High-order structure functions for passive scalar fed by a mean gradient

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Abstract

Transport equations for even-order structure functions are written for a passive scalar mixing fed by a mean scalar gradient, with a Schmidt number $Sc = 1$. Direct numerical simulations (DNS), in a range of Reynolds numbers $R_\lambda \in [88, 529]$ are used to assess the validity of these equations, for the particular cases of second-and fourth-order moments. The involved terms pertain to molecular diffusion, transport, production, and dissipative-fluxes. The latter term, present at all scales, is equal to: i) the mean scalar variance dissipation rate, $\langle \chi \rangle$, for the second-order moments transport equation; ii) non-linear correlations between $\chi$ and second-order moments of the scalar increment, for the fourth-order moments transport equation.

The equations are further analysed to show that the similarity scales (i.e., variables which allow for perfect collapse of the normalised terms in the equations) are, for second-order moments, fully consistent with Kolmogorov-Obukhov-Corrsin (KOC) theory. However, for higher-order moments, adequate similarity scales are built from $\langle \chi^n \rangle$. The similarity is tenable for the dissipative range, and the beginning of the scaling range.

Keywords:

1. Introduction

Fully developed turbulence is characterized by a large range of length scales, varying from the so-called integral length scale $l_t$, at which large velocity fluctuations occur on average, down to the smallest scale, the so-called Kolmogorov or dissipation scale $\eta$, at which turbulent fluctuations are dissipated. Until now, most understanding of turbulent flows has been gained from Kolmogorov’s scaling theory [Kolmogorov (1941a,b)], which was
later extended by Obukhov (1949) and Corrsin (1951) to passive scalars advected by a turbulent velocity field. The Kolmogorov-Obukhov-Corrsin (hereafter, KOC) theory postulates that, under the condition of sufficiently high Reynolds numbers, the small scales of the flow decouple from the large scales. The understanding is that there is a steady cascade from the large scales to the smallest scales, where the energy transfer rate is equal to the mean energy dissipation rate $\langle \varepsilon \rangle$. Kolmogorov hypothesized that the small scales should depend only on two parameters, namely the viscosity $\nu$ and the mean energy dissipation $\langle \varepsilon \rangle$. Because only two quantities with different physical units are involved, this was viewed as a claim of universality. If the notion that the small-scale motion is universal was strictly valid, then there would be realistic hope for a statistical theory of turbulence.

The local and non-local phenomena which are inherent to turbulent flows can be analyzed by the moments of the scalar increment $\Delta \phi$, the so-called structure functions, defined by

$$S_p(x, r) = \langle (\phi(x + r) - \phi(x))^p \rangle = \langle (\Delta \phi)^p \rangle, \quad (1)$$

where $r$ is the separation vector between the two points and the angular brackets denote an ensemble-average. In statistically homogeneous turbulence, structure functions are independent of the position $x$. Yaglom (1949) presented an exact transport equation for the second order scalar structure function in homogeneous isotropic turbulence, where the separation distance $r$ (the modulus of vector $r$) is the independent variable. i.e.

$$\frac{\partial}{\partial t} \langle (\Delta \phi)^2 \rangle + \frac{\partial}{\partial r_i} \langle (\Delta u_i)(\Delta \phi)^2 \rangle = 2D \frac{\partial^2}{\partial r_i^2} \langle (\Delta \phi)^2 \rangle - 2\langle \chi \rangle, \quad (2)$$

where $\Delta u_i = u_i(x + r) - u_i(x)$ denotes the velocity increment and $D$ the molecular diffusivity. Equation (2) uses Einstein’s summation convention, which implies summation over indices appearing twice. The mean scalar dissipation is defined as,

$$\langle \chi \rangle = 2D \left\langle \left( \frac{\partial \phi}{\partial x_i} \right)^2 \right\rangle. \quad (3)$$

Provided that the Reynolds number is high enough, Eq. (2) has two separate analytical solutions. One in the dissipative range for $r \to 0$, where the diffusive term and the scalar dissipation balance, i.e.

$$\langle (\Delta \phi)^2 \rangle = \frac{\langle \chi \rangle}{6D} r^2, \quad (4)$$
and one for the inertial range for $\eta \ll r \ll l_t$, where the transport term balances the scalar dissipation, i.e.

$$\langle (\Delta u_L)(\Delta \phi)^2 \rangle = -\frac{2}{3} \langle \chi \rangle r,$$  \hspace{1cm} (5)

with $\Delta u_L$ being the longitudinal velocity increment in the direction of $r$. These two results are of high significance. They are both exact and were derived from first-principles only under the assumptions of (local) isotropy and (local) homogeneity.

