# The effective diffusivity of cellular flows

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## 1 Advection-diffusion by cellular flows

In the previous chapter we dealt with unidirectional flows. Now we turn to the slightly more complicated case of incompressible two-dimensional cellular flows. The velocity field can be obtained from a streamfunction $\psi(x, y)$ according to our usual convention $\boldsymbol{u} = (u, v) = (-\psi_y, \psi_x)$. The domain is a periodic array of square cells, each with side $\ell$, so that the streamfunction has the periodicity $\psi(x + m\ell, y + n\ell) = \psi(x, y)$ where $m$ and $n$ are integers. We use the notation

$$\langle\theta\rangle \equiv \ell^{-2} \int_{\mathcal{S}} \theta \, \mathrm{d}^2\boldsymbol{x}, \tag{1}$$

to denote an average over an $\ell \times \ell$ square $\mathcal{S}$. We are assuming that the average of the flow over a cell vanishes, i.e., $\langle \boldsymbol{u} \rangle = 0$. The cell-average $\langle\rangle$ will play a role analogous to the cross-channel average of the previous sections. Thus we will be concerned with the 'large-scale' transport of passive tracer where 'large-scale' means a length which is much greater than the cell size $\ell$. The cell average is used to isolate the slowly varying part of the concentration.

As a illustrative example, start with the steady state advection-diffusion equation

$$J(\psi, c) = \kappa \nabla^2 c \,, \tag{2}$$

where $J(a, b) \equiv a_x b_y - a_y c_x$ is the Jacobian and $\kappa$ is the molecular diffusivity of the tracer. Following Childress (1979), Moffatt (1983) and many others we will use the prototypical example $\psi = \psi_{\max} \cos(kx) \cos(ky)$ where $k = 2\pi/\ell$ (see the left hand panel of figure 1).

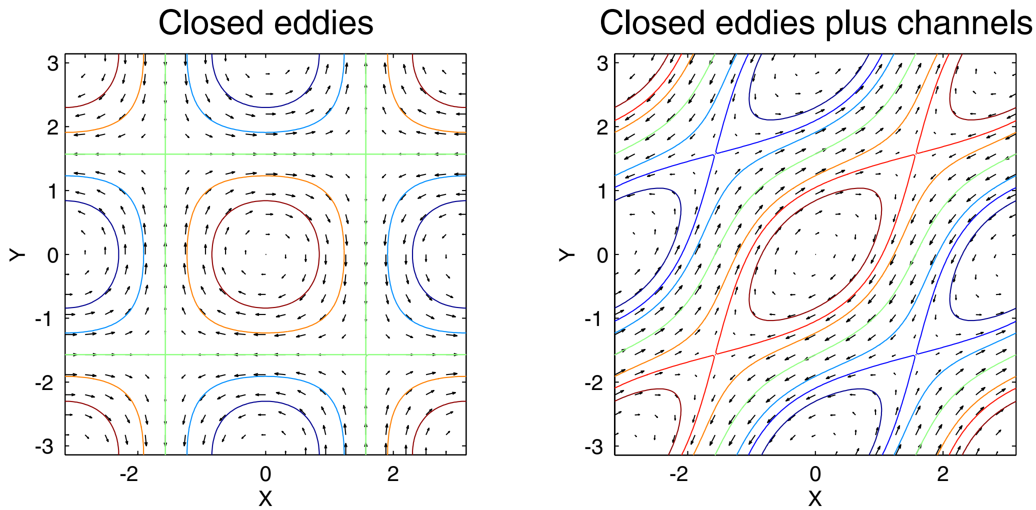


Figure 1: Examples of cellular flows. In left hand panel there are closed cells and large scale transport of tracer can only occur as a result of molecular diffusion. In this figure the cell size is $\ell = 2\pi$.

If we release some tracer into a steady cellular flow does the blob spread diffusively? Without molecular diffusivity ($\kappa = 0$) the answer is clearly 'no'. Each tracer particle will stay on its initial streamline, and if that streamline is closed then there can be no large-scale transport. But, with even very weak molecular diffusivity, molecules of tracer are not confined to streamlines and indeed there is an effective diffusivity characterizing large-scale transport. Instead of considering the initial value problem we can obtain the effective diffusivity using the $Gx$-trick. That is, we suppose that a large scale uniform gradient $\boldsymbol{G}$ is externally imposed and we then proceed to calculate the flux $\boldsymbol{F}$ which is associated with $\boldsymbol{G}$. This procedure enables us to bypass the initial value problem and deal with a simpler *steady state* problem.

Suppose that the system is in a big box containing $N \times N$ cells i.e. the box is a $N\ell \times N\ell$ square. On the wall at $x = 0$ we impose the boundary condition $c(0, y) = 0$ and on the wall at $x = N\ell$, we impose $c(N\ell, y) = GN\ell$. Further, suppose that there is no flux of $c$ through the boundaries at $y = 0$ and $y = N\ell$. If there is no advection ($\psi_{\max} = 0$) then the solution of (2) with these boundary conditions is $c = Gx$. the flux associated with this $\psi = 0$ solution is $F_0 = -\kappa G$.

Now consider the general case with $\psi_{\max} \neq 0$. Integrating (2) from $y = 0$

to $y = N\ell$ we find that

$$F = \frac{1}{N\ell} \int_0^{N\ell} uc - \kappa c_x \mathrm{d}y \tag{3}$$

is constant. $F$ is the *flux* which is passing from the high-$c$ source at $x = N\ell$ to the low-$c$ sink at $x = 0$. Our goal is determine $F$ in terms of imposed gradient $G$ and parameters such as the Péclet number

$$p \equiv \psi_{\max}/\kappa\,. \tag{4}$$

The Péclet number measures the stength of advection relative to diffusion; when $p$ is small the diffusive solution $c = Gx$ is only slightly distorted by advection.

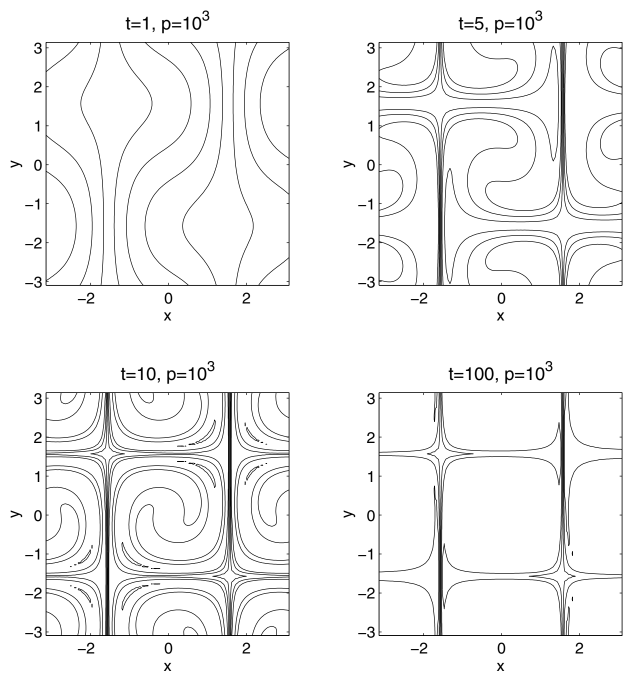


Figure 2: Steady concentration field, $x + c'(x, y)$, obtained numerically using $\psi = \psi_{\max} \cos kx \cos ky$, and various values of the Péclet number, $p = \psi_{\max}/\kappa$. (Thanks to Raffaele Ferrari.)

