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Author(s):

T. T. Clark, T-3
S.-Y. Chen, T-3
L. Turner, T-3
C. Zemach, T-3

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Turbulence and Turbulence Spectra in Complex Fluid Flows

Timothy T. Clark*, Shi-Yi Chen, Leaf Turner and Charles Zemach
Theoretical Division, Los Alamos National Laboratory

Abstract

This is the final report of a three-year, Laboratory Directed Research and Development (LDRD) project at Los Alamos National Laboratory (LANL). Our objective was to develop a theoretical model of fluid turbulence in parallel with a series of direct numerical simulations of increasingly complex test environments to establish limits of error and regimes of applicability, and to guide improvements. The aim is to produce methods of tested accuracy, with tractable numerical approximations, for turbulent fluids of constant density, and then for variable densities and multimaterial flows. We proceed from a recent spectral model that describes turbulent energy and stress densities in terms of a range of length scales. This should lead not only to improved engineering models, but also to a basic conceptual improvement because the spectral approach accounts for the variation of evolution rates with turbulence length scales.

Background and Research Objectives

Consider the evolution in time of a three-dimensional velocity field $u_i(\mathbf{x},t)$ for a fluid of constant density ρ and constant viscosity ν . Much of our work addresses such flows, the main exceptions being variable density incompressible flows with mixing fluid constituents and multimaterial flows. The Navier-Stokes equation

$$\frac{\partial u_i}{\partial t} + u_n \frac{\partial u_i}{\partial x_n} = -\frac{1}{\rho} \frac{\partial p}{\partial x_i} + \nu \frac{\partial^2 u_i}{\partial x_n \partial x_n} \quad (1)$$

is well recognized as the proper theoretical point of departure for a broad variety of fluid flows of practical importance, and its dynamics includes the phenomenon of turbulence. Because the advection term $u_n (\partial u_i / \partial x_n)$ is quadratic in the velocity, spatial variations of u_i interfere with one another, broadening the range of length scales. This nonlinear process is compounded over time and, unless it is offset by other physical factors, a flow pattern confined to a narrow spectrum of length scales is inherently unstable.

This advection-induced instability may generate (a) irregularity of flow patterns, i.e., in addition to scales of variation in time and space set by initial conditions, geometry

* Principal Investigator, email: ttc@lanl.gov

and applied forces, the fluid velocity and other fluid data acquire a continuous spectrum of scales in time and space characteristic of the instability mechanism itself, (b) mixing, i.e., initially disjoint regions of fluid are finely intermixed and diffusion processes are enhanced, and (c) unpredictability, i.e., small, physically unobservable change in fluid motion at one time leads to gross changes shortly thereafter. These are among the principal attributes of a region of fluid in a turbulent state.

The viscosity term in (1) offsets the advection term, diffusing concentrations of fluid momentum and dissipating fluid kinetic energy. When it dominates at all relevant scales (regime of low Reynolds number), the advection-induced instability is damped and the flow pattern is smooth. When the advection dominates (regime of high Reynolds number), the flow is turbulent. Even so, the viscosity always wins in the limit of rapid velocity oscillations, that is, of small length scales, because it multiplies the Laplacian of the velocity field. Thus, there is "dissipation length scale" (Kolmogorov scale); for velocity variations at smaller length scales, the main process is irreversible conversion of the fluid kinetic energy associated with such scales into heat.

If a fluid dynamics calculation is carried out on a numerical grid whose cell size is less than the dissipation scale, then the dynamics are "fully resolved" and any turbulence phenomena are included in the calculated results. This constitutes a direct numerical simulation (DNS). In most practical applications, a DNS is a hopeless goal. For example, at the current state of global ocean modeling, the grid size is about 50 kilometers while the dissipation scale is less than a centimeter.

In these cases, a standard alternative is to separate the velocity field into a mean part and a fluctuating (turbulent) part: $u_i = \langle u_i \rangle + \langle u'_i \rangle$. The mean is defined as an ensemble averaged over many experimental realizations with the same macroscopic initial and boundary conditions, but with random fine-scale conditions. In appropriate cases, this is equivalent to localized time or space averages of a single fluid configuration. The mean part $\langle u_i \rangle$ has scales of variation characteristic of the geometry of the problem, and satisfies a modified Navier-Stokes equation,

$$\frac{\partial \langle u_i \rangle}{\partial t} + \frac{\partial \langle u_n \rangle \langle u_i \rangle}{\partial x_n} = -\frac{1}{\rho} \frac{\partial \langle p \rangle}{\partial x_i} + \frac{\partial}{\partial x_n} \left\{ \nu \frac{\partial \langle u_i \rangle}{\partial x_n} - R_{in} \right\} \quad (2)$$