The paper is devoted to the analysis of $S_p$ for $p = 2$ and $p = 4$, in the context of transport equations obtained from the first principles, by considering a restricted number of additional hypotheses, such as self-preservation, cf. Danaila and Mydlarski (2001). Section 2 describes the main characteristics of the performed direct numerical simulations (DNS), on which the analysis is based. In Section 3 we present the theory of generalized scalar scale-by-scale structure functions for any even order. Next, we develop in Section 4 similarity scales based on the scale-by-scale budget equations for the second and fourth order moments. The similarity scales are then justified by using data from DNS with different Taylor length-scale based Reynolds numbers between 88 and 529. Concluding remarks are given in Section 5.

2. Direct numerical simulations

We study a passive scalar advected by a statistically homogeneous isotropic and incompressible turbulent velocity field. In the present study, we consider a passive scalar with unity Schmidt number $Sc = \nu / D$, so that the kinematic viscosity $\nu$ equals the molecular diffusivity $D$. A uniform mean gradient $\Gamma$ is imposed on the scalar field in $x_2$-direction. The mean gradient injects continuously energy into the scalar field and keeps statistics in a statistically steady state. The instantaneous scalar field can be decomposed in a mean part $\Gamma x_2$ and a scalar fluctuation $\phi$, namely

$$\Phi = \Gamma x_2 + \phi.$$  \hspace{1cm} (6)

The scalar fluctuations $\phi$ are statistically homogeneous and obey the equation

$$\frac{\partial \phi}{\partial t} + u_i \frac{\partial \phi}{\partial x_i} = D \frac{\partial^2 \phi}{\partial x_i^2} - \Gamma u_2,$$  \hspace{1cm} (7)
where $t$ is the time, $x_i$ the spatial coordinates, and $u_i$ denote the velocity field.

The three-dimensional incompressible Navier-Stokes equations in the vorticity formulation are solved together with Eq. (7) by a dealiased pseudo-spectral approach, cf. Canuto et al. (1988). Temporal integration is carried out by a second order semi-implicit Adams-Bashforth/Crank-Nicolson method. The integration domain is a triply periodic cube with length $2\pi$. An external stochastic forcing, see Eswaran and Pope (1988), is applied to the velocity field to maintain a statistically steady state. The forcing is statistically isotropic and limited to low wave-numbers so that the small scales are not affected by the forcing scheme. The simulations have been carried out with an in-house hybrid MPI/OpenMP parallelized simulation code on the supercomputer JUQUEEN at research center Jülich, Germany.

Characteristic parameters of the DNS are presented in table 1, where $N$ denotes the number of grid points along one coordinate axis, $Re_\lambda$ the Taylor based Reynolds number, $\langle k \rangle$ the mean kinetic energy, $\langle \varepsilon \rangle$ the mean energy dissipation, $\langle \phi^2 \rangle$ the mean scalar variance, $\langle \chi \rangle$ the mean scalar dissipation, and $\langle u_2 \phi \rangle$ the mean scalar flux. The production of scalar variance is $-2 \langle u_2 \phi \rangle \Gamma$. Ensemble-averages are denoted by angular brackets and are computed over the whole computational domain due to homogeneity and over a time frame $t_{avg}$ due to stationarity. The number of analyzed ensembles is in the range between $M = 6$ for case R5 up to $M = 189$ for case R0. Resolving the smallest scales by the numerical grid is important for the accuracy of the DNS. To ensure an appropriate resolution of the smallest scales, the number of grid points has been increased to as high as $4096 \times 4096 \times 4096$ for case R5. Following Ishihara et al. (2007) and Donzis et al. (2005), a resolution condition of $\kappa_{max} \eta > 2.5$ is maintained for all cases to accurately compute high-order statistics. Here, $\kappa_{max}$ denotes the highest resolved wavenumber and $\eta = \nu^{3/4} \langle \varepsilon \rangle^{-1/4}$ denotes the Kolmogorov length scale. Further details about the DNS are presented by Gauding et al. (2015) and Peters et al. (2016).