The first step is to make a simple substitution

$$c = Gx + c'(x, y)\,, \tag{5}$$

which separates $c$ into the large-scale uniform gradient and a flow-induced perturbation $c'$. Throwing (5) into (2) we obtain

$$J(\psi, c') - \kappa\nabla^2 c' = -Gu\,. \tag{6}$$

Once we have solved (6) we get $F$ by evaluating the integral in (3).

It is impossible to solve (6) exactly so instead we rely on a combination of numerical solution and analysis of the limits $p \ll 1$ and $p \gg 1$. Figure 2 shows the solution of (6) with $G = 1$ and four different Péclet numbers. The case with $p = 1$ shows that $c$ is distorted only slightly away from the diffusive solution $c = x$. When $p$ is large the solution exemplifies the Prandtl-Batchelor limit in which all of the variation in $c$ is compressed into thin layers at the eddy boundaries. Figure 3 shows how this boundary layer solution is established in an intial value problem starting with $c(x, y, 0) = x$.

The $p \ll 1$ case (weak advection) is particularly simple because to leading order we neglect the Jacobian on the left hand side of (6) and, since $u = k\psi_{\max}\cos(kx)\sin(ky)$, we quickly obtain

$$c' \approx -\left[\frac{\psi_{\max}}{2k\kappa}\cos kx \sin ky\right] G\,. \tag{7}$$

With $c'$ in hand, the final step is to calculate $F$ by evaluating the integral in (3). Because $F$ is a constant we can make this evaluation at any $x$ and get the same result. Alternatively, we can average over a cell to obtain

$$F = -\kappa G + \langle uc' \rangle\,, \tag{8}$$

or, using (7),

$$F \approx -\left[\kappa + \frac{\psi_{\max}^2}{8\kappa}\right] G\,. \tag{9}$$

The effect of weak advection ($p \ll 1$) is to slightly enhance the transfer of $c$.

It is convenient to describe the transport properties of a flow using nondimensional variables. The Nusselt number is the ratio

$$\mathrm{Nu} \equiv \frac{F}{F_0}\,, \tag{10}$$

where $F_0 = -\kappa G$ is the diffusive flux which occurs if $\psi_{\max} = 0$. For instance, from (9),

$$\mathrm{Nu} = 1 + \frac{p^2}{8} + O(p^4)\,, \tag{11}$$

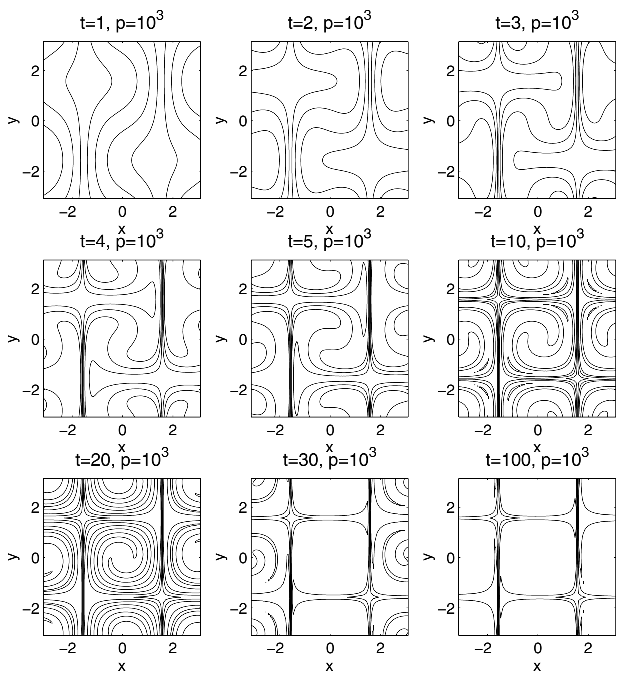


Figure 3: Unsteady concentration field obtained numerically using $\psi = \psi_{\max} \cos kx \cos ky$ with $p \equiv \psi_{\max}/\kappa = 1000$. The initial condition is $c(x, y, 0) = x$. The concentration within an eddy becomes uniform as $t \to \infty$. (Thanks to Raffaele Ferrari.)

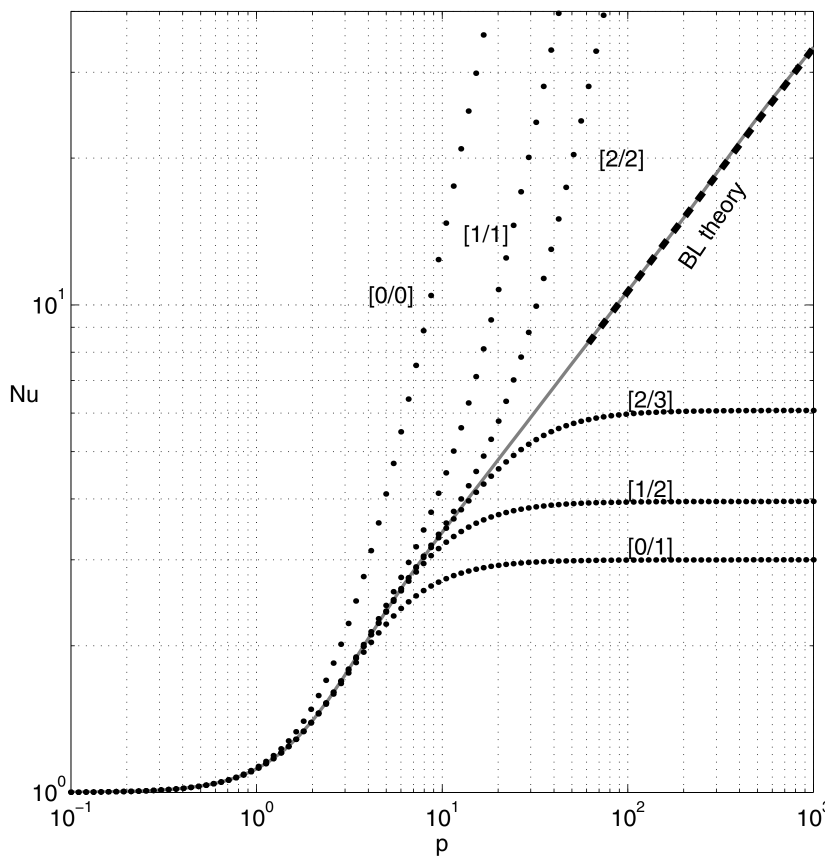


Figure 4: The Nusselt number defined in (10) as a function of Péclet number $p$. The solid curve is the result of a $128 \times 128$ spectral solution of (2). The dotted curve labelled [0/0] is the result in (11) and [0/1] is the result in (47) ; the other dotted curves labelled [1/1], [1/2] etcetera are the Padé sums discussed in section 3. The dashed line denoted "BL theory" is the prediction (12) which is based on the boundary layer theory of section 5. (Figure courtesy of Raffaele Ferrari and Aldo Manfroi.)

