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Diffusion-limited scalar cascades

By N. J. BALMFORTH[1] and W. R. YOUNG[2]

[1]Department of Applied Mathematics and Statistics, University of California, Santa Cruz, CA 95064, USA

[2]Scripps Institution of Oceanography, La Jolla, CA 92093-0213, USA

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We study advection–diffusion of a passive scalar, T, by an incompressible fluid in a closed vessel bounded by walls impermeable to the fluid. Variations in T are produced by prescribing a steady non-uniform distribution of T at the boundary. Because there is no flow through the walls, molecular diffusion, κ, is essential in 'lifting' T off the boundary and into the interior where the velocity field acts to intensify ∇T. We prove that as $\kappa \to 0$ (with the fluid velocity fixed) this diffusive lifting is a feeble source of scalar variance. Consequently the scalar dissipation rate χ – the volume integral of $\kappa|\nabla T|^2$ – vanishes in the limit $\kappa \to 0$. Thus, in this particular closed-flow configuration, it is not possible to maintain a constant supply of scalar variance as $\kappa \to 0$ and the fundamental premise of scaling theories for passive scalar cascades is violated.

We also obtain a weaker bound on χ when the transported field is a dynamically active scalar, such as temperature. This bound applies to the Rayleigh–Bénard configuration in which $T = \pm 1$ on two parallel plates at $z = \pm h/2$. In this case we show that $\chi \leqslant 3.252 \times (\kappa\varepsilon/\nu h^2)^{1/3}$ where ν is the viscosity and ε is the mechanical energy dissipation per unit mass. Thus, provided that ε and ν/κ are non-zero in the limit $\kappa \to 0$, χ might remain non-zero.

1. Introduction

An important process at the heart of many fluid phenomena in the physical and engineering sciences is the advection and diffusion of a passive scalar. One of the canonical idealizations of this process is the problem first broached by Zeldovich (1937), in which the scalar is advected inside a closed container by an incompressible fluid with an arbitrary velocity field. There is no source or sink of the scalar within the fluid, and its concentration is maintained in some fixed pattern on parts of the boundary, whilst other areas of the boundary are impermeable.

The mathematical formulation of Zeldovich's problem is the advection–diffusion equation for the scalar field, $T(\boldsymbol{x}, t)$, in a region of volume $\mathscr{V}$:

$$T_t + \boldsymbol{u} \cdot \nabla T = \kappa \nabla^2 T , \tag{1.1}$$

where κ is molecular diffusivity and $\boldsymbol{u}(\boldsymbol{x}, t)$ is a prescribed smooth velocity field satisfying $\nabla \cdot \boldsymbol{u} = 0$. There is no flow through the walls of the domain, and so $\boldsymbol{n} \cdot \boldsymbol{u} = 0$, where $\boldsymbol{n}$ is the outward unit normal (but we do not necessarily insist on the no-slip condition). Some part of the boundary may be insulating, i.e. $\boldsymbol{n} \cdot \nabla T = 0$, while on the remainder of the boundary T is prescribed. An example solution to this problem is presented in figure 1, which illustrates the filamentation of the tracer when κ is small.