3. Scale-by-scale transport equations for even order structure functions

Starting from Eq. (7), a transport equation for the even moments of the scalar increment can be derived by using a similar procedure as presented in Danaila et al. (1999) and Hill (2001). For homogeneous turbulence this
Table 1: Summary of different DNS cases. Reynolds number variation between $\text{Re}_\lambda = 88$ and $\text{Re}_\lambda = 529$.

|      | R0   | R1   | R2   | R3   | R4   | R5   |
|------|------|------|------|------|------|------|
| $N$  | 512$^3$ | 1024$^3$ | 1024$^3$ | 2048$^3$ | 2048$^3$ | 4096$^3$ |
| $\text{Re}_\lambda$ | 88 | 119 | 184 | 215 | 331 | 529 |
| $\nu$ | 0.01 | 0.0055 | 0.0025 | 0.0019 | 0.0010 | 0.00048 |
| $\langle k \rangle$ | 11.15 | 11.20 | 11.42 | 12.70 | 14.35 | 23.95 |
| $\langle \varepsilon \rangle$ | 10.78 | 10.52 | 10.30 | 11.87 | 12.55 | 28.51 |
| $\langle \phi^2 \rangle$ | 1.95 | 1.89 | 1.94 | 2.47 | 2.25 | 2.41 |
| $\langle \chi \rangle$ | 3.92 | 3.90 | 4.01 | 5.00 | 4.76 | 6.78 |
| $-2\Gamma \langle u_2 \phi \rangle$ | 3.93 | 3.98 | 4.03 | 4.95 | 4.79 | 5.76 |
| $t_{\text{avg}}/\tau$ | 100 | 30 | 30 | 10 | 10 | 2 |
| $M$ | 189 | 62 | 61 | 10 | 10 | 6 |
| $\kappa_{\text{max}} / \eta$ | 3.93 | 4.99 | 2.93 | 4.41 | 2.53 | 2.95 |

The equation reads

\[
\frac{\partial}{\partial t} \langle \Delta \phi^{2n} \rangle(r) + \frac{\partial}{\partial r_i} \left( \left( \Delta u_i \right) \langle \Delta \phi^{2n} \rangle(r) \right) + 2n \Gamma \langle \Delta u_2 \rangle \langle \Delta \phi^{2n-1} \rangle(r) = J_{2n}(r),
\]  

(8)

where $J_{2n}$ are the molecular-diffusion terms, i.e.

\[
J_{2n}(r) = nD \left( \Delta \phi \right)^{n-1} \left[ \frac{\partial^2 (\Delta \phi)}{\partial x_i^2} + \frac{\partial^2 (\Delta \phi)}{\partial x_j^2} \right].
\]  

(9)

The term $J_{2n}$ is a function of $r$ and remains finite even when $D$ tends to zero. Equation (8) is exact, which means that it is derived from the governing equations without any approximation beside of incompressibility and homogeneity. It is convenient to decompose $J_{2n}(r)$ by partial integration, i.e.

\[
J_{2n}(r) = 2D \frac{\partial^2}{\partial r_i^2} \left( \langle \Delta \phi^{2n} \rangle - n(2n-1) \langle \Delta \phi^{2n-2} \rangle \chi(x) \langle \chi(x + r) \rangle \right).
\]  

(10)

The terms of Eqs. (8) and (10) can be physically interpreted. The first term on the left-hand side is the temporal change of the moments of the scalar
increment. The second term $Tr_{2n}$ is a mixed velocity-scalar structure function and represents an inter-scale transport from large scale towards small scales. Therefore, it is hereinafter referred to as transport term. The third term $Pr_{2n}$ is proportional to the mean scalar gradient $\Gamma$ and can be interpreted as a production term that is mainly active at large scales. According to Eq. (10), term $J_{2n}$ splits up into two terms. The first is a diffusive transport term $D_{2n}$. The latter term is the so-called dissipation source term $E_{2n}$. The second order dissipation source term $E_{2}$ is independent of $r$ and simplifies to $2\langle \chi \rangle$. In this case, Eq. (5) reduces to the Yaglom equation for homogeneous, but anisotropic turbulence at finite Reynolds number, cf. Antonia et al. (1997). For higher orders, $E_{2n}$ is a multi-scale correlation between the local scalar difference $(\Delta \phi)^{2n-2}$ and the sum of the instantaneous scalar dissipation $\chi$ at two points separated by $r$.

Most theoretical works consider integrated formulations of Eq. (5), where an integration is carried out either over spheres of radius $r$ (when the data used comes from DNS, Casciola et al. (2003)), or along straight lines with a length $r$. This latter possibility is preferred by studies based on experimental data, because of the use of Taylor’s hypothesis. In this work we follow an approach introduced by Peters et al. (2016) and evaluate the terms of the scale-by-scale budget equations as given by Eq. (8). The transport and the diffusive terms involve derivatives in $r$-space. By using the rules of differentiation the $r$-derivative can be replaced by local spatial derivatives. For example, with homogeneity and incompressibility, the transport term is written as

$$\frac{\partial}{\partial r_i} \left\langle (\Delta u_i)(\Delta \phi)^{2n} \right\rangle = 2n \left\langle (\Delta u_i)(\Delta \phi)^{2n-1} \frac{\partial \phi}{\partial x_i} \right\rangle. \quad (11)$$

By using Eq. (11), the transport term can be easily computed from DNS data, as only a correlation between velocity and scalar increments with a local scalar derivative is required. The diffusive term can be computed in the same way. The temporal decay term is negligible, because the continuous forcing ensures stationary state of the mixing.

