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Cite as: Phys. Fluids **33**, 080403 (2021); https://doi.org/10.1063/5.0062933
Submitted: 09 July 2021 • Accepted: 19 July 2021 • Published Online: 04 August 2021

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Physics of Fluids EDITORIAL scitation.org/journal/phf

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Cite as: Phys. Fluids 33, 080403 (2021); doi: 10.1063/5.0062933
Submitted: 9 July 2021 · Accepted: 19 July 2021 ·
Published Online: 4 August 2021

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ABSTRACT

Professor Edward Ephraim O'Brien ("Ted") has made lasting contributions to the theory and modeling of scalar mixing and reaction in turbulent flows. With a doctoral dissertation at The Johns Hopkins University in 1960, entitled "On the Statistical Behavior of a Dilute Reactant in Isotropic Turbulence," supervised by the legend Stanley Corrsin, and in the company of notable pioneer of turbulence, John Leask Lumley, Ted's academic training propelled him through a prolific career. In the opening article of this Special Issue, we provide a review of some of Ted's contributions. First, a summary is presented of his work on the examination of the failure of the cumulant discard approximation for the scalar mixing. This is followed by a highlight of his impacts on other spectral theories of turbulence including Kraichnan's direct interaction approximation. His contributions to more modern theoretical/computational description of reactive turbulence are discussed next, including the transported probability density function (pdf) formulation, scalar-gradient pdf transport equation, scalar interfaces, and the filtered density function. Finally, some of his research on Direct Numerical Simulation of compressible turbulence is reviewed.

I. SETTING THE STAGE

The success of statistical theories of turbulence was apparent in the 1950s. The Johns Hopkins University (JHU) was a lighthouse in Fluid Mechanics and Turbulence in that and subsequent decades. Francis Clauser, Stan Corrsin, Owen Phillips, Les Kovasznay, Marc Morkovin, Bob Betchov, and Clifford Truesdell, among others, formed the avant-garde fostering innovative education and creative research in these fields. Ted O'Brien arrived at JHU amid this legendary atmosphere in 1957 and stayed there until 1961. John Lumley was also there during those years. Stan Corrsin and Ted O'Brien pioneered the formulation of initial ideas on the statistical treatment of turbulent reacting flows and set the stage for future developments in reactive and combusting systems. Ted focused most of his research on turbulent constant density fluid flows, which convect scalars of constant molecular diffusion coefficients. The scalar field, $\theta(\boldsymbol{x},t)$, obeys the conservation equation

$$\frac{\partial\theta}{\partial t}+u_j\frac{\partial\theta}{\partial x_j}=D\frac{\partial^2\theta}{\partial x_j\partial x_j}+\frac{\dot{\omega}(\theta)}{\rho}, \tag{1}$$

where u_j is the jth component of the turbulent solenoidal zero-mean velocity field, ρ is the constant fluid density, D stands for the constant Fickian molecular diffusion coefficient, and $\dot{\omega}(\theta)$ represents the reaction rate, dependent on $\theta(\boldsymbol{x},t)$ in a non-linear manner. Moreover, in most of his research, O'Brien assumed statistically homogeneous, and often isotropic, scalar, and zero mean turbulence fields. A statistically homogeneous scalar field, $\theta(\boldsymbol{x},t)$, with a mean, $\langle\theta\rangle(t)$, which is either a constant (for an inert scalar) or a time-dependent function (for a reactive scalar), was decomposed into its mean plus its fluctuations, $\theta'(\boldsymbol{x},t)$, as $\theta(\boldsymbol{x},t)=\langle\theta\rangle(t)+\theta'(\boldsymbol{x},t)$. Ted's work on turbulent mixing of passive scalars considered a variety of flows, including isotropic,[1] homogenous with a mean scalar,[2] turbulent boundary layers,[3] wakes,[4] and plumes.[5] His work on reactive turbulence was almost exclusively in homogeneous flows.[6–15] Below, a summary is provided of some of his key contributions in a nearly chronological manner.

II. SPECTRAL THEORIES

One of Ted's earlier contributions to the spectral theory of turbulence follows his doctoral studies at JHU[16] and pertains to the scalar field application of the quasi-normal approximation, originally proposed for turbulence.[17,18] The turbulence problem concerns the solution of the transport equation for the spectral energy $E(\boldsymbol{k},t)$ where $\boldsymbol{k}$ is the vector of wavenumbers in an isotropic field. The closure is

achieved with the assumption that the fourth-order cumulant of the non-Gaussian fluctuating velocity vanishes like for a Gaussian random variable. With this approximation, the fourth-order moments can be expressed as the sum of products of the second-order moments. A statistically homogeneous and isotropic scalar fields, advected by an isotropic turbulent field with a zero-mean velocity, is investigated. For this problem, the equation for the two-point scalar correlation field $\langle \theta'(\boldsymbol{x},t)\theta'(\boldsymbol{x}+\boldsymbol{r},t)\rangle$ is analyzed by Ted and Francis,[19] where $\boldsymbol{r}=\boldsymbol{x}'-\boldsymbol{x}$ is the spatial separation vector, with $G(k^2,t)$ as the isotropic spectral representation of this correlation. They also included the governing equations for three-point, third-order moments, $\langle \theta'(\boldsymbol{x},t)\theta'(\boldsymbol{x}+\boldsymbol{r},t)\boldsymbol{u}'(\boldsymbol{x}'',t)\rangle$, where $\boldsymbol{x}''=\boldsymbol{x}+\boldsymbol{r}'$, with a corresponding isotropic spectral representation of these moments by $\mathcal{L}(k,k',\mu,t)$, where $\mu=\frac{\boldsymbol{k}\cdot\boldsymbol{k}'}{|\boldsymbol{k}||\boldsymbol{k}'|}$. The governing equations for the third-order moments contain several fourth-order moments such as $\left\langle u_k'(\boldsymbol{x}'',t)\,u_j'(\boldsymbol{x},t)\,\theta'(\boldsymbol{x},t)\,\theta'(\boldsymbol{x}',t)\right\rangle$, with the spectral transform $\varphi_{jk}(\boldsymbol{k}')\,G(k^2)$, where $\varphi_{jk}(\boldsymbol{k}')$ is the Fourier transform of the fluctuating velocity correlation $\left\langle u_i'u_j'(\boldsymbol{r})\right\rangle$. This fourth-order moment, as an example, is approximated via a cumulant discard closure assumption, analogous to that for the turbulent field