where the "1-point Reynolds stress tensor," $R_{ij}(\mathbf{x}, t) = \langle u'_i(\mathbf{x}, t) u'_j(\mathbf{x}, t) \rangle$, is a second-order correlation function of the fluctuating part of the velocity. The turbulent kinetic

energy per unit mass $K(\mathbf{x},t)$ is related by $K(\mathbf{x},t)=R_{nn}(\mathbf{x},t)/2$. The fluid kinetic energy per unit mass separates into a mean kinetic energy per unit mass and a turbulent part:

$$\text{Total Kinetic Energy} = \frac{1}{2} \langle u_n(\mathbf{x},t) \rangle \langle u_n(\mathbf{x},t) \rangle + K(\mathbf{x},t) \quad (3)$$

The fluctuating velocity, u'_i is not calculated in detail, but its effect on the mean flow is sought through evaluation of R_{ij} , which is now a problem in both stochastic theory and fluid mechanics.

The essential features of a turbulent region of fluid are that (a) its overall state has a stochastic regularity and (b) its detailed motions are irregular, mixing, and unpredictable. This belies the understandable but too simple view that, because the dynamical law of the fluid is fully contained in the "well-known" Navier-Stokes equation, there is no remaining problem of principle and that predictive fluid dynamics may now be left to the computer programmer. The conceptual and methodological complexities of turbulence are comparable to those of quantum field theory.

Turbulence Spectra

The length-scale dependence of turbulent processes can be analyzed in wave-number space ($\mathbf{k}$ -space), proceeding from Fourier transforms such as

$$u(\mathbf{x},t) = \iiint \hat{u}(\mathbf{k},t) \exp(i \mathbf{k} \cdot \mathbf{x}) d\mathbf{k} \quad (4)$$

or other appropriate superpositions of modal functions such as $\exp(i \mathbf{k} \cdot \mathbf{x})$ with characteristic oscillation numbers. (The wave number k is the magnitude of the wave vector $\mathbf{k}$.) The correspondence with a characteristic length scale L is reciprocal: $L = 1/k$.

Similarly, there is a Fourier transform relation between the generalized (2-point) Reynolds stress tensor $R_{ij}(\mathbf{x}_1, \mathbf{x}_2, t) = \langle u_i(\mathbf{x}_1, t), u_j(\mathbf{x}_2, t) \rangle$ and the turbulent stress-energy spectrum $E_{ij}(\mathbf{x}, \mathbf{k}, t)$. The transform is from relative coordinate $\mathbf{x}_1 - \mathbf{x}_2$ to $\mathbf{k}$ with center coordinate $\mathbf{x} = (\mathbf{x}_1 + \mathbf{x}_2)/2$ held constant. The turbulent kinetic energy $K(\mathbf{x}, t)$ is then the sum over k -space modes,

$$K(\mathbf{x}, t) = \int_0^\infty E_{nn}(\mathbf{x}, k, t) dk \quad (5)$$

and $E_{nn}(\mathbf{x}, k, t)$ is the portion of the turbulent energy at $\mathbf{x}$ associated with fluctuations of length scale $1/k$.

The dynamic of turbulent interactions depends on the length-scale, or manner of distribution of length scales, of the interacting fields. The reaction rates for turbulent processes cannot be summarized by 1-point correlation data such as the aggregate turbulent kinetic energy $K(\mathbf{x},t)$ and the aggregate turbulent energy dissipation rate $\epsilon(\mathbf{x},t)$, except in the special regime of spectral equilibrium. This simplified regime may be relevant to many applications. Even in this regime, the experimentally fitted constants that are inserted into 1-point engineering models such as the $K - \epsilon$ model depend on the particular form of the equilibrated k-space spectra that is enforced by a particular mean-flow environment. The particular forms of the equilibrated spectra can only be discerned from a spectral viewpoint. We base this proposition on our work comparing spectral and other approaches to a variety of turbulence experiments as discussed below.

The turbulent processes here referred to include (a) energy transfer between mean flow and turbulent motion, driven by spatial variation of mean flow strain-rate and vorticity, and usually but not always increasing the turbulent energy, (b) transfer of turbulent energy within the wave number spectrum; in three dimensions this transfer is predominantly toward smaller length scales and higher wave numbers, (c) stress-energy exchange among the Reynolds stress components -- there is a stochastic tendency toward isotropy possibly offset by anisotropy in the influence of mean-flow gradients, (d) turbulent diffusion of inhomogeneity in the turbulent fields, which usually dominates the molecular diffusion, and (e) viscous dissipation of turbulent energy into heat at the high-k end of the spectrum, i.e., mostly at length scales smaller than the dissipation length.