where the $O(p^4)$ anticipates some later results in this lecture by indicating the higher order corrections.

The solid curve in figure 4 is a numerical calculation of $Nu(p)$ in the range $0.1 < p < 1000$ and the dashed curve labelled [0/0] is the small $p$ approximation in (11). The dashed line in figure 4, labelled "BL theory", is the prediction of a large-$p$ theory, namely

$$\mathrm{Nu} \sim 1.0655 p^{1/2} \,. \tag{12}$$

The asymptotic prediction (12) is the subject of section 5 and problem 1.1.

*Problem 1.1.* Using dimensional variables the large-$p$ result in (12) imples an effective diffusivity $D_{\text{eff}} \sim \sqrt{\kappa\psi_{\max}}$. Give a physically motivated scaling argument for this result.

*Solution.* Denote the boundary layer thickness in figure 2 by $\delta$. The jump in $c$ between two adjacent cells is $\Delta c \sim G\ell$ and since all of this varaition occurs in the boundary layer, the flux is

$$F \sim \kappa \frac{\Delta c}{\delta} \,. \tag{13}$$

To determine $\delta$, we argue that in the neighbourhood of the eddy boundary boundary the dominant balance in the advection diffusion equation is

$$-Xv'(Y)c_X + v(Y)c_Y = \kappa c_{XX} \,, \tag{14}$$

where the capitals denote local coordinates and $v(Y) = k\psi_{\max} \sin kY$. With $\partial_X \sim \delta^{-1}$ and $\partial_y \sim k \sim \ell^{-1}$ (14) implies a balance

$$k^2 \psi_{\max} \sim \kappa \delta^{-2} \quad \text{or} \quad \delta \sim \sqrt{\frac{\kappa}{\psi_{\max}}} \ell \,. \tag{15}$$

Putting (15) into (13) gives $F \sim \sqrt{\kappa\psi_{\max}} G$, or $D_{\text{eff}} \sim \sqrt{\kappa\psi_{\max}}$.

We can interpret the effective diffusivity $\sqrt{\kappa\psi_{\max}}$ as

$$D_{\text{eff}} = \ell \times k\psi_{\max} \times \frac{\delta}{\ell} \,. \tag{16}$$

The first factor $\ell$ on the RHS is the mixing length and the second, $k\psi_{\max}$, is the eddy velocity. The third factor is the fraction of "active" particles, meaning particles in the boundary layers.

# 2 The fundamental problem

Because (2) is linear, there must be a linear relation between the large scale concentration gradient, $\boldsymbol{G}$, and the flux $\boldsymbol{F}$. In other words, we anticipate that

$$\boldsymbol{F} = -\boldsymbol{K}\boldsymbol{G}. \tag{17}$$

where $\boldsymbol{K}$ is $2 \times 2$ diffusion tensor. One of our goals is to calculate $\boldsymbol{K}$ for a few simple cellular flows.

If $\boldsymbol{G}$ is not uniform then we should regard (17) as simply the first term in an expansion of the form $F_i = -K_{ij}G_j + L_{ijk}G_{j,k} + \cdots$ We will not trouble with higher order terms such as $L_{ijk}$ — obtaining the leading-order effect contained in $\boldsymbol{K}$ is our main goal.

The advection-diffusion equation (2) has a solution of the form

$$c(x, y, t) = \boldsymbol{G}\cdot\boldsymbol{x} + c'(x, y), \tag{18}$$

where $c'$, like $\psi$, is a cellular function. The first term on the RHS of (18) is the externally imposed, large-scale gradient; the second term $c'$ is the small-scale distortion created by the velocity $\boldsymbol{u}$ advecting the large-scale field $\boldsymbol{G}\cdot\boldsymbol{x}$.

Substituting (18) into (2) we obtain

$$\boldsymbol{u}\cdot\nabla c' - \kappa\nabla^2 c' = -uG_x - vG_y, \tag{19}$$

where $\boldsymbol{G} \equiv (G_x, G_y)$ is a constant vector. Because (19) is a linear equation it must be that

$$c' = -aG_x - bG_y, \tag{20}$$

where the cellular function $\boldsymbol{a} \equiv [a(x, y), b(x, y)]$ is determined by solving the *fundamental problem*:

$$\mathcal{L} \equiv \boldsymbol{u}\cdot\nabla - \kappa\nabla^2, \qquad \mathcal{L}\boldsymbol{a} = \boldsymbol{u}. \tag{21}$$

Simple prescriptions for $\boldsymbol{u}$ will often have symmetries which will enable us to deduce the solution of for $b$ from the solution for $a$, and vice-versa (examples follow).

The total flux is calculated using

$$\boldsymbol{F} \equiv \langle \boldsymbol{u}c - \kappa\nabla c\rangle = -\kappa\boldsymbol{G} + \langle \boldsymbol{u}c\rangle, \tag{22}$$

Solving the fundamental problem and constructing $c$ as a linear combination of $a$ and $b$ then gives

$$\begin{pmatrix} F_x \\ F_y \end{pmatrix} = -\begin{bmatrix} \kappa + \langle ua\rangle & \langle ub\rangle \\ \langle va\rangle & \kappa + \langle vb\rangle \end{bmatrix} \begin{pmatrix} G_x \\ G_y \end{pmatrix}. \tag{23}$$

The $2 \times 2$ matrix above is the effective diffusion tensor $\boldsymbol{K}$.