Even though Eqs. (5) and (10) are exact, they cannot be solved directly, because they are not closed. Nonetheless, all terms can be computed from DNS. This is displayed in fig. 1 where the terms of the transport equations for the second and fourth order scalar structure functions $\langle (\Delta \phi)^{2n} \rangle$ are shown for $Re_\lambda = 88$ and $Re_\lambda = 529$. Let us first briefly discuss the scale-by-scale budget for the second order scalar structure function. For the second order
Figure 1: Terms in Eq. (8) and (10) for the second (top) and fourth order scalar structure function equation. The left column is for case R0 and the right column is for case R5. The green squares represent the sum $Tr_{2n}(r) + Pr_{2n}(r) + D_{2n}(r)$, which balances the term $E_{2n}(r)$ for all scales. This indicates that the budget is satisfied. It is notable, that $E_2$ is independent of $r$ and simplifies to $2\langle \chi \rangle$. 
the sum $Tr_2 + Pr_2 + D_2$ is independent of $r$ and equals $2\langle\chi\rangle$. The diffusive terms $D_2$ is dominant in the dissipative range and tends to $2\langle\chi\rangle$ for $r \to 0$. The production term $Pr_2$ in dominant at large scales and equals $2\langle\chi\rangle$ for $r \to \infty$. The transport term is dominant in the inertial range, but attains the value $2\langle\chi\rangle$ only when the Reynolds number is large enough. For low Reynolds numbers, statistics in the inertial range are strongly affected by molecular diffusion and large scale effects originating from the mean scalar gradient. The width of the inertial range scaling regime increases only slowly with Reynolds number, which underlines that accounting for finite Reynolds number effects is important.

The scale-by-scale budget for the fourth order structure function $\langle(\Delta \phi)^4\rangle$ is significantly different. Here, the dissipative source term $E_4$ is a function of the separation distance, revealing two different scaling regimes for the dissipative and the inertial range. In the dissipative range $E_4(r)$ scales with $r^2$ and balances the diffusive term $D_4$. Term $E_4$ is proportional to $\langle(\Delta \phi)^2 (\chi(x) + \chi(x + r))\rangle$. Along any arbitrary direction $r_k$, a Taylor series development when $r_k \to 0$ for $(\Delta \phi)^2 = \left(\frac{\partial \phi}{\partial x_k}\right)^2 r^2$. Injecting this in the expression of $E_4$, and because the average applies to the product between $(\Delta \phi)^2$ and $\chi$, the small-scale limit of $E_4$ will be proportional to the average value of the square of the scalar dissipation. Finally, $E_4$ can be written in the limit $r_k \to 0$ as

$$E_4(r_k) = \frac{2\langle\chi^2\rangle}{D} r_k^2.$$  

The derivation of eq. (12) is detailed in Appendix A. In the inertial range, fig. indicates that $E_4$ is balanced by the transport term $Tr_4$, provided that the Reynolds number is high enough. Under this condition, $E_4$ and $Tr_4$ have the same inertial range scaling exponent $\zeta_4$ and the relation

$$E_4(r) = Tr_4(r) = c_4 r^{\zeta_4}$$  

is satisfied. Note that due to internal intermittency, neither $c_4$ nor $\zeta_4$ can be obtained from dimensional arguments, cf. Kolmogorov (1962). In the large scale limit, $E_4$ balances $Pr_4$ and becomes independent of $r$, as it tends to $12\langle\phi^2\chi\rangle$ for $r \to \infty$. These limits will be exploited in Section 4.2 to develop similarity scales for higher-order moments.
4. Similarity scales pertaining to the dissipative range

Kolmogorov-Obukhov-Corrsin (KOC) scales are built from the mean value of the scalar dissipation rate $\langle \chi \rangle$. As illustrated in figures 2 and 3, an adequate collapse after normalization using KOC scales only applies for the second-order moments, and for the third-order mixed velocity-scalar structure functions $\langle (\Delta u_i)(\Delta \phi)^2 \rangle$ when the Reynolds number is large enough. Figures 2 and 3 clearly emphasize that the mean dissipation $\langle \chi \rangle$ is not consistent with a small-scale collapse of the fourth-order structure function $S_4$, or transport term $Tr_4$. In the following, we use the transport equations derived in Section 3 to provide expressions for the similarity scales.