Importance to LANL's Science and Technology Base and National R&D Needs

Theoretical modeling of complex turbulent flows after decades of effort is still inadequate. The spectral approach provides a fundamental new capability to understand and to account for (in practical applications) the distributions of turbulence scales and the statistical effect of fluctuations at scales too small to be resolved by current fluid dynamics methods. The spectral approach gives a richness to the physical processes that the simpler models cannot provide. The more detailed theoretical models also serve a crucial role in the development of more tractable engineering models. The range of applicability of these simpler engineering models may be determined more easily than in the past, because the

assumptions and limitations required for their derivation are made obvious in the reduction from the spectral closures.

The need for advanced tractable models of turbulence is vast and varied. Virtually all fluid flows of commercial, industrial or environmental interest are turbulent, and hence beyond the reach of direct computation. Improved models should lead to improved predictions of the behavior of many fluid systems of interest including compression and ignition of inertial confinement fusion (ICF) capsules, flow of fuel and air in internal combustion engines, and dispersal of atmospheric or oceanic pollutants.

Scientific Approach and Accomplishments

The starting point for our research was the spectral turbulence model proposed by Besnard, Harlow, Rauenzahn and Zemach [1]. The model describes the evolution of the spectral tensor, $E_{ij}(\mathbf{x}, k, t)$ for circumstances of general inhomogeneous, anisotropic turbulence. Subsequent work by Clark [2] established many of the properties of the model, and determined appropriate values for the five undetermined model coefficients of the original derivation. The early phases of research focused on documenting extensive comparisons of this model, referred to as the Local-Wave-Number (or LWN) model because it represents the turbulent cascade phenomenon as a local advection and diffusion in k -space rather than as a nonlocal integro-differential transfer process as indicated by a more rigorous deduction from the exact Navier-Stokes equations. The results of the preliminary and early LDRD research suggested the following form for the LWN model:

$$\begin{aligned}
& \frac{\partial E_{ij}}{\partial t} + \frac{\partial U_n E_{ij}}{\partial x_n} + 2\nu k^2 E_{ij} = - \left\{ \frac{\partial U_i}{\partial x_n} E_{nj} + \frac{\partial U_j}{\partial x_n} E_{in} \right\} \\
& + c_b \left\{ \frac{\partial U_i}{\partial x_n} E_{nj} + \frac{\partial U_j}{\partial x_n} E_{in} - \frac{2}{3} \delta_{ij} \frac{\partial U_m}{\partial x_n} E_{mn} \right\} + \left(\frac{11}{5} - 3c_b \right) \left\{ \frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} \right\} E_{mn} \\
& + (8c_b - 6) \left\{ \frac{\partial U_n}{\partial x_i} E_{nj} + \frac{\partial U_n}{\partial x_j} E_{in} - \frac{2}{3} \delta_{ij} \frac{\partial U_m}{\partial x_n} E_{mn} \right\} \\
& + \left(1 - \frac{3}{2} c_b \right) \frac{\partial}{\partial k} \left\{ \left(\frac{\partial U_i}{\partial x_n} + \frac{\partial U_n}{\partial x_i} \right) k E_{nj} + \left(\frac{\partial U_j}{\partial x_n} + \frac{\partial U_n}{\partial x_j} \right) k E_{in} - \frac{4}{3} \delta_{ij} \frac{\partial U_m}{\partial x_n} k E_{mn} \right\} \\
& + \left(c_b - \frac{7}{10} \right) \left(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} \right) \frac{\partial k E_{nn}}{\partial k} + \left(\frac{7}{2} c_b - \frac{8}{3} \right) \frac{\partial U_m}{\partial x_n} \frac{\partial k E_{mn}}{\partial k} \\
& - \frac{3}{11} C_K^{-3/2} \frac{\partial}{\partial k} \left\{ k^2 \sqrt{k E_{nn}} \left[k \frac{\partial E_{ij}}{\partial k} - 2 E_{ij} \right] \right\} \\
& + \frac{26}{33} C_K^{-3/2} k \sqrt{k E_{nn}} \left\{ \frac{1}{3} \delta_{ij} E_{nn} - E_{ij} \right\} \\
& + c_d \frac{\partial}{\partial x_n} \left\{ \left[\int_0^\infty \frac{\sqrt{\zeta E_{nn}(\zeta)}}{\zeta^2} d\zeta \right] \frac{\partial E_{ij}}{\partial x_n} \right\}
\end{aligned} \tag{6}$$

