Notes on Ocean Effective Diffusivities

C. B. Rocha* & W. R. Young

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1 The Advection-Diffusion Equation

1.1 Preliminaries

We are concerned with the lateral advection and diffusion of a passive scalar (tracer) ϑ

$$\vartheta_t + \vec{u} \cdot \nabla \vartheta = \mathcal{S} + \kappa \triangle \vartheta \,, \tag{1}$$

where $\mathcal{S}$ represents sources, κ is the molecular diffusivity of the tracer ϑ, and the horizontal laplacian is $\triangle \overset{\text{def}}{=} \partial_x^2 + \partial_y^2$. Because the flow $\vec{u}$ is horizontally non-divergent, we define the streamfunction ψ such that

$$u = -\psi_y \,, \qquad \text{and} \qquad v = \psi_x \,, \tag{2}$$

and (1) can be re-written

$$\vartheta_t + \mathsf{J}(\psi, \vartheta)\vartheta = \mathcal{S} + \kappa \triangle \vartheta \,, \tag{3}$$

where the horizontal Jacobian is $\mathsf{J}(A, B) = A_x B_y - B_x A_y$.

1.2 X-averaged Equation

Introducing the Reynolds decomposition

$$\vartheta(x, y, t) = \bar{\vartheta}(y, t) + \vartheta'(x, y, t) \,,$$
$$\psi(x, y, t) = \bar{\psi}(y, t) + \psi'(x, y, t) \,, \tag{4}$$
$$\tag{5}$$

where

$$\bar{f}(y, t) = \frac{1}{L_x} \int_0^{L_x} f(x, y, t) \, \mathrm{d}x \,. \tag{6}$$

With periodicity in x, the $x-$averaged $y-$velocity vanishes $\bar{v} = \bar{\psi}_x = 0$. The $x-$averaged tracer equation is then

$$\bar{\vartheta}_t + \partial_y(\overline{v'\vartheta'}) = \bar{S} + \kappa \partial_y^2 \bar{\vartheta} \,. \tag{7}$$

For completeness, the equation for the perturbation about the $x-$averaged tracer is

$$\vartheta'_t + \partial_x(u'\vartheta') + \partial_y(v'\vartheta') + \partial_x(u'\bar{\vartheta}) + \partial_y(v'\bar{\vartheta}) - \partial_y(\overline{v'\vartheta'}) = S' + \kappa(\partial_y^2 \vartheta' + \partial_x^2 \vartheta) \,. \tag{8}$$

Introducing an eddy-difussivity parameterization for the $y-$direction trace flux $\overline{v'\vartheta'}$

$$\overline{v'\vartheta'} = -K \partial_y \bar{\vartheta} \,, \tag{9}$$

we obtain

$$\bar{\vartheta}_t = \bar{S} + D \partial_y^2 \bar{\vartheta} \,, \tag{10}$$

where the effective diffusivity is $D \overset{\text{def}}{=} K + \kappa$.

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*Scripps Institution of Oceanography, University of California, San Diego. E-mail: crocha@ucsd.edu

1.3 Variance budget

With harmless boundary conditions (e.g., double periodicity or no-flux across the boundaries) the tracer variance equation is

$$\frac{\mathrm{d}}{\mathrm{d}t} \int \tfrac{1}{2}\vartheta^2 \mathrm{d}A = \int \vartheta \mathcal{S} \mathrm{d}A - \kappa \int |\nabla \vartheta|^2 \mathrm{d}A \,. \tag{11}$$

2 Renovated Waves on a Lattice

To begin exploring the accuracy of different methods to estimate ocean effective diffusivities, we use a simple advection-diffusion model on a lattice first proposed by Pierrehumbert (2000). The idea is to break the advection and difussion in different steps. The advection step is further separated in two substeps: advection in the x-direction and y-direction. The advection substeps are performed on a lattice. That is, the advection in the x-direction corresponds to a shift in the x-direction, and the advection in the y-direction corresponds to a shift in the y-direction:

$$i_x^{n+1} = i_x^n - \mathrm{int}\left(u_n(y)\Delta t\right) \,, \tag{12}$$

and

$$i_y^{n+1} = i_y^n - \mathrm{int}\left(v_n(x)\Delta t\right) \,, \tag{13}$$

where the superscripts represent the iteration. Figure 2, adapted from Pierrehumbert, explains the advection steps better than any set of words. Notice that this "advection-scheme" exactly conserves the probability density of the tracer.