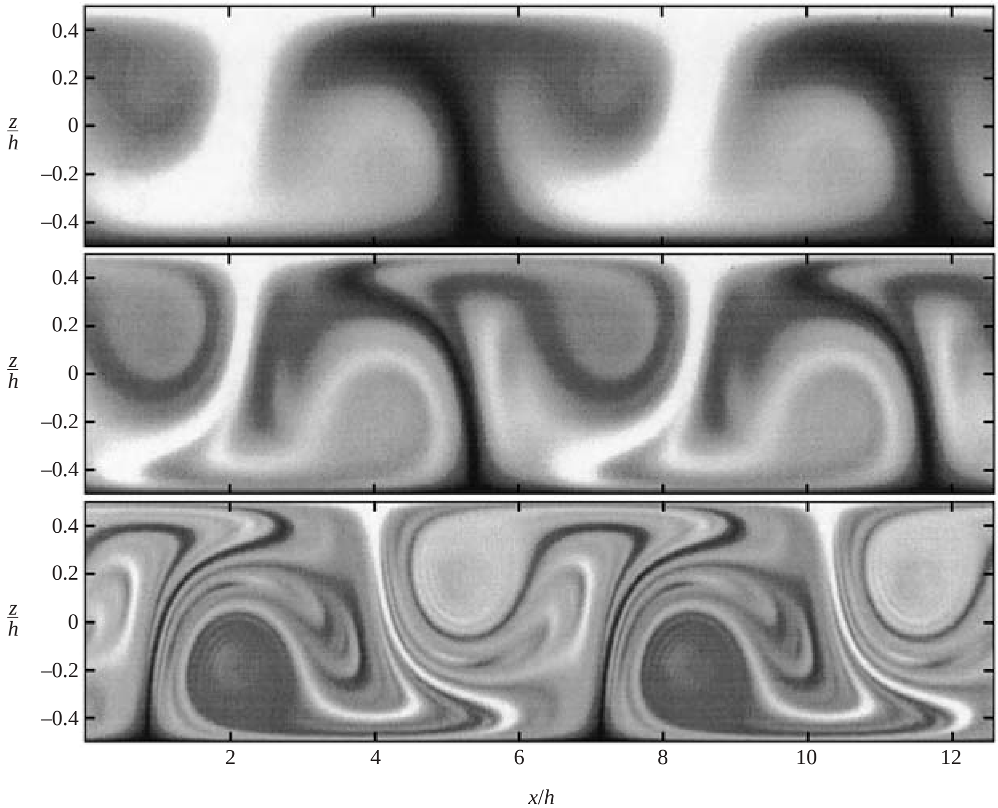

FIGURE 1. A solution of (1.1) using Solomon & Gollub's (1988) model of oscillating convection cells. (The velocity is defined by the streamfunction in (3.1) with $\alpha = 3h/2$.) The tracer is fixed at $T = +1$ on the top plate ($z = h/2$) and $T = -1$ on the bottom plate ($z = -h/2$.) The three panels show snapshots of $T(x, z, t)$ after transients have subsided for computations with three values of the Péclet number (10^2, 10^3 and 10^4, top to bottom). The concentration field is twisted into increasingly sharp filaments that are torn from the boundaries and wrapped around the sweeping cells. Intense gradients are created in boundary layers and filaments, but over most of the domain, the tracer is well mixed by the fluid motions.

Zeldovich's problem applies to many situations in oceanography, meteorology, astrophysics and engineering, and is a classical setting in which to study 'passive scalar turbulence' (the creation of complicated structure in the scalar field by fluid motion; e.g. Shraiman & Siggia 2000; Sreenivasan 1991; Warhaft 2000). The motivating idea here is that when the scalar is supplied at large scales, differential advection creates increasingly fine length scales so that molecular diffusion ultimately balances the advective intensification of scalar gradients (cf. figure 1). Obukhov, Corrsin and Batchelor argued that the link between the large-scale source of scalar variance and the small-scale sink is a turbulent cascade and dimensional analysis, much like Kolmogorov's theory of turbulence, is applicable (e.g. Sreenivasan 1996; Shraiman & Siggia 2000). The cascade rate,

$$\chi \equiv \kappa \langle |\nabla T|^2 \rangle \,, \tag{1.2}$$

plays a key role in these arguments. In (1.2) the angular brackets denote a volume and time average,

$$\langle Z \rangle \equiv \int_0^{t_\infty} \int Z(\boldsymbol{x}, t) \frac{\mathrm{d}V}{\mathscr{V}} \frac{\mathrm{d}t}{t_\infty}, \tag{1.3}$$

and t_∞ is sufficiently long to remove unsteady fluctuations in T forced by pulsations in $\boldsymbol{u}(\boldsymbol{x}, t)$. If T is the temperature of the fluid then, within the Boussinesq approximation, χ is the rate of entropy production.

The fundamental premise of Obukhov's, Corrsin's and Batchelor's theories of passive scalar cascades is that χ is independent of κ and enters as an external parameter in the dimensional analysis (Sreenivasan 1996; Shraiman & Siggia 2000). The main result of the current paper is that

$$\lim_{\kappa \to 0} \chi = 0, \tag{1.4}$$

for a fixed velocity field. Thus, the fundamental premise of the standard theory is violated in Zeldovich's problem.

