Large-eddy-simulation closures of passive scalar turbulence: a systematic approach

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The issue of the parameterization of small-scale ('subgrid') turbulence is addressed in the context of passive scalar transport. We focus on the Kraichnan advection model which lends itself to the analytical investigation of the closure problem. We derive systematically the dynamical equations which rule the evolution of the coarse-grained scalar field. At the lowest-order approximation in l/r, l being the characteristic scale of the filter defining the coarse-grained scalar field and r the inertial-range separation, we recover the classical eddy-diffusivity parameterization of small scales. At the next-leading order a dynamical closure is obtained. This outperforms the classical model and is therefore a natural candidate for subgrid modelling of scalar transport in generic turbulent flows.

1. Introduction

One of the most striking characteristics of hydrodynamic turbulence is the presence of a wide range of active length and time scales. These scales are strongly and nonlinearly coupled, a fact that makes analytical approaches, at best, impractical. The situation does not look better for direct numerical simulations of turbulent systems: to fully resolve a turbulent flow requires approximately $(L/\eta)^{3/4}$ grid points in each spatial direction (see, for example, Frisch 1995), L and η being the integral scale and the dissipation scale respectively. In the atmosphere, for instance, the ratio L/η may become of the order of 10^{10} ($\eta \sim 10^{-3}$ m and $L \sim 10^7$ m) thus requiring the dynamical description of 10^{22} degrees of freedom. This remains, up to now and probably also in the near feature, a prohibitive task.

To overcome the problem, 'coarse-grained' versions of the original hydrodynamic equations are often considered in order to describe large-scale features of the original full system. The large-eddy simulation (LES) technique is probably the most popular example (Meneveau & Katz 2000). The success of such a strategy is however strongly dependent on the realism of the description of small scales in terms of the large, explicitly resolved, scales. The problem of representing small unresolved scales in the absence of scale separation – the long-known *closure problem* – attracts a great deal of attention in many domains ranging from geophysics to engineering (McComb 1992), and is one among the many challenges of turbulence theory.

Our goal here is to shed some light on this aspect within the context of scalar turbulence where considerable progress has been achieved in the last few years (Shraiman & Siggia 2000; Falkovich, Gawędzki & Vergassola 2001). For this purpose

we will consider a particular model of scalar transport (Kraichnan 1968, 1994) where the LES strategy can be formulated and the problem of relating unresolved scales to resolved ones can be successfully attacked analytically.

In this respect, the Kraichnan model has some characteristics of paramount importance:

(i) Exact expressions for relevant statistical observables can be derived from first principles, that is from equation (2.1): this amounts to saying that the observables for the 'fully resolved case' are known. An example is the expression (3.3) for the second-order scalar structure function, an observable tightly related to the Fourier spectrum of the scalar field.

(ii) Closures for the large-scale dynamics can be derived in a systematical way (see §3), and their predictions can be analytically checked against the exact solution.

Those features make the Kraichnan model an ideal candidate for studying LES closures.

2. LES closures for passive scalar turbulence

Scalar transport is governed by the advection–diffusion equation

$$\partial_t \theta + \boldsymbol{v} \cdot \boldsymbol{\nabla} \theta = \kappa_0 \Delta \theta + f, \tag{2.1}$$

describing the evolution of a passive scalar field $\theta(\boldsymbol{x}, t)$ – e.g. temperature when buoyancy effects are negligible – advected by an incompressible velocity field $\boldsymbol{v}(\boldsymbol{x}, t)$. Scalar fluctuations are injected into the system at the large scale L by the forcing term f. Dissipation occurs at small scales η due to the molecular diffusivity κ_0.

The coarse-grained scalar and velocity fields, denoted by $\tilde{\theta}$ and $\tilde{\boldsymbol{v}}$ are obtained by convolving the original, fully resolved, fields with a filter G_l with characteristic scale l $(\eta \ll l \ll L)$:

$$\tilde{\theta}(\boldsymbol{x}, t) = \int G_l(\boldsymbol{x} - \boldsymbol{x}')\theta(\boldsymbol{x}', t)\, \mathrm{d}\boldsymbol{x}', \tag{2.2}$$

$$\tilde{\boldsymbol{v}}(\boldsymbol{x}, t) = \int G_l(\boldsymbol{x} - \boldsymbol{x}')\boldsymbol{v}(\boldsymbol{x}', t)\, \mathrm{d}\boldsymbol{x}'. \tag{2.3}$$

