) and (b) the scalar spectrum normalized by KOC variables. Instead of a flat region indicating KOC’s $k^{-5/3}$ law, a scaling range with slope $2/3$ appears suggesting a power law behavior of $k^{-1}$. It is noticed in Fig. 3.12(a) at $R_\lambda \approx 38$, the scaling range lies at scales larger than $\eta$; in Fig. 3.12(b) at $R_\lambda \approx 8$ for higher Schmidt numbers, the $k^{-1}$ range shifts toward scales smaller than $\eta$.

Figure 3.13(a) and (b) show the DNS data at $R_\lambda \approx 38$ and $R_\lambda \approx 8$ for the spectrum normalized by Batchelor variables (as a function of $k \eta_B$) and compared with the expressions of Batchelor and Kraichnan, where $q = 2\sqrt{5}$ is used according to Qian (1995). The data suggest the presence of $k^{-1}$ scaling for $k \eta_B < 0.1$. Kraichnan’s form is more accurate in the viscous-diffusive range, within which good agreement is found even for $Sc = 1$. To infer the value of $q$ needed for the best fit, the log-linear scale plot is also shown in the inset for the quantity $k E_B(k)(\langle \epsilon \rangle / \nu)^{1/2} / \langle \chi \rangle$ versus $k \eta_B$, such that $q$ would be the height of a plateau at $k \eta_B \ll 1$. It appears that the value of $q$ required for an optimum fit increases with $Sc$ somewhat, being about 3.5 for $Sc = 1$ but 5.5 for $Sc = 64$ at $R_\lambda \approx 38$. At $R_\lambda \approx 8$, the optimum fit for $q$ varies from 4.3 for $Sc = 64$ to 5.2 for $Sc = 1024$.

Although classical arguments suggest that the width of an apparent $k^{-1}$ scaling range is primarily contingent upon having a sufficiently high Schmidt number, it is of interest to ascertain whether there is also a Reynolds number dependence. To address this question, Fig. 3.14 compares the normalized spectra for three Reynolds and Schmidt number combinations. An increase of $Sc$ from 64 to 1024 with $R_\lambda$ held constant (at 8) produces, as expected, results closer to $k^{-1}$ scaling with a wider range. However, a similar effect can also be observed when $R_\lambda$ is increased (from 8 to 38) while $Sc$ is held constant (at 64). These results suggest that the actual requirement for high $Sc$ may be weakened (say, towards only
moderately large values) if the Reynolds number is high. The difference between the scalar spectrum at \( R_\lambda \approx 38 \), \( Sc = 64 \) and \( R_\lambda \approx 8 \), \( Sc = 1024 \) is that the \( k^{-1} \) scaling range lies more in the viscous-convective range between \( \eta_B \) and \( \eta \) for scalar of higher Schmidt number, whereas for scalar at higher Reynolds number with relatively low Schmidt number, the Batchelor scaling range shifts toward larger scales than those in the viscous-convective range.

The effects of Schmidt number on the scaling of second-order structure function for \( Sc > 1 \) are shown in Fig. 3.15(a) and (b). For small \( r \) the Taylor-series result (Eq. 3.4) in terms of Obukhov-Corrsin variables is seen to continue to hold, even for \( Sc \gg 1 \). Whereas an increase in Reynolds number has been seen (Fig. 3.3) to promote a plateau in the normalized structure function, an increase of Schmidt number apparently has no such effect. In the limit of large \( r \) the data conforms to Eq. 3.5 which is valid at all Schmidt numbers. Since the scaling used in Fig. 3.15 is chosen to produce a universal "collapse" at the small scales, the "fanning-out" of curves with increasing Schmidt number also reflects the existence of a wider range of scales in the scalar field at higher \( Sc \). It is noted that the second-order structure function for \( Sc = 256 \) from the \( 256^3 \) and \( 512^3 \) simulations almost coincides, similar as in Fig. 3.12(b).

Corresponding results for the mixed third-order structure function for high Schmidt numbers at \( R_\lambda \approx 38 \) and \( R_\lambda \approx 8 \) are shown in Fig. 3.16(a) and (b). It is interesting to note that, although Yaglom’s relation (Eq. 3.7) is traditionally associated with the inertial-convective range for \( Sc \leq 1 \) at high Reynolds number, the arguments leading to it are also increasingly valid at high \( Sc \). Indeed it can be seen that the results at high \( Sc \) appear to approach the limit of Yaglom’s relation for intermediate \( r \).

### 3.2 Local Isotropy: Schmidt number effects

Local isotropy is the central assumption in KOC scaling. In the limit of infinite Reynolds number and Schmidt number, scalar and velocity fields are assumed to be isotropic at small scales. Many indicators of varying degrees of sensitivity can be used as tests of local isotropy.
For example in Sec. 3.1, isotropy relations between spectra in one and three dimensions have been discussed, and it is noted that structure functions show some differences depending on the direction of the spatial separation. Here, the focus is mainly on statistics of scalar gradients parallel \( (\nabla_\parallel \phi) \) and perpendicular \( (\nabla_\perp \phi) \) to the mean gradient, including their relationships with velocity gradient fluctuations.

Because of reflectional symmetry in the plane perpendicular to the mean gradient, all odd-order moments of \( \nabla_\perp \phi \) are expected to be zero. Furthermore, local isotropy requires odd-order moments of \( \nabla_\parallel \phi \) to vanish, and even-order moments of \( \nabla_\parallel \phi \) and \( \nabla_\perp \phi \) to be equal. Table 3.3-3.5 show that the second-order moment of \( \nabla_\parallel \phi \) and \( \nabla_\perp \phi \) are very close to each other and without definite trend with Reynolds number or Schmidt number, suggesting that the second-order moment of scalar gradient is not a sensitive indicator of local isotropy. Figures 3.17(a), (b) and (c) show higher-order moments of scalar gradients as a function of Schmidt number at \( R_\lambda \approx 38 \) with \( Sc \) varying from 1/4 to 64 and \( R_\lambda \approx 8 \) with \( Sc \) from 1 to 1024 (also listed in Tables 3.3 and 3.5). The skewness of \( \nabla_\parallel \phi \) in Fig. 3.17(a) slightly increases at low \( Sc \) at both \( R_\lambda \), then for \( Sc \geq 1 \) at \( R_\lambda \approx 38 \) and \( Sc \geq 8 \) at \( R_\lambda \approx 8 \), the skewness decreases steadily as an approximate power law of \( Sc \). A weaker trend of decrease at high Peclet number may also be present in results by Holzer and Siggia (1994) based on two-dimensional synthetic velocity fields. Between \( Sc = 4 \) and 64, the skewness at \( R_\lambda \approx 38 \) and \( R_\lambda \approx 8 \) is close to each other, although it has a slightly faster decreasing rate at \( R_\lambda \approx 38 \). In Fig. 3.17(a), the skewness factors from Mydlarski and Warhaft (1998), Tong and Warhaft (1994) for grid turbulence at \( Pr = 0.71 \) for \( R_\lambda \) up to over 700 are also included for comparison and they are reasonably close to the DNS results. From Tables 3.3-3.5, it can be seen that the value of skewness of \( \nabla_\parallel \phi \) for \( Sc \leq 1 \) at all Reynolds numbers is typically between 1 and 2 with the smallest value (\( \sim 0.3 \)) occurring at the highest Schmidt number (\( Sc=1024 \)). This apparent trend of decreasing skewness at high Schmidt number is, however, just one facet of the deeper question of whether local isotropy would be recovered in the limit of infinite Schmidt number. In any case, the results suggest that local isotropy is a better approximation at high Schmidt number. This positive skewness itself is usually thought to be due to the occurrence of ramp-cliff structures of preferred orientation induced
by the mean gradient, e.g., Antonia and Van Atta (1978). If so, a reduction of skewness may be the result of the orientation of these structures in space becoming more randomized. The effects of high Schmidt number on these structures have not yet been investigated in detail though a beginning has been made in Schumacher (2003).

It is emphasized that the observed values of the skewness of $\nabla_{\parallel} \phi$ as shown in Tables 3.3-3.5 do not decrease with increasing Reynolds number, which is consistent with various results at high Reynolds number in the literature (Warhaft 2000). On the other hand, the flatness factors show increasing closeness between $\nabla_{\parallel} \phi$ and $\nabla_{\perp} \phi$ at high Schmidt numbers. It is also noted that the flatness of $\nabla_{\parallel} \phi$ and $\nabla_{\perp} \phi$ monotonically increases with Reynolds number. For a more complete picture, higher-order moments are also studied. Normalized third, fifth and seventh moments ($\mu_3, \mu_5, \mu_7$) of $\nabla_{\parallel} \phi$, shown in Fig. 3.17(c), seem to decrease with $Sc$. (The situation for moments of yet higher orders is unclear because they are subject to large uncertainties in statistical sampling.) The rates of decrease depend on the order of the moment. It is clear that, if the seventh order moment is to ultimately reach the isotropic value of zero, the Schmidt number would have to be extremely high. It is noticed that at small $Sc$ the odd-order moments of $\nabla_{\parallel} \phi$ are larger for higher Reynolds number, but as $Sc$ increases, the odd-order moments decrease faster at higher Reynolds number, which suggests that better approximation of local isotropy can be achieved in the limit of both high $Sc$ and $Re$.

A positive skewness for $\nabla_{\parallel} \phi$ as seen in Fig. 3.17(a) and 3.17(c) means that large positive fluctuations are more likely than negative ones. The probability density function (PDF) of $\nabla_{\parallel} \phi$ in normalized form is shown in Fig. 3.18(a) and (b) at $R_\lambda \approx 38$ and $R_\lambda \approx 8$ for various Schmidt numbers. The PDF becomes more nearly symmetric at higher $Sc$, which is consistent with the reduction in skewness noted above. Schmidt number effects appear to be primarily felt via increased probabilities for large negative fluctuations. The increasing “width” of the PDF at high Schmidt number also indicates increased non-Gaussianity and intermittency. Comparison of Fig. 3.18(a) and Fig. 3.18(b) shows that the PDF of scalar gradient is “wider” at higher Reynolds number, which suggests increased intermittency with Reynolds number and is consistent with the flatness of $\nabla_{\parallel} \phi$ shown in Tables 3.3-3.5. The
form of the PDF is apparently close to exponential in the range between 5 to 15 standard deviations. However, because of sampling limitations, the behavior at the extreme tails is somewhat uncertain.

Statistical relationships between velocity gradient and scalar gradient fluctuations expressed as “mixed” derivative moments are also relevant tests of isotropy. Similar to the mixed gradient skewness \( S_{u\phi} \) (Eq. 3.9), the mixed gradient flatness is defined by

\[
F_{u\phi} \equiv \left( \frac{\partial u}{\partial x} \right)^2 \left( \frac{\partial \phi}{\partial x} \right)^2 \left/ \left( \left( \frac{\partial u}{\partial x} \right)^2 \left( \frac{\partial \phi}{\partial x} \right)^2 \right) \right.
\]

(3.16)

Similar quantities \( S_{v\phi}, S_{w\phi} \) and \( F_{v\phi}, F_{w\phi} \) defined in the other \((y, z)\) coordinate directions are also calculated. Numerical values of \( S_{u\phi} \) and \( F_{u\phi} \) listed in Tables 3.1 and 3.2 show that the mixed skewness and flatness are generally larger in the direction of the mean scalar gradient. The contrast among different coordinate directions is strongest for low Schmidt number, but becomes less so at higher Reynolds number and/or Schmidt number. If gradients of velocity and scalar were statistically independent, the mixed skewness would be zero, and the mixed flatness would be unity. However, the data do not show a clear trend towards these asymptotic states.

In addition to single-point statistics presented above, it is useful to consider the degree of local isotropy as a function of scale size. In Fig. 3.19(a) and (b), it is shown that the skewness structure function

\[
\mu_3(r) \equiv \frac{\langle |\Delta_{\|} \phi(r)|^3 \rangle}{\langle |\Delta_{\|} \phi(r)|^2 \rangle^{3/2}}
\]

(3.17)

This is the skewness of the increment \( \Delta_{\|} \phi(r) \). Similar to measurements in grid turbulence with transverse temperature gradient (Mydlarski and Warhaft 1998), this function is found to be non-negative for all scale sizes \( r \). Furthermore, contrary to local isotropy, this skewness becomes larger as \( r \) becomes smaller. At \( r \) of order \( \eta_B \) or less, different curves are seen to approach plateaus of different heights, corresponding to the skewness of \( \nabla_{\parallel} \phi \) (see Tables 3.3-3.5). All curves approach zero for large \( r \), because \( \Delta_{\parallel} \phi(r) \) would then become a difference between two independent random variables. For high \( Sc \) (e.g., curve H for \( Sc = 64 \) and curve I for \( Sc = 1024 \)), there is some hint of an intermediate scaling range at the highest \( Sc \) for both cases, where the skewness becomes nearly independent of \( r \). This observation

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suggests the emergence of a viscous-convective range, where a small deviation from local isotropy exists at the level of the third-order moment.

### 3.3 Intermittency: effects for high Schmidt numbers

The small-scale intermittency of the passive scalar field is usually expressed in terms of the statistical properties and spatial structure of scalar gradients and the dissipation rate. The prime concern in this chapter is how the small-scale intermittency depend on the Schmidt number, with observations of Reynolds number dependence also providing a useful contrast. In Chapter 4, intermittency as a function of scale size is discussed through two-point statistics of dissipation.

Tables 3.3-3.5 also present several moments of the scalar dissipation rate, and of its logarithm. Because $\chi$ is a non-negative random variable, both its skewness and flatness factors are indicators of the occurrence of intense fluctuations that are large compared to the mean value. In addition, the ratio $\sigma_{\chi}/\langle \chi \rangle$ (where $\sigma_{\chi}$ is the standard deviation) as well as the variance of $\ln \chi$ provide information on intermittency characteristics (Monin and Yaglom 1975, Frish 1995). From Tables 3.3-3.5 it is clear that, for a fixed Schmidt number, intermittency increases with Reynolds number.

To interpret Schmidt number effects it is noted first that, for the same Reynolds number and Schmidt number, all measures of intermittency from simulations at higher grid resolutions are consistently stronger than those at lower resolutions. Such cases include $Sc = 16$ at $R_\lambda \approx 38$, $Sc = 64$ and $Sc = 256$ at $R_\lambda \approx 8$, which suggest that intermittency may be underestimated if the grid resolution is not sufficiently refined. In other words, it is likely that the intermittency at $Sc = 64$, $R_\lambda \approx 38$ and $Sc = 1024$, $R_\lambda \approx 8$ (as well as at $Sc = 1$ for $R_\lambda = 140, 240$ and 390) is somewhat stronger than suggested in Tables 3.3-3.5. The flatness of the scalar dissipation, which is highly intermittent, is also subject to substantial statistical uncertainty. However, it is worth noting that, although the ensemble-averaged moments individually depend on $Sc$, a scatter plot of the flatness versus skewness (with one data point for each realization) from all realizations at all Reynolds
number ($R_\lambda \approx 8, 38, 140, 240, 390$) and all Schmidt numbers ($Sc$ from $1/8$ to $1024$), as shown in Fig. 3.22, is essentially universal independent of $Sc$ and $R_\lambda$. In other words, despite the substantial variability expected for higher-order moments, all realizations obey a systematic trend, which in Fig. 3.22 is represented as a power-law variation with an exponent of 2.33 by least-square fit. It is interesting to note that all realizations at different Reynolds numbers and Schmidt numbers have similar scaling behavior, although some deviations appear for $R_\lambda \approx 8$ and $R_\lambda \approx 390$. In Yeung et al. (2002), results at the same $R_\lambda \approx 38$ appear to have better power law scaling.