2. Comparison functions and some bounds

Our goal is to place limits on the scalar dissipation rate, χ. If we multiply (1.1) by T and take a $\langle\rangle$-average we obtain a useful alternative to the definition in (1.2):

$$\chi = \kappa \int_0^{t_\infty} \int T T_n \frac{\mathrm{d}A}{\mathscr{V}} \frac{\mathrm{d}t}{t_\infty}. \tag{2.1}$$

The area integral above is over the boundary of $\mathscr{V}$ and $T_n \equiv \nabla T \cdot \boldsymbol{n}$. At first sight, (2.1) offers some explanation for why the scalar cascade rate should vanish in the limit $\kappa \to 0$. However, the limit is not completely trivial, since for complicated velocity fields one cannot exclude the possibility that scalar gradients at the walls become as large as κ^{-1} in the limit.

Because the advection–diffusion equation is linear, we may also normalize the prescribed boundary values of T to lie between $+1$ and -1. Then, by invoking the *extremum principle* for the advection–diffusion equation, the interior values of T are also constrained by $-1 < T(\boldsymbol{x}, t) < 1$. The main tools we use in this study are this extremum principle, together with the concept of a *comparison function*, $C(\boldsymbol{x})$. The comparison function satisfies the same boundary conditions as the scalar (on the insulating walls $T_n = C_n = 0$ and on the remainder of the boundary $C = T$), and is chosen to possess some other useful properties, outlined shortly. Because the prescribed boundary concentration is steady we can restrict ourselves to comparison functions which are independent of t. Given a comparison function C, we define

$$\chi_C \equiv \kappa \int C C_n \frac{\mathrm{d}A}{\mathscr{V}} \tag{2.2}$$

in analogy with (2.1).

2.1. *Zeldovich's lower bound*

Using Green's first theorem, and the boundary properties of C, one has

$$\int \nabla T \cdot \nabla C \, \mathrm{d}V = \int C C_n \, \mathrm{d}A - \int T \nabla^2 C \, \mathrm{d}V. \tag{2.3}$$

The integral identity above implies that

$$\kappa \langle \nabla T \cdot \nabla C \rangle = \chi_C - \kappa \langle T \nabla^2 C \rangle. \tag{2.4}$$

A simple example of bounding using comparison functions is provided by using (2.4) to replace the cross-term in $\kappa\langle|\nabla T - \nabla C|^2\rangle \geqslant 0$. This replacement gives

$$\chi \geqslant 2\chi_C - \kappa\langle|\nabla C|^2\rangle - 2\kappa\langle T\nabla^2 C\rangle\,. \tag{2.5}$$

If we now choose the particular comparison function which satisfies $\nabla^2 C = 0$ in $\mathscr{V}$ then (2.5) becomes $\chi \geqslant \chi_C$. In other words, using the conduction solution as a comparison function we obtain Zeldovich's result that χ is a minimum when the fluid is at rest.

2.2. *An identity and two inequalities*

Using Green's second theorem one has

$$\int T\nabla^2 C - C\nabla^2 T \,\mathrm{d}V = \int C C_n - T T_n \,\mathrm{d}A\,. \tag{2.6}$$

If we multiply (1.1) by C, take the $\langle\rangle$-average, and use (2.6), we obtain the fundamental identity

$$\chi = \chi_C - \langle T\boldsymbol{u}\cdot\nabla C\rangle - \kappa\langle T\nabla^2 C\rangle\,. \tag{2.7}$$

Since only T, and not ∇T, appears on the right-hand side of (2.7) we can invoke the extremum principle, $-1 < T < +1$, and extract the maximum value, $T = 1$, from the integrals to obtain

$$\text{Bound A}: \qquad \chi \leqslant \chi_C + \langle|\boldsymbol{u}\cdot\nabla C|\rangle + \kappa\langle|\nabla^2 C|\rangle\,. \tag{2.8}$$

Combining (2.7) with the inequality (2.5) we obtain $\chi \leqslant \kappa\langle|\nabla C|^2\rangle + 2\langle T\boldsymbol{u}\cdot\nabla C\rangle$. Again invoking the extremum principle we find the bound

$$\text{Bound B}: \qquad \chi \leqslant \kappa\langle|\nabla C|^2\rangle + 2\langle|\boldsymbol{u}\cdot\nabla C|\rangle\,. \tag{2.9}$$

2.3. *The bound for small* κ

Both (2.8) and (2.9) apply for arbitrary values of κ. To prove (1.4) we proceed by selecting C to be different from zero only in boundary layers which cling to walls of the vessel. The boundary layer thickness, δ, is much less than the characteristic length scale $\mathscr{V}^{1/3}$, which ensures that $\boldsymbol{u}\cdot\nabla C$ is small over most of the domain (more detail below). But δ cannot be made too small without promoting the other terms, which are all explicitly proportional to κ, but involve higher normal derivatives of C. Thus the optimal value of δ is obtained by making $\langle|\boldsymbol{u}\cdot\nabla C|\rangle$ the same order of magnitude as the other terms.