## Quadratic integrals

From (21) one can show using integration by parts that

$$\kappa\langle\nabla a\cdot\nabla a\rangle=\langle ua\rangle,\qquad \kappa\langle\nabla b\cdot\nabla b\rangle=\langle vb\rangle, \tag{24}$$

and

$$\langle\psi J(a,b)\rangle+\kappa\langle\nabla a\cdot\nabla b\rangle=\langle ub\rangle,\quad -\langle\psi J(a,b)\rangle+\kappa\langle\nabla a\cdot\nabla b\rangle=\langle va\rangle. \tag{25}$$

Using these quadratic integrals the symmetric and antisymmetric parts of $\boldsymbol{K}$ can then be written as

$$\boldsymbol{K}^{(s)}=\begin{bmatrix}\kappa+\kappa\langle\nabla a\cdot\nabla a\rangle & \kappa\langle\nabla a\cdot\nabla b\rangle\\ \kappa\langle\nabla a\cdot\nabla b\rangle & \kappa+\kappa\langle\nabla b\cdot\nabla b\rangle\end{bmatrix}, \tag{26}$$

and

$$\boldsymbol{K}^{(a)}=\begin{bmatrix}0 & \langle\psi J(a,b)\rangle\\ -\langle\psi J(a,b)\rangle & 0\end{bmatrix}. \tag{27}$$

With the Cauchy-Schwarz inequality, one can show that the matrix $\boldsymbol{K}^{(s)}$ is positive definite.

The antisymmetric part of $\boldsymbol{K}$ is equivalent to advection. To see what is meant by this, let $\phi\equiv-\langle\psi J(a,b)\rangle$ and $\boldsymbol{u}_\phi\equiv(-\phi_y,\phi_x)$. In a slowly varying situtation the averaged concentration evolves according to

$$\langle c\rangle_t=\nabla\cdot\boldsymbol{K}\nabla\langle c\rangle\,. \tag{28}$$

Using the decomposition $\boldsymbol{K}=\boldsymbol{K}^{(s)}+\boldsymbol{K}^{(a)}$, (28) can be rewritten as

$$\langle c\rangle_t+\boldsymbol{u}_\phi\cdot\nabla\langle c\rangle=\nabla\cdot\boldsymbol{K}^{(s)}\nabla\langle c\rangle\,. \tag{29}$$

Thus, the antisymmetric part of the diffusion tensor is equivalent to advection with a velocity $\boldsymbol{u}_\phi$.

*Problem 2.1.* Prove that if $a$, $b$ and $c$ are cellular functions then $\langle a\nabla^2 b\rangle=-\langle\nabla a\cdot\nabla b\rangle$ and $\langle aJ(b,c)\rangle=\langle cJ(a,b)\rangle=\langle bJ(c,a)\rangle$. Use these results to obtain (40) and (41). Prove that $\langle\nabla\psi\cdot\nabla a\rangle=\langle\nabla\psi\cdot\nabla b\rangle=0$.

*Problem 2.2.* How does the effective diffusion tensor $\boldsymbol{K}$ change if we flip the sign of the velocity $\boldsymbol{u}$?

*Solution.* Consider the differential operators:

$$\mathcal{L} \equiv \boldsymbol{u}\cdot\nabla - \kappa\nabla^2, \qquad \text{and} \qquad \mathcal{L}^\dagger \equiv -\boldsymbol{u}\cdot\nabla - \kappa\nabla^2. \tag{30}$$

$\mathcal{L}^\dagger$ is the differential adjoint of $\mathcal{L}$, and $\mathcal{L}^\dagger$ is also the operator associated with $\boldsymbol{u}^\dagger \equiv -\boldsymbol{u}$. In addition to the vector $\boldsymbol{a} = (a, b)$, we introduce $\boldsymbol{a}^\dagger = (a^\dagger, b^\dagger)$ defined as the solution of the †-problem. In other words,

$$\mathcal{L}\boldsymbol{a} = \boldsymbol{u}, \qquad \text{and} \qquad \mathcal{L}^\dagger\boldsymbol{a}^\dagger = -\boldsymbol{u}\,. \tag{31}$$

The flux-gradient relationship of the †-problem:

$$\begin{pmatrix} F_x^\dagger \\ F_y^\dagger \end{pmatrix} = -\begin{bmatrix} \kappa - \langle ua^\dagger\rangle & -\langle ub^\dagger\rangle \\ -\langle va^\dagger\rangle & \kappa + \langle -vb^\dagger\rangle \end{bmatrix} \begin{pmatrix} G_x \\ G_y \end{pmatrix}. \tag{32}$$

The $2 \times 2$ matrix above is the diffusion tensor of the reversed flow, $\boldsymbol{K}^\dagger$.

With assiduous integration by parts one can prove the identities:

$$\langle\theta\mathcal{L}\phi\rangle = \langle\phi\mathcal{L}^\dagger\theta\rangle \qquad \text{and} \qquad \langle\theta\mathcal{L}\theta\rangle = \langle\theta\mathcal{L}^\dagger\theta\rangle = \kappa\langle\nabla\theta\cdot\nabla\theta\rangle\,. \tag{33}$$

The identities above can be used to relate the terms in $\boldsymbol{K}^\dagger$ to those in $\boldsymbol{K}$. For example, consider $\langle a^\dagger u^\dagger\rangle = -\langle a^\dagger u\rangle$. Then $\langle a^\dagger u\rangle = \langle a^\dagger\mathcal{L}a\rangle = \langle a\mathcal{L}^\dagger a^\dagger\rangle = -\langle au\rangle$. In this fashion, working through the four different terms in $\boldsymbol{K}^\dagger$, we find that

$$\boldsymbol{K} = \boldsymbol{K}^{\dagger\mathrm{T}}, \tag{34}$$

where T denotes "transpose". Equation (34) shows that daggering undoes transposition.

*Problem 2.3.* A flow is said to be mirror symmetric if either $\psi(x,y) = -\psi(-x,y)$ or $\psi(x,y) = -\psi(x,-y)$. Prove that the diffusion tensor of a mirror symmetric flow is symmetric.

*Solution.* For mirror-symmetric flows the sign of $\boldsymbol{u}$ is an accident of the choice of the coordinate system. Consequently, using the notation of the previous problem, $\boldsymbol{K} = \boldsymbol{K}^\dagger$. Invoking (34) we conclude that $\boldsymbol{K} = \boldsymbol{K}^{\mathrm{T}}$.

*Problem 2.4.* Prove that if $\psi$ is mirror symmetric, and if the line of symmetry is taken to be a coordinate axis, then $\boldsymbol{K}$ is a diagonal tensor.

*Problem 2.5.* A flow is said to be parity invariant in $x$ if $\psi(x,y) = \psi(-x,y)$ and parity invariant in $y$ if $\psi(x,y) = \psi(x,-y)$. Show that if a flow has parity invariance in either $x$ or $y$ then $\langle ub\rangle = -\langle va\rangle$.