4.1. Similarity scales for the second-order moments transport equation

In the transport equation for the second-order moments, all terms depend on the spatial increment $r$. Therefore, anisotropy of the flow and mixing is accounted for. In the following, we address the question of self-similarity, as introduced by Townsend (1976) for the one-point energy budget equation, and later on by George (1992) for the two-point statistics in the spectral space, and Antonia et al. (2003) for two-point statistics in real space.

In order to examine the conditions under which Eq. (8) satisfies similarity, we need to assume functional forms for the terms in this equation. This equation, for the second-order moments, can be formally written as: $Tr_2 + Pr_2 + D_2 = (\langle \chi(x + r) \rangle + \langle \chi(x) \rangle)$, where $Tr_2$ is the transport term, $Pr_2$ is the production, and $D_2$ is the molecular term. Because anisotropy is accounted
for, and as the flow and mixing are stationary and spatially homogeneous, these terms depend on the vector $r$ and vary as a function of the energy injected in the flow, so say, on the Reynolds number of the flow. We thereby have to distinguish between functions which are Reynolds-dependent (and do not depend on the scale $r$) and the functions which depend on the spatial increment $r$. Following Antonia et al. (2003) and Burattini et al. (2005), we take

$$
\langle (\Delta \phi)^2 \rangle = c_1(Re) \cdot f(\xi)
$$

$$\frac{\partial}{\partial r_j} \langle \Delta u_j (\Delta \phi)^2 \rangle = c_2(Re) \cdot g(\xi),$$

$$\Gamma \langle \Delta u_2 \Delta \phi \rangle = c_3(Re) \cdot v(\xi),$$

$$\langle \chi \rangle^+ + \langle \chi \rangle^- = c_4(Re) \cdot w(\xi).$$

(14)

where $\xi = r/L$ and $L$ is a characteristic length scale, to be determined. The scale $L$ depends on $Re$, but also on the spatial direction of the separation vector $r$, say $e_r = r/|r|$. It is natural to identify $c_1 \sim \phi_{ref}^2$, where the index 'ref' stands for the 'reference'. Similarly, $c_2 \sim v_{ref} \phi_{ref}^2 / L$, $c_3 \sim \Gamma v_{ref} \phi_{ref}$ and $c_4 \sim \chi_{ref}$. A dependence on the initial conditions, as explained by George (1992) is also plausible. The separation between functions of $Re$ and $\xi$ allows solutions of the transport equation for which a relative balance among all of the terms is maintained for increasing Reynolds numbers. Upon substituting Eqs. (14) into Eq. (8), considering the viscous term $D \frac{D^2}{\partial r_j^2} \langle (\Delta \phi)^2 \rangle$.
as a reference, whose scaling is $D_{\text{ref}}^2$, we obtain

$$\frac{v_{\text{ref}} \cdot \mathcal{L}}{D} = K_1;$$ (15)

$$\frac{\langle \chi \rangle_{\text{ref}} \cdot \mathcal{L}^2}{D \cdot \phi_{\text{ref}}^2} = K_2;$$ (16)

$$\frac{D \cdot \phi_{\text{ref}}}{v_{\text{ref}} \Gamma \mathcal{L}^2} = K_3.$$ (17)

The constants $K_i$ are understood as such with respect to the variable $Re$. Combining these equations and considering that the similarity scale for the velocity field is, at least for the smallest scales, proportional to the Kolmogorov scale $\eta = (\nu^3 / \langle \varepsilon \rangle)^{1/4}$, then a characteristic scale of the scalar can be identified with $\phi_{\text{ref}} \equiv [Sc \tau_r(\chi)]^{1/2}$, where $\tau_r$ is the Kolmogorov time scale. Thus, the energy transport term $Tr_2$ should scale as $Tr_2 \sim v_{\text{ref}} \frac{\phi_{\text{ref}}^2}{\mathcal{L}} = \eta \frac{Sc \tau_r \langle \chi \rangle}{\eta} = Sc \cdot \langle \chi \rangle$. For our simulations, the Schmidt number is equal to 1, so term $Tr_2$ should scale as $\langle \chi \rangle$ when the energy injected in the flow varies. In other words, the ratio $Tr_2 / \langle \chi \rangle$ may vary as a function of the vectorial separation $\xi$, but must be a constant of the Reynolds number, if the similarity was to be valid. This is firmly confirmed by the excellent collapse of the normalized curves in Fig. 3 for the smallest scales. For increasing Reynolds numbers, the agreement is excellent over a wider and wider range of scales, thus validating our approach.