Given that C has a boundary-layer structure, we can make order-of-magnitude estimates of the terms on the right-hand sides of (2.8) and (2.9). Consider, for instance, the term $\langle|\boldsymbol{u}\cdot\nabla C|\rangle$. In the boundary layer, $\nabla C \sim \delta^{-1}\boldsymbol{n}$, where $\boldsymbol{n}$ is the normal to the boundary. Now $\boldsymbol{u}\cdot\boldsymbol{n}$ is zero on the walls, and increases linearly with distance from the boundary. Thus, provided that the boundary layer is sufficiently thin, $\boldsymbol{u}\cdot\nabla C \sim \boldsymbol{u}\cdot\boldsymbol{n}/\delta \sim \omega$ where ω is normal derivative of $\boldsymbol{u}\cdot\boldsymbol{n}$. Since the total volume of the boundary layer is $\mathscr{V}^{2/3}\delta$, the volume average gives $\langle|\boldsymbol{u}\cdot\nabla C|\rangle \sim \omega\delta/\mathscr{V}^{1/3}$. Analogous rough estimates of the other terms (namely $\kappa\langle|\nabla C|^2\rangle$, χ_C and $\kappa\langle|\nabla^2 C|\rangle$) in (2.8) and (2.9) show that these are all of order κ/δ. In summary, both (2.8) and (2.9) give bounds of the form

$$\chi \leqslant \mathscr{V}^{-1/3}\left[a_1\frac{\kappa}{\delta} + a_2\omega\delta\right], \tag{2.10}$$

where a_1 and a_2 are dimensionless positive constants, depending only on the geometry of the vessel.

The terms in square brackets on the right-hand side of (2.10), viewed as a function of δ, achieve their minimum value at $\delta = \sqrt{a_1\kappa/a_2\omega}$. Evaluating (2.10) at this optimal δ then gives

$$\chi \leqslant 2\mathscr{V}^{-1/3}\sqrt{a_1 a_2 \omega\kappa}\,, \tag{2.11}$$

and (1.4) follows.

If the velocity field also satisfies the no-slip condition at the wall (as in Ghosh, Leonard & Wiggins 1998) then the bound can be strengthened. Specifically, inside the boundary layer, $\boldsymbol{n}\cdot\boldsymbol{u}$ varies quadratically with distance from the wall. In these circumstances one can show that the optimal boundary layer scale is $\delta \propto \kappa^{1/3}$ and $\chi < O(\kappa^{2/3})$.

3. An example

A simple example is a fluid confined by two plates at $z = \pm h/2$. On the top plate we prescribe $T = +1$ and on the bottom plate $T = -1$. The domain is periodic in the x-direction and of length $2\pi h$. We consider a flow field with the streamfunction

$$\psi(x, z, t) = \phi \sin(X/h)\cos(\pi z/h)\,, \tag{3.1}$$

where $X = x + \alpha \sin t$. The model streamfunction has two parameters, α and ϕ; the Péclet number is ϕ/κ. Our sign convention is $(u, w) = (\psi_z, -\psi_x)$. This two-dimensional flow is a specific case of the model of unsteady convective rolls proposed by Solomon & Gollub (1988). Provided that $\alpha \neq 0$ this flow chaotically advects tracer particles.

As comparison functions we consider

$$C(z) = \frac{\sinh \mu z}{\sinh(\mu h/2)}\,, \tag{3.2}$$

where $\mu = 1/\delta$ is varied to determine the tightest bound. To use the inequalities in (2.8) and (2.9) we first calculate the following properties of (3.2):

$$\chi_C = 2\kappa h^{-2} m \coth(m/2)\,, \qquad \kappa\langle|\nabla^2 C|\rangle = 2\kappa h^{-2} m \tanh(m/4)\,, \tag{3.3}$$

$$\kappa\langle|\nabla C|^2\rangle = \frac{\kappa}{h^2}\frac{m(\sinh m + m)}{\cosh m - 1}\,, \tag{3.4}$$

where $m \equiv \mu h$. The term requiring most work is $\langle|\boldsymbol{u}\cdot\nabla C|\rangle = \langle|w|C_z\rangle$:

$$\langle|wC_z|\rangle = \frac{4\phi}{h^2}\frac{m\coth(m/2)}{\pi^2 + m^2}\,, \tag{3.5}$$

which is independent of α.