$$\begin{aligned}\left\langle u_k'(\boldsymbol{x}'',t)\,u_j'(\boldsymbol{x},t)\,\theta'^{(\boldsymbol{x},t)}\theta'(\boldsymbol{x}',t)\right\rangle &= \left\langle u_k'(\boldsymbol{x}'',t)\,u_j'(\boldsymbol{x},t)\right\rangle\left\langle\theta'^{(\boldsymbol{x},t)}\theta'(\boldsymbol{x}',t)\right\rangle \\ &+\left\langle u_k'(\boldsymbol{x}'',t)\,\theta'(\boldsymbol{x},t)\right\rangle\left\langle u_j'(\boldsymbol{x},t)\,\theta'(\boldsymbol{x}',t)\right\rangle \\ &+\left\langle u_k'(\boldsymbol{x}'',t)\,\theta'(\boldsymbol{x}',t)\right\rangle\left\langle u_j'(\boldsymbol{x},t)\,\theta'(\boldsymbol{x},t)\right\rangle. \end{aligned} \tag{2}$$

O'Brien and Francis[19] numerically solved the spectral decay of $G(k^2,t)$ and $\mathcal{L}(k,k',\mu',t)$, together with the equation governing spectral scalar energy transfer

$$2\pi\int_0^\infty\int_{-1}^{+1}\mathcal{L}(k,k'',\mu,t)k''^2\,dk''d\mu' = T\left(k^2,t\right).$$

The initial conditions are as follows:

$$G\left(k^2,0\right)=Be^{-k^2},\quad E\left(k'^2,0\right)=E\left(k'^2,t\right)=\left(3\pi^{3/2}\right)^{-1}k'^2e^{-k'^2},\quad \text{and}\quad T\left(k^2,0\right)=0, \tag{3}$$

where $\varphi_{ij}(\boldsymbol{k}')=\varphi(k'^2)\left[\delta_{jk}-\frac{k_j'k_k'}{k'^2}\right]$, and E is the spectrum energy density for the turbulence. The solution shows that the scalar spectrum develops incorrect negative values after a time of approximately $2l/u_{rms}$, where l is the integral length scale of the energy-containing components of the turbulence, and $u_{rms}=\left(\langle u'^2\rangle\right)^{1/2}$ is the root-mean-square turbulent velocity fluctuation. To address this problem, Orszag[20] proposed the addition of a damping term to the physical viscosity in the evolution equation for the third-order moments in spectral space, leading to the Eddy-Damped Quasi-Normal (EDQN) approximation. This approach, although producing a more physically acceptable solution, does not guarantee realizability, or the positiveness of the energy spectrum in all situations. This prompted another modification,[21] often referred to as Markovianization, wherein the augmented viscous exponent in the third-order moment equations is assumed to vary with a characteristic time, much smaller than the characteristic evolution time of the sum of products of the second-order moments used to approximate the fourth-order moments. This level of the quasi-normal theory is referred to as the Eddy-Damped Quasi-Normal Markovian (EDQNM) approximation. Although the EDQNM may yield acceptable solutions in the inertial and dissipative ranges of the energy spectrum, it is questionable in the energy-containing range where both times are of a comparable order of magnitude. Leslie[22] proposed a remedy for this in a subsequent study.

The failure of the cumulant discard closure approximation for the scalar mixing problem[19,23] provided the motivation to explore the direct interaction approximation (DIA). Kraichnan[24] applied the DIA theory to the scalar quantity convective problem, deriving the set of equations under Gaussian initial conditions. Lee[25] investigated the decay of scalar quantity fluctuations in a simplified statistically stationary velocity field and reported the physical plausibility of the solutions. However, in a quantitative test of DIA, O'Brien[8] showed that the application to the problem of isotropic mixing of a reactant undergoing an isothermal second-order reaction fails to preserve an important invariance. Namely, in the absence of molecular diffusion, the decay of single-point statistical functions of the concentration should be independent of the turbulence. Thus, whereas $\langle\theta\rangle(t)$ and $\langle\theta'^2\rangle(t)$ were found to be insensitive to the approximation over the time interval used to integrate for Damkhöler number, $Da\in[0,\,100]$, but that $\langle\theta'^3\rangle(t)$ showed a marked variation with Da. This problem with $\langle\theta'^3\rangle(t)$ is expected to influence the behavior of the lower moments significantly at later times.

Partly because of the non-invariance of the DIA under random Galilean transformations, the procedure does not give a Kolmogorov $k^{-5/3}$ in the inertial range, but rather a $k^{-3/2}$. Kraichnan[26] thus proposed a heuristic Lagrangian history direct interaction approximation (LHDIA). In a subsequent study on LHDIA, O'Brien[9] derived the equations describing the behavior of the passive reactant when its concentration is decaying owing to an isothermal reaction of second order, and when it is advected by a turbulent flow. Within the Lagrangian framework, the scalar equation in the form

$$\left(\frac{\partial}{\partial t}-D\nabla^2\right)\theta(\boldsymbol{x},t)=-\boldsymbol{u}(\boldsymbol{x},t|t_r)\cdot\nabla\theta(\boldsymbol{x},t)-c\theta^2(\boldsymbol{u},t) \tag{4}$$

was investigated, where θ is the instantaneous scalar field and $\boldsymbol{u}(\boldsymbol{x},t|t_r)$ is the velocity measured at time t_r within the fluid element, which passes through $\boldsymbol{x}$ at time t. The analogous scalar field definition is $\theta(\boldsymbol{x},t|t_r)$, which is equal to $\theta(\boldsymbol{x},t_r)$. O'Brien[9] was able to establish that the decay of one-point statistical functions of the concentration field occurs at a rate that is independent of the turbulence when molecular diffusion is neglected, or $D=0$. Under this condition, turbulence plays no direct role in decreasing the scalar intensity. It is noteworthy that this invariance was not consciously built into LHDIA. The DIA and LHDIA theories are not widely used today, and it is unclear whether they are superior to EDQNM.[22] The EDQNM was later used by Ted's student, Jiang, for modeling reactive turbulent flows.[27]

III. TRANSPORTED PROBABILITY DENSITY FUNCTION (PDF) FORMULATIONS

Ted and his Ph.D. student (C.D.) initiated a systematic study leading to what is known today as the transported pdf modeling.