We may preclude that in flows where similarity is tenable at the smallest scales only, then the unique solution of the problem that emerges is the Kolmogorov velocity and length scales, and KOC scale for the scalar itself.

4.2. Similarity scales for the higher-order moments transport equations

A similar analysis may be performed for the transport equation of the higher-order moments. The development is done here for the 4-th order moments, but the generalization is then straightforward for arbitrary higher-order moments.

The transport term $Tr_4$, scales as $Tr_4 \sim v_{\text{ref}} \frac{\phi_{\text{ref}}^4}{\mathcal{L}}$. An important point to be underlined here is that, similarity scales for high-order moments are not the same as those for the second-order and third-order moments. For the sake of simplicity, we keep however the notation $v_{\text{ref}}$ and $\mathcal{L}$. The molecular term scales as $D_4 \sim D_{\text{ref}}^{\phi_{\text{ref}}^4 \mathcal{L}}$, the production term behaves as $Pr_4 \sim v_{\text{ref}} \Gamma \phi_{\text{ref}}^3$. Lastly, the dissipation source term scales as $E_4 \sim \langle \phi^2 \cdot \chi \rangle_{\text{ref}}$. Note that the latter term was not decomposed in a product of two terms, and further
reliable closures will be required to progress towards clear scaling laws within the inertial range. For the similarity to be valid, ratios between any two terms should be real constant (i.e., not functions of the Reynolds number, nor the scale). Therefore, several results may be deduced, such as \( T_{r4}/P_{r4} = \text{const.} \), which translates in

\[ \phi_{\text{ref}} \sim \Gamma L, \quad (18) \]

or, the ratio \( T_{r4}/D_{4} = \text{const.} \) which is perfectly consistent with Eq. (15). Further information on the similarity scale can be inferred for the dissipative range, so when \( r \to 0 \). For these scales,

\[ E_{4} \sim \frac{\langle \chi^{2} \rangle L^{2}}{D}, \quad (19) \]

which should be proportional to the molecular term, as these two terms are dominant in the dissipative range and they balance each other, cf. Eq. (12). Therefore,

\[ D \frac{\phi_{\text{ref}}^{4}}{L^{2}} \sim \frac{\langle \chi^{2} \rangle L^{2}}{D}, \quad (20) \]

which leads to

\[ \phi_{\text{ref}}^{4} \sim \frac{\langle \chi^{2} \rangle L^{4}}{D^{2}}. \quad (21) \]

Note the clear dependence on \( \langle \chi^{2} \rangle \), which is different from the square of \( \langle \chi \rangle \). Furthermore, scalings for all the other terms in the dissipative range may be inferred, such as, for example, the transport term \( T_{r4} \), which writes

\[ T_{r4} \sim \frac{v_{\text{ref}} \phi_{\text{ref}}^{4}}{L}. \quad (22) \]

After some straightforward manipulations, and if the similarity scale is the same as that of the velocity field, so \( L = \eta \), then

\[ T_{r4} \sim \tau_{\eta} S c^{2} \langle \chi^{2} \rangle. \quad (23) \]

This scaling is reasonably supported by fig. 4 at least for the smallest scales, and for the value \( S c = 1 \) of our simulations. The non-perfect collapse is most likely due to the fact that the best adapted similarity length scale, \( L \), should be built from higher-order moments of the energy dissipation rate, so from \( \langle \varepsilon^{2} \rangle \), and not from \( \langle \varepsilon \rangle \) itself. This hypothesis is being explored and is subject of future publication.
Figure 4: Fourth order transport term $T_{r_4}$ normalized by similarity scales $\langle \chi^2 \rangle / \tau_\eta$ from eq. (23).

The scaling of the dissipation source term $E_4$ is of special interest, because this term depends on the scale $r$ and it balances one of the other terms of Eq. (8). Figure 5 shows the term $E_4$ for the different Reynolds numbers under consideration, where $E_4$ is normalized by the classical KOC quantities (left) and by the similarity scales for the fourth order moment (right) obtained from Eq. (19). The normalization by the KOC quantities leads to a staggered agreement where the normalized $E_4(r)$ clearly depends on the Reynolds number. This behavior was already expected by Landau and Lifshitz (1959), who argued that $\langle \varepsilon \rangle$ (and $\langle \chi \rangle$ for the scalar) could not be the relevant normalization quantity for higher orders. However, the modified scaling from Eq. (19) reveals an excellent collapse of the curves independently of Reynolds number. It is notable that the collapse is not limited to the dissipative range, but extends up to the inertial range. Thus, Eq. (19) predicts correctly the Reynolds number dependence of the dissipation source term $E_4(r)$. Note also that, for the range of investigated Reynolds numbers, DNS reveals that $\zeta_4$ is close to 0.3, cf. fig. 5.