Substituting the results above into (2.8) and (2.9) gives the bounds

$$\text{Bound A}: \qquad \chi \leqslant 2\frac{\kappa}{h^2} m\left[\coth\left(\frac{m}{2}\right) + \tanh\left(\frac{m}{4}\right)\right] + 4\frac{\phi}{h^2}\frac{m\coth(m/2)}{\pi^2 + m^2}\,, \tag{3.6}$$

$$\text{Bound B}: \qquad \chi \leqslant \frac{\kappa}{h^2}\frac{m(\sinh m + m)}{(\cosh m - 1)} + 8\frac{\phi}{h^2}\frac{m\coth(m/2)}{\pi^2 + m^2}\,. \tag{3.7}$$

Finally, with fixed κ and ϕ, we minimize these bounds by finding the optimal value of m (see figure 2). When κ/ϕ is small the optimal m is $O(\kappa/\phi)^{-1/2}$ and both (3.6) and (3.7) reduce to (2.10). If κ/ϕ becomes large, on the other hand, m approaches zero and the bounds converge to the conduction solution, $\chi = 4\kappa/h^2$.

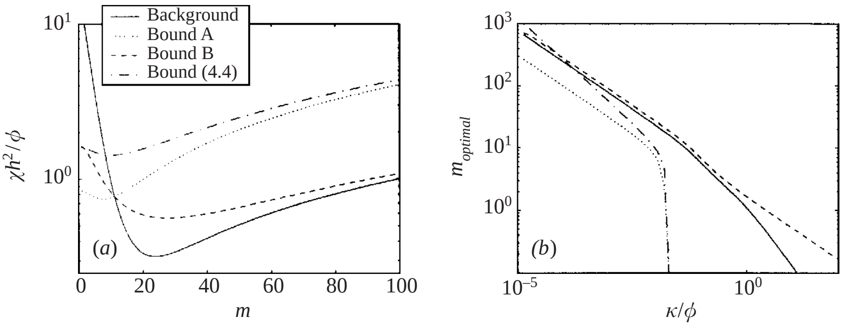

FIGURE 2. Construction of bounds using C in (3.2). (*a*) A plot of the upper bound on χ as a function of m for $\kappa/\phi = 0.01$, and (*b*) the optimal m as a function of κ/ϕ. Shown are computations for the two bounds A and B in (3.6) and (3.7), the bound from the background method in (A 10), and the bound in (4.4).

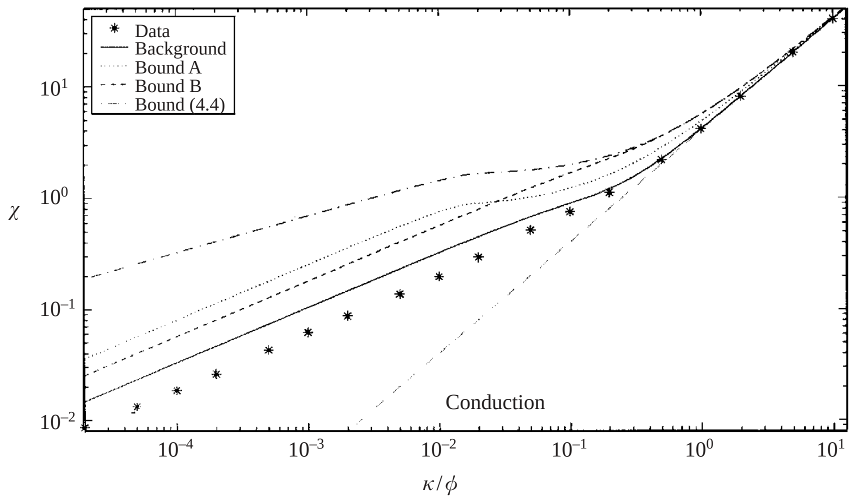

FIGURE 3. The bounds on χ, computed from (3.6), (3.7), (A 10), and (4.4), together with some data points obtained by numerically integrating (1.1). Shown also is the conduction solution (for which $\chi = 4\kappa/h^2$).