Some general conclusions on Schmidt number dependence can be drawn. It has been seen in Tables 3.3-3.5 and Fig. 3.17(b) that the flatness factor of scalar gradients increases with $Sc$ for low values of $Sc$, but varies little at higher $Sc$. Overall, it can be said that, consistent with other works in the literature (Bogucki et al. 1997, Vedula et al. 2001), all measures of intermittency for scalar dissipation at $Sc = 1$ are more pronounced than those for energy dissipation. In addition, it seems clear that the flatness of scalar gradient stops increasing for $Sc$ greater than $\sim 10$. This saturation of the flatness data suggests that some asymptotic state is reached as $Sc \to \infty$. Data on the skewness of $\ln \chi$ indicate that $\chi$ is more symmetric or closer to lognormal at higher Reynolds numbers: $\mu_3(\ln \chi)$ remains between $-0.2$ to $-0.5$ at $R_\lambda \approx 8$ and 38, whereas its magnitude is less than 0.1 at higher Reynolds number cases. Theories (Chertkov et al. 1998) based on rapidly varying Gaussian velocity fields suggest that $\chi$ has a stretched-exponential PDF in the limit of very high Schmidt number.

Finally, before a more detailed discussion on intermittency in inertial-convective range and viscous-convective range in the next chapter, let us consider intermittency as a function of scale size in terms of scalar structure functions for the quantities $\Delta_\parallel \phi(r)$ and $\Delta_\perp \phi(r)$ with separation distance taken in the parallel and perpendicular directions, respectively, as shown in Fig. 3.20 and 3.21 for $R_\lambda \approx 38$ and $R_\lambda \approx 8$ respectively. It can be seen that although, for $Sc > 4$ at $R_\lambda \approx 38$ and higher $Sc$ at $R_\lambda \approx 8$, the increasing trend ceases to hold for small scales, it does persist for intermediate scale sizes. This is especially true in the parallel direction. At $R_\lambda \approx 8$, the flatness structure function curves are closer at high
$Sc$ indicating closer approximation of high $Sc$ limit. At lower Schmidt numbers $\Delta_{||}\phi(r)$ is more intermittent than $\Delta_{\perp}\phi(r)$, but this difference (which is an indication of anisotropy at scale size $r$) appears to vanish in the $Sc \gg 1$ limit.

In this Chapter, discussions have been given for the DNS results on scalar spectrum and structure functions at Reynolds numbers that are high enough to have inertial-convective range. The DNS data support the KOC $-5/3$ scaling in inertial-convective range. The scalar spectrum at high Schmidt numbers appears to have a Batchelor $k^{-1}$ scaling range. Discussions on the issues of local isotropy and small-scale intermittency at high Schmidt numbers are also given through statistics of scalar gradient and scalar dissipation. Local isotropy appears to be a better approximation at high Schmidt numbers and small-scale intermittency tends to approach an asymptotic level in the high Schmidt limit.
Table 3.1: Mixed gradient skewness and flatness at $R_\lambda$ up to 390.

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**Table 3.2:** Mixed gradient skewness and flatness at $R_\lambda \approx 8$.

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41
Table 3.3: Statistical moments of scalar gradients and the scalar dissipation at $R_\lambda \approx 38$.

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Table 3.4: Statistical moments of scalar gradients and the scalar dissipation at $R_\lambda$ up to 390.

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FIG. 3.1. Compensated spectrum according to Obukhov-Corrsin variables (Eq. 3.1) for passive scalars at different Schmidt numbers (open symbols for $1/8$, closed symbols for 1.0). Triangles, circles and squares denote Reynolds number at 90, 140 and 240 respectively. Cross and plus denote $Sc = 1$ and $1/8$, respectively, at $R_\lambda \approx 390$. Dashed line at 0.67 is for comparison with experiments.
FIG. 3.2. Compensated one-dimensional spectrum for scalars of $Sc = 1/8$ (triangles) and $Sc = 1$ (circles) at $R_\lambda \approx 390$. Dashed line at 0.4 is for comparison with experiments (Sreenivasan 1996). Also shown for comparison are: Squares for one-dimensional longitudinal energy spectrum in DNS, and unmarked solid line for data on scalar spectrum from Mydlarski & Warhaft (1998) at $R_\lambda \approx 582$ and Prandtl number of 0.71.
FIG. 3.3. Obukhov-Corrsin scaling of component-averaged second-order structure function of passive scalars at different Schmidt numbers (open symbols for $1/8$, closed symbols for 1.0). Triangles, circles and squares denote Reynolds number at 90, 140 and 240 respectively. Cross and plus denote $Sc = 1$ and $1/8$, respectively, at $R_\lambda \approx 390$. The dotted line shows the small $r$ asymptote (Eq. 3.4). Dashed line at 1.608 is for comparison with experiments. The inset shows second-order structure function normalized by the scalar variance (which is not dependent on $r$), with dashed line at the value 2.0.
FIG. 3.4. Scaling of mixed third-order velocity-scalar structure function, compared with Yaglom’s relation (Eq. 3.7). Symbols are same as in Fig. 3.3. Dashed line at 2/3 is for comparison with Yaglom’s exact result.
FIG. 3.5. Normalized third-order velocity-scalar structure function for $Sc = 1$ at $R_\lambda \approx 390$, with separation distance $r$ taken in different coordinate directions (triangles, circles and squares for $x$, $y$, $z$, respectively).
FIG. 3.6. Even-order compensated scalar structure functions. Curves A and B are at $R_\lambda \approx 240$ for $Sc = 1/8$ and $Sc = 1$, respectively. Curves C and D are at $R_\lambda \approx 390$ for $Sc = 1/8$ and $Sc = 1$, respectively. Compensation power law exponents for $Sc = 1$ at $R_\lambda \approx 390$ are $\zeta_2^\phi = 0.6$, $\zeta_4^\phi = 0.85$, $\zeta_6^\phi = 1.0$ and $\zeta_8^\phi = 1.1$. 

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FIG. 3.7. Odd-order compensated scalar structure functions, where the notations for each curve are the same as FIG. 3.6. $\zeta^\phi_3 = 0.75$, $\zeta^\phi_5 = 0.95$, and $\zeta^\phi_7 = 1.05$ for $Sc = 1$ at $R_\lambda \approx 390$. 
FIG. 3.8. Even-order compensated longitudinal velocity structure functions. Curves A, B and C are at $R_\lambda \approx 140$, $R_\lambda \approx 240$ and $R_\lambda \approx 390$, respectively. Compensation power law exponents at $R_\lambda \approx 390$ are $\zeta_2 = 0.68$, $\zeta_4 = 1.26$, $\zeta_6 = 1.75$ and $\zeta_8 = 2.15$. 
FIG. 3.9. Same as FIG. 3.8 for odd-order structure functions. $\zeta_3 = 1$, $\zeta_5 = 1.5$, and $\zeta_7 = 1.96$. 
FIG. 3.10. Scaling exponents for scalar structure functions and longitudinal velocity structure functions. Triangles and squares are DNS results at $R_\lambda \approx 390$, for scalar structure functions and longitudinal velocity structure functions, respectively. Circles are for scalar structure functions at $R_\lambda \approx 461$ and $Pr \approx 0.71$ from Mydlarski and Warhaft (1998) for temperature field in grid turbulence. Crosses are for longitudinal velocity structure functions at $R_\lambda \approx 536$ from Anselmet et al. (1984) for a turbulent jet. Dashed line with a slope of 1/3 is shown to represent KOC prediction. Solid circles are from p.166(c) of Dasi (2004) for $Sc \approx 1000$ at $Re10000$, $x = 2m$ for turbulent boundary layers.
FIG. 3.11(a). Three-dimensional spectra at $R_\lambda \approx 38$ for scalars of Schmidt numbers 1/4, 1, 4, 8, 16, 32, 64 (lines A to G respectively). The dashed line has a slope of $-1$ on logarithmic scales.
FIG. 3.11(b). Three-dimensional spectra at $R_\lambda \approx 8$ for scalars of Schmidt numbers 64, 128, 256 ($256^3$) and 256, 512, 1024 ($512^3$) (lines A to F respectively). The dashed line has a slope of $-1$ on logarithmic scales.
FIG. 3.12(a). Three-dimensional spectra normalized by Kolmogorov scaling. Same data as FIG. 3.11(a). The dashed line has a slope of 2/3.
FIG. 3.12(b). Same as FIG. 3.12(a), except at $R_\lambda \approx 8$ for $Sc = 64, 128, 256$ (256$^3$) and $Sc = 256, 512, 1024$ (512$^3$) (line A to F, respectively).
FIG. 3.13(a). Three-dimensional scalar spectrum normalized by Batchelor variables at \( R_\lambda \approx 38 \) for \( Sc = 1, 4, 8, 16, 32, 64 \) (lines A-F, respectively). Dotted curve for Batchelor’s expression (Eq. 3.13), dashed curve for Kraichnan’s (Eq. 3.14). Inset shows the same data in log-linear scales.
FIG. 3.13(b). Same as FIG. 3.13(a), except at $R_\lambda \approx 8$ for $Sc = 64, 128, 256 \ (256^3)$ and $256, 512, 1024 \ (512^3)$ (lines A-F, respectively).
FIG. 3.14. Same as FIG. 3.13(a), except for \( R_\lambda \approx 38 \) and \( Sc = 64 \) (triangle), \( R_\lambda \approx 8 \) and \( Sc = 64 \) (square) and \( R_\lambda \approx 8 \) and \( Sc = 1024 \) (circle).
FIG. 3.15(a). Scaling of second-order scalar structure function (similar to FIG. 3.3) for scalars of $Sc = 1, 4, 8, 16, 32, 64$ (lines A-F, respectively) at $R_\lambda \approx 38$. 

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FIG. 3.15(b). Same as FIG. 3.15(a) except for $Sc = 64, 128, 256 \ (256^3)$ and $Sc = 256, 512, 1024 \ (512^3)$ at $R_\lambda \approx 8$ (lines A-F, respectively).
FIG. 3.16(a). Scaling of mixed third-order velocity-scalar structure function (similar to FIG. 3.4) for scalars with $Sc = 1, 4, 8, 16, 32, 64$ (lines A-F, respectively) at $R_\lambda \approx 38$. 
FIG. 3.16(b). Same as FIG. 3.16(a) except for $Sc = 64, 128, 256 (256^3)$ and $Sc = 256, 512, 1024 (512^3)$ at $R_\lambda \approx 8$ (lines A-F, respectively).
FIG. 3.17(a). Skewness of scalar gradients in the direction parallel to the mean scalar gradient. Close symbols are for $R_\lambda \approx 38$, and open symbols for $R_\lambda \approx 8$. Solid and open squares from Mydlinski & Warhaft (1998) at $R_\lambda \approx 217,731$ for Pr=0.71, Solid circle from Tong & Warhaft (1994) at $30 < R_\lambda < 130$.  

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FIG. 3.17(b). Kurtosis of scalar gradients. Triangles are for $\Delta_\parallel \phi$ and squares are for $\Delta_\perp \phi$. Close symbols are for $R_\lambda \approx 38$, and open symbols for $R_\lambda \approx 8$. 
FIG. 3.17(c). Normalized odd-order moments of scalar gradients. Triangles are for $\mu_3$, squares are for $\mu_5$ and circles are for $\mu_7$. Close symbols are for $R_\lambda \approx 38$, and open symbols for $R_\lambda \approx 8$. 
FIG. 3.18(a). Standardized probability density function (shown as base-10 logarithm) of $\nabla_{\parallel} \phi$ for scalars of Schmidt numbers 1, 4, 8, 16, 32, 64 (lines A to F respectively) at $R_\lambda \approx 38$. Dashed curve shows a Gaussian distribution for comparison.
FIG. 3.18(b). Standardized probability density function (shown as base-10 logarithm) of $\nabla_{||} \phi$ for scalars of Schmidt numbers 1, 8, 64 (lines A-C, 128$^3$), 64, 128, 256 (lines D-F, 256$^3$) and 256, 512, 1024 (lines G-I, 512$^3$) at $R_{\lambda} \approx 8$. Dashed curve shows a Gaussian distribution for comparison.
FIG. 3.19(a). The skewness structure function of $\nabla_\parallel \phi$ (Eq. 3.17) as a function of separation on Batchelor scales, for scalars of Schmidt numbers $1/4$, $1/2$, 1, 4, 8, 16, 32, 64 (lines A to H respectively) at $R_\lambda$ 38. Dashed line shows Gaussian value of 0.
FIG. 3.19(b). Same as FIG. 3.19(a), except for Schmidt numbers 1, 8, 64 (lines A-C, 128$^3$), 64, 128, 256 (lines D-F, 256$^3$) and 256, 512, 1024 (lines G-I, 512$^3$).
FIG. 3.20(a). The flatness structure function of $\nabla_\parallel \phi$ with symbols same as FIG. 3.19(a). Dashed line shows Gaussian value of 3.
FIG. 3.20(b). The flatness structure function of $\nabla_\perp \phi$ with symbols same as FIG. 3.20(a).
FIG. 3.21(a). The flatness structure function of $\nabla_\parallel \phi$ with symbols same as FIG. 3.19(b).
FIG. 3.21(b). The flatness structure function of $\nabla_\perp \phi$ with symbols same as FIG. 3.19(b).
FIG. 3.22. Plot of flatness versus skewness for the scalar dissipation. Each data point represents one realization taken from our data sets at various Reynolds numbers of $R_\lambda \approx 8$, $R_\lambda \approx 38$, $R_\lambda \approx 140$, $R_\lambda \approx 240$ and $R_\lambda \approx 390$. The dashed line is a least-square fit, with a slope of 2.33.
CHAPTER IV

INTERMITTENCY EXPONENTS OF ENERGY AND SCALAR DISSIPATION

In this chapter, the two-point statistics of energy and scalar dissipation are studied, which contain information on intermittency at different scale sizes. The effects of Schmidt number and Reynolds number on the intermittency properties are discussed through intermittency exponent, which is the power law exponent of the two-point statistics in a certain scaling range.

4.1 Background

Inertial range intermittency in turbulence has been found in many experimental and numerical investigations, which show discrepancies of scaling exponents from the prediction of self-similar theories of Kolmogorov (1941), Obukhov (1949) and Corrsin (1951). Kolmogorov (1962) introduced the log-normal model for energy dissipation, which provides adjustment to the scaling exponent of local energy dissipation \( \epsilon_r \) averaged over a sphere of diameter \( r \). Inclusion of intermittency effects will affect the scaling of spectrum in wavenumber space, structure functions and the two-point statistics of dissipation.

In the literature (Sreenivasan and Kailasnath 1993) several related definitions for intermittency exponents have been used. Three definitions of the intermittency exponent are considered, two of which are based on the local average \( \epsilon_r \), and one is derived from the two-point correlators of \( \epsilon \) evaluated at spatial separations in the inertial range. Kolmogorov (1962) conjectured that the second-order moments of local energy dissipation has scaling behavior

\[
\langle \epsilon_r^2 \rangle \sim r^{-\mu_1},
\]

where \( \mu_1 \) is a positive constant that is usually referred to as the intermittency exponent. It
follows from the lognormal assumption that the \( n^{th} \) order moment of \( \epsilon_r \) scales as

\[
\langle \epsilon_r^n \rangle \sim r^{-(n-1)\mu_1/2},
\]

(4.2)

The corresponding structure functions scale as

\[
\langle (\Delta_r u)^n \rangle \sim r^{n[1-1/6\mu_1(n-3)]/3},
\]

(4.3)

where the term containing \( \mu_1 \) is the intermittency correction to the Kolmogorov’s (1941) \( r^{n/3} \) scaling. The inertial range spectrum will also be modified according to

\[
E(k) \sim k^{-(5/3+\mu_1/9)}.
\]

(4.4)

Hence, determination of the intermittency exponent \( \mu_1 \) is useful for assessing intermittency correction to the energy spectrum, structure functions and the two-point statistics of dissipation. The behavior of \( \epsilon_r \) and the value of \( \mu_1 \) is often of great interest in various intermittency models such as the multifractal model (Meneveau and Sreenivasan 1987, 1991) and the mapping closure model (She and Orszag 1991), to name a few. The general relation between the structure functions and moments of local energy dissipation that is independent of specific intermittency model is

\[
\langle (\Delta_r u)^m \rangle \sim r^{m/3}\langle \epsilon_r^{m/3}\rangle,
\]

(4.5)

i.e., \( \zeta_m = m/3 + \tau_m/3 \), where \( \langle (\Delta_r u)^m \rangle \sim r^{\zeta_m} \) and \( \langle \epsilon_r^m \rangle \sim r^{-\tau_m} \).