The equation for $\tilde{\theta}$ derived from (2.1) is

$$\partial_t \tilde{\theta} + \tilde{\boldsymbol{v}} \cdot \boldsymbol{\nabla} \tilde{\theta} = \kappa_0 \Delta \tilde{\theta} + \tilde{f} - (\mathscr{L} + \tilde{\mathscr{S}}), \tag{2.4}$$

where $\mathscr{L}$ is analogous to the Leonard stress

$$\mathscr{L} \equiv \widetilde{\tilde{\boldsymbol{v}} \cdot \boldsymbol{\nabla} \tilde{\theta}} - \tilde{\boldsymbol{v}} \cdot \boldsymbol{\nabla} \tilde{\theta}, \tag{2.5}$$

and $\mathscr{S}$ is defined as

$$\mathscr{S} \equiv \boldsymbol{v}' \cdot \boldsymbol{\nabla} \tilde{\theta} + \boldsymbol{v}' \cdot \boldsymbol{\nabla} \theta' + \tilde{\boldsymbol{v}} \cdot \boldsymbol{\nabla} \theta'. \tag{2.6}$$

The small-scale fields θ' and $\boldsymbol{v}'$ are defined as $\theta' \equiv \theta - \tilde{\theta}$ and $\boldsymbol{v}' \equiv \boldsymbol{v} - \tilde{\boldsymbol{v}}$.

The purpose of LES closures is to express $\mathscr{L}$ and $\tilde{\mathscr{S}}$ in terms of the large-scale fields $\tilde{\theta}$ and $\tilde{\boldsymbol{v}}$. Once this goal is accomplished, (2.4) can be numerically integrated on a mesh of spacing l, rather than η as would be required for the integration of the full system (2.1), with an enormous gain in memory and CPU time requirements.

Unfortunately, no general closed expression for $\mathscr{L}$ and $\tilde{\mathscr{S}}$ in terms of $\tilde{\theta}$ and $\tilde{\boldsymbol{v}}$ is available. A remarkable exception is the case where there is a marked scale separation

between velocity and scalar length and time scales. It is then possible to show (see, e.g., Biferale *et al.* 1995; Mazzino 1997) that the effect of unresolved scales is just the renormalization of the molecular diffusion coefficient κ_0 to an enhanced eddy-diffusivity κ^{eff} (generally speaking, an eddy-diffusivity tensor $\kappa_{ij}^{\mathrm{eff}}$). General expressions for the eddy diffusivity as a function of the flow properties do not exist, and in most cases κ^{eff} can be determined only numerically.

Here, our aim is to consider the challenging situation where there is no scale separation between velocity and scalar and explore, in such a context, the existence of effective equations for $\tilde{\theta}$.

Our procedure to derive the closed coarse-grained dynamical equations is the following:

(i) starting from first principles, that is from (2.1), we take advantage of the distinctive aspects of the Kraichnan model to derive an exact, yet unclosed, statistical equation for the correlation function of the filtered scalar field $\langle\tilde{\theta}(\boldsymbol{x}, t)\tilde{\theta}(\boldsymbol{x} + \boldsymbol{r}, t)\rangle$;

(ii) the statistical averages appearing in this equation, which involve small-scale fields, are then expressed in terms of correlations of large-scale fields only, at a given order of approximation in l/r;

(iii) from the statistically closed equations we consistently infer the dynamical closed equations for $\tilde{\theta}$.

No supplementary assumptions are made in performing this procedure. Although the method relies heavily on distinctive characteristics of the Kraichnan model, we believe that the results are relevant to generic passive scalar turbulence as well. Our claim is supported by numerical and analytical evidence gathered in the past few years showing that most of the phenomenology of scalar turbulence is captured by the Kraichnan model. For an exhaustive review on this aspect see, e.g., Falkovich *et al.* (2001).

To illustrate the power of our approach we anticipate here the main results of this paper, postponing their derivation to the following sections.

Carrying out the procedure at the lowest significant order in l/r yields the following effective equation for the coarse-grained field:

$$\partial_t\tilde{\theta} + \tilde{\boldsymbol{v}}\cdot\boldsymbol{\nabla}\tilde{\theta} = \kappa^{\mathrm{eff}}\Delta\tilde{\theta} + \tilde{f}, \qquad \kappa^{\mathrm{eff}} \equiv \kappa_0 + \kappa_1, \tag{2.7}$$

where κ_1 is a constant depending on the flow properties that can be explicitly calculated within the Kraichnan model. Equation (2.7) is just the long-known *constant eddy-diffusivity closure*.

At the next-leading order we find

$$\partial_t\tilde{\theta} + \tilde{\boldsymbol{v}}\cdot\boldsymbol{\nabla}\tilde{\theta} = \kappa_{\alpha\beta}^{T}\nabla_\alpha\nabla_\beta\tilde{\theta} + \tilde{f}, \tag{2.8}$$

with $\kappa_{\alpha\beta}^{T}(\boldsymbol{x}, t) = \delta_{\alpha\beta}\kappa^{\mathrm{eff}} - al^2\, e_{\alpha\beta}$, and $e_{\alpha\beta} = \frac{1}{2}(\nabla_\alpha\tilde{v}_\beta + \nabla_\beta\tilde{v}_\alpha)$. The filter-dependent factor a can be determined analytically within the Kraichnan model. Equation (2.8) is the passive scalar analogue (see, e.g., Kang & Meneveau 2001) of the so-called 'mixed-model' (nonlinear closure plus scalar eddy viscosity) used in Navier–Stokes turbulence (see, e.g., Borue & Orszag 1998). Such a mixed model was also invoked by Kang & Meneveau (2001) to reproduce the correct amount of anisotropy in heated turbulent jets.