where the arguments are dropped for brevity, and $U_i = \langle u_i \rangle$. The first line of eqn. (6) is an exact deduction from the Navier-Stokes equations. It consists of (from left to right) the time rate of change, advection, molecular diffusion, and (to the right of the equal sign) production and destruction due to coupling with mean flow. The second and third lines are intended to model the effects of the pressure-strain correlations in the exact moment equations, and serve to produce or destroy E_{ij} in a manner that doesn't directly affect the trace of E_{ij} . The fourth and fifth lines model the effects of the mean velocity field in distorting the spectrum due to the different strain histories felt at different parts of the turbulent flow field. The sixth line represents the cascade of E_{ij} from large scales (i.e., low wave numbers) to small scales (i.e., high wave numbers) and is the source of the description "Local Wave Number." The seventh line represents the tendency of the turbulent field to "erase" its own "directionality" and thus tend to a nondirectional, or "isotropic," form. The final line represents the tendency of the turbulent field to diffuse itself from regions of high intensity turbulence into regions of low intensity turbulence.

The choices of coefficients were first determined by Clark [2] and detailed discussions are presented in Clark and Zemach [3]. The results are briefly summarized here. The coefficient C_K is the Kolmogorov constant, a fundamental constant of turbulence theory and is related to the cascade process in Fourier space. An exact value is not known, but its approximate value is taken to be 1.5 in the present work. The coefficient c_b is dependent on the structure of the energy spectrum in the neighborhood of $k=0$. Given a power law form for the spectrum in this region,

$$\lim_{k \rightarrow 0} E_m(k, t) = e_0 k^n$$

where e_0 has dimensions $[L^{(3-n)}T^{-2}]$ and may be a function of time, then the coefficient c_b depends on the power-law exponent, n ;

$$c_b \leq \frac{8n}{11n-1}.$$

Comparisons of model predictions with experiments and direct numerical simulations indicate that the value of c_b should be taken to be as large as possible. Values of n may vary from 1 to 4. The coefficient c_d in the above model was shown earlier [1] to be approximately 0.5125.

In addition to presenting derivations of the model and coefficients for the circumstance of homogeneous anisotropic turbulence, Clark and Zemach [3] also presented extensive comparisons to experimental data, thus demonstrating the adequacy of eqn. (6) and the above coefficients for predicting many real-world flows. Clark and Zemach demonstrated that the so-called return-to-isotropy is necessarily incomplete--the largest scales of the turbulent field will possess a persistent anisotropy that eventually "imprints" the finer scale, producing a final state of decaying turbulence with a constant level of anisotropy. This result was shown by both numerical solution of the LWN equations as well as by group-theoretic arguments. Clark and Zemach also used the simple group-theoretic arguments to demonstrate the possibility of two distinctly different forms for a fully self-similar spectral tensor, one for the case of decaying anisotropic turbulence, and the other for homogeneous turbulence subjected to homogeneous mean flow velocity gradients. It also was shown that the LWN model predictions displayed the emergence of these forms. These two forms have been used in the LWN model to derive two distinctly different forms for the well-known K - ϵ models, with two different regimes of validity [1 and (report in progress)]. The group-theoretic arguments have also been used to

understand the emergence of self-similar forms for decaying isotropic turbulence [4]. This effort unifies much of the work by previous researchers regarding this fundamental issue.

Equation (6) serves as the starting point for much subsequent research. A first step was to improve the model predictions for cases of homogeneous incompressible turbulence. Although the model was shown to produce excellent agreement with experimental results, a known flaw of the model is that the turbulent time-scales ($\tau_i^{-1}(k, t) = k\sqrt{kE_m(k, t)}$) used in the cascade and return-to-isotropy terms vanish at high wave numbers in the so-called dissipation range where viscous effects dominate. Two additional motivations existed to improve this approximation: (1) comparisons of LWN and the Eddy-Damped Quasi-Normal Markovian (EDQNM) model to direct numerical simulations of the truncated Euler equations indicated a deficiency in the LWN time-scales when the spectrum is not near an equilibrium scaling of $k^{-5/3}$ and (2) extensions of the LWN model to the case of passive scalar diffusion and variable density turbulence failed to produce the correct scaling for the scalar-scalar (or density-density) correlations in the dissipation range as functions of Schmidt number. A more reasonable form for the turbulent time-scale (suggested initially by J. Herring [5]) was substituted;

$$\tau_i(k, t) = \left[\int_0^k \zeta^2 E_m(\zeta, t) d\zeta \right]^{-1/2}.$$

This time-scale (in conjunction with appropriately modified versions of the cascade terms) allowed for better prediction of the dissipation scales, slightly improved predictions of the evolution of the truncated Euler equations, and the improved predictions of the behavior of the dissipation range for passive scalar correlations.