*Solution.* Suppose that the parity invariance is in $x$ so that

$$\psi(x,y) = \psi(-x,y) \quad \Rightarrow \quad a(x,y) = -a^\dagger(-x,y), \quad b(x,y) = b^\dagger(-x,y)\,. \tag{35}$$

Then:

$$\begin{aligned} \langle u(x,y)b(x,y)\rangle &= \langle u(-x,y)b(-x,y)\rangle, \\ &= \langle u(x,y)b^\dagger(x,y)\rangle, \quad \text{(parity invariance in } x) \\ &= -\langle v(x,y)a(x,y)\rangle, \quad (\ \boldsymbol{K} = \boldsymbol{K}^{\dagger\mathrm{T}}). \end{aligned} \tag{36}$$

*Problem 2.6.* Suppose that $\psi(x,y) = \psi(y,x)$. Prove that $\langle ua\rangle = \langle vb\rangle$.

# 3 The diffusive limit: $p \ll 1$.

The fundamental problem (21) can be nondimensionalized with

$$\hat{\boldsymbol{x}} \equiv (2\pi/\ell)\boldsymbol{x}\,, \quad \psi = \psi_{\max}\hat{\psi}\,, \quad \hat{\boldsymbol{a}} \equiv (2\pi/p\ell)\boldsymbol{a}\,, \quad \boldsymbol{K} = \kappa\hat{\boldsymbol{K}}\,. \tag{37}$$

In these nondimensional variables the cell size is $2\pi \times 2\pi$ and the diffusion tensor is

$$\hat{\boldsymbol{K}} = \begin{bmatrix} 1 + p^2\langle \hat{u}\hat{a}\rangle & p^2\langle \hat{u}\hat{b}\rangle \\ p^2\langle \hat{v}\hat{a}\rangle & 1 + p^2\langle \hat{v}\hat{b}\rangle \end{bmatrix}, \tag{38}$$

where $p \equiv \psi_{\max}/\kappa$ is Péclet number.

Dropping the decoration on the nondimensional variables, the fundamental problem is

$$\nabla^2 \boldsymbol{a} = -\boldsymbol{u} + pJ(\psi, \boldsymbol{a})\,. \tag{39}$$

and the nondimensional symmetric and antisymmetric parts of $\boldsymbol{K}$ are

$$\boldsymbol{K}^{(s)} = \begin{bmatrix} 1 + p^2\langle \nabla a \cdot \nabla a\rangle & p^2\langle \nabla a \cdot \nabla b\rangle \\ p^2\langle \nabla a \cdot \nabla b\rangle & 1 + p^2\langle \nabla b \cdot \nabla b\rangle \end{bmatrix}, \tag{40}$$

and

$$\boldsymbol{K}^{(a)} = p^3 \begin{bmatrix} 0 & \langle \psi J(a,b)\rangle \\ -\langle \psi J(a,b)\rangle & 0 \end{bmatrix}. \tag{41}$$

If $p \ll 1$ is small we can solve (39) iteratively and explicitly calculate $\boldsymbol{K}$. Specifically, the expansion $\boldsymbol{a} = \boldsymbol{a}_0 + p\boldsymbol{a}_1 + \cdots$ leads to

$$\nabla^2 \boldsymbol{a}_0 = -\boldsymbol{u}, \qquad \nabla^2 \boldsymbol{a}_n = J(\psi, \boldsymbol{a}_{n-1}) \quad (n \geq 1). \tag{42}$$

Examples of the algebra are given in the problems at the end of this section.

These perturbation expansions result in power series representations of $\boldsymbol{K}$. For example, with $\psi = \sin x \sin y$, there are so many symmetries that $\boldsymbol{K} = \mathrm{Nu}\boldsymbol{I}$ where $\boldsymbol{I}$ is the identity matrix and Nu is the Nusselt number defined in (10). From (57), $\mathrm{Nu}(p)$ has the expansion

$$\mathrm{Nu}(p) = 1 + 2q\left[1 - q + \frac{6}{5}q^2 - \frac{381}{250}q^3 + O(p^8)\right], \tag{43}$$

where $q \equiv (p/4)^2$. How can we extract maximum information from this hard-won series? The answer is Padé summation.

The philosophy is that the radius of convergence of the series in (43) is limited by a singularity in the complex-$q$ plane. For instance, consider

$$\frac{1}{1+q} = 1 - q + q^2 + \cdots \tag{44}$$

The function on the left hand side has a pole at $q = -1$ and consequently the series on the right hand side does not converge if $|q| > 1$. In fact, the series in the square bracket on the right hand side of (43) slightly resembles (44), and this suggests that (43) is a convergence-limiting singularity somewhere near $q = -1$. Following this heuristic argument we "resum" the terms within the square bracket in (43) using (44):

$$\mathrm{Nu}(p) = 1 + 2q \left[\frac{1}{1+q}\right] + O(p^6)\,. \tag{45}$$

We refer to the result above as a "[0/1]" Padé approximant because the rational function in the square bracket has a polynomial of order zero upstairs and a polynomial of order one downstairs. This approximation is dotted curve labelled [0/1] in figure 4. Our expectation is that the rational approximations, such as (45), have a greater range of validity than the naked series in (43). Comparison with the numerical solution gratifyingly affirms this hope.

We improve on (45) by matching more terms in the series (43). Thus, we expand a more general rational function, with three undetermined coefficients,

$$\begin{aligned} \frac{1+aq}{1+bq+cq^2} = {} & 1 + (a-b)q + (b^2 - ab - c)q^2 \\ & + \left[c(b-a) + b(c + ab - b^2)\right] q^3 + O(q^4)\,. \end{aligned} \tag{46}$$

Matching up terms in (46) with the series in (43) then gives

$$\mathrm{Nu}(p) = 1 + 2q \left[\frac{50 + 31q}{50 + 81q + 21q^2}\right] + O\left(p^{10}\right)\,. \tag{47}$$

This is a [1/2]-approximant because the numerator is a first order polynomial and the denominator is second order. Figure 4 also shows two higher order Padé approximants, [2/2] and [2/3]. Using Padé approximants of fairly modest order we have obtained pretty accurate results to beyod $p = 10$ using a $p \ll 1$ expansion.

The denominator in (47) has zeros at $p = \pm 4\sqrt{16/21}\mathrm{i}$ and $\pm 4\sqrt{65/21}\mathrm{i}$. This suggests that $\mathrm{Nu}(p)$, viewed as a function of complex-$p$, has pole singularities close to these same points. Padé summation is rolling over the convergence problems presented by the poles of $\mathrm{Nu}(p)$ by using rational functions as approximants. Ineed, if we could *prove* that the only singularities of $\mathrm{Nu}(p)$ are poles then we would have a compelling motivation for trusting extrapolation based on Padé summation. Figure 4 shows how successively higher order Padé approximants provide alternately upper and lower bounds on the exact answer. Thus in this particular problem Padé summation is a potent computational tool.