Kolmogorov (1962) also suggests that the variance of \( \ln \epsilon_r \) varies with \( r \) in the form

\[
\sigma_{\ln \epsilon_r}^2 = A + \mu_2 \ln(L/r), \quad (\eta \ll r \ll L),
\]

(4.6)

where \( L \) is a large-eddy length scale, and \( A \) is a coefficient dependent on the large scales. However, accurate evaluation of the statistics of \( \epsilon_r \) is difficult because averaging over many data points is required to produce each sample of \( \epsilon_r \), especially in three dimensions. It is easier to use the two-point correlator

\[
\langle \epsilon(x)\epsilon(x+r) \rangle \sim \langle \epsilon \rangle^2 (r/L)^{-\mu_3}, \quad (\eta \ll r \ll L),
\]

(4.7)
which expresses the statistical relationships between fluctuations of \( \epsilon \) at two points at distance \( r \) apart in space. If a line average is used to define \( \epsilon_r \), then an exact relationship applicable for homogeneous turbulence is (Monin & Yaglom 1975, p. 618)

\[
\langle \epsilon(x) \epsilon(x + r) \rangle = \frac{1}{2} \frac{d^2}{dr^2} \left( r^2 \langle \epsilon_r^2 \rangle \right). \tag{4.8}
\]

This relation implies that if a well-defined scaling range exists then \( \mu_1 \) and \( \mu_3 \) should be equivalent to each other, although not necessarily equal to \( \mu_2 \).

Most of the known results in the literature (Sreenivasan et al. 1993, Sreenivasan & Antonia 1997) suggest intermittency exponent \( \mu_1 \) and \( \mu_3 \) for the energy dissipation rate to be about \( 0.25 \pm 0.05 \), with no strong dependence on the Reynolds number. A considerable fraction of the known data on this subject has been derived from experiments, where, because of measurement limitations, one-dimensional surrogates (e.g. the squared velocity gradient, \( (\partial u/\partial x)^2 \)) are typically studied in place of the full dissipation rate, and Taylor’s frozen turbulence hypothesis is often invoked to convert time derivatives to space derivatives. However, there is no guarantee that the full dissipation rate would have the same behavior.

Recent work comparing longitudinal and transverse velocity structure functions (e.g. Chen et al. 1997, Shen & Warhaft 2000) also suggest that longitudinal and transverse velocity gradients have different scaling exponents. Exponents for symmetric and anti-symmetric components of the velocity gradient tensor leading to energy dissipation and enstrophy (vorticity squared) respectively may also differ, at least at moderate Reynolds numbers.

A detailed understanding of possible differences in inertial-range intermittency of different components of velocity gradients is thus important, and would also help resolve the issue (Nelkin 1999) of whether observed differences in the intermittency of enstrophy and energy dissipation would vanish in the high Reynolds number limit. In addition to the velocity field, important questions also arise in characterizing the intermittency of the dissipation rate of passive scalar fluctuations as a function of the Schmidt number which can vary widely in applications.

For the scalar dissipation rate, the scaling range of interest depends on the Schmidt number. In particular, two ranges are considered: (a) the inertial-convective range \( \{n, n_{IC} \} \leq \)
$r \leq L$ based on the Obukhov-Corrsin scale $\eta_{OC} = \eta Sc^{-3/4}$ for scalars with $Sc = O(1)$ or less at high Reynolds number, and (b) the viscous-convective range $\eta > r > \eta_B$ based on the Batchelor scale $\eta_B = \eta Sc^{-1/2}$ for scalars with $Sc \gg 1$.

In Sec. 4.2, discussions of results on intermittency exponents of the velocity field for energy dissipation and enstrophy and issues of one-dimensional surrogacy for energy dissipation are given. Section 4.3 provides discussions on intermittency exponents of scalar dissipation, including the issues of Reynolds number and Schmidt number effects and the properties of one-dimensional surrogates represented by one component of scalar gradient.

### 4.2 Velocity field intermittency

In this section, basic results are presented on inertial-range intermittency exponents of the energy dissipation rate and enstrophy at different Reynolds numbers. The effects of surrogacy and dimensionality of local averaging are also studied.

For some background information, it is necessary to refer to several one-point statistics of the dissipation as given in Table 4.1. The mean dissipation rate is mainly set by forcing parameters (i.e. energy input at the large scales) and hence almost the same in the higher Reynolds number runs where the viscosity has been varied while the forcing parameters are kept fixed. The increase of intermittency with Reynolds number can be seen directly via the ratio $\langle \epsilon^2 \rangle / \langle \epsilon \rangle^2$, as well as the skewness and flatness of $\epsilon$, which reflect the emergence of wide tails in the probability density function (PDF) of the dissipation rate. The variance of $\ln \epsilon$ also increases with Reynolds number. Although the log-normality hypothesis is known to be inaccurate for high-order moments, the skewness and flatness values of $\ln \epsilon$ are closer to Gaussian (0 and 3 respectively) at higher Reynolds number.

Fig. 4.1(a,b,c) shows the quantities $\sigma_{\ln \epsilon_r}^2$, $\langle \epsilon_r^2 \rangle$ and $\langle \epsilon(x) \epsilon(x+r) \rangle$ (normalized by $\langle \epsilon \rangle^2$) as a function of Kolmogorov-scaled separation at different Reynolds numbers. In principle, in the limit of $r \to 0$ these quantities should approach the single-point moments in Table 4.1, with both $\langle \epsilon_r^2 \rangle / \langle \epsilon \rangle^2$ and $\langle \epsilon(x) \epsilon(x+r) \rangle / \langle \epsilon \rangle^2$ approaching the dimensionless ratio $\langle \epsilon^2 \rangle / \langle \epsilon \rangle^2$.

The DNS results at low Reynolds number agree with this expectation since data points
for \( r \) a few times smaller than the Kolmogorov scale are available. In the higher Reynolds number cases, the resolution is \( \Delta x \approx 2\eta \) which is not fine enough to reach the small \( r \) limit for the second-order moments. This indicates that dissipation fluctuations are highly localized in space and their full resolution demands \( \Delta x \ll \eta \) which unfortunately cannot be readily accommodated using the resources available. At the other extreme, as \( r \) approaches the size of the solution domain, \( \epsilon_r \) approaches the global average \( \langle \epsilon \rangle \), and \( \langle \epsilon(x)\epsilon(x+r) \rangle / \langle \epsilon \rangle^2 \) approaches unity as the values of \( \epsilon \) at two points far apart become statistically independent.

Plots in the form of Fig. 4.1 (giving \( \mu_1, \mu_2 \) and \( \mu_3 \) from parts (a), (b) and (c) of the figure respectively) are used to evaluate intermittency exponents, i.e., the slopes of linear segments in the range of \( r/\eta \) that provides the closest resemblance of inertial range behavior. Because a wide scaling range is not expected at Reynolds numbers currently reachable in DNS, the range of \( r/\eta \) for measuring exponents must be chosen very carefully. Based on Anselmet et al. (1984), the third-order velocity structure function (whose classical inertial-range form is described by an exact expression free of empirical constants) are used. The DNS results of \( \langle (\Delta_r u)^3 \rangle / r \) (e.g. Fig. 7 in Yeung & Zhou 1997) are plotted and for each curve a range of \( r \) is selected such that it appears to be closest to a plateau and also satisfies the condition \( \eta \ll r \ll L \). The scaling exponents are taken as the slope of a straight line approximated by least-square method for the data points in the chosen scaling range. The intermittency exponents are also calculated by the method of logarithmic derivatives, i.e.,

\[
\frac{\text{dlog}\langle \epsilon^2 \rangle}{\text{dlog}(r/\eta)}
\]

(Praskovsky and Oncley 1997). Results from these two procedures are quite similar. The inset in Fig. 4.1(c) for the two-point correlator at \( R_\lambda 390 \) shows the logarithmic slopes as a function of \( r/\eta \) where \( \mu_3 \) is taken as the value of the logarithmic slope at \( r/\eta \approx 80 \) where the curve is seen to flatten slightly.

The best estimates of the intermittency exponents for energy dissipation and enstrophy (to be discussed later) at \( R_\lambda \approx 140,240 \) and 390 are given in Table 4.2. The ranges of \( r/\eta \) where these exponents are measured are also included. As expected, the applicable scaling range widens with increasing Reynolds number. The exponent \( \mu_3 \) obtained from the two-point correlator shows a significant increase with the Reynolds number, which is consistent with data trends found in experiments by Mydlarski & Warhaft (1998) but may also be
an effect of moderate Reynolds number in DNS. For the case of highest \( R_\lambda \) (390), the exponents \( \mu_1 \) and \( \mu_3 \) obtained from Fig. 4.1(b) and (c) are 0.2 – 0.23 and 0.17 – 0.21, which are somewhat less than, but still reasonably close to the mid-range value 0.25 in Sreenivasan \textit{et al.} (1993). Furthermore, it can be seen that \( \mu_1, \mu_2 \) and \( \mu_3 \) become closer together at higher \( R_\lambda \), which is consistent with the development of a wider and better-defined scaling range.

As noted in Sec. 1, the dimensionality of the averaging domain may affect the statistics of the local dissipation \( \epsilon_r \). In Fig. 4.2 Comparisons are made for \( \langle \epsilon_r^2 \rangle \) obtained by averaging in 1D, 2D and 3D respectively. The data trends seen in parts (a) and (b) of the figure for \( R_\lambda \approx 140 \) and 390 are quite similar except that the latter exhibits a wider range of scales and stronger intermittency overall. For all values of \( r \) the value of \( \langle \epsilon_r^2 \rangle \) is found to become smaller with increasing averaging dimensions. This is because, for a given value of \( r \), averaging in two- and three-dimensions involve progressively more grid points in each sample of \( \epsilon_r \), such that contributions from highly localized fluctuations are diluted somewhat by lower values of \( \epsilon \) elsewhere in the domain of averaging. The effect is more pronounced at intermediate values of \( r \), and would be more so if higher-order moments were considered. It appears that the intermittency exponents are slightly larger by three-dimensional averaging than two and one-dimensional averaging, though the dependence is rather weak.

Because of the widespread (and often inevitable) use of the one-dimensional surrogate \( \epsilon' = 15\nu(\partial u/\partial x)^2 \) in investigations of dissipation intermittency, it is important to determine the nature of differences between results based on \( \epsilon' \) and \( \epsilon \). Some past efforts at resolving this issue include the DNS studies in Chen (1993) and Wang \textit{et al.} (1996), and more recently Cleve \textit{et al.} (2003) which is based on measurements of more than one velocity gradient component in an atmospheric boundary layer. The results in Cleve \textit{et al.} suggest that although the statistics of \( \epsilon \) and \( \epsilon' \) differ at the small scales their intermittency exponents are almost the same. Figure 4.3(a,b) show, at two different Reynolds numbers, the normalized two-point correlators of the full energy dissipation, and the squares of longitudinal and transverse velocity gradients. (Note the directions along which \( r \) is taken, as stated in the figure captions.) It can be seen that at the small scales, both \( (\partial u/\partial x)^2 \) and \( (\partial u/\partial y)^2 \)
are more intermittent than $\epsilon$, which can be understood by noting that $\epsilon$ is the sum of contributions from both longitudinal and transverse velocity gradients. In the inertial range the normalized two-point correlators of $\epsilon$ and $(\partial u/\partial x)^2$ are almost the same, especially at high Reynolds number, which suggests that the use of longitudinal gradients squared as a 1-D surrogate for energy dissipation in inferring intermittency exponents is acceptable. However, it should be noted that the transverse gradient $(\partial u/\partial y)^2$ is more intermittent and has a much shorter scaling range. These results are consistent with Cleve et al. (2003).

For completeness, results of two-point correlator for different coordinate components of the velocity gradient squared are also included, which in general can be written as 
\[ \langle (\partial u_\alpha/\partial x_\beta)^2(x) (\partial u_\alpha/\partial x_\beta)^2(x+r_{\gamma}) \rangle, \] 
with summation taken over repeated Greek subscripts and normalization based on the mean square of $\partial u_\alpha/\partial x_\beta$. If local isotropy is assumed, then there are five statistically distinct combinations, namely (i) $\alpha = \beta = \gamma$; (ii) $\alpha = \beta \neq \gamma$; (iii) $\alpha \neq \beta, \alpha = \gamma$; (iv) $\alpha \neq \beta, \beta = \gamma$; (v) $\alpha \neq \beta \neq \gamma$. Cases (i) and (iv) correspond to the data in Fig. 4.3. All five combinations are shown in Fig. 4.4, at $R_\lambda \approx 390$. Except for the case of (v), it is found that, as in Fig. 4.3, the differences are mainly significant at the small scales and they tend to become smaller in the inertial range. This suggests the use of one-dimensional surrogates in experiments may give adequate results at sufficient high Reynolds number.

Another indirect method for obtaining the dissipation intermittency exponent is through the sixth-order velocity structure function. It is based on a scaling relation suggested by Frisch et al. (1978), namely
\[ \langle \epsilon(x)\epsilon(x + r) \rangle \sim \langle (\Delta_r u)^6 \rangle / r^2 \]  
(4.9)

where $\Delta_r u$ is a longitudinal velocity increment over a distance $r$ in the inertial range. Frisch (1978) noted that this relation may be justified in part by estimates of energy transfer in the inertial range, and that it is satisfied by both the lognormal (Kolmogorov 1962) and the $\beta$-models (Frisch et al. 1978) of intermittency. Figure 4.5 shows the normalized sixth-order structure function at $R_\lambda \approx 140, 240,$ and 390. The logarithmic slope shown in the inset illustrates clearly the trend towards a wider scaling range as the Reynolds number
increases. The intermittency exponent inferred from this figure is close to 0.25 (as marked by the dashed line), which is consistent with the values in preceding figures obtained by other means. The utility of Eq. 4.9 is that (despite challenges in sampling) sixth-order velocity structure functions are easier to measure than the full, three-dimensional dissipation rate. However, it has no analog for other flow variables such as enstrophy and scalar dissipation.

Finally, Fig. 4.6(a,b,c) show results for enstrophy $\Omega \equiv \omega^2$ similar as in Fig. 4.1. At small $r$ the highest values seen in these curves compared to those in Fig. 4.1 indicate that enstrophy is more intermittent than dissipation as measured by single-point moments: e.g. $\langle \Omega^2 \rangle / \langle \Omega \rangle^2$ is larger than $\langle \epsilon^2 \rangle / \langle \epsilon \rangle^2$. However, the inertial-range intermittency exponents obtained in Table 4.1 are close to those for the energy dissipation, especially if viewed in terms of $\mu_2$ based on the logarithms of the local averages. The DNS data also support some suggestions in the literature (Nelkin 1999) that the scaling of dissipation and enstrophy become similar in the inertial range at high Reynolds number.