Dopazo and O'Brien[28–30] formally examined linear equations in functional derivatives[31–33] and applied them to the dynamically passive turbulent mixing of two reactants undergoing a one-step, second-order, irreversible, exothermic, and constant temperature, chemical reaction in homogeneous turbulence. Under some simplifying assumptions and through the projection of the functional equation[34,35] into a finite dimensional space, one- and two-point temperature pdf transport equations were obtained. The reaction rate term, product of concentrations, and the Arrhenius exponential dependence on temperature became variable coefficients in probability space. The derivation of the pdf transport equation can be straightforwardly applied also to variable density fluid flows.[36]

For a statistically homogeneous zero-mean velocity turbulence of a constant density fluid stirring a statistically homogeneous scalar field, the one-point pdf, $P(\Theta;t)=\langle\delta[\Theta-\theta(\boldsymbol{x},t)]\rangle$, is governed by the two equivalent transport equations

$$\frac{\partial P}{\partial t}=-\frac{\partial}{\partial\Theta}\left\{\left\langle D\frac{\partial^2\theta}{\partial x_j\partial x_j}\middle|\theta(\boldsymbol{x},t)=\Theta\right\rangle P\right\}-\frac{\partial}{\partial\Theta}\left[\frac{\dot\omega(\Theta)}{\rho}P\right], \quad (5)$$

$$\frac{\partial P}{\partial t}=-\frac{\partial^2}{\partial\Theta^2}\left[\langle\varepsilon_\theta|\theta(\boldsymbol{x},t)=\Theta\rangle P\right]-\frac{\partial}{\partial\Theta}\left[\frac{\dot\omega(\Theta)}{\rho}P\right]. \quad (6)$$

Θ stands for $\theta(\boldsymbol{x},t)$ in the probability space. $\delta[\Theta-\theta(\boldsymbol{x},t)]$ is the Dirac delta function, which defines the fine-grained pdf.[37–39] Angular brackets denote, for example, ensemble average or any other type of averaging operator. Note that convection does not explicitly enter the equation because of the assumptions of solenoidality and statistical homogeneity. The first terms on the right side represent the molecular diffusion of pdf, whereas the last one expresses the effect of the chemical reaction on the pdf. Both terms imply transport in scalar space.

The term $\left\langle D\frac{\partial^2\theta}{\partial x_j\partial x_j}\middle|\theta(\boldsymbol{x},t)=\Theta\right\rangle$ in Eq. (5) is the molecular diffusion rate, conditioned on $\theta(\boldsymbol{x},t)=\Theta$. This is the so-called micro-mixing term and has been the stumbling block in the transported pdf methodology for almost fifty years. Note that the scalar dissipation rate, conditional upon the scalar value $\theta(\boldsymbol{x},t)=\Theta$, $\langle\varepsilon_\theta|\theta(\boldsymbol{x},t)=\Theta\rangle$, is a non-negative variable.

The second derivative with respect to Θ in Eq. (6) implies diffusion in the Θ-domain with a negative variable diffusivity. This corresponds to the physical fact that for asymptotically large times probability tends to concentrate about the mean with a vanishing variance. The issue of diffusion equations with negative diffusivities has been investigated, for example, in light squeezing research to reduce quantum noise[40] and in the simultaneous backward diffusion of boron and point defects in Si.[41]

Note that, as previously mentioned, the non-linearity of $\frac{\dot\omega(\theta)}{\rho}$ in physical space becomes a nonlinear variable coefficient, $\frac{\dot\omega(\Theta)}{\rho}$, in the pdf transport equations (5) and (6). Equating the right sides of these two equations, a relationship between the conditional dissipation, the conditional diffusion, and $P(\Theta;t)$ can be established. Dopazo and O'Brien[29] proposed a model, known as the Linear Mean Square Estimation (LMSE), for the unclosed conditional diffusion $\left\langle D\frac{\partial^2\theta}{\partial x_j\partial x_j}|\theta(\boldsymbol{x},t)=\Theta\right\rangle$. This term was rephrased as $D\lim_{\boldsymbol{x}'\to\boldsymbol{x}}\nabla^2_{\boldsymbol{x}'}\langle\theta(\boldsymbol{x}',t)|\theta(\boldsymbol{x},t)=\Theta\rangle$, which was approximated using a Linear Mean Square Estimation (LMSE), namely, $\langle\theta(\boldsymbol{x}',t)|\theta(\boldsymbol{x},t)=\Theta\rangle=\langle\theta\rangle(t)+\rho(\boldsymbol{r},t)[\Theta-\langle\theta\rangle(t)]$, where $\rho(\boldsymbol{r},t)=\langle[\theta(\boldsymbol{x},t)-\langle\theta\rangle(t)][\theta(\boldsymbol{x}+\boldsymbol{r},t)-\langle\theta\rangle(t)]\rangle/\sigma^2_\theta(t)$ is the scalar autocorrelation coefficient and $\sigma^2_\theta(t)=\left\langle[\theta(\boldsymbol{x},t)-\langle\theta\rangle(t)]^2\right\rangle=\langle\theta'^2\rangle$ is the variance of scalar fluctuations. For a statistically isotropic scalar field, $\rho(\boldsymbol{r},t)$ is only a function of $r=|\boldsymbol{r}|$, the distance separating the two points. Then, the conditional diffusion was formally recast as

$$\left\langle D\frac{\partial^2\theta}{\partial x_j\partial x_j}\middle|\theta(\boldsymbol{x},t)=\Theta\right\rangle=-3D[\Theta-\langle\theta\rangle(t)]\left\{-\left[\frac{\partial^2\rho(r,t)}{\partial r^2}\right]_{r=0}\right\}. \quad (7)$$