The nonlinear closure can also be derived starting from a Taylor expansion in the spirit of Leonard (1974) performed on a modified Leonard term (see, e.g., Horiuti 1997). A purely dissipative effective-viscosity model is usually added because the sole nonlinear model does not suffice, its dissipation being far too low. Here, the constant eddy diffusivity plus the nonlinear model follow from first principles
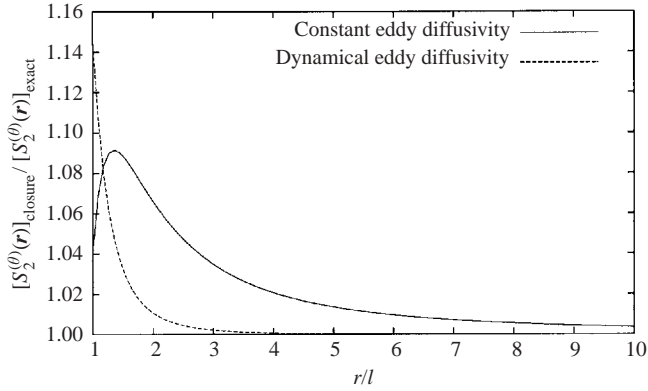
FIGURE 1. The coarse-grained structure functions obtained from the constant eddy-diffusivity closure, and the dynamical eddy-diffusivity model, normalized with respect to the exact filtered structure function (3.4).

without additional requirements. The turbulent eddy-diffusivity κ^T depends on the coarse-grained velocity field: for this reason we will dub this model *dynamical eddy-diffusivity closure.*

In order to compare the performances of the various models we will explicitly compute the structure function $S_2^{(\theta)}(r) = \langle [\tilde{\theta}(\boldsymbol{x} + \boldsymbol{r}, t) - \tilde{\theta}(\boldsymbol{x}, t)]^2 \rangle$ of the coarse-grained scalar field according to (2.7) or to (2.8) and compare them with the exact value obtained from the solution of (2.1) upon filtering. The result is shown in figure 1: the dynamical eddy-diffusivity closure gives a structure function that is already almost indistinguishable from the exact result at scales $r \approx 2l$ whereas the constant eddy diffusivity is not very effective in the range $r \lesssim 10 l$.

3. A systematic approach to LES closure

3.1. *The Kraichnan model*

In order to carry out our analysis, we need to specialize (2.1) to a class of random velocity fields. To be more specific, the velocity field is assumed here to be Gaussian, of zero mean, statistically stationary, homogeneous and isotropic, δ-correlated in time and with inertial-range power-law behaviour. Its statistics is fully determined by the correlation function

$$\langle [v_\alpha(\boldsymbol{x}_1, t) - v_\alpha(\boldsymbol{x}_2, t)][v_\beta(\boldsymbol{x}_1, 0) - v_\beta(\boldsymbol{x}_2, 0)] \rangle = 2D_{\alpha\beta}^{(v)}(\boldsymbol{x}_1 - \boldsymbol{x}_2)\delta(t), \qquad (3.1)$$

where $D_{\alpha\beta}^{(v)}(\boldsymbol{r}) \equiv D_0 \, r^\xi [(d + \xi - 1)\delta_{\alpha\beta} - \xi r_\alpha r_\beta / r^2]$, $r \equiv |\boldsymbol{r}| = |\boldsymbol{x}_2 - \boldsymbol{x}_1|$ and d is the space dimension. The assumption of δ-correlation in time is of course far from the reality, but it has the remarkable feature of leading to closed equations for equal-time correlation functions $C_n^{(\theta)} \equiv \langle \theta(\boldsymbol{x}_1, t) \dots \theta(\boldsymbol{x}_n, t) \rangle$ of any order n (see, e.g., Falkovich *et al.* 2001). The parameter ξ governs the roughness of the velocity field, whose Hölder exponent is $\xi/2$. Due to the white-in-time character of the flow, the Kolmogorov value is $\xi = 4/3$. A convenient choice for the forcing term is to take f random, Gaussian, statistically homogeneous and isotropic, white in time, of zero mean and with correlation function

$$\langle f(\boldsymbol{x}_1, t) f(\boldsymbol{x}_2, 0) \rangle = F(r/L) \delta(t) \qquad (3.2)$$

with $F(r/L)$ decreasing rapidly for $r \gg L$. Since $l \ll L$ we have $\tilde{f} \simeq f$.