As demonstrated before, the classical KOC scaling is not valid for higher-order structure functions. Following the similarity scales for higher-order moments, cf. Eq. (21), a scaling relation can be derived for scalar structure functions of any even order

$$\frac{\langle (\Delta \phi)^{2n} \rangle}{\langle \chi \rangle^{n} / \tau_n} = C_{2n} \frac{\langle \chi^n \rangle}{\langle \chi \rangle^n} \left( \frac{r}{\eta} \right)^{2n}, \quad (24)$$

The prefactor $C_{2n} \langle \chi^n \rangle / \langle \chi \rangle^n$ on the right-hand side accounts for the depen-
Figure 5: Fourth order dissipation source term $E_4$ normalized by the KOC scaling variables $(\chi)^2 \tau_\eta$ (left) and the higher-order similarity scales $\langle \chi^2 \rangle \tau_\eta$ (right).

Figure 6: Higher order scalar structure functions $\langle (\Delta \phi)^{2n} \rangle$ normalized according to Eq. (24).

The dependence of the normalized $2n$-th order structure function on the Reynolds number. The constant $C_{2n}$ is a function of the order $n$, but not of the Reynolds number. For $n = 1$, eq. (24) reduces to the classical KOC scaling. The scaling from Eq. (24) is supported by fig. 6, where the normalized structure functions $\langle (\Delta \phi)^{2n} \rangle$ are shown for the second, fourth and sixth order. By using Eq. (24), the quality of the collapse of the higher-order structure functions is as good as the collapse for the second order, and significantly improved compared to fig. 2 (right). We want to emphasize that it is not possible to derive Eq. (24) from pure dimensional arguments, because $\langle \chi^2 \rangle$ and $\langle \chi^2 \rangle$ have the same dimensions.
5. Conclusions

Transport equations for even-order structure functions were written for a passive scalar mixing fed by a mean scalar gradient, with a Schmidt number $Sc = 1$. Direct numerical simulations (DNS), in a range of Reynolds numbers $R_{\lambda} \in [88, 529]$ were performed and used to assess the validity of these equations, for the particular cases of second-order and fourth-order moments. The involved terms pertain to molecular diffusion, transport, production, and dissipative-fluxes. The latter term, present at all scales, was shown to be equal to:

i) the mean scalar variance dissipation rate, $\langle \chi \rangle$, for the second-order moments transport equation;

ii) non-linear correlations between the instantaneous $\chi$ and the second-order scalar increment, for the fourth-order moments transport equation.

The equations were further analysed to show that the similarity scales (i.e., variables which allow for perfect collapse of the normalised terms in the equations) are, for second-order moments, fully consistent with KOC theory. However, for higher-order moments, adequate similarity scales are built from $\langle \chi^n \rangle$. The similarity is tenable for the dissipative range, and the beginning of the scaling range (or, inertial range).

Finding the similarity variables for larger scales requires reliable closures of two other terms: the transport term $(Tr_{2n})$, as well as of term $E_{2n}$. The latter term is exactly closed only for $n = 1$, so for the second-order moments. For larger values of $n$, the coupling between the instantaneous dissipation rate $\chi$ (specific of the small scales) and the large-scale moments $(\Delta \phi)^{(2n-2)}$ reflects a direct correlation between large and small scales, and it admits to an exact analytical development for the small scales only. For larger scales, modelling is needed.

Another comment is devoted to the observation that, the passive scalar being transported by the velocity field, characteristic scales of the scalar and of the dynamic field, act together. Our concern being on mixing at $Sc = 1$, our reasonable assumption was that the characteristic scales were the same for both the scalar and dynamic fields. Nonetheless, as already noted, these scales depend on the order $2n$ of the investigated moments, as clearly shown analytically and proven by our DNS results. This does not comply with the idea of complete self-preservation (which requires a single length/velocity/scalar scale, Townsend (1976)). Therefore, albeit the value of the Schmidt number is $Sc = 1$, and despite the fact that the investigated
Reynolds number is as high as 529, this flow and mixing are only incomplete self-preserving, i.e. only small scales may be self-similar, when normalized with respect to quantities adequately chosen. Their expressions are deduced basically from the first principles, and in particular from transport equations of high-order moments.