With more effort, a superior bound can be obtained using the Constantin–Doering–Hopf method of the background field (see the Appendix). This approach gives a third bound, presented in (A 10), which lowers the constraint on χ by a factor of roughly 2, but offers no improvement over (3.6) and (3.7) in the scaling of the bound at small or large κ. All of the bounds are summarized in figure 3 and compared with results obtained by numerically integrating the advection–diffusion equation with initial condition, $T(x, z, 0) = \sinh(4z/h)/\sinh(2)$. (We verified that the precise form of the initial condition had an insignificant effect on the computed value of χ.)

4. Boundary-layer velocity fields and dynamically active scalars

A key restriction on our earlier results is that $\boldsymbol{u}$ is independent of both κ and C. Looking back over our estimates, this crucial assumption has enabled us to argue that as $\kappa \to 0$, the scale of $\boldsymbol{u}$ near the wall is much greater than the thickness of the comparison-function boundary layer. In this section we lift this restriction and present a bound, weaker than (2.11), but with the important advantage of encompassing velocity fields with fine-scale structure near the wall. This includes dynamical problems, in which T is not a passive scalar, and also the possibility that as $\kappa \to 0$ the velocity $\boldsymbol{u}$ also forms a comparably sharp boundary layer (for example, because the Prandtl number is fixed).

We use only bound A in (2.8) and we consider the parallel plate geometry of § 3, with $T = \pm 1$ on $z = \pm h/2$. Thus the following estimates apply to the standard Rayleigh–Bénard convection problem in which the temperature T determines the buoyancy of the fluid. However, a similar approach can be used with more general boundary conditions on the parallel plates.

As a comparison function, we can again use $C(z)$ in (3.2). Some of the integrals we need are in (3.3). The difficult term is always $\langle |\boldsymbol{u} \cdot \nabla C| \rangle = \langle |w| C_z \rangle$. To bound $\langle |w| C_z \rangle$, without making restrictive assumptions about w, we invoke Howard's (1972) *Lemma 1* that

$$w^2 \leqslant \left(\frac{h^2}{4} - z^2 \right) \int_{-h/2}^{h/2} w_z^2 \, \frac{\mathrm{d}z}{h} \,. \tag{4.1}$$

The inequality (4.1) requires only that w is continuous and w_z is square integrable. Using (4.1) we obtain

$$\langle |w| C_z \rangle \leqslant \omega_1 \int_{-h/2}^{h/2} \sqrt{\frac{h^2}{4} - z^2} \; C_z \, \frac{\mathrm{d}z}{h} \,, \tag{4.2}$$

where $\omega_1 \equiv \sqrt{\langle w_z^2 \rangle}$. Evaluating the integral in (4.2) using C in (3.2) gives

$$\langle |w| C_z \rangle \leqslant 2\omega_1 \frac{I_1(m/2)}{\sinh(m/2)} \,, \tag{4.3}$$

where I_1 is the modified Bessel function and $m \equiv \mu h$.

Inserting (3.3) and (4.3) into (2.8) gives an inequality valid for all κ and all m:

$$\chi < \frac{2\kappa}{h^2} \left[m \coth\left(\frac{m}{2} \right) + m \tanh\left(\frac{m}{4} \right) + \frac{\omega_1 h^2}{\kappa} \frac{I_1(m/2)}{\sinh(m/2)} \right] . \tag{4.4}$$

If $\kappa / h^2 \omega_1 \ll 1$ then the terms in square brackets on the right-hand side of (4.4), viewed as a function of m, achieves its minimum value at $m = O(\kappa/\omega_1 h^2)^{-2/3}$. In this case one can use asymptotic simplifications to compute the minimum value so that finally

$$\chi < 5.162 \times \kappa^{1/3} \omega_1^{2/3} h^{-2/3} \qquad (\kappa/\omega_1 h^2 \ll 1) \,. \tag{4.5}$$

Since the bound is $O(\kappa^{1/3})$ this is weaker than our earlier $O(\kappa^{1/2})$ estimates.