4.3 **Intermittency of scalars**

In this section, the intermittency of scalar dissipation is studied via the scaling behavior of quantities analogous to those for energy dissipation, namely the logarithmic variance $\sigma_{\ln \chi}^2$, the mean-squared box average $\langle \chi^2 \rangle$, and the two-point correlator $\langle \chi(x)\chi(x+r) \rangle$. Although many studies of scalar gradient and scalar dissipation statistics (e.g. Antonia & Chambers 1980, Overholt & Pope 1996, Wang, Chen & Brasseur 1999, Vedula, Yeung & Fox 2001) show that the scalar field is more intermittent than the velocity, the value of the scalar dissipation intermittency exponent obtained from the quantities above, and as a function of Schmidt number, is not well determined in the literature. It is necessary to distinguish between two scaling ranges, namely the inertial-convective range at high Reynolds number, and the viscous-convective range at high Schmidt number. Before presenting detailed results for the scalar dissipation, the issue of scalar gradient surrogacy for scalar dissipation, which may be affected by deviations of scalar field from local isotropy, is also reviewed.

A. **Scalar gradient surrogacy for scalar gradients**
The square of a scalar gradient component is often used as a one-dimensional surrogate for the scalar dissipation although Sreenivasan et al. (1977) has pointed out that direct measurement of $\chi$ is not as difficult as $\epsilon$ since only three separate components are involved. The latter can be defined as $\chi_{\alpha} = 2D(\partial \phi / \partial x_{\alpha})^2$ for $\alpha = 1, 2, 3$, whose characteristics may depend on orientation relative to the direction of the mean scalar gradient in the flow. From the identity $\chi = \sum_{\alpha=1}^{3} \chi_{\alpha}$, it can be written the two-point correlator of $\chi$ as the sum of three terms of the form $\langle \chi_{\alpha}(x) \chi_{\alpha}(x+r) \rangle$ and six “cross” terms of the form $\langle \chi_{\alpha}(x) \chi_{\beta}(x+r) \rangle$ (with $\alpha \neq \beta$).

Figure 4.7(a,b) compare the two-point correlators of the scalar dissipation, where components parallel and perpendicular to the mean gradient are distinguished as $\chi_{\parallel}$ and $\chi_{\perp}$, respectively. For $\chi$, average is taken for the two-point correlator over $r$ in three coordinate directions, whereas for $\chi_{\parallel}$ and $\chi_{\perp}$, $r$ is chosen in the same direction as the gradient component. To put the results in the context of local isotropy (or deviation therefrom), the following data sets have been chosen: (a) a high $R_{\lambda}$ data set at $Sc = 1$ which deviates substantially from local isotropy, and (b) high $Sc$ data sets for which (Yeung et al. 2002, 2004) local isotropy holds substantially better. It is clear that the observed differences among $\chi$, $\chi_{\parallel}$ and $\chi_{\perp}$ for the high Schmidt number case are smaller. As the sum of three intermittent random variables, scalar dissipation $\chi$ is expected to be less intermittent than its individual components. This is reflected in the normalized two-point correlators for $\chi$ being at lower values than those of $\chi_{\parallel}$ and $\chi_{\perp}$ in the limit of small $r$. For values of $r$ slightly larger in the dissipation range the two-point correlators for both $\chi_{\parallel}$ and $\chi_{\perp}$ decay more rapidly than $\chi$ until they become close at values of $r$ much larger than $\eta_B$ (or $\eta$ in the case of $Sc = 1$).

Measurements of intermittency exponents for $\chi$ and its three component surrogates were previously reported by Sreenivasan et al. (1977) for the case of a heated boundary layer, based on $Var(\ln \chi_{r})$ with one-dimensional averaging. Figure 4.8(a,b) show the DNS results for $Var(\ln \chi_{r})$ (and similar for $\chi_{\parallel}$ and $\chi_{\perp}$, with three-dimensional averaging over a cube). As in Fig. 4.7, two data sets have been chosen, one at high Reynolds number, and one at high Schmidt number, with different degrees of departure from local isotropy. The DNS results are consistent with Sreenivasan et al. (1977) in indicating stronger intermittency.

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for the components of χ as seen via larger values of the logarithmic variance at small r. At intermediate values of r the data suggest that use of one-dimensional surrogates may lead to a slight overestimate of the intermittency exponents in the inertial-convective range (in the case of high $R_\lambda$) and more so in the viscous-convective range (in the case of high $Sc$). Comparisons with other data sets (not shown) suggest that high Reynolds number tends to reduce differences in the inertial-convective range. On the other hand, in Fig. 4.8(b), it can be seen that results for $\chi_\parallel$ and $\chi_\perp$ at high Schmidt number become almost equivalent, but both possess larger intermittency exponents than the results of $\chi$.

In viewing Fig. 4.7 and 4.8 together it seems that the effects of component surrogacy are manifested in the two-point correlators and logarithmic variances in different ways. This is not fully understood, but may be the result of the same physical processes that contribute to contrasts between results obtained by these two methods as noted elsewhere (Wang, Brasseur & Chen 1999). Also less understood is the effect of the orientation of the spatial separation vector (relative to the mean scalar gradient) on the two-point correlator, which can be generalized as $\langle \chi_\alpha(x) \chi_\alpha(x + r_\alpha) \rangle$. In the configuration of the simulations four distinct combinations of the set $\{\alpha, \beta\}$ are possible, with the situation becoming more complex yet in anisotropic turbulence where preferred orientations in the mean velocity field will also have an effect.

B. Reynolds number effects in inertial-convective range

The primary requirement for an inertial-convective range is sufficiently high Reynolds number. Fig. 4.9(a,b,c) show the functions $\sigma_{in,\chi}^2$, $\langle \chi^2 \rangle$ and $\langle \chi(x) \chi(x + r) \rangle$ at $Sc = 1$ for the three highest Reynolds numbers ($R_\lambda \approx 140, 240$ and $390$) in the simulations. Compared to results for energy dissipation in Fig. 4.1, stronger intermittency in the scalar field compared to the velocity is indicated by larger values of these normalized functions at the small scales, and by steeper negative slopes at intermediate scales. However, since the slopes of these curves are more sensitive to the choice of scaling range, great care is needed in order to obtain reliable values of the intermittency exponents. A range of $r$ is chosen such that it best approximates the so-called Yaglom relation for the mixed velocity-scalar

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third-order structure function, i.e. \( \langle \Delta r \Delta r \phi^2 \rangle = -(2/3) \langle \chi \rangle r \) for \( \eta, \eta_{OC} \ll r \ll L \). The scaling range available in the simulations is limited by the Reynolds number, and inherently narrower for scalars with \( Sc < 1 \) for which \( \eta_{OC} > \eta \). Additional ambiguities may also arise due to deviations from local isotropy, although this is in part alleviated by averaging results for \( r \) in three coordinate directions.

With the caveats noted above, the best estimates for the scalar dissipation intermittency exponents are given in Table 4.3, for scalars with \( Sc = 1/8 \) and \( Sc = 1 \). As expected from standard arguments, an increase in Reynolds number gives a wider scaling range which is also shifted towards scales increasingly large compared to \( \eta \). Because the scalar statistics scale with \( \eta_{OC} \) for \( Sc \leq 1 \) an increase in \( Sc \) from \( 1/8 \) to \( 1 \) produces the opposite trend (towards smaller \( r/\eta \)) as \( \eta_{OC} \) becomes smaller. The results agree with Wang et al. (1999) that the variance of the logarithm gives systematically larger values of the intermittency exponent. Larger intermittency exponents reflecting stronger intermittency are also expected at higher Reynolds and Schmidt numbers (at least when \( Sc = O(1) \)). However, the data in Table 4.3 do not reveal a systematic trend, presumably because the effect is weak and easily masked by uncertainties inherent in the tasks of choosing a precise scaling range and measuring the slopes of curves. Nevertheless, exponents obtained for both \( \langle \chi^2 \rangle \) and \( \langle \chi(x) \chi(x + r) \rangle \) are within the range 0.3-0.4, which is in reasonable agreement with both 0.38-0.46 in Sreenivasan et al. (1977) and 0.2-0.3 by Mydlarski & Warhaft (1998) in grid turbulence experiments.

Although the Reynolds number is the main parameter of concern in studies of the inertial-convective range, understanding of Schmidt number effects is also important. Figure 4.10 compares normalized two-point correlators of the scalar dissipation at \( Sc = 1/8 \) and \( Sc = 1 \) obtained from the \( R_\lambda \approx 390 \) simulation. In parts (a) and (b) of this figure, the distance \( r \) has been expressed in Kolmogorov and Obukhov-Corrsin scaling, respectively. In the limit \( r \to 0 \) the function shown should approach the ratio \( \langle \chi^2 \rangle / \langle \chi \rangle^2 \), which is (see Table 4.3) larger for \( Sc = 1 \) than for \( Sc = 1/8 \). This is not obvious from (a), where the normalized two-point correlator appears to be larger for \( Sc = 1/8 \) at fixed \( r \), and results for \( Sc = 1 \) do not show a clear trend towards the small \( r \) asymptote. These features arise
because the Kolmogorov scale does not (except for $Sc = 1$) represent the size of the small scales in the scalar field, and because the grid spacing is not sufficiently fine to fully resolve the small-scale content of the scalar dissipation fluctuations. (A critical discussion of local resolution requirements is given recently by Sreenivasan 2004.) The Schmidt number scaling is much clearer in (b) where $\eta_{OC}$ is used as the normalizing scale instead. In this modified scaling the normalized two-point correlators at $Sc = 1/8$ and $Sc = 1$ are seen to be very similar in shape. However a comparison of the respective intermittency exponents is still very sensitive to the chosen scaling range.

C. Schmidt number effects in viscous-convective range

Recent studies of high-Schmidt-number mixing using DNS have provided direct evidence that although both increasing $R_\lambda$ and $Sc$ produce a wider range of scales in the scalar field, their effects are very different in nature. In particular, Yeung et al. (2002, 2004) showed that high Schmidt number causes a return towards local isotropy and a saturation of intermittency while the value of $Sc$ needed for the asymptotic behavior to emerge appears to decrease with Reynolds number. Schmidt number effects are discussed in the context of dissipation statistics in the viscous-convective range i.e., for length scales $r$ such that $\eta_{B} < r < \eta$.

Fig. 4.11(a,b,c) shows the functions $\text{Var}(\ln \chi_r), \langle \chi_r^2 \rangle$ and $\langle \chi(x)\chi(x + r) \rangle$ for a range of Schmidt numbers (1 to 64) at fixed $R_\lambda$ (38), with scale size $r$ normalized by $\eta_{B}$. At the smaller scales (say $r < 10\eta_{B}$) data trends are not very well defined in $\text{Var}(\ln \chi_r)$. However, for the other two quantities it is apparent that except for $Sc = 1$ the differences between curves for different Schmidt numbers are small at small $r$. In other words, the Schmidt number dependence becomes diminished at high $Sc$, which is consistent with a trend towards saturation of intermittency in single-point statistics in the high Schmidt number limit. It is found that most curves display a scaling range roughly between $2\eta_{B}$ and $2\eta$, with a steeper slope than in the intermediate scales (say beyond $10\eta_{B}$) where all curves fall more slowly at increasing Schmidt numbers.

Intermittency exponents for the viscous-convective range obtained from the data in
Fig. 4.11 are shown in Table 4.4. In order to illustrate possible effects of inadequate resolution at the small scales, data have been included for $Sc = 16$ from two simulations at $256^3$ and $512^3$ resolution, respectively. (Only the latter, which is believed to be more accurate, is actually shown in Fig. 4.11.) The comparison suggests that a degree of resolution of $k_{\text{max}} \eta_B = 1.5$ (at $256^3$) may not be sufficient and can lead to underestimation of intermittency. (This effect is similar to that for the flatness factor of intermittent signals in space, where insufficient resolution can be considered as a local smoothing which causes some extreme fluctuations not fully captured.) With this limitation considered (and presumably applicable also to the $Sc = 64$ case at the bottom of the Table), it can be said that there are systematic trends in Schmidt number overall. The exponent obtained from the two-point correlator decreases with $Sc$, which is qualitatively consistent with experimental data by Sreenivasan & Prasad (1989). At higher Schmidt numbers it seems that these two exponents agree more closely with each other, which may be an indication of the attainment of a better-defined scaling range. Differences in the behavior of this scaling exponent from the others remain to be understood although they have been reported before (e.g. Wang, Brasseur & Chen 1999, figures 11 and 12 therein).

An inherent limitation in the results of Fig. 4.11 and Table 4.4 for $Sc$ up to 64 is that the viscous-convective range is not well-defined because of relatively small $\eta/\eta_B$. This consideration provided the motivation for simulations of even higher $Sc$ of up to 1024 (Yeung et al. 2004) albeit at even lower Reynolds number, namely $R_\lambda \approx 8$. Fig. 4.12 shows the results, scaled in the same manner as in Fig. 4.11, with corresponding scaling exponents shown in Table 4.5. For reasons similar to those noted in the discussion of Table 4.3, data at $Sc = 64$ and 256 on $128^3$ and $256^3$ grids respectively are regarded as less accurate and hence omitted from Fig. 4.12. Figure 4.13 shows the intermittency exponents for high Schmidt numbers at $R_\lambda \approx 38$ and $R_\lambda \approx 8$. The data are based on Table 4.4 and 4.5 and average value is taken whenever applicable. The intermittency exponent $\mu_3$ obtained from the two-point correlator decreases with $Sc$ and it is almost independent of $R_\lambda$ at small $Sc$. Exponent $\mu_1$ for $\langle \chi_f^2 \rangle$ slightly decreases with $Sc$ for $Sc \geq 32$. The data show that $\mu_1$ is generally smaller than $\mu_3$, but $\mu_1$ and $\mu_3$ become closer at high $Sc$. It is noted that the calculated $\mu_1$ at
small $Sc$ is subject to uncertainty arising from the low resolution and fewer data points in viscous-convective range available for the purpose of exponent calculation. The inset of Fig. 4.13 shows $\mu_2$ for $Var(\ln \chi_r)$. The results suggest that $\mu_2$ is normally larger than $\mu_1$ and $\mu_3$ but also tends to be independent of $Sc$ at high $Sc$. These various intermittency exponents suggest that intermittency shows no increasing trend in viscous-convective range at high $Sc$.

In this chapter, scalings of energy dissipation, enstrophy and scalar dissipation have been studied based on the DNS data sets for Reynolds number up to $R_\lambda \approx 390$ and $Sc$ up to 1024. Various intermittency exponents have been calculated, including those indicated by $\langle Y(x)Y(x + r)\rangle$, $\langle Y_r^2 \rangle$ and $Var(\ln Y_r)$, where $Y$ represents particularly energy dissipation, scalar dissipation and enstrophy. It is found that the velocity intermittency exponents in inertial range increase with Reynolds number, and has the value of about 0.2 in the highest Reynolds number case of $R_\lambda \approx 390$. This value is reasonably close to 0.25 cited in Sreenivasan et al. (1993). It is possible that the intermittency exponent becomes closer to 0.25 for even high Reynolds number. The velocity intermittency exponents $\mu_1$, $\mu_2$ and $\mu_3$ become closer at high Reynolds number. In calculation of $\langle Y_r^2 \rangle$, averaging over three dimensions gives slightly larger value of intermittency exponent than averaging in one dimension. Scalar intermittency exponents in the inertial-convective range are larger than those of velocity field, suggesting that the scalar field is more intermittent than the velocity field. In the viscous-convective range, scalar intermittency exponents tend to have a weak dependence on $Sc$ in the limit of high Schmidt number. The intermittency exponents $\mu_1$ and $\mu_3$ become closer at high $Sc$, however, $\mu_2$ is significantly larger than $\mu_1$ and $\mu_3$. 