In this framework the expression for the second-order correlation function $C_2^{(\theta)}$ can be derived analytically (Falkovich *et al.* 2001). In the inertial range $\eta \ll r \ll L$ the exact second-order structure function of the scalar field $S_2^{(\theta)}(r) \equiv \langle [\theta(\boldsymbol{x}_1, t) - \theta(\boldsymbol{x}_2, t)]^2 \rangle$ is

$$S_2^{(\theta)}(r) = \frac{2F(0)}{\zeta_2(d-1)dD_0} r^{\zeta_2}, \qquad \zeta_2 = 2 - \xi, \tag{3.3}$$

where $F(0)$, defined in (3.2), is the average injection rate of scalar variance. The exponent ζ_2 coincides with the predictions based on dimensional arguments, and is $\zeta_2 = 2/3$ for $\xi = 4/3$, according to the Kolmogorov–Obukhov–Corrsin scaling.

From now on, we will confine ourselves to space dimension $d = 3$ and specialize G_l to a top-hat filter, that is $G_l(r) = 3/(4\pi l^3)$ if $r < l$ and 0 otherwise.

To provide a benchmark for the various closures, we first evaluate the exact value of the coarse-grained structure function $S_2^{(\tilde{\theta})} \equiv \langle [\tilde{\theta}(\boldsymbol{x}_1, t) - \tilde{\theta}(\boldsymbol{x}_2, t)]^2 \rangle$. A double integration of (3.3) yields

$$\left[S_2^{(\tilde{\theta})}(r) \right]_{\text{exact}} = S_2^{(\theta)}(r) \left[1 + \frac{(2-\xi)(3-\xi)}{5} \left(\frac{l}{r} \right)^2 + O \left(\frac{l}{r} \right)^4 \right]. \tag{3.4}$$

Clearly, as the separation r increases and becomes much greater than the filter scale l the unfiltered result is recovered. Equation (3.4) represents, therefore, the best result that can be achieved by means of a closure.

3.2. *Exact statistical equations for unfiltered and filtered fields*

As a first step, we derive the exact equations for the two-point correlation function of the filtered and of the unfiltered field. It is more convenient to start the analysis from (2.1) by substituting $\boldsymbol{v} = \tilde{\boldsymbol{v}} + \boldsymbol{v}'$ and $\theta = \tilde{\theta} + \theta'$ in the advective term $\boldsymbol{v} \cdot \nabla \theta$. Equation (2.1) takes then the form

$$\partial_t \theta(\boldsymbol{x}_2, t) + \tilde{\boldsymbol{v}}(\boldsymbol{x}_2, t) \cdot \nabla \tilde{\theta}(\boldsymbol{x}_2, t) = \kappa_0 \Delta \theta(\boldsymbol{x}_2, t) + f(\boldsymbol{x}_2, t) - \mathscr{S}(\boldsymbol{x}_2, t), \tag{3.5}$$

from which we can immediately derive the equation for $C_2^{(\theta)}(r, t) = \langle \theta(\boldsymbol{x}_1, t)\theta(\boldsymbol{x}_2, t) \rangle$:

$$\partial_t C_2^{(\theta)}(r, t) + 2\langle \theta(\boldsymbol{x}_1, t)\tilde{\boldsymbol{v}} \cdot \nabla \tilde{\theta}(\boldsymbol{x}_2, t) \rangle - 2\kappa_0 \Delta C_2^{(\theta)}(r, t) = F(r) - 2\langle \theta(\boldsymbol{x}_1)\mathscr{S}(\boldsymbol{x}_2) \rangle. \tag{3.6}$$

A double convolution of the above equation with the filter G_l yields the exact equation for the correlation of the filtered field:

$$\partial_t C_2^{(\tilde{\theta})}(r, t) + 2\langle \tilde{\theta}(\boldsymbol{x}_1, t)\widetilde{\tilde{\boldsymbol{v}} \cdot \nabla \tilde{\theta}}(\boldsymbol{x}_2, t) \rangle - 2\kappa_0 \Delta C_2^{(\tilde{\theta})}(r, t) = F(r) - 2\langle \tilde{\theta}(\boldsymbol{x}_1)\tilde{\mathscr{S}}(\boldsymbol{x}_2) \rangle. \tag{3.7}$$

This is the starting point for our systematic procedure to construct closure approximations. It contains two terms, the second one on the left-hand side and the last one on the right-hand side, which are not expressed as functions of large-scale fields only. In the following, we will find approximate closed expressions for the unclosed terms perturbatively in l/r.

3.3. *Constant eddy-diffusivity closure*

In order to calculate the second term on the left-hand side of (3.7), let us start from $\langle \theta(\boldsymbol{x}_1)\mathscr{S}(\boldsymbol{x}_2) \rangle$. Its expression can be easily obtained by exploiting, e.g., the Furutsu–Novikov functional Gaussian integration (see, e.g., Frisch 1995), which holds for Gaussian velocities and forcings. It is

$$\langle \theta(\boldsymbol{x}_1)\mathscr{S}(\boldsymbol{x}_2) \rangle = \frac{F(0)2^{\xi+2}(3-\xi)}{(4+\xi)(6+\xi)} \left(\frac{l}{r} \right)^{\xi} - \frac{F(0)}{30}\xi^2 \left(\frac{l}{r} \right)^2 + O \left(\frac{l}{r} \right)^{2+\xi}. \tag{3.8}$$