We recall that[42] $-\left[\frac{\partial^2\rho(r,t)}{\partial r^2}\right]_{r=0}=\frac{2}{\lambda^2_\theta(t)}$, where $\lambda^2_\theta(t)$ is the scalar fluctuations equivalent to the Taylor micro-scale, $\lambda(t)$, in turbulence. $\lambda^2_\theta(t)$ is more consistently defined as a characteristic scalar fluctuation–dissipation timescale, $\tau_\theta(t)=\frac{\lambda^2_\theta(t)}{D}=6\frac{\sigma^2_\theta(t)}{\langle\varepsilon_\theta\rangle(t)}$. $\langle\varepsilon_\theta\rangle(t)=D\left\langle\frac{\partial\theta}{\partial x_j}\frac{\partial\theta}{\partial x_j}\right\rangle$ is the average scalar fluctuation–dissipation rate. Therefore,

$$\left\langle D\frac{\partial^2\theta}{\partial x_j\partial x_j}\middle|\theta(\boldsymbol{x},t)=\Theta\right\rangle=-6\frac{\Theta-\langle\theta\rangle(t)}{\tau_\theta(t)}. \quad (8)$$

Corrsin[43] had shown that for turbulent scalar mixing $\lambda^2_\theta(t)/D=2\lambda^2(t)/\nu=2\tau$, where ν is the kinematic viscosity and τ stands for a characteristic turbulent kinetic energy dissipation time. However, in turbulent reacting flows both the scalar autocorrelation coefficient and its associated length micro-scale must display an explicit dependence on the reaction rate. Obviously, the chemical reaction contributes to either the enhancement or the destruction of pre-existing scalar gradients and hence to $\langle\varepsilon_\theta\rangle(t)$. For small Karlovitz numbers,[44] the two variables will strongly depend on the characteristic chemical time, whereas for high Karlovitz numbers, Corrsin's relationship will be accurate and the characteristic micro-mixing time will be proportional to the turbulent kinetic energy dissipation time. Therefore, in the limit of high Karlovitz numbers, the conditional scalar diffusion is modeled as

$$\left\langle D\frac{\partial^2\theta}{\partial x_j\partial x_j}\middle|\theta(\boldsymbol{x},t)=\Theta\right\rangle=-3\frac{\Theta-\langle\theta\rangle(t)}{\tau}. \quad (9)$$

The LMSE micro-mixing model can also be justified based on the Laplacian operator finite differencing or its approximation in terms of the scalar average in a volume element around the point where $\theta(\boldsymbol{x},t)=\Theta$. The LMSE closure $\langle\theta(\boldsymbol{x}',t)|\theta(\boldsymbol{x},t)=\Theta\rangle$ can be replaced by a non-linear stochastic approximation, including higher order statistical correlations; the added complications of a non-linear model are not justified by the higher accuracy gained. The conditional diffusion can alternatively be approximated in terms of the scalar gradient magnitude and the local mean curvature of the iso-scalar surface $\theta(\boldsymbol{x},t)=\Theta$. Mixing models with two different time scales, accounting for the "explicit coupling between mixing and reaction,"[45] have been recently proposed by several authors.[46–50]

The LMSE implies a relaxation of any scalar value toward its mean. After 47 years of the first publication of this micro-mixing model, some of its flaws have been disclosed.

However, the model is still being widely used due to its simplicity. It has become apparent that the hyperbolic type pdf transport equation maintains the positiveness of the distribution but does not

change the initial shape of the distribution.[49] The addition of a stochastic term to the LMSE relaxation model allows modifying the initial pdf shape, although with incorrect asymptotic behavior.[50–52] Another class of micro-mixing closures, which overcome this problem, was inspired by droplet interaction models. Janicka *et al.*[53] and Dopazo[49] independently proposed essentially the same model. The issue on non-localness of the LMSE[45] has been addressed by Subramaniam and Pope.[54]

Ted and co-workers showed that one-point one-scalar pdf transport equations are computable. However, it soon became apparent that when dealing with joint pdfs of multi-species and temperature or species and velocity, the dimensionality in composition space was too high to use conventional finite-difference, finite-volume, or finite-element numerical techniques. Monte Carlo particle simulation methods had been applied to compute turbulent reactive flows.[55] The computational work in Monte Carlo methods is proportional to the number of independent variables, whereas, for example, in finite volume methods it grows exponentially with that number. Pope[36,56] demonstrated the feasibility of a sequential Monte Carlo simulation by the simple use of time-splitting or fractional-step techniques, which involve the separate and consecutive application of differential or discretized operators representing physical processes. A Monte Carlo field method, proposed by Valino[57] as an alternative to Monte Carlo particle techniques and applied by Sabel'nikov and Soulard[58] to turbulent reacting flows, has proved successful in Large Eddy Simulation (LES)/PDF methodologies.[59,60]

Calculation of the first and the second scalar derivatives in the conservation equation requires the knowledge of the scalar value in two and three points, respectively. This translates into a closure problem in the pdf transport equation. We recall that the conditional diffusion was rephrased in terms of the local scalar average, conditioned on the scalar value at a neighboring point.[28,61] This average can be obtained from the two-point one-time scalar pdf, $P_2(\Theta,\Theta';\mathrm{x},\boldsymbol{x}',t) = \left\langle \delta\left[\Theta-\theta(\boldsymbol{x},t)\right]\delta\left[\Theta'-\theta(\boldsymbol{x}',t)\right]\right\rangle$ or, alternatively, from the conditional pdf $P(\Theta|\Theta';\boldsymbol{x},\boldsymbol{x}',t) = P_2(\Theta,\Theta';\boldsymbol{x},\boldsymbol{x}',t)/P(\Theta';\boldsymbol{x}',t)$. P_2 also yields the scalar gradient statistics.