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Table 4.1: Intermittency exponents for energy dissipation and enstrophy

<table>
<thead>
<tr>
<th>Statistics</th>
<th>$R_{\lambda}140$</th>
<th>$R_{\lambda}240$</th>
<th>$R_{\lambda}390$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Grid</td>
<td>256$^3$</td>
<td>512$^3$</td>
<td>1024$^3$</td>
</tr>
<tr>
<td>$\langle \epsilon \rangle$</td>
<td>1.2</td>
<td>1.25</td>
<td>1.3</td>
</tr>
<tr>
<td>$\langle \epsilon^2 \rangle/\langle \epsilon \rangle^2$</td>
<td>1.8</td>
<td>2.8</td>
<td>3.7</td>
</tr>
<tr>
<td>$L/\eta$</td>
<td>98</td>
<td>195</td>
<td>442</td>
</tr>
<tr>
<td>Measure range</td>
<td>(31-65)$\eta$</td>
<td>(47-100)$\eta$</td>
<td>(45-125)$\eta$</td>
</tr>
<tr>
<td>$\langle \epsilon^2 \rangle$</td>
<td>0.17</td>
<td>0.16-0.21</td>
<td>0.2-0.23</td>
</tr>
<tr>
<td>$\sigma_{in\epsilon, r}^2$</td>
<td>0.17</td>
<td>0.17-0.22</td>
<td>0.2-0.24</td>
</tr>
<tr>
<td>$\langle \epsilon(x)\epsilon(x+r) \rangle$</td>
<td>0.09-0.17</td>
<td>0.12-0.18</td>
<td>0.17-0.21</td>
</tr>
<tr>
<td>$\langle \Omega_{r}^2 \rangle$</td>
<td>0.21</td>
<td>0.17-0.22</td>
<td>0.22-0.29</td>
</tr>
<tr>
<td>$\sigma_{in\Omega, r}^2$</td>
<td>0.23</td>
<td>0.18-0.29</td>
<td>0.22-0.32</td>
</tr>
<tr>
<td>$\langle \Omega(x)\Omega(x+r) \rangle$</td>
<td>0.09-0.18</td>
<td>0.12-0.19</td>
<td>0.17-0.23</td>
</tr>
<tr>
<td>$\langle (\Delta u)^6 \rangle/r^2$</td>
<td>0.2-0.3</td>
<td>0.2-0.28</td>
<td>0.21-0.28</td>
</tr>
<tr>
<td></td>
<td>(60-71$\eta$)</td>
<td>(92-122$\eta$)</td>
<td>(80-170$\eta$)</td>
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</table>
Table 4.2: Intermittency exponents for scalar dissipation at higher Reynolds numbers

<table>
<thead>
<tr>
<th>$R_\lambda$</th>
<th>Grid</th>
<th>Sc</th>
<th>Range</th>
<th>$\langle \chi(x)\chi(x + r) \rangle$</th>
<th>$\langle \chi_r^2 \rangle$</th>
<th>$\sigma_{m\chi_r}^2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>140</td>
<td>$256^3$</td>
<td>1/8</td>
<td>(29-57)$\eta$</td>
<td>0.31-0.45</td>
<td>0.45-0.51</td>
<td>0.65-0.70</td>
</tr>
<tr>
<td>140</td>
<td>$256^3$</td>
<td>1</td>
<td>(17-31)$\eta$</td>
<td>0.29-0.41</td>
<td>0.42</td>
<td>0.63</td>
</tr>
<tr>
<td>240</td>
<td>$512^3$</td>
<td>1/8</td>
<td>(45-85)$\eta$</td>
<td>0.41-0.47</td>
<td>0.45-0.51</td>
<td>0.7-0.82</td>
</tr>
<tr>
<td>240</td>
<td>$512^3$</td>
<td>1</td>
<td>(19-51)$\eta$</td>
<td>0.31-0.47</td>
<td>0.40-0.50</td>
<td>0.57-0.7</td>
</tr>
<tr>
<td>390</td>
<td>$1024^3$</td>
<td>1/8</td>
<td>(76-128)$\eta$</td>
<td>0.42-0.48</td>
<td>0.48</td>
<td>0.78</td>
</tr>
<tr>
<td>390</td>
<td>$1024^3$</td>
<td>1</td>
<td>(41-93)$\eta$</td>
<td>0.33-0.36</td>
<td>0.34-0.39</td>
<td>0.52-0.61</td>
</tr>
</tbody>
</table>

Table 4.3: Intermittency exponents for scalar dissipation at $R_\lambda \approx 38$

<table>
<thead>
<tr>
<th>$R_\lambda$</th>
<th>Grid</th>
<th>Sc</th>
<th>Range</th>
<th>$\langle \chi(x)\chi(x + r) \rangle$</th>
<th>$\langle \chi_r^2 \rangle$</th>
<th>$\sigma_{m\chi_r}^2$</th>
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</thead>
<tbody>
<tr>
<td>38</td>
<td>$256^3$</td>
<td>4</td>
<td>$2\eta_B - 2\eta$</td>
<td>0.56-0.6</td>
<td>0.4</td>
<td>0.59</td>
</tr>
<tr>
<td>38</td>
<td>$256^3$</td>
<td>8</td>
<td>$2.8\eta_B - 2\eta$</td>
<td>0.52-0.56</td>
<td>0.37</td>
<td>0.69</td>
</tr>
<tr>
<td>38</td>
<td>$256^3$</td>
<td>16</td>
<td>$4\eta_B - 2\eta$</td>
<td>0.47-0.52</td>
<td>0.38</td>
<td>0.64</td>
</tr>
<tr>
<td>38</td>
<td>$512^3$</td>
<td>16</td>
<td>$2\eta_B - 2\eta$</td>
<td>0.51-0.57</td>
<td>0.37-0.45</td>
<td>0.61-0.82</td>
</tr>
<tr>
<td>38</td>
<td>$512^3$</td>
<td>32</td>
<td>$2.8\eta_B - 2\eta$</td>
<td>0.47-0.51</td>
<td>0.35-0.43</td>
<td>0.68-0.85</td>
</tr>
<tr>
<td>38</td>
<td>$512^3$</td>
<td>64</td>
<td>$4\eta_B - 2\eta$</td>
<td>0.43-0.46</td>
<td>0.35-0.39</td>
<td>0.61-0.72</td>
</tr>
</tbody>
</table>
Table 4.4: Intermittency exponents for scalar dissipation at $R_\lambda \approx 8$

<table>
<thead>
<tr>
<th>$R_\lambda$</th>
<th>Grid</th>
<th>Sc</th>
<th>Range</th>
<th>$\langle \chi(x) \chi(x + r) \rangle$</th>
<th>$\langle \chi_r^2 \rangle$</th>
<th>$\sigma_{m_{\chi_r}}^2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>8</td>
<td>128$^3$</td>
<td>4</td>
<td>$\eta_B - \eta$</td>
<td>0.58</td>
<td>0.2</td>
<td>0.37</td>
</tr>
<tr>
<td>8</td>
<td>128$^3$</td>
<td>8</td>
<td>$1.4\eta_B - \eta$</td>
<td>0.57</td>
<td>0.28</td>
<td>0.47</td>
</tr>
<tr>
<td>8</td>
<td>128$^3$</td>
<td>16</td>
<td>$2\eta_B - \eta$</td>
<td>0.47-0.52</td>
<td>0.35</td>
<td>0.59</td>
</tr>
<tr>
<td>8</td>
<td>128$^3$</td>
<td>32</td>
<td>$2.8\eta_B - \eta$</td>
<td>0.46-0.49</td>
<td>0.37</td>
<td>0.66</td>
</tr>
<tr>
<td>8</td>
<td>128$^3$</td>
<td>64</td>
<td>$4\eta_B - \eta$</td>
<td>0.43</td>
<td>0.35</td>
<td>0.62</td>
</tr>
<tr>
<td>8</td>
<td>256$^3$</td>
<td>64</td>
<td>$2\eta_B - 2\eta$</td>
<td>0.44-0.55</td>
<td>0.34-0.42</td>
<td>0.61-0.76</td>
</tr>
<tr>
<td>8</td>
<td>256$^3$</td>
<td>128</td>
<td>$2.8\eta_B - 2\eta$</td>
<td>0.41-0.50</td>
<td>0.34-0.38</td>
<td>0.68-0.77</td>
</tr>
<tr>
<td>8</td>
<td>256$^3$</td>
<td>256</td>
<td>$4\eta_B - 2\eta$</td>
<td>0.37-0.40</td>
<td>0.33-0.35</td>
<td>0.57-0.66</td>
</tr>
<tr>
<td>8</td>
<td>512$^3$</td>
<td>256</td>
<td>$2.4\eta_B - \eta$</td>
<td>0.39-0.48</td>
<td>0.33-0.38</td>
<td>0.65-0.79</td>
</tr>
<tr>
<td>8</td>
<td>512$^3$</td>
<td>512</td>
<td>$3.4\eta_B - \eta$</td>
<td>0.35-0.45</td>
<td>0.32-0.35</td>
<td>0.71-0.79</td>
</tr>
<tr>
<td>8</td>
<td>512$^3$</td>
<td>1024</td>
<td>$4.8\eta_B - \eta$</td>
<td>0.30-0.40</td>
<td>0.31-0.32</td>
<td>0.60-0.67</td>
</tr>
</tbody>
</table>
FIG. 4.1 The functions (a) $\text{Var}(\ln \epsilon_r)$, (b) $\langle \epsilon_t^2 \rangle / \langle \epsilon \rangle^2$, and (c) $\langle \epsilon(x) \epsilon(x+r) \rangle / \langle \epsilon \rangle^2$ used to infer intermittency exponents for the energy dissipation. Lines A-E represent results at Taylor-scale Reynolds numbers $R_\lambda \approx 8$ (on $256^3$ grid), 38 ($256^3$), 140 ($256^3$), 240 ($512^3$), and 390 ($1024^3$), respectively. Inset in (c) shows use of slope of line E to evaluate the exponent $\mu_3$ at $R_\lambda \approx 390$. Dashed lines are at 0.17 and 0.21, respectively.
FIG. 4.2. Comparison of the mean-squared local energy dissipation $\langle \epsilon_r^2 \rangle / \langle \epsilon \rangle^2$, at (a) $R_\lambda$ 140, (b) $R_\lambda$ 390, for averages taken in one, two- and three-dimensions respectively (lines A-C).
FIG. 4.3. Comparisons of two-point correlators of energy dissipation and its one-dimensional surrogates at (a) $R_\lambda 140$, (b) $R_\lambda 390$. Triangles for full 3-D dissipation ($Y = \epsilon$) averaged over distance $r$ in three directions; circles for longitudinal velocity with longitudinal separation distance (e.g. $Y = (\partial u_1/\partial x_1)^2$ with $r = r_1$), squares for transverse velocity with transverse separation distance (e.g. $Y = (\partial u_1/\partial x_2)^2$ with $r = r_3$).
FIG. 4.4. Comparisons of two-point correlators of different velocity gradients squared $(\partial u_\alpha / \partial x_\beta)^2$, with distance $r$ taken along the axis $x_\gamma$. Open triangle: $\alpha = \beta = \gamma$, open circle: $\alpha = \beta \neq \gamma$, open square: $\alpha = \gamma \neq \beta$, close triangle: $\alpha \neq \beta = \gamma$, close circle: $\alpha \neq \beta \neq \gamma$. 
FIG. 4.5. Normalized sixth-order longitudinal velocity structure function. $R_{\lambda} \approx 140, 240$ and 390 (lines A-C respectively). The inset shows the slopes of the curves, with a dashed line corresponding to an intermittency exponent 0.25 for reference.
FIG. 4.6(a,b,c). Same as Fig. 4.1(a,b,c), but for the enstrophy ($\Omega = \omega_i \omega_i$).
FIG. 4.7 Comparisons of two-point correlators of scalar dissipation and its scalar gradient surrogates for (a) $R_\lambda \approx 390$, $Sc = 1$ and (b) $R_\lambda \approx 38$, $Sc = 64$. Triangles for full scalar dissipation ($\chi$) averaged over distance $r$ in three directions; circles and squares for components parallel ($\chi_\parallel$) and perpendicular ($\chi_\perp$) to direction of mean gradient respectively.
FIG. 4.8. Same as Fig. 4.7, but for local averages taken over three-dimensional boxes of length $r$ on each side.
FIG. 4.9(a,b,c). Same as Fig. 4.1(a,b,c), but for scalar dissipation at $Sc = 1$ for the same Reynolds numbers.
FIG. 4.10. Comparison of two-point correlators for scalar dissipation at $Sc = 1/8$ and 1 (lines A and B) $R_\lambda 390$, with distance $r$ normalized by (a) Kolmogorov scale and (b) Obukhov-Corrsin scale.
FIG. 4.11(a,b,c). Same as Fig. 4.1(a,b,c), but for scalar dissipation at $R_{\lambda}$ 38, for Schmidt numbers $Sc = 1, 4, 8$ (lines A-C, 256$^3$) and 16,32,64 (lines D-F, 512$^3$).
FIG. 4.12(a,b,c). Same as Fig. 4.11(a,b,c), but at $R_\lambda$ 8, for $Sc = 1, 4, 16$ (lines A-C, $128^3$), 64 (line D, $256^3$), and 256,1024 (lines E-F, $512^3$).
FIG. 4.13 Intermittency exponents as a function of $Sc$: closed symbols at $R_\lambda \approx 38$, open symbols at $R_\lambda \approx 8$; squares ($\mu_1$), circles ($\mu_2$), triangles ($\mu_3$).
CHAPTER V

DIFFERENTIAL DIFFUSION AND SCALAR SPECTRAL TRANSFER

In this chapter of the thesis, basic properties of differential diffusion between weakly diffusive scalars are discussed. The later part of the chapter describes single scalar spectral transfer and subgrid transfer for a given cut-off wavenumber $k_c$. The work in this chapter may be considered as an extension of previous work at $Sc = 1$ or less (Yeung, 1996, 1998, Yeung and Zhou 1996) to the high $Sc$ regime.