As stated above, one of the motivations for this new choice of the turbulent time-scales was the extension of the LWN model to variable-density incompressible turbulence [6]. The development of the spectral form of the variable-density equations began by construction of a symmetrized form of a two-point generalization of the mass-averaged (Favre-averaged) Reynolds stress tensor;

$$R_{ij}(\mathbf{x}_1, \mathbf{x}_2, t) = \frac{1}{2} \left\langle [\rho(\mathbf{x}_1, t) + \rho(\mathbf{x}_2, t)] u_i''(\mathbf{x}_1, t) u_j''(\mathbf{x}_2, t) \right\rangle,$$

where the velocity has been decomposed as $u_i = \bar{U}_i + u_i''$ and $\bar{\rho} \bar{U}_i = \overline{\rho u_i}$ and $\overline{\rho u_i''} = 0$. The salient correlations arising in this development all have single-point counterparts seen in previous variable-density models, such as that of Besnard, Harlow, Rauenzahn and Zemach [7]. The actual definition of these terms and their evolution equations (exact and

modeled) for statistically homogeneous variable density turbulence subjected to accelerations are presented by Clark and Spitz [6]. (The initial formulation of this model occurred prior to this LDRD project, but subsequent development, documentation, refinement and testing of the model were performed under the project.) In the limit of small density fluctuations, this model gives predictions that are in reasonable agreement with the isotropic diffusion of passive scalars in an isotropic turbulent field. The model has also been tested by comparisons to direct numerical simulations of variable density turbulence [8,9,10]. These results indicate that the spectral model provided much better predictions than the one-point closure of Besnard et al. [7], principally because the spectral closure does not require any of the spectral self-similarity assumptions implicit in a one-point closure. Instead, a spectral closure permits the self-similarities to emerge naturally as a response of the turbulence field to the environment [10]. The variable-density spectral model applied to homogeneous turbulence did not demonstrate the emergence of a self-similar form--a prerequisite for formal validity of a single-point closure. In the absence of any source for density fluctuations, the spectrum for the fluctuating density-specific volume correlations either decays (due to molecular diffusion) or "piles-up" at a given wave number region due to unspecified "particle-size" or "bubble-size" limitations. However, the spectra for the energy and turbulence mass flux start at zero, attain extremal values at some time, and then decay as the fluctuating density correlations vanish. Under these circumstances, there is no "equilibration" of the various spectra with respect to each other and no full self-similarity emerges. In the case of a mean-field density gradient, as in the case of the Rayleigh-Taylor mixing layer, a full self-similarity may emerge. (See below.)

The variables and equations derived for the variable-density extension of the LWN model have provided a basis for subsequent variable-density spectral closure developments by Steinkamp, Clark and Harlow [11,12], as well as by French researchers at the Centre d'Etudes de Limeil-Valenton [13]. Steinkamp, Harlow and Clark [11,12] extended the modeling to the strongly inhomogeneous Rayleigh-Taylor Instability. An important aspect of the model of Steinkamp et al. is the development of an explicitly integral formulation of the pressure terms. Previous modeling efforts (including ALL one-point developments, as well as the LWN model and the model of Clark and Spitz [6]) treat the fluctuating pressure-strain correlations as "local" differential terms, despite the fact that they exert an influence over the entire turbulent field in a "nonlocal" integral fashion. Although differential models can be exact for homogeneous turbulence, the exact form is impractical for engineering applications. In addition, if the field is strongly inhomogeneous, as in the case of the Rayleigh-Taylor instability, the assumption of homogeneity implicit in the differential

formulation is strongly suspect. Thus this particular aspect of the model of Steinkamp et al. is novel, and may point the way to more advanced closures for the pressure-strain correlations. (The issue of proper modeling of pressure-strain correlations will be discussed in greater detail below.)

The Steinkamp et al. model demonstrated good agreement with experimental data, although it must be admitted that the available experimental data was of insufficient detail to provide a comprehensive and conclusive test of the model. This model did show the emergence of approximately self-similar spectra, suggesting a reduction to a particular single-point form, presented in [12]. Current work is ongoing at LANL (under other auspices) to compare this model's predictions with the highly detailed data now available from the Linear Electric Motor (LEM) Rayleigh-Taylor experiments currently conducted at Lawrence Livermore National Laboratory. Vasseur [13] extended the modeling to compressible turbulence, but no comparisons of this development with either experiment or direct numerical simulations have been made.

An additional extension of the LWN model was the case of isotropic turbulence with helicity [14]. The possibility of modeling helical turbulence with a relatively simple closure like the LWN model suggests that models similar to the LWN model might be constructed usefully for circumstances wherein turbulent helicity may play an important role, such as turbulent plasmas. Much work remains to be done along these lines, but our initial effort suggests a fruitful future for this approach.