The physical signification of the second-order moments is the energy at scales smaller or equal to $r$ (see also Danaila et al. (2012)). The physical parameters describing their evolution are the viscosity, the Prandtl (or Schmidt) number, and the mean value of the dissipation, in agreement with the classical KOC theory. The fourth-order moments pertain to the variance of the variance of the signal, thus having a much more refined insight into the temporal activity of the flow. The theory shows that, at least for the smallest scales of the mixing, it is the mean value of the square of the dissipation which must be accounted for, corresponding to the dissipation of the variance of the variance at a given scale $r$. At least for the range of Reynolds numbers investigated in this paper, the scale for four-order moments is clearly different from the classical KOC scale. Whether or not these scales become equivalent in the limit of larger and larger Reynolds numbers, remains for now an open issue.

We are honored to dedicate this paper to Prof. Andrew Pollard, for the celebration of his whole career, including impressive scientific contributions, editor work, as well as the organisation of many congresses. L.D. acknowledges extended fruitful discussions on quantifying internal intermittency from measurements with flying hot wires.

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Appendix A. Exact relations between the moments of the scalar dissipation and the scalar gradients

In this appendix we derive Eq. (12) under the assumptions of local isotropy and homogeneity. With the Taylor series expansion $(\Delta \phi)^2 = \left( \frac{\partial \phi}{\partial x_1} \right)^2 r^2$ and $\chi = 2D \left( \frac{\partial \phi}{\partial x_i} \right)^2$, term $E_4(r)$ can be written in the limit $r \to 0$ as

$$E_4(r) = 24D \left( \left( \frac{\partial \phi}{\partial x_1} \right)^2 \left[ \left( \frac{\partial \phi}{\partial x_1} \right)^2 + \left( \frac{\partial \phi}{\partial x_2} \right)^2 + \left( \frac{\partial \phi}{\partial x_3} \right)^2 \right] \right) r^2, \quad (A.1)$$

where we assumed without loss of generality that the separation vector $r$ is aligned with the $x_1$ axis. The fourth-order derivatives appearing in Eq. (A.1) can be directly related to $\langle \chi^2 \rangle$. Under the assumption of local isotropy the general form of a fourth order gradient tensor reads (e.g. Siggia (1981))

$$\langle \frac{\partial \phi}{\partial x_i} \frac{\partial \phi}{\partial x_j} \frac{\partial \phi}{\partial x_k} \frac{\partial \phi}{\partial x_l} \rangle = \alpha \delta_{ij} \delta_{kl} + \beta \delta_{ik} \delta_{jl} + \gamma \delta_{il} \delta_{jk}. \quad (A.2)$$

The value of this generic tensor must be invariant under permutations of its components which leads to

$$\left\langle \left( \frac{\partial \phi}{\partial x_1} \right)^4 \right\rangle = 3 \left\langle \left( \frac{\partial \phi}{\partial x_1} \right)^2 \left( \frac{\partial \phi}{\partial x_2} \right)^2 \right\rangle = 3 \left\langle \left( \frac{\partial \phi}{\partial x_1} \right)^2 \left( \frac{\partial \phi}{\partial x_3} \right)^2 \right\rangle, \quad (A.3)$$

and consequently

$$\lim_{r \to 0} E_4(r) = 40D \left\langle \left( \frac{\partial \phi}{\partial x_1} \right)^4 \right\rangle r^2. \quad (A.4)$$

Equation (A.2) further implies that the second moment of the scalar dissipation can be written as

$$\langle \chi^2 \rangle = 20D^2 \left\langle \left( \frac{\partial \phi}{\partial x_1} \right)^4 \right\rangle, \quad (A.5)$$

which gives with Eq. (A.4) the final result

$$\lim_{r \to 0} E_4(r) = 2\frac{\langle \chi^2 \rangle}{D} r^2. \quad (A.6)$$
A generalization of Eq. (A.5) to higher order moments is straightforward, and exact relations between the moments of the scalar derivatives and the scalar dissipation are found, i.e.

\[ \left\langle \left( \frac{\partial \phi}{\partial x_1} \right)^{2n} \right\rangle = C_n \left( \frac{\chi^n}{D^n} \right), \tag{A.7} \]

where the \( C_n \) are Reynolds number independent coefficients. A confirmation of Eq. (A.7) is shown in fig. A.7 for a wide Reynolds numbers range and for \( n \) between 1 and 4. Figure A.7 also indicates that the assumption of local isotropy is well justified for the present DNS.
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