These observations suggest two problems. First, can we systematically obtain more terms in the series (43), and obtain higher order Padé approximants (see Baker & Graves-Morris, 1996)? Following this route we can obtain even more accurate approximations of $\boldsymbol{K}(p)$ and accumulate more evidence as to the nature of the singularities in the $p$-plane. Second, instead of gropping in the dark, what can we prove about the analytic structure of $\boldsymbol{K}(p)$ (see Avellenda & Majda 1991)?

*Problem 3.1.* Prove that the diagonal terms of $\boldsymbol{K}^{(s)}$ in (40) are given perturbatively by

$$\langle \nabla f \cdot \nabla f \rangle = \langle \nabla f_0 \cdot \nabla f_0 \rangle - p^2 \langle \nabla f_1 \cdot \nabla f_1 \rangle + p^4 \langle \nabla f_2 \cdot \nabla f_2 \rangle + \cdots \tag{48}$$

where $f$ is either $a$ or $b$. Show that the off-diagonal terms of $\boldsymbol{K}^{(s)}$ are

$$\langle \nabla a \cdot \nabla b \rangle = \langle \nabla a_0 \cdot \nabla b_0 \rangle - p^2 \langle \nabla a_1 \cdot \nabla b_1 \rangle + p^4 \langle \nabla a_2 \cdot \nabla b_2 \rangle + \cdots \tag{49}$$

*Solution.* Taking $\langle a_m \text{ (42)} \rangle$ and integrtating by parts gives

$$\langle \nabla f_m \cdot \nabla g_n \rangle = -\langle \nabla f_{m+1} \cdot \nabla g_{n-1} \rangle = -\langle \nabla f_{m-1} \cdot \nabla g_{n+1} \rangle, \tag{50}$$

where $f$ and $g$ are either $a$ or $b$. With $f = g = a$, repeatedly applying identity (50) shows that

$$\begin{aligned} m-n \text{ odd:} \quad & \langle \nabla a_m \cdot \nabla a_n \rangle = 0, \\ m-n \text{ even:} \quad & \langle \nabla a_m \cdot \nabla a_n \rangle = (-1)^{(m-n)/2} \langle \nabla a_{(m+n)/2} \cdot \nabla a_{(m+n)/2} \rangle \,. \end{aligned} \tag{51}$$

Substituting $a = a_0 + p a_1 + \cdots$ into $\langle \nabla a \cdot \nabla a \rangle$ and invoking (51), the sums collapse so that

$$\langle \nabla a \cdot \nabla a \rangle = \langle \nabla a_0 \cdot \nabla a_0 \rangle - p^2 \langle \nabla a_1 \cdot \nabla a_1 \rangle + p^4 \langle \nabla a_2 \cdot \nabla a_2 \rangle + \cdots \tag{52}$$

There is an analogous identity for $\langle \nabla b \cdot \nabla b \rangle$.

Similar manipulations, with $f = a$ and $g = b$ in (50), give

$$\langle \nabla a \cdot \nabla b \rangle = \langle \nabla a_0 \cdot \nabla b_0 \rangle - p^2 \langle \nabla a_1 \cdot \nabla b_1 \rangle + p^4 \langle \nabla a_2 \cdot \nabla b_2 \rangle + \cdots \tag{53}$$

Using (52) and (53) one can deduce higher order terms in the expansion of $\boldsymbol{K}^{(s)}$ from lower order terms in the expansion of $a$ and $b$. This trick saves a lot of calculation in the next examples.

*Problem 3.2.* The antisymmetric part of the diffusion tensor, $\boldsymbol{K}^{(a)}$ in (41) contains only one element; show that this element is given perturbatively by

$$\langle \psi J(a,b) \rangle = \langle \nabla a_0 \cdot \nabla b_1 \rangle - p^2 \langle \nabla a_1 \cdot \nabla b_2 \rangle + p^4 \langle \nabla a_2 \cdot \nabla b_3 \rangle + \cdots \tag{54}$$

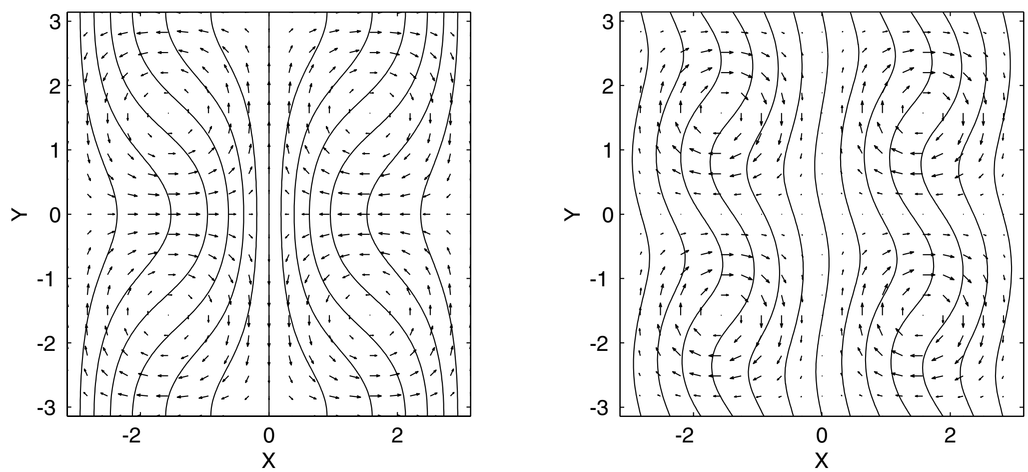


Figure 5: Concentration field obtained using the $p \ll 1$ expansion with $p = 2$. Left hand panel shows $\psi = \sin x \sin y$ and the right hand panel shows $\psi = \sin^2 x \sin^2 y$.

*Problem 3.3.* Consider the streamfunction $\psi = \sin x \sin y$ (see figure 5). Find a few terms in the small-$p$ expansion of $\boldsymbol{K}$.

*Solution.* Because of the mirror symmetry of $\psi$, $\langle au \rangle = \langle bv \rangle$ and $\langle av \rangle = \langle bu \rangle = 0$ so that $\boldsymbol{K}$ is isotropic. From (42) we find

$$a_0 = -\frac{1}{2}\sin x \cos y, \qquad a_1 = -\frac{1}{16}\sin 2x, \qquad a_2 = -\frac{1}{16}a_0 - \frac{1}{160}\sin 3x \cos y, \tag{55}$$

and

$$a_3 = \frac{3}{640}\sin 2x - \frac{1}{2560}\sin 4x + \frac{1}{1280}\sin 2x \cos 2y - \frac{1}{6400}\sin 4x \cos 2y. \tag{56}$$

Invoking the identity (52) we get

$$\langle ua \rangle = \frac{1}{8} - \frac{p^2}{128} + \frac{3p^4}{5120} - \frac{381p^6}{500 \times 2^{14}} + O(p^8). \tag{57}$$

*Problem 3.4.* Consider the streamfunction $\psi = \sin^2 x \sin^2 y$ (see figure 5). Find a few terms in the small-$p$ expansion of $\boldsymbol{K}$.