The first application of the LWN model to inhomogeneous turbulence was presented by Besnard et al. [1] and consisted of calculations of a temporally evolving free-shear layer. Two features of these calculations deserve special mention. First, the model displayed the emergence of a self-similar form wherein the scaled spectra appeared to be constant functions of their scaled distance from the shear plane. This feature is well documented by Besnard et al. [1], and implies that the turbulence anisotropy is a constant function of the distance from the center of the shear plane and of time. Second, the results were highly sensitive to the particular choice of the coefficient c_d . For values of c_d that are slightly larger or smaller than $c_d = 0.5125$ (e.g., 0.65 or 0.35), the model produced physically implausible solutions at late times. Subsequent analysis has indicated that both of these features are products of the simple form for the turbulence self-diffusion model (the last line of eqn. (6)). The specifics of this analysis have been prepared for publication.

The results of the model computations and analysis of the temporally evolving free-shear layer suggested that the turbulence self-diffusion term (last line of eqn. (6)) must be refined. This term represents the configuration space effects of the triple-velocity

correlations arising from the advective terms of the Navier-Stokes. Since the single-point triple-velocity correlation $\langle u'_i u'_j u'_k \rangle$ is symmetric in its indices, it is reasonable to require a similar tensorial property for the spectral model of this term after integrating it over all wave numbers. The simple form of the diffusion closure fails this test, although it must be noted that the two-point triple-velocity correlation does not satisfy such a simply indicial symmetry. It has been argued that similar effects arise from the fluctuating pressure-velocity correlations that do not satisfy the indicial symmetry, and that inclusion of the effect of these terms may render a form in agreement with that shown in eqn. (6). Our analysis has indicated that inclusion of the pressure-velocity correlations does not yield the given form. (This analysis is being prepared for publication.)

As part of the effort to determine the correct form of the model for the triple velocity correlations and pressure-velocity correlations, a DNS computer code was developed and implemented for the case of inhomogeneous turbulence--turbulent flow between two free-slip walls. A total of 16 statistically independent computations were performed to simulate diffusive inhomogeneous turbulence in the absence of any mean-flow velocity gradients. The resolution of these runs was $80 \times 120 \times 80$. These 16 computations form an "ensemble" of computations with which to compute statistics of the second-, third- and fourth-order velocity correlations as well as pressure-velocity correlations. The results indicate the importance of maintaining the proper symmetric tensor form of the triple-velocity correlations. In addition, the results indicate that the effects of the pressure-velocity correlations are small compared to the triple correlations except in the vicinity of the wall. In addition, no clean differential formulation of the effects of the pressure-velocity correlations appeared to improve the fidelity of the model calculations. The results of these simulations are being prepared for inclusion in our analysis of the triple-velocity correlations described above.

On the basis of the analysis of the triple velocity correlations and the results of the direct numerical simulations, an additional series of computations were performed using the LWN model with the symmetric form of the triple correlation as proposed by Besnard et al. [1], as well as variants of this form. The symmetric form given by Besnard et al. [1] is

$$Turb. Diff. = \frac{\partial}{\partial x_n} \left\{ D_{ni} \frac{\partial E_{ij}}{\partial x_i} + D_{ji} \frac{\partial E_{ni}}{\partial x_i} + D_{ii} \frac{\partial E_{jn}}{\partial x_i} \right\} \quad (7.a)$$

where

$$D_{ij} = \int_0^\infty \frac{E_{ij}}{\tau_i} dk \quad (7.b)$$

is a diffusivity tensor and τ_t is a k -space dependent turbulent time-scale, either the form originally proposed by Besnard et al. [1], or the modified form discussed above. The computations with the fully symmetric form produced self-similar solutions that were physically more plausible than the original nonsymmetric form. The scaled spectral shapes were constant in time, but were now functions of the scaled distance from the shear plane. Hence the turbulence anisotropy now varies across the shear layer. Figures 1-4 show the variations of the spectral shapes as functions of the scaled distance (y) from the shear plane. Note that the scaling is based on the characteristic length scale, $L(t) = 1/k_{max}(t)$ where $k_{max}(t)$ is the wave number where $E_{nn}(0, k, t)$ attains its maximum value. Figure 5 shows the variation of the turbulence anisotropy across the shear plane. Note that the anisotropy tensor is defined as

$$b_{ij} = \frac{\langle u'_i u'_j \rangle}{\langle u'_n u'_n \rangle} - \frac{1}{3} \delta_{ij}.$$

The self-similar form observed in this free-shear-layer computation can be exploited profitably in the derivation of more tractable single point closures. The results of this examination of turbulent diffusion also have implications for the spectral modeling effort in the variable density case, since similar terms describing similar physical processes also arise in the variable density case. Constraints have not permitted us to pursue this further under this LDRD project, but the research is now ongoing at LANL under other auspices.