Now we can rewrite (4.5) in a more useful form by invoking the inequality

$$\left\langle w_z^2 \right\rangle \leqslant \tfrac{1}{4} \langle \| \nabla \boldsymbol{u} \|^2 \rangle \tag{4.6}$$

(Doering & Constantin 1994), where $\| \nabla \boldsymbol{u} \|^2 = u_x^2 + u_y^2 + \cdots + w_z^2$ is the deformation rate. Since the energy dissipation per unit mass is $\varepsilon \equiv \nu \langle \| \nabla \boldsymbol{u} \|^2 \rangle$, where ν is the viscosity, we can write (4.5) in the form

$$\chi \leqslant 3.252 \times \left(\frac{\kappa \varepsilon}{\nu h^2} \right)^{1/3} . \tag{4.7}$$

Thus the scalar cascade rate is bounded in terms of the mechanical energy dissipation rate and the Prandtl number, $Pr = \nu/\kappa$. We can conclude that χ goes to zero with

$\kappa^{1/3}$ only if ε and ν are fixed. But, if ε is finite and Pr is fixed as $\kappa \to 0$, we can only conclude that χ is bounded from above by a constant.

Finally, for the Rayleigh–Bénard configuration, we note that the total flux of T through the layer, F, is given by the average of $-\kappa T_z(x, y, \pm h/2, t)$ over x, y and t. It follows from (2.1) that $F = -h\chi/2$. Hence, all of the bounds on χ in §§ 3 and 4 also apply to the flux. In particular, if $\chi \to$ as $\kappa \to 0$, we conclude that the flux of the scalar into the fluid must likewise vanish. In fact, it is this diffusive limitation of the supply of the scalar at large scales that constrains the cascade.

5. Conclusion

We have placed upper bounds on the scalar cascade rate, χ, in the advection–diffusion problem posed by Zeldovich in 1937. The bounds prove that $\chi \to 0$ as $\kappa \to 0$ for a fixed velocity field, which is contrary to the requirements of the scaling theories of Obukhov, Corrsin and Batchelor. Zeldovich's problem runs counter to these theories because, in the closed vessel, molecular diffusion plays a dual role: κ provides the dissipation at the end of the cascade, but κ is also responsible for 'lifting' T off the walls. Thus, as $\kappa \to 0$, the scalar cannot diffuse away from the boundaries sufficiently quickly to provide a non-zero source of variance; the cascade is diffusion-limited. Many problems discussed previously for passive scalar turbulence escape this predicament since the scalar is introduced by either a volume source, or by advecting the scalar into the domain with fluid inflow (the system is not closed). In our closed system we can also avoid a diffusively limited cascade if the velocity field is not independent of κ in the limit. This is possible if T is an active scalar (such as temperature), or if the Prandtl number is fixed. In those situations, our bound in (4.7) on χ is weaker, so that if the mechanical energy dissipation rate, ε, remains finite in the limit $\kappa \to 0$, then we can only prove that χ is bounded from above by a constant.

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Appendix. The background method

Tighter bounds on χ can be constructed using the Constantin–Doering–Hopf method for the background field (Doering & Constantin 1994). This approach avoids the crudest part of the comparison-function method, namely the replacement of T with its maximal value in $\langle T\boldsymbol{u}\cdot\nabla C\rangle$. Let

$$T(x, y, z, t) = \mathscr{T}(x, y, z) + \theta(x, y, z, t), \tag{A 1}$$

where the time-independent 'background field', $\mathscr{T}$, satisfies the same boundary conditions as T and the unsteady remainder, θ, has homogeneous boundary conditions. Putting (A 1) into (1.1) gives an inhomogeneous advection–diffusion equation for $\theta(\boldsymbol{x}, t)$ from which one can obtain the 'power integral':

$$\kappa\langle|\nabla\theta|^2\rangle + \langle\theta\boldsymbol{u}\cdot\nabla\mathscr{T}\rangle - \kappa\langle\theta\nabla^2\mathscr{T}\rangle = 0\,. \tag{A 2}$$

Also in terms of $\mathscr{T}$ and θ, the entropy-production functional is

$$\chi[\theta] = \kappa\langle|\nabla\mathscr{T}|^2\rangle - 2\kappa\langle\theta\nabla^2\mathscr{T}\rangle + \kappa\langle|\nabla\theta|^2\rangle. \tag{A 3}$$