Lundgren,[62] Ievlev,[63] and Ted along with his students, Kuo[64] and Jiang[65] investigated multipoint pdf transport equations. While the closure approximations are cumbersome and not easy to test, the advantages of this strategy are not evident. Pope[66] and Kollmann and Wu[67] used two-time pdf transport equations at a single point. Using stochastic models, Kollmann and Wu[67] solved the transport equation for $P_2(\boldsymbol{V},\boldsymbol{V}';\boldsymbol{x},t,t') = \langle\delta[\boldsymbol{V}-\boldsymbol{u}(\boldsymbol{x},t)]\delta[\boldsymbol{V}'-\boldsymbol{u}(\boldsymbol{x},t')]\rangle$, evaluating the integral timescale and the kinetic energy dissipation rate. External specification of a timescale is not necessary and the agreement of predictions with available experimental data for a mixing layer is satisfactory. The hierarchy of multipoint pdf transport equations in compressible turbulence has been investigated, among others, by Fox[68] and more recently by Praturi *et al.*[69]

IV. SCALAR-GRADIENT PDF TRANSPORT EQUATION

The importance of the scalar fluctuation–dissipation rate in turbulent reacting flows had been remarked by Bilger.[70] Meyers and O'Brien[71] and Gao and O'Brien[72] scrutinized the joint statistics of one scalar, $\theta(\boldsymbol{x},t)$, and its gradient, $\nabla\theta(\boldsymbol{x},t)$, namely, $P_2(\Theta,\boldsymbol{G};\boldsymbol{x},t) = \langle\delta\left[\Theta-\theta(\boldsymbol{x},t)\right]\delta\left[\boldsymbol{G}-\nabla\theta(\boldsymbol{x},t)\right]\rangle$. A relaxation model (LMSE) toward mean values, θ and $\nabla\theta$, was proposed *a priori* for contributions of molecular transports. On the other hand, a white noise Kubo approximation for the convective term was used. The effects of mean velocity, molecular mixing, chemistry, and turbulent transport on the statistics of a scalar and its gradient were scrutinized. It was shown that as the Reynolds number increases the joint statistical dependence of the scalar and its gradient magnitude, $|\nabla\theta|$, becomes less significant, and $P_2(\Theta,G;\boldsymbol{x},t) \approx P(\Theta;\boldsymbol{x},t)P_g(G;\boldsymbol{x},t)$. This supported previous assumptions for non-premixed flames.[70] An analogy between transport in composition space due to chemical reaction and mass conservation in compressible gas dynamics was invoked to suggest a methodology for determining the statistical dependence induced by the chemical reaction. The model was then applied to the turbulent convection of an isotropic scalar gradient field, showing that it yields a transition probability for the logarithm of the magnitude of the gradient, which is a simple random walk with outward drift. The timescale of both the drift velocity and the variance was determined.[71,73] The explicit effect of turbulence on $P_2(\Theta,G;\boldsymbol{x},t)$ enters its transport equation as the average of the flow strain rate normal to the iso-scalar surface $\theta(\boldsymbol{x},t)=\Theta$, conditional upon the scalar value and its gradient magnitude, $\langle a_N|\theta(\boldsymbol{x},t)=\Theta,|\nabla\theta|(\boldsymbol{x},t)=G\rangle$. This is an unclosed term and requires a model.

The amplitude mapping closure (AMC) is an alternative methodology to construct approximations for the joint statistics of a scalar and its gradient undergoing molecular diffusion under stirring by a statistically isotropic turbulent velocity field. The closure is obtained by taking a Gaussian reference scalar field and distorting it locally in physical space through a mapping to exhibit the statistics of the actual scalar variable.[74–76] It is worth noting that the LMSE closure is an exact model for the molecular diffusion of a Gaussian scalar field. Gao and O'Brien[77,78] and Pope[79] compared AMC and DNS results and extended the method to model molecular diffusion in a multispecies turbulent flow. Valino *et al.*[80] generalized the AMC to time-dependent Gaussian fields, obtained analytical solutions for symmetric binary mixing, and produced numerical results combining a Monte Carlo simulation and the analytic solution. O'Brien and Jiang[81] show that a necessary and sufficient condition for the conditional scalar dissipation rate to be independent of scalar value is that its one-point pdf is Gaussian, which obtain for an initially symmetric double-delta pdf a separable (scalar and time dependences) closed-form solution, which agree with DNS results. Ted and Sahay[82] show unsatisfactory asymptotic properties in the scalar binary mixing problem of the AMC, which predicts a conditional expectation that shows both a persistent symmetry when the pdf is not symmetric and an unphysical permanence for the original scalar bounds. The incorrect asymptotic behavior of the AMC for unsymmetric binary mixing is also shown by He and Rubinstein.[83] Raissi *et al.*[84] use deep learning (DL) to discover models for the conditional expected diffusion and the conditional expected dissipation of a scalar undergoing a Fickian diffusion described by its transported single-point PDF equation and the discovered model is appraised against the exact solution derived by the AMC/Johnson–Edgeworth translation model of binary scalar mixing in homogeneous turbulence.[85] The philosophy behind the recent deformation of Gaussian fields (RDGF) closure[86] to investigate the evolution of velocity gradients in turbulence and the multiscale turnover Lagrangian map (MTLM) procedure[87] to generate non-Gaussian synthetic turbulence fields is somewhat similar to that of the AMC.

Conditioned scalar dissipation and chemical reaction rates are directly connected.[88] Conditional dissipation also appears as one of the essential variables of quasi-stationary normalized scalar pdf.[89,90] Ted's Ph.D. students, Gao and Jiang, conducted further investigations on the AMC.[91,92]

The pdf transport methods have been extensively reviewed by O'Brien,[61,93,94] Pope,[36,95–97] Kollmann,[98] Dopazo,[99] Fox,[50] Haworth,[100] Haworth and Pope,[101] among others.