A chief difficulty in the modeling efforts described above (as well as in all one-point modeling efforts) is the inability to rigorously treat the diffusive "nonlocal" effects of the triple-velocity correlations and of the fluctuating pressure-strain and pressure-velocity correlations. The triple correlations have been the object of much theoretical scrutiny because they form the crux of the closure problem: evolution equations for an n^{th} -order correlation require $(n+1)^{\text{th}}$ -order correlations. Theoretical developments to treat the triple correlations are typically based on the assumption that the turbulent fluctuations are nearly statistically Gaussian. For example, the EDQNM model assumes that the triple correlations are nonzero, but then invokes a Gaussian assumption for the fourth order correlations, thus closing the hierarchy of equations. Unfortunately, most of the previous theoretical work regarding the triple correlations has been for a homogeneous isotropic turbulence where the diffusive effects of the turbulence upon itself are irrelevant. The correlations involving fluctuating pressure can be succinctly expressed as convolution integrals over the turbulent field. These integrals involve the two-point second-order and third-order correlations. The correlations involving fluctuating pressure provide no additional closure problem in

principle beyond that posed by the third-order two-point correlations. However, the resulting formulations typically are nearly intractable except in the simplest circumstances, e.g., isotropic turbulence. The second and third lines of eqn. 6 are models of the pressure-strain correlations--a two-point second-order correlation--deduced from the full three-dimensional convolution. This is not a precise representation of the actual physical process because much information regarding the directionality of the correlation has been lost in order to make the model a function of scalar- k rather than vector- $\mathbf{k}$. This was done for reasons of tractability. Thus it appears that modeling at the level of the LWN model (and including recent work by other researchers (LaPorta [15] and Burden [16])) still requires the invocation of heuristic assumptions, which may have profound effects on the predicted self-similarities of the modeled equations. This was precisely the circumstance discussed above regarding the free-shear-layer computations.

One route to avoiding the use of additional heuristic assumptions for inhomogeneous circumstances beyond those required to close the velocity-moment hierarchy of equations is to construct the model from basis functions appropriate to the flow-field geometry wherein the convolutions required by the correlations with the fluctuating pressure become simple multiplications. Thus the diffusive effects of turbulence in an inhomogeneous circumstance are produced simply from the nature of the closure assumption (e.g., nearly Gaussian fluctuations) and without resort to additional heuristic arguments such as those invoked in LWN. Such an approach was first suggested by Kraichnan using the Direct Interaction Approximation [17] and using the Test Field Model [18]. Due to the complexity of these formulations, these initial suggestions were never pursued.

In an effort to elucidate the nature of the turbulent diffusion processes and the influence of the correlations involving pressure fluctuations, Turner has constructed an Eddy-Damped Quasi-Normal Markovian (EDQNM) model using basis functions appropriate for turbulence between two free-slip walls. The methodology for determining these basis functions was first proposed by Turner and Christiansen [19] and then refined by Turner under the auspices of this LDRD project, first for homogeneous anisotropic turbulence [20] and then for the case of inhomogeneous anisotropic turbulence [21]. The precise definition of the basis functions is not important for the present discussion, and is presented in [21]. Using the Navier-Stokes equations expressed in terms of these basis functions as a starting point, the EDQNM model can be derived in virtually the same manner as for homogeneous anisotropic turbulence. However, one additional statistical assumption is required: that the states described by the basis functions be statistically

independent. This assumption is referred to as the random phase approximation (RPA)[21] and can be expressed succinctly as

$$\langle c(\mathbf{k}, t) c(\mathbf{k}', t) \rangle = \delta(\mathbf{k} + \mathbf{k}') U(\mathbf{k}, t),$$

where the c -functions are the coefficients of the basis states and U is the correlation function, (not the velocity). The RPA does not need to be invoked explicitly for homogeneous turbulence. It is a consequence of the translational symmetry of the homogeneous environment. For the present inhomogeneous case, the RPA seems physically plausible.