Our first claim is that, at order $(l/r)^2$, with an error of order $(l/r)^{2+\xi}$ we have

$$\langle \theta(\boldsymbol{x}_1)\mathscr{S}(\boldsymbol{x}_2)\rangle = \langle \tilde{\theta}(\boldsymbol{x}_1)\tilde{\mathscr{S}}(\boldsymbol{x}_2)\rangle = \langle \tilde{\theta}(\boldsymbol{x}_1)\mathscr{S}(\boldsymbol{x}_2)\rangle, \tag{3.9}$$

$$\langle \tilde{\theta}(\boldsymbol{x}_1, t)\widetilde{\tilde{\boldsymbol{v}} \cdot \boldsymbol{\nabla}\tilde{\theta}}(\boldsymbol{x}_2, t)\rangle = \langle \tilde{\theta}(\boldsymbol{x}_1, t)\tilde{\boldsymbol{v}} \cdot \boldsymbol{\nabla}\tilde{\theta}(\boldsymbol{x}_2, t)\rangle. \tag{3.10}$$

The derivation of (3.9) and (3.10) is postponed to the Appendix. Before proceeding further, some comments on (3.10) are in order. It tells us that the Leonard-type term does not contribute, at $O((l/r)^2)$, to the equation for the second-order coarse-grained scalar correlation function. Since our closures are derived from this equation, it follows that the Leonard-type term will not contribute to small-scale parameterizations. This fact is not a consequence of the Kraichnan advection model but rather seems to hold for general advection models. Indeed, a standard expansion in the spirit of Leonard (1974) (see also, e.g., Horiuti 1997) performed on $\langle \tilde{\theta}(\boldsymbol{x}_1)\mathscr{L}(\boldsymbol{x}_2)\rangle$ with $\mathscr{L}$ given by (2.5) yields at the lowest order in the filter width the expression

$$\langle \tilde{\theta}(\boldsymbol{x}_1)\mathscr{L}(\boldsymbol{x}_2)\rangle \sim l^2 \Delta \langle \tilde{\theta}(\boldsymbol{x}_1, t)\tilde{\boldsymbol{v}} \cdot \boldsymbol{\nabla}\tilde{\theta}(\boldsymbol{x}_2, t)\rangle. \tag{3.11}$$

This expression is trivially zero, since $\langle \tilde{\theta}(\boldsymbol{x}_1, t)\tilde{\boldsymbol{v}} \cdot \boldsymbol{\nabla}\tilde{\theta}(\boldsymbol{x}_2, t)\rangle$ is the flux of scalar variance, which is independent of $r = |\boldsymbol{x}_2 - \boldsymbol{x}_1|$ provided that r falls in the inertial range of scales.

For standard closure models based on single-point quantities, the contribution from the Leonard stress in the parameterizations is, generally speaking, non-zero.

Let us now focus on consequences of relations (3.9) and (3.10) for (3.7) evaluated at order $(l/r)^\xi$. At this order, from (3.8) and (3.9) we have

$$-2\langle \tilde{\theta}(\boldsymbol{x}_1)\tilde{\mathscr{S}}(\boldsymbol{x}_2)\rangle = 2\kappa_1 \Delta C_2^{(\tilde{\theta})}(r, t). \tag{3.12}$$

The above expression follows by comparing (3.8) at order $(l/r)^\xi$ with the contribution coming from the diffusive term, $2\kappa_0 \Delta C_2^{(\tilde{\theta})}(r, t) = -F(0)\kappa_0(3-\xi)/(3D_0 r^\xi)$. We immediately realize that the term of order $(l/r)^\xi$ in (3.8) corresponds to an effective diffusive term with an eddy diffusivity $\kappa_1 \equiv l^\xi[2^\xi 24 D_0]/[(\xi + 4)(\xi + 6)]$. This gives rise to an effective dissipative scale comparable to l:

$$\eta^{\text{eff}} \equiv \left[(2l)^\xi \left(\frac{24}{(\xi + 4)(\xi + 6)} \right) + \eta_0^\xi \right]^{1/\xi}, \tag{3.13}$$

where $\eta_0 \equiv (\kappa_0/D_0)^{1/\xi}$ is the molecular dissipation scale.