*Solution.* Because all the eddies rotate the same way, the mirror symmetry is broken. However, because of parity invariance in either $x$ or $y$, we can conclude that $\langle vb \rangle = \langle ua \rangle$ and $\langle ub \rangle = -\langle va \rangle$. From (52) we find that

$$a_0 = -\frac{1}{8}\sin 2y + \frac{1}{16}\cos 2x \sin 2y\,, \tag{58}$$

and

$$\begin{aligned} a_1 = -\frac{3}{128}\sin 2x + \frac{1}{512}\sin 4x + \frac{1}{64}\sin 2x \cos 2y \\ - \frac{1}{640}\sin 4x \cos 2y - \frac{1}{640}\sin 2x \cos 4y\,. \end{aligned} \tag{59}$$

The higher order terms become increasingly cumbersome. Using the identity (52) we have

$$\begin{aligned} \langle ua \rangle &= \frac{5}{128} - \frac{269p^2}{163840} + \frac{505021p^4}{6815744000} - \frac{337081764493p^6}{100257958461440000} + O(p^8)\,, \\ &= 0.0391 - 0.0263q + 0.0190q^2 - 0.0138q^3 + O(p^8)\,, \end{aligned} \tag{60}$$

where we have approximated the coefficients at the fourth decimal digit and used $q \equiv (p/4)^2$. Using (**??**) we find

$$\langle va \rangle = -\frac{p}{128} + \frac{57p^3}{163840} - \frac{53743p^5}{3407872000} + \frac{14358445251p^7}{20051591692288000} + O(p^9)\,. \tag{61}$$

*Problem 3.5.* Consider the streamfunction $\psi = \sin x \sin y + \mu \cos x \cos y$. Calculate a few term in the small-$p$ expansion of the $\boldsymbol{K}$.

*Solution.* Using symmetry arguments $\langle au \rangle = \langle bv \rangle$ and $\langle av \rangle = \langle bu \rangle$. Explicit calculation from (42) gives

$$a_0 = -\frac{1}{2}\sin x \cos y + \frac{1}{2}\mu \cos x \sin y, \qquad a_1 = -\frac{1}{16}\sin 2x + \frac{1}{16}\mu^2 \sin 2x, \ldots \tag{62}$$

Using (52) we then have

$$\begin{aligned} \langle ua \rangle \;&=\; \frac{1}{8}\left(1+\mu^2\right) - \frac{1}{128}\left(1-\mu^2\right)^2 p^2 + \frac{3}{5120}\left(1+\mu^2\right)\left(1-\mu^2\right)^2 p^4 \\ &-\; \frac{3}{8192000}\left(127 + 562\mu^2 + 127\mu^4\right)\left(1-\mu^2\right)^2 p^6 + O(p^8), \end{aligned} \tag{63}$$

and

$$\langle ub \rangle = \frac{\mu}{4} - \frac{\mu}{1024}\left(1-\mu^2\right)^2 p^4 + O(p^4). \tag{64}$$

# 4 Mathematical stuff?

To justify Padé summation we must understand the singularity structure of $\boldsymbol{K}(p)$. We give a gentleman's account, beginning with a folk theorem that the spectrum of $\mathcal{L} \equiv pJ(\psi, ) - \nabla^2$ is discrete and consists of a countable number of eigenvalues $\lambda_k$, $k = 1, 2, \ldots$ each of finite multiplicity. The corresponding eigenfunctions,

$$\mathcal{L}\phi_k = \lambda_k \phi_k \,, \tag{65}$$

of $\mathcal{L}$ are complete. $\mathcal{L}$ is not self-adjoint and we must also consider the adjoint operator $\mathcal{L}^\dagger = -pJ(\psi, ) - \nabla^2$. The eigenvalues of $\mathcal{L}^\dagger$ are the same as those of $\mathcal{L}$, but the eignefunctions are different,

$$\mathcal{L}^\dagger \phi_k^\dagger = \lambda_k \phi_k^\dagger \,. \tag{66}$$

There is an orthogonality condition, namely if $\lambda_m \neq \lambda_n$ then

$$\langle \phi_m^\dagger \phi_n \rangle = \delta_{mn} \,. \tag{67}$$

If we possessed $\phi_k$ and $\phi_k^\dagger$ then solving $\mathcal{L}a = u$ would be a triviality i.e.

$$a = \sum_{k=1}^{\infty} \lambda_k^{-1} \langle \phi_k^\dagger u \rangle \phi_k \quad \text{and} \quad \langle au \rangle = \sum_{k=1}^{\infty} \lambda_k^{-1} \langle u \phi_k^\dagger \rangle \langle u \phi_k \rangle \,. \tag{68}$$

Even without $\phi_k$ and $\phi_k^\dagger$, we see that the flux $\langle au \rangle$ can only be singular if $\mathcal{L}$ has zero as an eigenvalue: then there is a zero divisor in the series (68). If the eigenfunctions are nondegenerate this singularity is a pole.

We can locate the values of $p$ in the complex plane at which zero divisors in (68) appear by setting $\lambda_k = 0$ in (65) and regarding $p$ itself as an eigenvalue in the resulting generalized eigenproblem:

$$p_m J(\psi, \phi_m) = \nabla^2 \phi_m \,. \tag{69}$$

Numerical solution of (69) gives $p_1 = \gimel \mathrm{i}$, $p_2 = \daleth \mathrm{i}$ etcetera. These poles on the imaginary $p$-axis limit the radius of convergence of the $p \ll 1$ expansion.

*Problem 4.1.* Prove that the eigenvalues $p_m$ of the generalized eigenproblem (69) are imaginary.

# 5 The advective limit: $p \gg 1$

# 6 The packed eddy model

Consider a uniform chiral medium with a diffusivity tensor

$$\boldsymbol{K}^* = \begin{pmatrix} \kappa^* & \mu^* \\ -\mu^* & \kappa^* \end{pmatrix}, \tag{70}$$

and suppose that distant boundaries impose a concentration field $C = Gx$ with a uniform gradient $\boldsymbol{G} = G\hat{\boldsymbol{x}}$. Then the flux through the medium is

$$\boldsymbol{F} = -G\kappa^* \hat{\boldsymbol{x}} + G\mu^* \hat{\boldsymbol{y}}. \tag{71}$$

Imagine that in this medium we insert a circular eddy (radius $a$) with a streamfunction $\psi = p\kappa(\ln r/a)$; $\kappa \neq \kappa^*$ is the isotropic diffusivity within the eddy. Can we adjust the parameters so that the solution $C = Gx$ outside the eddy is undisturbed?