5.1 Differential diffusion

In this section, high-Sc DNS data are examined on basic statistical quantities involving two scalars $\phi_\alpha$ and $\phi_\beta$ with different molecular diffusivity $D_\alpha$ and $D_\beta$ advected by the same turbulent flows. The two scalars have zero fluctuations at time $t = 0$ and they evolve according to the scalar transport equation Eq. 2.3. A fundamental statistic that characterizes differential diffusion between $\phi_\alpha$ and $\phi_\beta$ is the correlation coefficient $\rho_{\alpha\beta}$ defined as

$$\rho_{\alpha\beta} = \frac{\langle \phi_\alpha \phi_\beta \rangle}{\langle \phi_\alpha^2 \rangle^{1/2} \langle \phi_\beta^2 \rangle^{1/2}}.$$  \hspace{1cm} (5.1)

Figure 5.1 shows the evolution of the correlation coefficient $\rho_{\alpha\beta}$ at $R_\lambda \approx 38$ and $R_\lambda \approx 8$ for scalar pairs with different Schmidt numbers. The coefficient $\rho_{\alpha\beta}$ starts from 1 at time $t = 0$ when the two scalars both have zero fluctuations. Subsequently, the two scalars begin to evolve differently as a result of difference in their respective molecular diffusivities and therefore, they become less perfectly correlated. Ultimately, $\rho_{\alpha\beta}$ tends to a stationary level as the turbulent fluctuations become stationary. Fig. 5.1(a) and (b) show correlation coefficients for scalar pairs with $Sc$ ratio 2 and 4 at $R_\lambda \approx 38$ and $R_\lambda \approx 8$, respectively. Scalar pairs in Fig. 5.1(a) are combinations of scalars with $Sc = \{16, 32, 64\}$ and those in Fig. 5.1(b) are from $Sc = \{256, 512, 1024\}$. It can be seen that the level of $\rho_{\alpha\beta}$ in stationary
state for both (a) and (b) is very close to each other for scalar pair with the same $Sc$ ratio. This suggests that at high Schmidt numbers, the scalar correlation coefficient mainly depends on the $Sc$ ratio between the two scalars and its dependence on Reynolds number is rather weak, whereas in Yeung (1998), it is found that for low $Sc$ ($= 1/8, 1$), scalars tend to be more correlated at higher Reynolds number. Fig. 5.1(c) shows $\rho_{a\beta}$ for scalars with larger $Sc$ ratios of 8 and 64 from combinations of $Sc = \{1, 8, 64\}$. It can be seen that larger $Sc$ ratio tends to de-correlate scalar fluctuations further because scalars with large $Sc$ ratio have more disparate scales. It is also noticed in Fig. 5.1(b) that scalar pairs with the same $Sc$ ratio but have different magnitude of $Sc$'s (line A for $Sc = \{1, 8\}$ and B for $Sc = \{8, 64\}$) have considerable difference compared with $Sc$ ratio of 2 in (a) and (c). Overall, Fig. 5.1 suggests that the asymptotic value of the correlation coefficient between two scalars at high $Sc$'s mainly depends on the $Sc$ ratio and large $Sc$ ratios tend to de-correlate scalar pair. For large $Sc$ ratio, $\rho_{a\beta}$ tends to be more correlated for scalar pairs with $Sc$'s of larger magnitude, but for smaller $Sc$ ratio, the magnitude of the $Sc$'s of the scalar pair has little effect on the correlation coefficient.

Also of interest here is the correlation of scalars at smaller scales, which can be quantified by the correlation coefficient of scalar gradient between two scalars, i.e.,

$$g_{a\beta} = \frac{\langle \frac{\partial \phi_a}{\partial x_i}, \frac{\partial \phi_\beta}{\partial x_i} \rangle}{\left( \langle \left( \frac{\partial \phi_a}{\partial x_i} \right)^2 \right) \left( \langle \left( \frac{\partial \phi_\beta}{\partial x_i} \right)^2 \rangle \right)^{1/2}},$$  \tag{5.2}

where $x_i$ can be any of the three Cartesian coordinates. Yeung (1998), Fox (1999) and Chakravarthy & Menon (2001) derived a model estimate for $g_{a\beta}$ based on a local isotropy assumption for the “joint dissipation” $\chi_{a\beta} = (D_\alpha + D_\beta)\langle (\partial \phi_\alpha/\partial x_i)(\partial \phi_\beta/\partial x_i) \rangle$, where the large time limit is

$$g_{a\beta} \approx 2\left( \frac{D_\alpha}{D_\beta} + \frac{D_\beta}{D_\alpha} + 2 \right)^{-1/2}. \tag{5.3}$$

Equation 5.3 indicates that the large time limit of $g_{a\beta}$ is only a function of the ratio of molecular diffusivities and is independent of the large scale parameter of Reynolds number. Figure 5.2 show correlation coefficient of scalar gradients in the direction of mean scalar gradient for various $Sc$-ratio and Reynolds number combinations. Dotted line represents the large time limit given by Eq. 5.3. Indeed, the stationary state $g_{a\beta}$ agrees with the
estimate of Eq. 5.3 for $Sc$ ratio (hence the ratio of molecular diffusivities) from 2 to 64 in Fig. 5.2. In contrast with scalar correlation coefficient $\rho_{\alpha\beta}$ in Fig. 5.1(b), $g_{\alpha\beta}$ for $Sc = \{1, 8\}$ and $\{8, 64\}$ does not show systematic difference. For $Sc = \{1, 64\}$, $g_{\alpha\beta}$ reaches 0.25 at large times. It is expected for $D_\alpha/D_\beta \rightarrow \infty$, $g_{\alpha\beta}$ will tend to zero. Figure 5.2(c) shows for $g_{\alpha\beta}$ at $R_\lambda \approx 140,240$ and 390 for $Sc = \{1/8, 1\}$, and the result suggests that large time limit of $g_{\alpha\beta}$ does not depend on Reynolds number, which is consistent with the small scale universality of K41 theory. In contrast, the larger scale correlation coefficient $\rho_{\alpha\beta}$ increases with Reynolds number (Yeung 1998). The results suggest that high Reynolds number tends to reduce differential diffusion at relatively large scales, but differential diffusion remains important at the small scales. It is also worth noting that differences among $g_{\alpha\beta}$ in the three coordinate directions are negligible suggesting that local isotropy is a good approximation for Eq. 5.3. Figure 5.2 at high Schmidt numbers and various Reynolds number agrees very well with the model prediction of Eq.5.3.

The scale dependency of the correlation between two scalars can be represented by the coherency spectrum, defined as

$$
\rho_{\alpha\beta}(k) \equiv \frac{E_{\alpha\beta}(k)}{[E_{\alpha\alpha}(k)E_{\beta\beta}(k)]^{1/2}}, \tag{5.4}
$$

where $E_{\alpha\beta}(k) \equiv 1/2(\hat{\phi}_\alpha \hat{\phi}_\beta^* + \hat{\phi}_\alpha^* \hat{\phi}_\beta)$ is the co-spectrum between $\phi_\alpha$ and $\phi_\beta$, where “hat” denotes the corresponding Fourier transform and “asterisk” the complex conjugate. $E_{\alpha\alpha}$ and $E_{\beta\beta}$ are scalar spectrum ($\equiv \langle \hat{\phi}\hat{\phi}^* \rangle$). Equation 5.4 suggests that the coherency is essentially a correlation coefficient in Fourier space, which conveys the information of scalar correlation at different scales. Figure 5.3 shows the coherency spectrum as a function of wavenumber normalized by the Batchelor scale $\eta_B$ of the less diffusive scalar based on the data sets for high $Sc$'s at $R_\lambda \approx 38$ and $R_\lambda \approx 8$. In Fig. 5.3, $\rho_{\alpha\beta}$ shows a rough “collapse” among data from intermediate to small scales according to $Sc$ ratios ($D_\alpha/D_\beta = 2, 4, 8, 64$) and there is little differential diffusion at large scales. It can be seen that stronger differential diffusion occurs for larger $Sc$ ratio, which is the major factor affecting differential diffusion at high $Sc$'s. The magnitude of Schmidt numbers and Reynolds number plays minor role in coherency spectrum at high $Sc$'s.

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The correlation between two scalars as a function of scale size can also be characterized in wavenumber space, where at each fixed wavenumber vector $\mathbf{k}$, the following can be computed

$$r_{\alpha\beta}(\mathbf{k}) = \frac{1}{\sqrt{\phi_{\alpha}(\mathbf{k})} \phi_{\beta}(\mathbf{k})} \cos[\theta_{\alpha}(\mathbf{k}) - \theta_{\beta}(\mathbf{k})], \quad (5.5)$$

with $\theta_{\alpha}$ and $\theta_{\beta}$ being the phase angles of $\phi_{\alpha}(\mathbf{k})$ and $\phi_{\beta}(\mathbf{k})$ in the complex plane. Hence, the spectral coherency between two scalars can be interpreted as their phase alignment in Fourier space. Fig. 5.4 shows the probability density function (PDF) of the phase angle difference between two scalars for Schmidt number ratio 2, 4, 8 and 64. It can be seen that the PDFs tend to be flatter at high wave numbers and for high $Sc$ ratio scalar pair, which suggests that scalars are more uncorrelated at small scales and for high $Sc$ ratios. This is consistent with the trend for coherency spectrum in Fig. 5.3.

A direct measure of differential diffusion at different scales is the spectrum of the difference between two scalars, defined as

$$F_{\alpha\beta}(\mathbf{k}) = E_{\alpha\alpha}(\mathbf{k}) - 2E_{\alpha\beta}(\mathbf{k}) + E_{\beta\beta}(\mathbf{k}), \quad (5.6)$$

where we have $\int k F_{\alpha\beta}(k) dk = \langle (\phi_{\alpha} - \phi_{\beta})^2 \rangle$. Figure 5.5 shows the difference spectrum normalized by Batchelor variables with $\eta_B$ chosen to be the Batchelor scale of the less diffusive scalar at $R_\lambda \approx 8$ with $Sc$ up to 1024 and $Sc$ ratio up to 64. At high wavenumbers, the dominating term in Eq. 5.6 is the scalar spectrum of the less diffusive scalar $E_{\beta\beta}(k)$, because the co-spectrum $E_{\alpha\beta}$ is negligible at small scales according to Fig. 5.3 where $\rho_{\alpha\beta}$ drops fast at high wavenumbers and $E_{\alpha\beta}$ drops faster that $E_{\beta\beta}$. The less diffusive scalar $\phi_{\beta}$ has more small-scale content than the more diffusive scalar $\phi_{\alpha}$. Therefore, it is likely that the difference spectrum at small scales can be described by Batchelor scaling based on parameters of the less diffusive scalar. Indeed, the difference spectrum $F_{\alpha\beta}$ in Fig. 5.5 “collapse” at high wavenumbers for all scalar pairs with different $Sc$ ratio. At intermediate to large scales, the co-spectrum becomes more important and $F_{\alpha\beta}$ “collapse” according to $Sc$ ratios with larger $Sc$ scalar pair having a higher difference spectrum at large scales. It is interesting to note that for the scalar pair $Sc = \{1, 64\}$ with the highest $Sc$ ratio 64 (curve B), there is an emerging flat region suggesting the difference spectrum for high $Sc$-ratio
scalar pair may also exhibiting a $k^{-1}$ scaling range. Results at even higher $Sc$ ratio will provide more evidence.

5.2 Scalar spectral transfer

Scalar transfer spectrum $T_\phi(k)$ serves as a redistributive ($\int_k T_\phi(k)d\mathbf{k} = 0$) term in the evolution equation of scalar spectrum

$$\frac{\partial E_\phi(k)}{\partial t} = T_\phi(k) + G_\phi(k) - 2Dk^2 E_\phi(k),$$

(5.7)

where $D$ is the molecular diffusivity and $G_\phi(k)$ accounts for the mean scalar gradient contribution. The scalar transfer spectrum $T_\phi(k)$ is defined as a non-linear triadic interaction between two scalar modes with scale size of $1/k$ and $1/q$ and one velocity mode of scale size $1/p$ in Fourier space. Here, the wavenumber vectors $\mathbf{k}$, $\mathbf{p}$ and $\mathbf{q}$ form a triangle, i.e., $\mathbf{p} + \mathbf{q} = \mathbf{k}$. In particular, $T_\phi(k)$ is given by

$$T_\phi(k) = 2k_j Im \left[ \langle \hat{\phi}^*(k) \int_{k=p+q} \hat{u}_j(p) \hat{\phi}(q)d\mathbf{p} \rangle \right],$$

(5.8)

where $Im$ denotes the imaginary part and the asterisk denotes a complex conjugate. In order to understand the details of spectral transfer process, the transfer spectrum can be decomposed into contributions from different velocity modes $\mathbf{p}$ and scalar modes $\mathbf{q}$

$$T_\phi(k) = \sum_p V_\phi(k|p) = \sum_q S_\phi(k|q),$$

(5.9)

and $V_\phi(k|p)$ and $S_\phi(k|q)$ can be further decomposed as

$$V_\phi(k|p) = \sum_q T_\phi(k|p, q),$$

(5.10)

and

$$S_\phi(k|q) = \sum_p T_\phi(k|q, p).$$

(5.11)

Qualitatively, many features of scalar spectral transfer at high Schmidt numbers are similar to those seen in previous work (Yeung 1996). The classical forward cascade behavior is observed: $T_\phi(k)$ and $V_\phi(k|p)$ are negative at low wavenumbers and positive at high wavenumbers; $S_\phi(k|q)$ is negative below the midpoint of each $q$ range and positive above it.
with maximum values occurring at the two ends of the $q$ range. At high wavenumbers, the
dominant contributions to velocity-scalar interactions (see Fig. 5.7) are nonlocal involving
a lower wavenumber velocity mode, suggesting that the large-scale motion affects the small-
scale scalar field. However, results for $S_\phi(k|q)$ and $T_\phi(k|p,q)$ show that scalar transfer at
high wavenumbers are local, which means that scalar fluctuations at large scales do not
affect the small scales. On the other hand, at low wavenumbers, velocity-scalar interactions
are more local in nature and scalar transfer is moderately non-local.

In order to compare the rate of scalar spectral transfer at different Reynolds and
Schmidt numbers, the scalar variance is normalized to unity in all cases such that the
magnitude reflects the relative rate of spectral transfer. Fig. 5.6 and 5.7 show the scalar
spectral transfer $T_\phi(k)$ (dashed line) and its decomposition into contribution from different
velocity modes $V_\phi(k|p)$, where each solid curve corresponds to the logarithmically spaced
wavenumber ranges separated by vertical dashed lines. Fig. 5.6 shows $V_\phi(k|p)$ at $R_\lambda \approx 8$
for $Sc = 1, 8, 64$ and 1024. Spectral transfer mainly comes from the two lowest velocity
modes ($1 \leq p \leq 4$). The forward cascading process is observed, indicated by $T_\phi(k)$ and
$V_\phi(k|p)$ that they are negative at low wavenumbers and become positive at high wavenum-
ers. The transition wavenumber where spectral transfer becomes positive increases with
$Sc$, which suggests that some spectral content is taken out from smaller scales to the high
wavenumbers at high $Sc$.

In general, spectral transfer rate at low to moderate wavenumbers decreases with
Schmidt number. As $Sc$ increases, the transfer spectrum curve tends to spread out to-
wards the high wavenumbers. It is seen from Fig. 5.7 that strong non-local velocity-scalar
interactions occur at high wavenumbers where velocity mode $2 \leq p \leq 4$ contributes the
most. The transfer rate at high wavenumbers increases with $Sc$ up to $Sc = 64$, and $V_\phi(k|p)$
at $Sc = 1024$ is smaller than $Sc = 64$. However, the DNS results for $Sc = 256, 512, 1024$
(not shown) indicate that $T_\phi(k)$ at high wavenumbers increases with $Sc$. The reason why
this trend is not monotonic from $Sc = 64$ ($128^3$) to $1024$ ($512^3$) might be due to the resolu-
tion difference. It can be inferred that the transfer rate at high wavenumbers increases with
$Sc$, which is opposite to the trend at low wavenumbers. This is consistent with the findings
in scalar spectrum where scalars at high Sc has more high wavenumber content. By comparison with results for $V_\phi(k|p)$ at high Reynolds number $R_\lambda \approx 38$ and $R_\lambda \approx 90$ in Yeung (1996), it is found that turbulent motions of intermediate scales tend to be significant for scalar spectral transfer at high Reynolds numbers, which is consistent with previous finding that velocity modes near the peak of the energy dissipation spectrum contribute the most to the transfer.

Fig. 5.8(a) and (b) show the decompositions of $V_\phi(k|p)$ for the most significant modes $1 \leq p \leq 4$ into $T_\phi(k|p,q)$ where different curves represent different scalar modes $q$. Strong mutual cancellation between adjacent scalar modes at moderate to high wavenumbers can be observed. At high wavenumbers, scalar transfer is local, i.e., the dominant contributions are from scalar mode $q$ very close to $k$. Scalar transfer becomes weaker for high Sc at intermediate scales and scalar transfer from high wavenumber modes becomes more significant, because scalars of high Sc have more high wavenumber content. The peaks of the transfer occur at the boundaries between adjacent wavenumber ranges and the “spikes” become narrower at high wavenumbers, which means that scalar transfer becomes more local as it cascades to the small scales. Fig. 5.8(c) and (d) show $S_\phi(k|q)$, the contributions to the spectral transfer from different scalar modes $q$. Qualitatively, $S_\phi(k|q)$ is very similar to $T_\phi(k|p,q)$. As Sc increases, the scalar mode with the highest peak increases.