V. SCALAR INTERFACES

Interfaces separating two regions of the flow domain with different levels of a variable are examples of non-material surfaces. Corrsin[102] unveiled the large scale or external intermittency of shear flow turbulence and what was termed "superlayer," namely, the thin layer separating the turbulent flow, with high vorticity or enstrophy levels, and the irrotational region outside it. For scalar fields, the iso-surface $\theta(\boldsymbol{x},t)=0^+$, where 0^+ denotes a constant infinitesimal value of $\theta(\boldsymbol{x},t)$, separates the two flow domains $\theta(\boldsymbol{x},t)<0^+$ and $\theta(\boldsymbol{x},t)>0^+$. The iso-surface $\theta(\boldsymbol{x},t)=0^+$ obeys the equation[103]

$$\frac{\partial\theta}{\partial t}+u_j^{\theta}\frac{\partial\theta}{\partial x_j}=0. \tag{10}$$

The local velocity of $\theta(\boldsymbol{x},t)=0^+$ is given by $u_j^{\theta}(\boldsymbol{x},t)=u_j(\boldsymbol{x},t)+V(\boldsymbol{x},t)n_j(\boldsymbol{x},t)$. $u_j(\boldsymbol{x},t)$ is the local flow velocity, and $V(\boldsymbol{x},t)n_j(\boldsymbol{x},t)$ is the local normal velocity vector relative to the iso-surface (see Fig. 1). Then,

$$\frac{\partial\theta}{\partial t}+u_j\frac{\partial\theta}{\partial x_j}=-V|\nabla\theta|=V^e|\nabla\theta|=D\frac{\partial^2\theta}{\partial x_j\partial x_j}+\frac{\dot\omega(\theta)}{\rho}. \tag{11}$$

The right side is the source of $\theta(\boldsymbol{x},t)$, and $-V=V^e$ is termed the entrainment velocity of fluid from region $\theta(\boldsymbol{x},t)<0^+$ to region $\theta(\boldsymbol{x},t)>0^+$, across the interface $\theta(\boldsymbol{x},t)=0^+$. An indicator function $I(\boldsymbol{x},t)$ can be defined as a generalized function,[104] such that $I(\boldsymbol{x},t)=0$ for $\theta(\boldsymbol{x},t)<0^+$ and $I(\boldsymbol{x},t)=1$ for $\theta(\boldsymbol{x},t)>0^+$. Note that the defined scalar interface is analogous to an iso-scalar surface within a turbulent premixed flame, where V plays the role of the normal displacement speed, S_d. $I(\boldsymbol{x},t)=H\left[\theta(\boldsymbol{x},t)-0^+\right]$, where H is the Heaviside function (Fig. 1).

A transport equation for $I(\boldsymbol{x},t)$ is readily derived

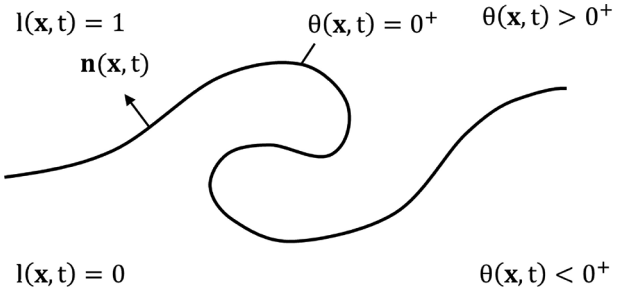

FIG. 1. Scalar interface, $\theta(\boldsymbol{x},t)=0^+$, separating regions where $\theta(\boldsymbol{x},t)<0^+$ from regions with $\theta(\boldsymbol{x},t)>0^+$. The zone indicator function is zero and unity, respectively, in those regions.

$$\frac{\partial I}{\partial t}+u_j\frac{\partial I}{\partial x_j}=V^e|\nabla\theta|\delta\left[\theta(\boldsymbol{x},t)-0^+\right]. \tag{12}$$

Equation (12) with an unknown source term on its right side had been postulated by Libby.[105,106] A different expression for the source term had been proposed by Dopazo.[107] Intermittency functions were also used in the experimental investigation of turbulent shear flows, for example, by Kovasznay *et al.*[108] Equation (12) can be used to condition any flow equation to the region where either $I(\boldsymbol{x},t)=0$ or $I(\boldsymbol{x},t)=1$. For example, the equation of $\theta(\boldsymbol{x},t)$, multiplied by $I(\boldsymbol{x},t)$, yields

$$\begin{aligned}\frac{\partial\langle I\theta\rangle}{\partial t}+\frac{\partial\langle Iu_j\theta\rangle}{\partial x_j}=&D\frac{\partial^2\langle I\theta\rangle}{\partial x_j\partial x_j}+\left\langle I\frac{\dot\omega(\theta)}{\rho}\right\rangle\\&+\left\langle\theta V^e|\nabla\theta|\delta\left[\theta(\boldsymbol{x},t)-0^+\right]\right\rangle\\&-\left\langle\varepsilon_\theta\left\{\theta\delta'\left[\theta(\boldsymbol{x},t)-0^+\right]-2\delta\left[\theta(\boldsymbol{x},t)-0^+\right]\right\}\right\rangle\\&-\left\langle\theta D\frac{\partial^2\theta}{\partial x_j\partial x_j}\delta\left[\theta(\boldsymbol{x},t)-0^+\right]\right\rangle.\end{aligned} \tag{13}$$

This is the conservation equation for $\theta(\boldsymbol{x},t)$, conditioned to region $I(\boldsymbol{x},t)=1$. $\delta'\left[\theta(\boldsymbol{x},t)-0^+\right]$ is a generalized Dirac delta function derivative.[104] The scalar conditional mean in region $I(\boldsymbol{x},t)=1$, $\langle\theta\rangle_1$, is obtained from $\langle I\theta\rangle=\langle I\rangle\langle\theta\rangle_1$; $\langle I\rangle$ is the scalar intermittency factor, which quantifies the probability of point $\boldsymbol{x}$ being at region $I(\boldsymbol{x},t)=1$ at time t. Terms involving Dirac delta functions and its derivative represent the interaction between regions $I(\boldsymbol{x},t)=1$ and $I(\boldsymbol{x},t)=0$ at the interface $\theta(\boldsymbol{x},t)=0^+$ to generate $\theta(\boldsymbol{x},t)$ in the zone $I(\boldsymbol{x},t)=1$. Multiplication by $[1-I(\boldsymbol{x},t)]$ yields the conditioned equation for zone $I(\boldsymbol{x},t)=0$. The addition of the two zone-conditioned equations yields the unconditioned conservation equation for $\langle\theta(\boldsymbol{x},t)\rangle$. Note that $|\nabla\theta|\delta\left[\theta(\boldsymbol{x},t)-0^+\right]$ in Eq. (12) has dimensions of $(\text{length})^{-1}$ normal to the iso-surface. For an infinitesimal volume, $dV=dS\left[|\nabla\theta|\delta\left[\theta(\boldsymbol{x},t)-0^+\right]\right]^{-1}$, centered at the interface