At order $(l/r)^\xi$, (3.7) is thus closed in the large-scale fields and, moreover, due to (3.10) it has the same structure as the equation for $C_2^{(\theta)}$ but with an effective diffusivity, $\kappa_0 + \kappa_1$. Equation (2.4) thus takes the form

$$\partial_t \tilde{\theta} + \tilde{\boldsymbol{v}} \cdot \boldsymbol{\nabla}\tilde{\theta} = \kappa^{\text{eff}} \Delta\tilde{\theta} + \tilde{f}, \qquad \kappa^{\text{eff}} \equiv \kappa_0 + \kappa_1. \tag{3.14}$$

Starting from (2.7) one can deduce the equation for the correlation function $C_2^{(\tilde{\theta})}$ exploiting the Furutsu–Novikov functional Gaussian integration. In doing that, the next step will consist in comparing the resulting expression for $S_2^{(\tilde{\theta})}$ with (3.4). After some simple but quite lengthy algebra, the calculation leads to

$$S_2^{(\tilde{\theta})} = S_2^{(\theta)} \left[1 + \frac{(2 - \xi)(3 + \xi)}{5} \left(\frac{l}{r} \right)^2 + O\left(\frac{l}{r} \right)^4 \right]. \tag{3.15}$$

By comparison with (3.4), the above expression permits the error to be quantified, which occurs at order $(l/r)^2$, on the second-order structure function due to the

closure (3.14). The degree of accuracy of the constant eddy-diffusivity description can be perceived by looking at figure 1, obtained for $\xi = 4/3$, corresponding to the Kolmogorov scaling law for the advecting velocity field.

3.4. *Dynamical eddy-diffusivity closure*

Our aim is now to improve the eddy-diffusivity closure, exact at order $(l/r)^\xi$, by introducing a new closure which is accurate up to order $(l/r)^2$. It is not difficult, although quite lengthy, to verify that the large-scale equation has the form (2.8):

$$\partial_t \tilde\theta + \tilde{\boldsymbol v} \cdot \boldsymbol\nabla \tilde\theta = \kappa^T_{\alpha\beta} \nabla_\alpha \nabla_\beta \tilde\theta + \tilde f, \qquad \kappa^T_{\alpha\beta}(\boldsymbol x, t) = \delta_{\alpha\beta} \kappa^{\text{eff}} - al^2 e_{\alpha\beta}, \qquad (3.16)$$

with $e_{\alpha\beta} = \frac{1}{2}(\nabla_\alpha \tilde v_\beta + \nabla_\beta \tilde v_\alpha)$. The filter-dependent factor $a = \int \mathrm{d}^3 r\, G_l(r) r^2/(3l^2)$. For the top-hat filter one immediately obtains $a = 1/5$.

The equation for $\langle \tilde\theta^2 \rangle$, deduced from (3.16), at the statistically stationary state, is (remember that $\tilde f = f$)

$$F(0) = 2\kappa^{\text{eff}} \langle (\nabla \tilde\theta)^2 \rangle - al^2 \langle e_{\alpha\beta} \nabla_\alpha \tilde\theta \nabla_\beta \tilde\theta \rangle, \qquad (3.17)$$

which states the energy balance between production (controlled by $F(0)$) and dissipation. The fact that the first term on the right-hand side of (3.17) gives a dissipative contribution is evident. This is actually the case also for the second term. To show that, let us start from simple physical considerations. Transforming to the principal coordinates, $\boldsymbol x'$, of $e_{\alpha\beta}$, the term $-al^2 e_{\alpha\beta} \nabla_\alpha \tilde\theta \nabla_\beta \tilde\theta$ becomes

$$-al^2(c_1 \nabla_{1'} \tilde\theta \nabla_{1'} \tilde\theta + c_2 \nabla_{2'} \tilde\theta \nabla_{2'} \tilde\theta + c_3 \nabla_{3'} \tilde\theta \nabla_{3'} \tilde\theta). \qquad (3.18)$$

Because of incompressibility one has $c_1 + c_2 + c_3 = 0$, and stretching in a given direction is always accompanied by compression along, at least, one other direction. By virtue of the fact that strong scalar gradients are expected to be aligned along the direction of maximum compression (corresponding to negative c_i), it then follows that, on average, (3.18) is expected to be positive. This is the mechanism which leads to the well-known ramp-and-cliff structure observed in passive scalar turbulence both for Navier–Stokes velocity fields and for the Kraichnan ensemble (see, e.g., Celani *et al.* 2001).

The above arguments can be substantiated within the Kraichnan model. Indeed, exploiting the Furutsu–Novikov functional Gaussian integration by parts, one obtains

$$-al^2 \langle e_{\alpha\beta} \nabla_\alpha \tilde\theta \nabla_\beta \tilde\theta \rangle = a\frac{l^2}{6} \langle (\nabla_i \tilde v_j)^2 \rangle \langle (\nabla \tilde\theta)^2 \rangle. \qquad (3.19)$$

However, it is clearly possible to observe, locally in space and time, positive values of $e_{\alpha\beta} \nabla_\alpha \tilde\theta \nabla_\beta \tilde\theta$, or, in other words, backscattering events responsible for negative contributions to the scalar energy flux (see, e.g., Borue & Orszag 1998 for discussions on backscattering events in hydrodynamics turbulence).