To gain more confidence in the validity of the RPA, the DNS results from the inhomogeneous spectral Navier-Stokes simulation code continue to be analyzed by Clark under other auspices. In these DNS results, the inhomogeneous direction lies along the axis $y=x_2$. The other two directions in the simulation are periodic ("homogeneous")--this is consistent with the inhomogeneous EDQNM model development. The significant correlation is

$$\langle c(k_1, k_2, k_3, t) c(-k_1, k'_2, -k_3, t) \rangle = \delta(k_2 + k'_2) U(\mathbf{k}, t).$$

This statistic, for a variety of values of k_1 and k_3 , was computed by averaging over sixteen realizations corresponding to a time of between one and two initial eddy turnover times. In order to compensate for background noise, the correlation was normalized as follows,

$$F(k_1, k_2; k'_2, k_3, t) = \frac{\langle c(k_1, k_2, k_3, t) c(-k_1, k'_2, -k_3, t) \rangle \langle c(k_1, k_2, k_3, t) c(-k_1, k'_2, -k_3, t) \rangle^*}{\langle c(k_1, k_2, k_3, t) c(-k_1, -k_2, -k_3, t) \rangle \langle c(k_1, k'_2, k_3, t) c(-k_1, -k'_2, -k_3, t) \rangle}$$

where the star denotes complex conjugation. The results of this calculation are presented in Figure 6, and seem to provide strong support for the validity of the RPA.

This model development provides the opportunity to determine if the fundamental statistical assumptions of current theoretical models are sufficient to describe the difficult circumstance of inhomogeneous turbulence, or if *ad hoc* (or heuristic) corrections are required. It has been asserted often by researchers that one profitably can assume "local homogeneity" in many inhomogeneous turbulence, and then invoke various results from homogeneous theories to solve inhomogeneous problems. While this may be true in some circumstances, it has never been rigorously demonstrated. This new model development allows us to test these assertions. It is important to note that, although the development of a formal theoretical description for a single inhomogeneous turbulent field may seem limited, prior rigorous applications of these theories almost exclusively have been for purely homogeneous turbulence, and usually for isotropic turbulence. We expect that study of the inhomogeneous EDQNM formulation will shed much more light on general

inhomogeneous fields than is possible with the homogeneous formulations used in the past. Hence, we expect that further work with this model will suggest fundamentally new approaches to development of more tractable engineering models by shedding new light on the processes that lead to the phenomenon of turbulent self-diffusion.

Numerous additional accomplishments include:

- Development of a new approach to initialize direct numerical simulations of isotropic turbulence to control initial anisotropy and helicity.
- Development of a new method for computing the radial distributions of turbulence spectra which have been calculated on a rectangular lattice.
- Development of new technology for analyses and computations of the EDQNM model applied to isotropic turbulence.
- Derivation and study of a chaotic system related to the triadic interactions of the Navier-Stokes equations as used by Turner [22].
- Construction of a simple algebraic model of passive scalar flux [23].

All of these developments have been catalogued in previous LDRD progress reports, and much of it is being prepared for submission, or currently submitted, to technical journals.

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Figure 1. Shape of $E_{nn}(y,k,t)$ at $t=1024.0$

{Note: $\xi(y,t) = k/k_{max}(y,t)$; $k_{max}(y,t)$ is value of k where $E_{nn}(y,k,t)$ is maximal.
 $L(t)$ is inverse of k where $E_{nn}(0,k,t)$ is maximal.}

Figure 2. Shape of $\bar{E}_{11}(y,k,t) = E_{11}(y,k,t) - E_{nn}(y,k,t)/3$ at $t=1024.0$

{ $\xi(y,t) = k/k_{max}(y,t)$; $k_{max}(y,t)$ is value of k where $\bar{E}_{11}$ is extremal.
 $L(t)$ is inverse of k where $E_{nn}(0,k,t)$ is maximal.}

Figure 3. Shape of $E_{12}(y, k, t)$ at $t=1024.0$

{ $\xi(y, t) = k/k_{\max}(y, t)$; $k_{\max}(y, t)$ is value of k where E_{12} is extremal.
 $L(t)$ is inverse of k where $E_{\min}(y, k, t)$ is maximal.}

Figure 4. Shape of $\tilde{E}_{22}(y, k, t) = E_{22}(y, k, t) - E_{\min}(y, k, t)/3$ at $t=1024.0$

{ $\xi(y, t) = k/k_{\max}(y, t)$; $k_{\max}(y, t)$ is value of k where $\tilde{E}_{22}$ is extremal.
 $L(t)$ is inverse of k where $E_{\min}(0, k, t)$ is maximal.}

Figure 5. Anisotropy Tensor Components versus Distance (y) from the Shear Plane at $t=1024.0$. {The anisotropy tensor, b_{ij} is defined in the text.}

Figure 6. Correlation of $c(k_1, k, k_3)$ and $c(-k_1, k', -k_3)$ averaged over 16 realizations and normalized as discussed in the text of this report. The diagonal line, representing the maximal correlation, demonstrates the RPA. Details are discussed in the text.