To answer the preceeding question in the affirmative, we consider the tracer conservation equation in the eddy. We use a polar coordinate system, $(r, \theta)$ centered on the eddy. Thus the conservation equation (**??**) becomes

$$pr^{-2}C_\theta = \nabla^2 C, \qquad C(a, \theta) = Ga\cos\theta. \tag{72}$$

The boundary condition above ensures that the concentration is continuous at the perimeter of the eddy. To ensure that the eddy does not produce an external, disturbance the normal component of the flux is continuous at $r = a$:

$$G\kappa^* \cos\theta - G\mu^* \sin\theta = \kappa C_r(a, \theta). \tag{73}$$

The problem in (72) is easy to solve explicitly because of the simple and unrealistic eddy velocity field.

The problem in (72) has the solution

$$C(r, \theta) = Ga\left(\frac{r}{a}\right)^{\lambda_r} \cos\left[\lambda_i \ln(r/a) + \theta\right], \tag{74}$$

where

$$\lambda_r + \mathrm{i}\lambda_i \equiv \sqrt{1 + \mathrm{i}p} = \sqrt{\frac{\sqrt{1+p^2}+1}{2}} + \mathrm{i}\sqrt{\frac{\sqrt{1+p^2}-1}{2}}. \tag{75}$$

Next, we apply the flux boundary condition in (73). This gives

$$\kappa\lambda_r = \kappa^*, \qquad \kappa\lambda_i = \mu^* \tag{76}$$

# 7 The multiscale method

As advertised at the beginning of the lecture, we now try to derive the eddy diffusivity based on a more general method which can be applied to cases where the tracers are dynamically active. We first write the most general two-dimensional advection-diffusion equation for a passive tracer:

$$c_t + J(\psi, c) - \kappa \nabla^2 c = s, \quad \epsilon \equiv l_\psi / l_s; \tag{77}$$

where $s$ is the source term for the tracer, $l_\psi$ is the eddy size (or the size of cellular pattern in the previous examples), and $l_s$ can be seen as the scale over which the source term varies. Here $l_s$ is assumed to be much larger than $l_\psi$ ($\epsilon \ll 1$). First nondimensionalizing the equation by scaling the distance to $l_\psi$, time to $\kappa / l_\psi$, and velocity to $\psi_0 / l_\psi$, we obtain the following equation:

$$c_t + pJ(\psi, c) = \nabla^2 c + \frac{s l_\psi^2}{\kappa}, \tag{78}$$

where $p \equiv \psi_0 / \kappa$ is the Péclet number. Our goal here is to separate time and spatial scales via the small parameter $\epsilon$, and to do this we rewrite the derivatives as follows:

$$\partial_x \to \partial_x + \epsilon \partial_\xi, \quad \partial_y \to \partial_y + \epsilon \partial_\eta, \quad \partial_t \to \epsilon^2 \partial_\tau. \tag{79}$$

Since we are interested in passive scalar transport over scale much larger than the eddy size, in our analysis $\psi$ is only a function of $(x, y)$, i.e., $\psi$ varies with the "fast variables" only. We also assume that $l_\psi^2 / \kappa \sim \mathcal{O}(\epsilon^2)$, and equation (78) now takes the following form:

$$\epsilon^2 c_\tau + p(\psi_x c_y - \psi_y c_x) + \epsilon p(\psi_x c_\eta - \psi_y c_\xi) - [(\partial_x + \epsilon \partial_\xi)^2 + (\partial_y + \epsilon \partial_\eta)^2] c = \epsilon^2 s. \tag{80}$$

The cell-averaged equation is

$$\epsilon^2 \langle c \rangle_\tau + \epsilon p \langle \psi_x c_\eta - \psi_y c_\xi \rangle - \epsilon^2 \langle c \rangle_{\xi\xi} - \epsilon^2 \langle c \rangle_{\eta\eta} = \epsilon^2 s, \tag{81}$$

and in this case it serves as a solvability condition as any constant can be a solution to equation (80) at zeroth order. Expanding $c$ in $\epsilon$:

$$c = c_0 + \epsilon c_1 + \epsilon^2 c_2 + \cdots,$$

we are now ready to derive $c_i$'s order by order. To zeroth order, we have

$$\mathcal{L}c_0 = 0,\ \mathcal{L} \equiv p(\psi_x\partial_y - \psi_y\partial_x) - (\partial_x^2 + \partial_y^2). \tag{82}$$

In terms of velocity fields, $\mathcal{L} = p\mathbf{u}\cdot\nabla - \nabla^2$, which is exactly what we have in the previous analysis (except here it is nondimensionalized). The only nontrivial solution to equation (81) is $c_0 = f(\xi, \eta, \tau)$. At next order ($\mathcal{O}(\epsilon)$), we have

$$\mathcal{L}c_1 = -p(\psi_x c_{0\eta} - \psi_y c_{0\xi}) - 2c_{0x\xi} - 2c_{0y\eta} = -p(\psi_x f_\eta - \psi_y f_\xi). \tag{83}$$

This is the fundamental problem again and we can use the previous analysis to get the solution for $c_1$. At this point we can bridge two analyses together by identifying $\mathbf{G}$ with the "slow gradient" $(f_\xi, f_\eta)$. Putting both $c_0$ and $c_1$ into equation (81), at order $\mathcal{O}(\epsilon^2)$ we obtain the diffusion equation for $\langle c_0\rangle$:

$$\langle c_0\rangle_\tau + p\langle\psi_x c_{1\eta} - \psi_y c_{1\xi}\rangle - \langle c_0\rangle_{\xi\xi} - \langle c_0\rangle_{\eta\eta} = s. \tag{84}$$

# References


[1] M. Avellaneda and A.J. Majda. An integral representation and bounds on the effective diffusivity in passive advection by laminar and turbulent flows. *Commun. Math. Phys.*, 138:339–391, 1991.

[2] G.A. Baker and P. Graves-Morris. *Padé Approximants, second edition.* Cambridge University Press, Cambridge, 1996.

[3] S. Childress. Alpha-effect in flux ropes and sheets. *Phys. Earth Planetary Interiors*, 20:172–180, 1979.

[4] S. Childress and A. Soward. Scalar transport and alpha-effect for a family of cat's-eye flows. *J. Fluid Mech.*, 205:99–133, 1989.

[5] H.K.Moffatt. Transport effects associated with turbulence with particular attention to the influence of helicity. *Rep. Prog. Phys.*, 46:621–664, 1983.