Focusing now on the unfiltered field, the balance equation has the well-known form

$$F(0) = 2\kappa_0 \langle (\nabla\theta)^2 \rangle. \qquad (3.20)$$

Equating the left-hand sides of (3.17) and (3.20), and recalling the inequality $\kappa^{\text{eff}} + l^2/60 \langle (\nabla_i \tilde v_j)^2 \rangle \gg \kappa_0$, one concludes that the gradients of the large-scale scalar field are smaller than the gradients of the unfiltered field. This is consistent with an effective dissipative scale comparable to l and thus much larger than η by definition.

To prove (3.16), let us start by rewriting (3.7) with $\langle \tilde{\theta}(\boldsymbol{x}_1)\tilde{\mathscr{I}}(\boldsymbol{x}_2) \rangle$ expressed in terms of (3.8). Using (3.9) we obtain

$$\partial_t C_2^{(\tilde{\theta})}(r, t) + 2\langle \tilde{\theta}(\boldsymbol{x}_1, t)\tilde{\boldsymbol{v}} \cdot \boldsymbol{\nabla}\tilde{\theta}(\boldsymbol{x}_2, t) \rangle - 2\kappa^{\text{eff}}\Delta C_2^{(\tilde{\theta})}(r, t) - F(r) = \frac{F(0)\xi^2}{15}\left(\frac{l}{r}\right)^2 \quad (3.21)$$

where the contribution of order $(l/r)^{\xi}$ in (3.8) has been incorporated in the eddy-diffusivity term. From (2.8) we immediately obtain the equation for $C_2^{(\tilde{\theta})}$:

$$\partial_t C_2^{(\tilde{\theta})}(r, t) + 2\langle \tilde{\theta}(\boldsymbol{x}_1, t)\tilde{\boldsymbol{v}} \cdot \boldsymbol{\nabla}\tilde{\theta}(\boldsymbol{x}_2, t) \rangle - 2\kappa^{\text{eff}}\Delta C_2^{(\tilde{\theta})}(r, t) - F(r)$$
$$= -2al^2 \langle \tilde{\theta}(\boldsymbol{x}_1)e_{\alpha\beta}\nabla_\alpha\nabla_\beta\tilde{\theta}(\boldsymbol{x}_2) \rangle + O[(l/r)^{2+\xi}], \quad (3.22)$$

with $a = 1/5$. We finally need to show that the right-hand side of (3.21) and the right-hand side of (3.22) coincide up to order $(l/r)^2$. In order to evaluate the right-hand side of (3.22) we need to exploit again the Furutsu–Novikov functional Gaussian integration by parts. One thus needs to compute the functional derivative $\delta\tilde{\theta}(\boldsymbol{x}, t)/\delta\tilde{\boldsymbol{v}}(\boldsymbol{x}'', t'')$ which can be easily obtained from (2.8). Accounting for the δ-correlation in time and utilizing the expansions

$$D_{\alpha\beta}^{(\tilde{v})}(\boldsymbol{r}) = D_{\alpha\beta}^{(v)}(\boldsymbol{r})\left\{1 + O\left[\left(\frac{l}{r}\right)^{\xi}\right]\right\}, \quad S_2^{(\tilde{\theta})}(r) = S_2^{(\theta)}(r)\left\{1 + O\left[\left(\frac{l}{r}\right)^2\right]\right\}, \quad (3.23)$$

one ends up exactly with the right-hand side of (3.21). Exploiting once more the Furutsu–Novikov functional Gaussian integration by parts, it is not difficult (although quite lengthy) to verify that the expression (3.4) for $S_2^{(\tilde{\theta})}$ is obtained from (2.8). The remaining error is at the order $(l/r)^4$.

4. Conclusions and perspectives

Summarizing, a systematic procedure to derive closed dynamical equations for a coarse-grained passive scalar field in the statistical steady state has been obtained in the framework of the Kraichnan advection model.

The question that naturally arises is whether those results are relevant to realistic advection models. The answer is given by the outcome of the procedure itself. We recover from first principles two well-known closures that are commonly used in applications: the constant eddy-diffusivity parameterization of small scales, and the passive scalar version of the nonlinear eddy-viscosity closure used in hydrodynamic turbulence. Of course, the value of the effective diffusivity κ^{eff} and of the numerical parameter a that appear in these closures can be analytically computed only in the Kraichnan model. However, we believe that the form of the parameterization can be exported without modifications to real situations as well. Clearly, in this case the free parameters (e.g. κ^{eff} and a) have to be determined *a posteriori* by some empirical procedure. The validity of this approach can be checked by direct numerical simulations.