To find an upper bound on χ, we recast the problem as a variational one and search through the set of functions which satisfy the power integral (A 2) and the homogeneous boundary conditions (this set contains the actual solution and, of course, many other functions). We search systematically by considering the functional,

$$\mathscr{F}[\theta] = \chi[\theta] - b[\kappa\langle|\nabla\theta|^2\rangle + \langle\theta \boldsymbol{u}\cdot\nabla\mathscr{T}\rangle - \kappa\langle\theta\nabla^2\mathscr{T}\rangle], \tag{A 4}$$

where b is a Lagrange multiplier which enforces the power-integral constraint. Thus, if θ_* denotes the function that extremizes $\mathscr{F}$, it must satisfy the Euler–Lagrange equation obtained by functional differentiation of (A 4):

$$\nabla^2\theta_* = \frac{b}{2\kappa(b-1)}\boldsymbol{u}\cdot\nabla\mathscr{T} - \frac{(b-2)}{2(b-1)}\nabla^2\mathscr{T}. \tag{A 5}$$

It follows from (A 5) that

$$\langle|\nabla\theta_*|^2\rangle = -\frac{b}{2\kappa(b-1)}\langle\theta_*\boldsymbol{u}\cdot\nabla\mathscr{T}\rangle + \frac{b-2}{2(b-1)}\langle\theta_*\nabla^2\mathscr{T}\rangle. \tag{A 6}$$

Now we decompose θ into the optimal field plus a deviation: $\theta = \theta_* + \hat{\theta}$. Using (A 5) and (A 6), the functional (A 4) can then be written in the compact form

$$\mathscr{F}[\theta_* + \hat{\theta}] = \kappa\langle|\nabla\mathscr{T}|^2\rangle + \kappa(b-1)\langle|\nabla\theta_*|^2\rangle - \kappa(b-1)\langle|\nabla\hat{\theta}|^2\rangle. \tag{A 7}$$

In other words, provided $b > 1$,

$$\chi = \mathscr{F}[\theta_* + \hat{\theta}] \leqslant \mathscr{F}[\theta_*] = \kappa\langle|\nabla\mathscr{T}|^2\rangle + \kappa(b-1)\langle|\nabla\theta_*|^2\rangle. \tag{A 8}$$

This shows that the functional $\mathscr{F}$, evaluated at a solution of the Euler–Lagrange equation (A 5), is an upper bound on the entropy production, χ. One can now adopt a specific $\boldsymbol{u}$, select a background field, $\mathscr{T}$, and solve (A 5) for θ_*. The strongest upper bound on χ is then given by optimizing $\mathscr{F}[\theta_*]$ with respect to b, and any further parameters in $\mathscr{T}$.

We can execute this program using the flow field (3.1) from § 3. We take the background field, $\mathscr{T}$, to be the comparison function in (3.2). We solve the Euler–Lagrange equation (A 5) exactly and we discover that the optimal choice is $b = 2$. The optimal solution is

$$\theta_* = 2\pi\,\frac{\phi\cos(X/h)m^2}{\kappa\Lambda\sinh(m/2)}\left[\frac{\sinh(m/2)\cosh(z/h)}{\cosh(1/2)} - \sinh(mz/h)\sin(\pi z/h) - \frac{m^2-\pi^2-1}{2\pi m}\cosh(mz/h)\cos(\pi z/h)\right], \tag{A 9}$$

where $m \equiv \mu h$ and $\Lambda(m) \equiv (m^2+\pi^2)^2 + 1 - 2m^2 + 2\pi^2$. Then, after some algebra,

$$\chi \leqslant \frac{\kappa m(m+\sinh m)}{h^2(\cosh m - 1)} + \frac{2\phi^2\pi^2 m^3}{\kappa h^2\Lambda(\cosh m-1)}\left\{\frac{\sinh(m/2)}{\cosh(1/2)}\left[\frac{\cosh(m+1)/2}{\pi^2+(m+1)^2} + \frac{\cosh(m-1)/2}{\pi^2+(m-1)^2}\right] - \frac{\sinh m}{4(m^2+\pi^2)} - \frac{m^2-\pi^2-1}{8\pi^2 m}\left[1+\frac{\pi^2\sinh m}{m(m^2+\pi^2)}\right]\right\}. \tag{A 10}$$

The final step is to minimize the right-hand side of (A 10) by finding the optimal value of m for each κ. The resulting bound is shown as the solid curve in figure 3.

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