$$\begin{aligned}\theta V^e|\nabla\theta|\delta\left[\theta(\boldsymbol{x},t)-0^+\right]&=\frac{1}{V}\iiint dV\theta V^e|\nabla\theta|\delta\left[\theta(\boldsymbol{x},t)-0^+\right]\\&=\frac{1}{V}\iint dS\theta V^e=\theta V^e\Sigma.\end{aligned} \tag{14}$$

dS is the surface area element on the iso-surface $\theta(\boldsymbol{x},t)=0^+$, and Σ is the local surface density $\left(m^2/m^3\right)$ of the iso-scalar surface.[109] $\theta V^e|\nabla\theta|\delta\left[\theta(\boldsymbol{x},t)-0^+\right]$ represents the entrainment of $\theta(\boldsymbol{x},t)$ across the interface from the region $I(\boldsymbol{x},t)=0$ to the region $I(\boldsymbol{x},t)=1$. Dopazo and O'Brien[110] used this zone conditioning technique to obtain entrainment profiles of mass and momentum in turbulent jets and wakes in the self-preservation region.

O'Brien and Dopazo[103] applied this technique to obtain the transport equation of the conditioned scalar pdf, $\langle I_{\wp}\rangle=\left\langle I\delta\left[\Theta-\theta(\boldsymbol{x},t)\right]\right\rangle=\langle I\rangle P_1(\Theta;\boldsymbol{x},t)$. $P_1(\Theta;\boldsymbol{x},t)$ is the scalar pdf restricted to the zone $I(\boldsymbol{x},t)=1$. The equation was applied to the similarity region of a two-dimensional turbulent wake, where extensive conditioned moment measurements were available.[111] The asymptotic forms of the pdf were found for low and high intermittency regions, showing good agreement with experimental data. A connection

between the rate of entrainment of scalar-free fluid into the scalar containing the zone and the pdf of the scalar at small positive values of $\theta(\boldsymbol{x}, t)$ was established. The calculated zone-conditioned mean and variance of the scalar field also showed to be compatible with available experimental data.

Byggstoyl and Kollmann[112] and Janicka and Kollmann[113] applied this zone conditioning methodology to compute intermittent turbulent shear flows. Enstrophy and scalar interfaces of a methane–air turbulent premixed turbulent annular jet flame stabilized on a bluff-body burner have been recently examined using a high-fidelity, flame-resolved, three-dimensional simulation;[114] the enstrophy and the scalar interfaces have been characterized by their displacement speeds relative to the flow, and mean values, conditioned on the reaction progress variable, have been obtained.

VI. FILTERED DENSITY FUNCTION (fdf)

With increased capabilities of supercomputing technology and easier access to large computational platforms, Ted dedicated a portion of his research in the 1990s to large-scale simulations (including DNS and LES) of reactive turbulence. One of his pioneering works in this regard is the development of the filtered density function (fdf) methodology for LES.[115] In this methodology, the subgrid-scale fluctuations of the underlying scalars' array, $\theta(\boldsymbol{x}, t)$, involving N_s species are considered in a probabilistic manner. In this context, the fdf, denoted by P_L, is formally defined as[95]

$$P_L(\boldsymbol{\Theta}; \boldsymbol{x}, t) = \int_{-\infty}^{+\infty} \wp[\boldsymbol{\Theta}, \theta(\boldsymbol{x}', t)] G(\boldsymbol{x}' - \boldsymbol{x}) d\boldsymbol{x}', \tag{15}$$

$$\wp\big[\boldsymbol{\Theta}, \theta(\boldsymbol{x}, t)\big] = \delta\big[\boldsymbol{\Theta} - \theta(\boldsymbol{x}, t)\big] = \prod_{\alpha=1}^{N_s} \delta\big[\Theta_\alpha - \theta_\alpha(\boldsymbol{x}, t)\big]. \tag{16}$$

δ denotes the Dirac delta function and $\boldsymbol{\Theta}$ stands for the composition domain of the scalar array. $\wp\big[\boldsymbol{\Theta}, \theta(\boldsymbol{x}, t)\big]$ is the "fine-grained" density,[61] and Eq. (15) implies that the fdf is the spatially filtered value of the fine-grained density. Thus, P_L gives the density in the composition space of the fluid around $\mathbf{x}$ weighted by the filter G. With the condition of a positive filter kernel, P_L has all the properties of the pdf.

The idea of using pdf methods for LES had been suggested by many authors in the past, but Gao and O'Brien[115] were the first who developed a transport equation for the fdf and paved the way for future developments of the methodology for LES of chemically reactive flows. Within the past 30 years, the popularity of the methodology has been growing steadily. Within the past decade, especially, there has been a significant increase in the number of investigators who have contributed to its continuing developments and utilization. In this period, we have witnessed significant progress in fine-tuning of the fdf sub-closures, and the procedure by which the fdf is solved numerically. The modeling strategy is naturally influenced by the procedure by which the simulations are conducted. The extent of the fdf popularity can be perhaps measured by the relatively large number of participants at a recent mini-symposium devoted to this methodology.[116] This is also reflected in the number of tutorials and survey articles devoted to the subject. Just within the last decade, detailed review articles have been provided by Givi,[117] Haworth,[100] Pope,[97] Yilmaz *et al.*,[118] Ren *et al.*,[119] Miller and Foster,[120] and Sammak *et al.*[121]

Because of its demonstrated capabilities, the fdf is now being covered in text books[96,122] and is being steadily built into commercial software and packages. As examples of computer codes currently in use are the ANSYS Fluent,[123,124] the Siemens[125] in Zhang and Haworth,[126] the OpenFoam[127] in Mokhtarpoor *et al.*,[128] Turkeri *et al.*,[129,130] Galindo-Lopez *et al.*[131] and Zhao *et al.*,[132] and most recently the Nektar++ spectral/hp element[133,134] by Sammak *et al.*[135] and in AMRex code[136] by Aitzhan.[137] The development of the Graphic Processing Units (GPU) simulator of the fdf has just been completed,[138] and "futuristic" fdf/pdf computations on quantum computers are shown to be feasible.[139–141] Obviously, the methodology is here to stay. Therefore, it will surely benefit from all of the expected developments in all of the constituents of reactive flow modeling and simulation, most of which were initiated by Ted.