Let us conclude by mentioning a possible generalization of our work. Our analysis has been carried for the second-order correlation function of the scalar field. There are two reasons for this choice. First, the second-order correlation function is the Fourier transform of the spectrum of scalar variance, a widely used statistical indicator to characterize most of the statistical properties of scalar turbulence. Second, for the Kraichnan model only the second-order correlation function has a simple, closed analytical expression. For higher-order correlation functions only perturbative

expressions (for example in the limit of small ξ) are available (see Falkovich *et al.* 2001). However, should have we focused on a higher-order correlation function, how would our results change? Although the analysis appears much more cumbersome than the one presented here, the procedure described in §3 can be completed as well: it is still possible to obtain a closed equation for the coarse-grained correlation function at any order in l/r, from which one can identify the corresponding dynamical equations for the large-scale scalar field. The question is: will the latter dynamical equation have the same structure of the coarse-grained scalar equation derived from the second-order correlation? And if this is the case, will the coefficients be the same? Even if the functional form of the closure is preserved, a modification of the effective coefficients would mean that strong small-scale fluctuations – associated with higher-order correlation functions – must be described by parameters different from the ones used for less intense fluctuations. That would call into question the applicability of closure models to the description of the statistics of turbulent fields such as temperature or concentration, which are characterized by a wide range of fluctuation intensities. This challenging issue is left for future research.

Appendix. Proof of (3.9) and (3.10)

Let us write, from (3.8), $\langle\theta(\boldsymbol{x}_1)\mathscr{S}(\boldsymbol{x}_2)\rangle = A(l/r)^\xi + B(l/r)^2$. By direct calculation it is easily checked that, for any filter G_l (normalized and isotropic), the following relations hold up to the second order in l/r:

$$\langle\tilde{\theta}(\boldsymbol{x}_1)\mathscr{S}(\boldsymbol{x}_2)\rangle = \int \mathrm{d}^3 s\, G_l(s)\langle\theta(\boldsymbol{x}_1 + \boldsymbol{s})\mathscr{S}(\boldsymbol{x}_2)\rangle$$

$$= \int \mathrm{d}^3 s\, G_l(s)\left[A\left(\frac{l}{|\boldsymbol{r} + \boldsymbol{s}|}\right)^\xi + B\left(\frac{l}{|\boldsymbol{r} + \boldsymbol{s}|}\right)^2\right] + O\left(\frac{l}{r}\right)^{\xi+2}$$

$$= A\left(\frac{l}{r}\right)^\xi \int \mathrm{d}s\, s^2 G_l(s)\int_{-1}^{1} \mathrm{d}(\cos\vartheta)\int_{0}^{2\pi} \mathrm{d}\varphi\left[1 - \xi\cos\vartheta\frac{s}{r} + O\left(\frac{s}{r}\right)^2\right]$$

$$+ B\left(\frac{l}{r}\right)^2 \int \mathrm{d}s\, s^2 G_l(s)\int_{-1}^{1} \mathrm{d}(\cos\vartheta)\int_{0}^{2\pi} \mathrm{d}\varphi\left[1 - 2\cos\vartheta\frac{s}{r} + O\left(\frac{s}{r}\right)^2\right]$$

$$+ O\left(\frac{l}{r}\right)^{\xi+2}$$

$$= A\left(\frac{l}{r}\right)^\xi + B\left(\frac{l}{r}\right)^2 + O\left(\frac{l}{r}\right)^{\xi+2}$$

$$= \langle\theta(\boldsymbol{x}_1)\mathscr{S}(\boldsymbol{x}_2)\rangle + O\left(\frac{l}{r}\right)^{\xi+2}.$$

Similarly, convolving also over $\boldsymbol{x}_2$, one finds

$$\langle\tilde{\theta}(\boldsymbol{x}_1)\tilde{\mathscr{S}}(\boldsymbol{x}_2)\rangle = \langle\tilde{\theta}(\boldsymbol{x}_1)\mathscr{S}(\boldsymbol{x}_2)\rangle + O\left(\frac{l}{r}\right)^{\xi+2} = \langle\theta(\boldsymbol{x}_1)\mathscr{S}(\boldsymbol{x}_2)\rangle + O\left(\frac{l}{r}\right)^{\xi+2}. \quad \text{(A 1)}$$

To prove (3.10), let us now consider (3.7) and the equation obtained from (3.6) with the sole convolution over x_1. Because of stationarity all time derivatives vanish and for r in the inertial range the two-point terms proportional to molecular diffusivity κ_0 are negligible. We thus obtain

$$2\langle\tilde{\theta}(\boldsymbol{x}_1)\widetilde{\tilde{\boldsymbol{v}}\cdot\boldsymbol{\nabla}\tilde{\theta}(\boldsymbol{x}_2)}\rangle = F(r) - 2\langle\tilde{\theta}(\boldsymbol{x}_1)\tilde{\mathscr{S}}(\boldsymbol{x}_2)\rangle \tag{A 2}$$

$$2\langle\tilde{\theta}(\boldsymbol{x}_1)\tilde{\boldsymbol{v}}\cdot\boldsymbol{\nabla}\tilde{\theta}(\boldsymbol{x}_2)\rangle = F(r) - 2\langle\tilde{\theta}(\boldsymbol{x}_1)\mathscr{S}(\boldsymbol{x}_2)\rangle. \tag{A 3}$$

Subtracting (A 3) from (A 2), and using (3.9), we conclude that $\langle\tilde{\theta}\mathscr{L}\rangle = O[(l/r)^{\xi+2}]$. This proves (3.10).

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