Furthermore, $S_\phi(k|q)$ can be decomposed into $T_\phi(k|q,p)$ as shown in Fig. 5.9 for $q$ at low to moderate wavenumbers. The largest contributions from velocity modes are the lowest couple of wavenumber ranges, the same as results for $V_\phi(k|p)$ in Fig. 5.6 and 5.7. The shape of $T_\phi(k|q,p)$ is very similar to $S_\phi(k|q)$ and they peak at the same wavenumber $k$. Unlike the mutual cancellation of $T_\phi(k|p,q)$, contributions from different velocity modes $T_\phi(k|q,p)$ are in phase and add up to $S_\phi(k|q)$.

### 5.3 Scalar subgrid transfer

In Large Eddy Simulation (LES), only large scales of turbulent motions are simulated whereas the dynamics of the small scales are modeled by the subgrid-scale (SGS) models.
Similarly, in the LES approach to studying scalars, corresponding scalar SGS models have to be used. One means of incorporating passive scalar transport into LES is to introduce turbulent Schmidt number $Sc_t$ and closure is obtained when either $Sc_t$ is specified as a model parameter or is estimated using a dynamic procedure (Pullin 2000). This turbulent Schmidt number can be obtained using DNS. Based on the methodology of studying SGS energy (Domaradzki et al. 1987, 1990) and scalar transfer (Yeung and Zhou 1996) by DNS, data are obtained for SGS scalar transfer and related SGS parameters at high Schmidt numbers in an effort to have more complete understanding of the physical process of scalar SGS transfer for a wider range of Schmidt numbers.

In the DNS approach to studying SGS transfer, a fictitious cutoff wavenumber $k_c$ is introduced, which separates the scales into resolvable ($k \leq k_c$) and subgrid ($k > k_c$) ranges. The scalar transfer spectrum for the resolvable scales can be written as

$$T_\phi(k) = T^{\leq}(k|k_c) + T^{>}(k|k_c) + T^{>}(k|k_c),$$

where $T^{\leq}(k|k_c)$ is the fully resolvable scale transfer for triadic interaction with $k, p, q \leq k_c$, $(k, p, q$ are defined in Eq. 5.8), $T^{>}(k|k_c)$ is the resolvable-subgrid transfer with one of $p$ and $q$ in the resolvable range and the other in the subgrid range, $T^{>}(k|k_c)$ is the fully subgrid transfer with both $p, q > k_c$. The total subgrid transfer $T^{s}(k|k_c)$ is written as

$$T^{s}(k|k_c) = T^{<}(k|k_c) + T^{>}(k|k_c).$$

Subgrid transfer $T^{s}(k|k_c)$ is the rate at which scalar is transferred into and out of the resolvable range due to interactions with subgrid scales. In SGS models, the SGS transfer is modeled by the subgrid diffusivity, defined as

$$D_c(k|k_c) = -\frac{T^{s}(k|k_c)}{2k^2E_\phi(k)}.$$  

Similarly, some SGS models use turbulent Schmidt number (or Prandtl number) as the input parameter, which is defined as

$$Sc(t|k_c) = \frac{\nu + \nu_c(k|k_c)}{D + D_c(k|k_c)},$$

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where \( \nu \) and \( D \) are viscosity and molecular diffusivity, respectively, and \( \nu_e(k|k_c) \) is the turbulent eddy viscosity similarly defined as the ratio of energy transfer and energy spectrum

\[
\nu_e(k|k_c) = \frac{T(k|k_c)}{2k^2E(k)}.
\]

(5.16)

In a forward cascade process, the net effect of the subgrid scales on the resolvable scales is to transfer the scalar fluctuations towards smaller scales and the eddy diffusivity is positive. When inverse transfer occurs, i.e., the net scalar fluctuations are transferred towards larger scales, the eddy diffusivity becomes negative. Usually, both forward and inverse transfer occur among different wavenumber modes.

To give an idea how different types of triadic interactions as shown in Eq. 5.12 contribute to the total spectral transfer, Figure 5.10 shows the decomposition of scalar spectral transfer for \( Sc = 1 \) and \( Sc = 64 \) at \( R_\lambda \approx 38 \). At low wavenumbers, subgrid transfer is almost zero because local triadic interactions dominate. Negative resolved-subgrid scale transfer emerges at wavenumbers close to the cutoff wavenumber \( k_c \). This negative subgrid transfer suggests a net effect of forward cascade process that transfers scalar fluctuations to the smaller scales with \( k > k_c \). It also implies a moderately non-local transfer. The fully subgrid transfer with \( p, q > k_c \) are negligible compared to other contributions which means few non-local triadic interactions. The spectral transfer in the resolved range also shows a forward cascade with the resolved and the total transfer being negative at low wavenumbers and positive at high wavenumbers. It can be seen that subgrid transfer is important only in the resolved range that are close to the cutoff wavenumber. For the high \( Sc \) case in Fig. 5.10(b), the magnitude of spectral transfer is less than the low \( Sc \) case in (a) and there is strong mutual cancellation of the resolved transfer and the resolved-subgrid transfer at close to \( k_c \).

The cutoff wavenumber \( k_c \) is an important parameter in LES and SGS transfer. Intuitively, higher \( k_c \) in LES gives more accurate results and requires higher resolution and the SGS transfer will be restricted to a narrower region close to \( k_c \). Lower \( k_c \) in LES corresponds to a coarser grid simulation. Fig. 5.11 shows the resolved transfer, the subgrid transfer and the corresponding sub-grid diffusivity for scalar \( Sc = 64 \) at \( R_\lambda \approx 38 \) for different \( k_c \). As \( k_c \)
increases, the range of scales in the resolvable region increases as shown in (a). For high 
k_c, subgrid transfer and subgrid diffusivity become less and appear confined in a narrower 
region.

As Sc increases, the scalar spectrum at high wavenumbers will increase and the subgrid transfer 
will subsequently increase. But the subgrid diffusivity depends on the ratio of subgrid transfer and 
the scalar spectrum (as in Eq. 5.14) and will be determined by the relative strength of these two factors. Fig. 5.12 shows the subgrid transfer and subgrid diffusivity for Sc = 1, 8 and 64 at R_\lambda \approx 8 and k_c = 8 and 16. In Fig. 5.12(a) and (b), 
the subgrid transfer at close to k_c indeed increases with Sc. The subgrid diffusivity in 
Fig. 5.12(c) and (d), however, shows much less dependence on Sc, especially at higher 
k_c. At k_c = 8, subgrid diffusivity at close to k_c shows slightly decreasing trend with Sc, 
indicating that the increase of scalar spectrum with Sc at high wavenumbers dominates 
that of the transfer spectrum.

It is expected the turbulent Schmidt number will be very sensitive to the cutoff wavenumber k_c, because in the definition in Eq. 5.15, Sc_t(k|k_c) has non-linear relation with the 
subgrid eddy viscosity and subgrid diffusivity, which depend on both the spectrum and the 
transfer spectrum. Fig. 5.13 shows the turbulent Schmidt number for Sc = 16, 32 and 64 
at k_c = 4, 16, 32 and 64. It is seen that as k_c increases from Fig. 5.13(a) to (d), Sc_t(k|k_c) 
becomes closer to the actual Schmidt number at low wavenumber numbers. This is because 
both subgrid viscosity and diffusivity approaches zero at low wavenumbers as k_c increases. 
At wavenumber close to k_c for relatively high k_c = 16, 32, 64, the subgrid viscosity and 
diffusivity dominate the viscosity and molecular diffusivity, respectively. Furthermore, subgrid diffusivity increases with wavenumber faster than subgrid viscosity because the scalar 
has more high wavenumber contents than the velocity field. This will make the turbulent Schmidt number decreases at k close to k_c. This trend is reversed for Sc < 1 as in Yeung 
and Zhou (1996) where subgrid viscosity increases faster than subgrid diffusivity. Fig. 5.13 
may provide some criteria as to how high the cutoff number should be in a LES in order to 
obtain reasonably accurate results.
Subgrid transfer can also be decomposed into contributions from modes of forward and inverse transfer, i.e., the modes with negative and positive transfers, respectively. The spectral transfers and subgrid diffusivities shown in the previous figures are the net results from contributions from both forward and inverse transfer. Figure 5.14 shows the forward, the inverse and the net transfer and the corresponding subgrid diffusivity to see their relative strength. This figure suggests that although the net subgrid transfer is a forward cascading process, there are significant inverse transfer contributions, i.e., transfer from subgrid scales to the resolved scales. Similarly, the decomposition of the fully subgrid transfer shown in Fig. 5.15 suggests that at higher $k_c$, the forward and inverse transfer for non-local triadic interactions are almost equally likely.

In this chapter, several aspects of the DNS results have been examined, including differential diffusion, between two scalars with different molecular diffusivity advected by the same turbulent flow, the scalar spectral transfer and the subgrid scalar transfer. It is found that Schmidt number ratio (also the ratio of molecular diffusivity) between the two scalars at high $Sc$ is an important parameter in differential diffusion and the higher this ratio is, the two scalars tend to be more uncorrelated. The magnitude of the $Sc$'s of the two scalars and Reynolds numbers are less important. Scalar spectral transfer at high Schmidt numbers undergoes the forward transfer process and it becomes weaker at moderate to large scales as $Sc$ increases, but the transfer increases with $Sc$ at small scales. Subgrid scalar transfer is dominated by forward transfer process although there are also significant transfer contributions. Subgrid transfer weakens with increasing cutoff wavenumber and becomes stronger with increasing $Sc$. 

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FIG. 5.1(a) Evolution of the scalar correlation coefficient $\rho_{\alpha \beta}$. Line A, B, and C represent scalar pairs with (a). $Sc = \{16, 32\}$, $Sc = \{16, 64\}$ and $Sc = \{32, 64\}$ at $R_\lambda \approx 38$. (b). $Sc = \{256, 512\}$, $Sc = \{256, 1024\}$ and $Sc = \{512, 1024\}$ at $R_\lambda \approx 8$. (c). $Sc = \{1, 8\}$, $Sc = \{1, 64\}$ and $Sc = \{8, 64\}$ at $R_\lambda \approx 8$. 
FIG. 5.2 Evolution of the scalar gradient (\(\nabla\parallel\phi\)) correlation coefficient \(g_{\alpha\beta}\). Line A, B, and C represent scalar pairs with (a) \(Sc = \{16, 32\}\), \(Sc = \{16, 64\}\) and \(Sc = \{32, 64\}\) at \(R_\lambda \approx 38\). (b) \(Sc = \{1, 8\}\), \(Sc = \{1, 64\}\) and \(Sc = \{8, 64\}\) at \(R_\lambda \approx 8\). (c) \(Sc = \{1/8, 1\}\) at \(R_\lambda \approx 140, 240\) and 390. Dashed line represents the large time limit in Eq. 5.3.
FIG. 5.3 Coherency spectrum as defined in Eq. 5.4, where we normalized wavenumber by $\eta_B$ of the less diffusive scalar. Lines A-F represent scalar pairs with $Sc = \{4,8\}, \{4,16\}, \{8,16\}, \{16,32\}, \{16,64\}, \text{and} \{32,64\} \text{ at } R_\lambda \approx 38$. Lines G-R represent scalar pairs with $Sc = \{1,8\}, \{1,64\}, \{8,64\}, \{4,16\}, \{4,32\}, \{16,32\}, \{64,128\}, \{64,256\}, \{128,256\}, \{256,512\}, \{256,1024\}, \text{and} \{512,1024\}, \text{respectively, at } R_\lambda \approx 8$. The curves “collapse” according to $Sc$ ratio of the scalar pair.
Log$_{10}$PDF of phase angle

\[ \theta_\alpha - \theta_\beta \]

FIG. 5.4 PDFs of the difference in phase angle at $R_\lambda \approx 8$ between scalars: (a) $Sc = \{512,1024\}$, (b) $Sc = \{256,1024\}$, (c) $Sc = \{1,8\}$, (d) $Sc = \{1,64\}$. (a), (b) lines A-F represent $k = 6,46,86,126,166,206$, respectively. (c), (d) lines A-F represent $k = 2,12,22,32,42,52$, respectively.
FIG. 5.5 Difference spectrum as defined in Eq. 5.6, where we normalized wavenumber by \( \eta_B \) of the less diffusive scalar. Lines A–L represent scalar pairs with \( Sc = \{1, 8\}, \{1, 64\}, \{8, 64\}, \{4, 16\}, \{4, 32\}, \{16, 32\}, \{64, 128\}, \{64, 256\}, \{128, 256\}, \{256, 512\}, \{256, 1024\} \) and \( \{512, 1024\} \), respectively, at \( R_\lambda \approx 8 \).
FIG. 5.6 Decomposition of the scalar transfer spectrum into contributions $T_\phi(k|p)$ from velocity modes $p$ in the logarithmic spaced ranges A-F in (a), (b), (c) and A-H in (d), where dashed lines are the overall scalar transfer $T_\phi(k)$. All from DNS data sets at $R_\lambda \approx 8$. (a) $Sc = 1$, $128^3$. (b) $Sc = 8$, $128^3$. (c) $Sc = 64$, $128^3$. (d) $Sc = 1024$, $512^3$. 

$k$

$T_\phi(k|p)$
\[ T_\phi(k|p) \]

(a) \hspace{2cm} (b)

(c) \hspace{2cm} (d)

\[ k \]

FIG. 5.7 The same as FIG. 5.6, shown only for high wavenumbers.
FIG. 5.8 Decomposition of scalar spectral transfer at $R_\lambda \approx 38$. (a) $T_\phi(k|p, q)$, $Sc = 1$, dashed line for $T_\phi(k|p)$, $1 \leq p \leq 2$, solid curves correspond to $q$ at different ranges, (b) same as (a) for $Sc = 64$, (c) $T_\phi(k|q)$, $Sc = 1$, dashed line for $T_\phi(k)$, (d) same as (c) for $Sc = 64$. 
\[ T_\phi(k|q, p) \]

FIG. 5.9 Decomposition of scalar spectral transfer \( T_\phi(k|q, p) \) at \( R_\lambda \approx 38 \). (a) \( Sc = 1 \), dashed line for \( T_\phi(k|q) \) with \( 2 \leq q \leq 4 \). (b) same as (a) for \( Sc = 64 \).
FIG. 5.10 Decomposition of scalar transfer spectrum $T_{\phi}(k)$ (dashed line) into fully resolvable transfer $T_{\phi}^{\leq}(k|k_c)$ (line A), resolvable-subgrid transfer $T_{\phi}^{<}(k|k_c)$ (line B) and fully subgrid transfer $T_{\phi}^{>}(k|k_c)$ (line C). (a) $Sc = 1$ at $R_\lambda \approx 38 (256^3)$, $k_c = 8$, (b) $Sc = 64$ at $R_\lambda \approx 38 (512^3)$, $k_c = 22.$
\[ T_0^\leq(k|k_c), T_0^b(k|k_c), D_c(k|k_c) \]

(a) \[ \begin{array}{cc}
\text{.30} & \text{.25} \\
\text{.20} & \text{.15} \\
\text{.10} & \text{.05} \\
\text{.00} & \text{.00} \\
\text{.00} & \text{.00} \\
\end{array} \]

(b) \[ \begin{array}{cc}
\text{.02} & \text{.01} \\
\text{.00} & \text{.00} \\
\text{.00} & \text{.00} \\
\end{array} \]

(c) \[ \begin{array}{cc}
\text{.14} & \text{.13} \\
\text{.12} & \text{.11} \\
\text{.10} & \text{.09} \\
\text{.08} & \text{.07} \\
\text{.06} & \text{.05} \\
\text{.04} & \text{.03} \\
\text{.02} & \text{.01} \\
\text{.00} & \text{.00} \\
\end{array} \]

\[ k/k_c \]

FIG. 5.11 (a) Fully resolvable transfer \( T_0^\leq(k|k_c) \) for \( Sc = 64 \) at \( R_\lambda \approx 38 \) at \( k_c = 4, 16, 32, 64 \) (lines A-D, respectively). (b) Same as (a) for subgrid transfer \( T_0^b(k|k_c) \). (c) Same as (a) for subgrid eddy diffusivity \( D_c(k|k_c) \).
FIG. 5.12 (a) Subgrid transfer $T_g^s(k|k_c)$ for $Sc = 1, 8, 64$ (lines A-C) at $R_\lambda \approx 8$, $k_c = 8$. (b) Same as (a) at $k_c = 16$. (c) Subgrid diffusivity $D_c(k|k_c)$ with the same parameters as (a). (d) Same as (c) at $k_c = 16$. 