VII. DNS OF COMPRESSIBLE TURBULENCE

In the last few years of his research career, Ted concentrated on DNS of compressible turbulent flows. The overall goal of his research was to provide a better understanding of high-speed air-breathing aerospace propulsion systems in which combustion is inherently diffusion-limited. In collaboration with his colleague, Ladenide, and Ph.D. student, Cai, they constructed one of the first Essentially Non-Oscillatory (ENO)-based DNS codes.[142,143] This code proved novel at this time because of its very low numerical errors (dispersion and dissipation). Therefore, it allowed high-fidelity DNS of high Reynolds number flows with sharp discontinuities, due to shock waves and/or flame fronts. Ladeinde *et al.*[142] employed DNS to calculate the scalar fluctuation correlations in polytropic, homogeneous turbulence for which the initial conditions, including the Reynolds and the Mach numbers, were chosen to produce three types of flows: (i) a nearly incompressible flow dominated by vorticity, (ii) a nearly purely acoustic turbulence dominated by compression, and (iii) a nearly statistical equipartition of the longitudinal (compressible) and transverse (solenoidal) energy components. The simulated results were used to assess the performance of the EDQNM in estimating the evolution of the fluctuation correlations. It was found that the predictions via the use of the solenoidal component of turbulence energy, rather than the total (compressible) turbulence energy, provide the best overall agreement with DNS data. In another DNS, Cai *et al.*[144] showed that the compressible turbulence modes are less efficient than the incompressible ones in transporting scalar spectral energy from large to small scales. This effect is attributed to the reduced size of the integral length scale of the compressible velocity components vis-a-vis that of the incompressible flow field. The results also explain the experimentally observed ineffectiveness of the dilatational velocity modes in determining the scalar flux in homogeneous, compressible turbulence with a uniform mean scalar gradient.

Cai *et al.*[145] conducted DNS of a decaying, isotropic, compressible turbulence with the initial temperature fluctuations larger than those of the pressure. The initial turbulent Mach number was kept at subsonic levels (0.3–0.7) and the magnitudes of the initial compressible kinetic energy to total kinetic energy were kept in the ranges of very low to unity. The simulated results indicated that only at the lowest values of initial turbulent compressible Mach number (M_t) and energy ratio do thermodynamic scalings with M_t follow the predictions in the literature. For example, Zank and Matthaeus[146] predicted fluctuating pressures of $\mathcal{O}(M_t)$ and the associated anticorrelation

between the fluctuating temperature and density, in their nearly incompressible energy theory for compressible turbulence. For turbulent Mach numbers above 0.3, or for finite values of the kinetic energy ratio, the scalings are more complex and the reported anticorrelation[146] is lost.

Ladeinde *et al.*[147] conducted DNS of turbulent shear flows and investigated the effects of the convective Mach number on several flow statistics such as the Reynolds stresses, the dissipation tensor, the pressure strain, and the triple correlation tensor. The short-time behaviors of some of these quantities were shown to be similar to those suggested by Sarkar.[148] The relative magnitudes and signs of the unclosed terms in the Reynolds stress transport equations provided very useful information for second-order closures of compressible turbulent flows. The results of these theoretical studies are in accord with those previously attained via DNS.[149]

VIII. ORGANIZATION OF THIS SI

We are very pleased to have 53 papers from over 200 researchers, including some of the leading experts from all over the world, to contribute to this special issue. This enthusiastic response is another indication of the respect Ted O'Brien has within the international research community of turbulence and reactive flows. These contributions are on diverse topics including combustion instability,[150,151] scalar mixing,[152–156] homogeneous isotropic turbulence,[157–160] turbulent premixed flames,[161–171] turbulent non-premixed flames,[172–175] wall-bounded turbulence,[176–178] turbulent combustion modeling,[179–181] FDF/PDF,[182–192] and two-phase turbulent flows.[193–202]

IX. CONCLUDING REMARKS

Being recognized as one of the outstanding problems of the physical sciences, turbulence has been the subject of intense investigations by many leading scientists, engineers, and mathematicians for over a century. With the continuing research in this field, a large variety of strategies have emerged, and the research community continues the search for more accurate, reliable, and systematic methodologies. The models developed within the past century range from very practical and engineering-oriented, to highly fundamental and theoretical. Ted's contributions, tending to be more on the latter side, elicited some of the most intricate physics of turbulent scalar mixing and reaction. His contributions have paved the way for some of the success we are enjoying today. His fundamental findings have also led to the developments of some of the practical tools for engineering predictions.

His PDF method has been widely recognized as the most systematic means of estimating the mean rate of reactants conversion in Reynolds-averaged simulations. His classical tutorial on the subject (O'Brien, 1980) remains as one of the most useful and widely cited pedagogical references on the subject. The counterpart of this method, the fdf, is now widely recognized as the most accurate tool for subgrid-scale modeling in LES of reacting flows. Because of this wide visibility, the fdf usually has its own sessions at most fluid dynamics conferences, including APS-DFD. In both pdf and fdf methods, the LMSE model of Dopazo–O'Brien continues to be the simplest and most popular, yet susceptible of improvement, closure for scalar micro-mixing.

Professor O'Brien will be remembered as one of the most influential pioneers of turbulent mixing and reacting flow research. His legacy will remain forever, not just through his publications, but also through his Ph.D. students (and their subsequent students, and so on) who are, and will be, making advancements in these fields. The works of some of these students are featured in this Special Issue.

ACKNOWLEDGMENTS

We are indebted to Ted for his mentorship, leadership, and friendship. All of us had the honor and pleasure of working with him closely, and we feel our research careers have been greatly enhanced because of our interactions with him. The current research of PG on modeling and simulation of reactive turbulence is being sponsored by NSF Grant No. CBET-2042918 and NASA Grant No. 80NSSC18M0150 at Pitt.

DATA AVAILABILITY

Data sharing is not applicable to this article as no new data were created or analyzed in this study.

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