$k/k_c$
FIG. 5.13 Subgrid turbulent Schmidt number $Sc_t(k/k_c)$ for $Sc = 16, 32, 64$ (lines A-C) at $R_\lambda \approx 38$.
Decomposition of $T_{\phi}(k|k_c)$ and $D_e(k|k_c)$

(a) \hspace{1cm} (b)

(c) \hspace{1cm} (d)

$k/k_c$

FIG. 5.14 (a) Subgrid transfer $T_{\phi}(k|k_c)$ (line A), its positive (line B) and negative contribution (line B and C) for $Sc = 64$ at $Re \approx 38$, $k_c = 4$. (b) Same as (a) at $k_c = 16$. (c) Corresponding decomposition of subgrid diffusivity $D_e(k|k_c)$ with the same parameters as (a) (d) Same as (c) at $k_c = 16$. 

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Decomposition of $T_{\phi}^{>\nu} (k|k_c)$

![Graph](image)

FIG. 5.15 Same as FIG. 5.14 (a) and (b), respectively, for decomposition of fully subgrid transfer.
CHAPTER VI

CONCLUSION

In this work, properties of passive scalars at high Schmidt numbers in stationary isotropic turbulence are studied by Direct Numerical Simulation (DNS). Schmidt numbers (Sc) as high as 1024 were achieved at Taylor-scaled Reynolds number $R_\lambda \approx 8$, in addition to $Sc = 64$ at $R_\lambda \approx 38$. The main objective is to contribute to the physical understanding of the scalar behavior in the limit of high Schmidt number.

Direct numerical simulation of stationary isotropic turbulence is performed on a cubic domain using a parallel code based on Rogallo’s (1981) pseudo-spectral algorithm. Turbulent velocity field is made statistically stationary by a stochastic forcing scheme (Eswaran and Pope 1988) acting at large scales. The scalar field is also maintained stationary by a uniform mean scalar gradient. The instantaneous velocity and scalar field saved at different times are analyzed and ensemble averages at different times are taken as different realizations. The results for high Sc come from simulations using up to $512^3$ grid points at $R_\lambda \approx 38$ and $R_\lambda \approx 8$ for $Sc$ up to 64 and 1024, respectively. Results at $R_\lambda \approx 90, 140, 240, 390$ are also obtained for $Sc = 1/8$ and 1 using up to $1024^3$ grid points.

In addition to the insights gained from the limited analyses of the DNS data, the DNS database also provided detailed information for further use as new theories and models come up. In the following section, summary of the results from Chap.III-V is given and possible future work that can provide additional understanding of scalar mixing at high Schmidt numbers is given.

6.1 Principal results

Chapter III presents results on the properties of moderately and weakly diffusive scalars through the scalar spectrum, structure functions and statistics of scalar gradient and scalar
dissipation. Moderately diffusive scalars with $Sc = 1/8$ and 1 appear to have inertial-
convective ranges with Obukhov-Corrsin’s $k^{-5/3}$ scaling from $R_\lambda \approx 140$ to 390 and the
inertial-convective range widens with increasing Reynolds number. The Obukhov-Corrsin
constant supported by the results is about 0.4 for $1 - D$ scalar spectrum, which is in agree-
ment with experimental value from Sreenivasan (1996). Comparisons of scalar structure
functions of up to order 8 with those of velocity structure function show that the scaling
exponents of scalar structure functions in inertial range deviate more from the classical
scaling than the corresponding velocity structure functions. This suggests that scalar field
is more intermittent than velocity field in inertial range and agrees with similar finding by
other researchers. The velocity-scalar mixed third-order structure function shows sustaining
trend of approaching Yaglom’s exact relation (1949) as Reynolds number increases. The
mixed structure function at low Reynolds numbers ($R_\lambda \approx 38$ and 8) also approaches Ya-
glom’s relation as $Sc$ increases even though there is no inertial range at such low Reynolds
numbers. The DNS results on scalar spectral at high $Sc$ agree with Batchelor (1959) and
Kraichnan (1968)’s models, both of which give a $k^{-1}$ scaling range. Kraichnan’s model
works better in capturing the spectrum in the diffusive range. Unlike the moderately dif-
fusive scalars at higher Reynolds number, the second-order scalar structure function for
$Sc > 1$ at $R_\lambda \approx 38$ and 8 does not show a classical 2/3 scaling range. The results for
small-scale scalar statistics, such as odd-order moments and probability density function of
scalar gradients do not support Kolmogorov’s hypothesis of local isotropy. However, the
normalized odd-order moments decreases with $Sc$ suggesting that local isotropy is a better
approximation at high $Sc$. Kurtosis (flatness) of scalar gradients and scalar dissipation
shows that small-scale intermittency tends to an asymptotic level at high $Sc$.

In Chapter IV, intermittency exponents manifested by the two-point statistics of scalar
dissipation are studied, including the two-point correlator $\langle \chi(x)\chi(x + r) \rangle$, the second-
order moment of local dissipation $\langle \chi^2 \rangle$ and the variance of the logarithmic local dissipation
$Var(\ln \chi_r)$. Comparisons are made for scalar dissipation with those of energy dissipation
and enstrophy. A major challenge is to compute $\langle \chi(x)\chi(x + r) \rangle$ with local average taken over
a three-dimensional cube of size $r$. It is found that the intermittency exponents obtained by
3-D averaging is larger than those obtained by 1-D averaging. The intermittency exponent for energy dissipation in inertial range increases with Reynolds number and reaches about 0.2 at \( R_\lambda \approx 390 \), which is close to the commonly cited value of 0.25. The three types of intermittency exponents for energy dissipation from the three two-point statistics mentioned above become closer to each other as Reynolds number increases. However, for scalar dissipation, the intermittency exponent of the variance of the logarithmic local dissipation is significantly larger than the other two types at high \( Sc \). Intermittency exponents for scalar dissipation in inertial range are larger than those of the energy dissipation, indicating that scalar field is more intermittent in inertial range. The intermittency exponents of scalar dissipation in viscous-convective range has weak dependence on \( Sc \) at high \( Sc \).

Results have been obtained for differential diffusion between two scalars transported by the same turbulent flow, scalar spectral transfer and subgrid transfer in Chapter V. The ratio of Schmidt number (also molecular diffusivity) between two scalars is an important parameter in differential diffusion and the two scalars tend to be more uncorrelated with increasing \( Sc \) ratio. The magnitude of \( Sc \) of the two scalars is less important than the \( Sc \) ratio. Scalar coherency spectrum and scalar difference spectrum “collapse” according to \( Sc \) ratios. Scalar spectral transfer at high Schmidt numbers has the same forward transfer process as that at low Schmidt numbers. The transfer becomes weaker at low to moderate wavenumbers as \( Sc \) increases, while the trend is reversed at high wavenumbers, suggesting that scalar spectral transfer at small scales is more important for scalars with high \( Sc \). Subgrid-scale scalar transfer is dominated by forward transfer process and there are also significant portion of inverse transfer. Subgrid transfer becomes weaker with increasing cutoff wavenumber and stronger with increasing \( Sc \).

6.2 Future research

In this concluding section, possible extensions of the current work and further investigations of scalars at high Schmidt numbers in other types of turbulent flows are discussed. These possibilities can be summarized as follows: (a) Schmidt number effects in turbulent shear flow, (b) scalar mixing in rotating turbulence, (c) scalar conditional statistics related to
mixing models, (d) Lagrangian statistics of passive scalars.

Discussions have been given on issues of local isotropy and intermittency in isotropic turbulence in Chap.III and IV. Compared to isotropic turbulence, shear flow adds a source of anisotropy to turbulence velocity field. Whether this velocity anisotropy affects the local isotropy of scalar field and to what extent can be of interests. Whether Schmidt number plays a significant role in local isotropy compared to turbulent shears will also assist in a better understanding.

An important application of scalar mixing in rotating turbulence is in jet engines, where the velocity field is subjected to a uniform solid-body rotation. Strong local anisotropy has been found (Yeung and J.Xu 2004) due to Coriolis forces, and where the one-dimensional scalar spectrum in the direction of rotation is very different from that in the other two directions. The question remains whether Batchelor’s $k^{-1}$ scaling still holds for 1-D scalar spectrum in any direction and whether increasing Schmidt number will promote a return to isotropy of the statistics of scalar gradient fluctuations.

Research on the geometric structure of passive scalars has been conducted by several authors (Schumacher etal. 2003, Brethouwer etal. 2003). The alignment between the most compressive strain rate and the largest scalar gradient is believed to cause the formation of sheet-like scalar fronts. The effects of velocity field on the passive scalars can be partly quantified via scalar statistics conditional on the energy dissipation (Vedula etal. 2001). Scalar conditional statistics are essential in scalar mixing models. DNS has been proved to be an effective way to study such detailed statistics. Study of the scalar conditional statistics and the alignment between strain rate and scalar gradient will provide additional understanding on the scalar mixing at high Schmidt numbers.

Finally, a Lagrangian approach to study scalar mixing at high Schmidt numbers will provide a different perspective. Lagrangian statistics of the trajectories of fluid and scalar particles are essential in stochastic modeling of turbulent dispersion problems and DNS is a very useful and convenient tool in studying Lagrangian statistics. Our DNS data for the trajectories of scalar particles at high Schmidt numbers can be analyzed to obtain
various one-scalar statistics and two-scalar dispersion statistics that are needed in stochastic modeling.
Appendix A


Abstract

We study by DNS the effects of Schmidt number (Sc) on passive scalars mixed by forced isotropic turbulence. The scalar field is maintained statistically stationary by a uniform mean gradient. We consider the scaling of spectra, structure functions, local isotropy and intermittency. For moderately diffusive scalars with $Sc = 1/8$ and 1, the Taylor-scale Reynolds number analyzed is either 140 or 240. A modest inertial-convective range is obtained in the spectrum, with a one-dimensional Obukhov-Corrsin constant of about 0.4, consistent with experimental data. However, the presence of a spectral bump makes a firm assessment somewhat difficult. The viscous-diffusive range is universal when scaled by Obukhov-Corrsin variables. In a second set of simulations we keep the Taylor-scale Reynolds number fixed at 38 but vary $Sc$ from 1 to 64, roughly by factors of 2. We observe a gradual evolution of a $-1$ roll-off in the viscous-convective region as $Sc$ increases, consistent with Batchelor's predictions. In the viscous-diffusive range the spectra follow Kraichnan's form well, with a coefficient that depends weakly on $Sc$. The breakdown of local isotropy manifests itself through differences between structure functions with separation distances in directions parallel and perpendicular to the mean scalar gradient, as well as through finite values of odd-order moments of scalar gradient fluctuations and of mixed velocity-scalar gradient fluctuations. However, all these indicators show, to varying degrees, an increasing tendency to isotropy with increasing $Sc$. The moments of scalar gradients and the scalar dissipation rate peak at $Sc \approx 4$. The intermittency exponent for the scale-range between the Kolmogorov and Batchelor scales is found to decrease with $Sc$, suggesting qualitative consistency with previous dye experiments in water ($Sc = O(1000)$).
Appendix B

Simulations of three-dimensional turbulent mixing for Schmidt

Abstract

We report basic results from new numerical simulations of passive scalar mixing at Schmidt numbers ($Sc$) of the order of 1000 in isotropic turbulence. The required high grid-resolution is made possible by simulating turbulence at very low Reynolds numbers, which nevertheless possesses universality in dissipative scales of motion. The results obtained are qualitatively consistent with those based on another study (Yeung et al. 2002) with a less extended Schmidt number range and a higher Reynolds number. In the stationary state maintained by a uniform mean scalar gradient, the scalar variance increases slightly with $Sc$ but scalar dissipation is nearly constant. As the Schmidt number increases, there is an increasing trend towards $k^{-1}$ scaling predicted by Batchelor (1959) for the viscous-convective range of the scalar spectrum; the scalar gradient skewness approaches zero; and the intermittency measured by the scalar gradient flatness approaches its asymptotic state. However, the value of $Sc$ needed for the asymptotic behavior to emerge appears to increase with decreasing Reynolds number of turbulence. In the viscous-diffusive range, the scalar spectrum is in better agreement with Kraichnan’s (1968) result than with Batchelor’s.
 Appendix C


Abstract

Basic results on the evolution of shape and size of three- and four-particle Lagrangian clusters are reported from direct numerical simulations at Taylor-scale Reynolds numbers between 90 and 400 in isotropic turbulence. At early times shape distortion by viscous effects is such that both the area and volume increase less rapidly than the two-particle separation. Later-time behavior is characterized by power-law increases and a self-similar shape distribution. Reynolds number effects are more prominent in measures of size than in shape parameters.
Appendix D


Abstract

Effects of molecular diffusion are implicitly neglected when Lagrangian statistical models for fluid particle motion are used to describe contaminant dispersion in turbulence. However, they are important at small times or close to localized contaminant sources. Here we use direct numerical simulations (DNS) to study this process, by tracking the paths of molecules undergoing Brownian motion relative to the fluid, at a rate according to diffusivities giving Schmidt numbers from 0.01 to 1000. The statistics of molecules of a single “species” (at a given Schmidt number) are well described in the framework of Saffman (1960, J. Fluid Mech. 8, 273), with the major modeling parameter being an integral timescale for the fluid velocity autocorrelation sampled along the molecular trajectory. We present two-species statistics measuring how molecules of species with different Schmidt number become dispersed from each other, with the separation distance being more intermittent if the Schmidt numbers involved are high. The two-species substance cross-correlation corresponding to the single-species autocorrelation is found to be very small. The DNS results are compared with a new Lagrangian stochastic model for relative dispersion including molecular Brownian motion. Implications for high Reynolds numbers are discussed.
REFERENCES


VITA

Shuyi Xu was born in a small town in the Northeast of China where her father, who was originally from southern China, settled down in his late twenties. Shuyi Xu was admitted to Beijing University of Aeronautics and Astronautics in 1992 and obtained her Bachelor of Engineering degree in Aerospace Engineering of Jet Propulsion in 1996. Since 1998, she has been pursuing graduate studies in School of Aerospace Engineering at the Georgia Institute of Technology.

Shuyi Xu has broad interests in mathematics, sciences, humanities, music and arts. Through years of study and research, she came to realize that she has a better intuition and “feel” in mathematical approach to things than physical one. She is still trying to find the “perfect” niche for a career where her strength, passion and sense of self-accomplishment meet.