We represent the velocity field as linear combination of waves with random phase:

$$u_n(y) = C \sum_{j=j_{min}}^{j_{max}} \left(\frac{j}{j_{min}}\right)^{-p/2} \cos\left(\frac{2\pi y}{L_y}j + \phi_n\right) \,, \tag{14}$$

$$v_n(x) = C \sum_{j=j_{min}}^{j_{max}} \left(\frac{j}{j_{min}}\right)^{-p/2} \cos\left(\frac{2\pi x}{L_x}j + \psi_n\right) \,, \tag{15}$$

where L_x and L_y are the dimensions of the periodic domain, ψ_n and ϕ_n are random phases drawn from a uniform distribution on $[0, 2\pi]$. Because these random phases are changed every iteration, this simple velocity field is termed renovated wave model. Note that in this generalized renovated wave model the kinetic energy spectrum of the flow follows a j^{-p} power-law. Also in (14) and (15), C is a normalization constant, determined so that the root-mean square velocity is prescribed

$$C = u_{rms} \left(\sum_{j=j_{min}}^{j_{max}} \left(\frac{j}{j_{min}}\right)^{-p}\right)^{-1/2} \,. \tag{16}$$

Pierrehumbert performs the diffusion step in physical space, as a simple average of neighboring points, corresponding to a second-order finite-difference approximation for the laplacian operator. Here we take advantage of the periodicity of this model, and perform the diffusion step more accurately in Fourier space:

$$\hat{\vartheta}_{k,l}^{n+1} = \hat{\vartheta}_{k,l}^n \mathrm{e}^{-\kappa(k^2+l^2)\Delta t} \,. \tag{17}$$
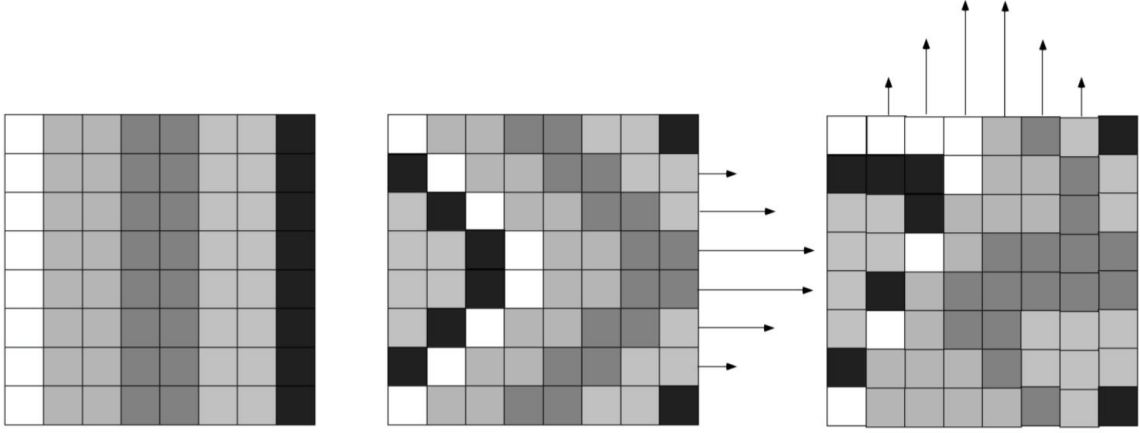
Figure 1: Schematic representing the advection substeps with single sinusoidal velocity fields. Adapted from Pierrehumbert (2000).

2.1 Advection-diffusion with a simple large-scale source

We employ a simple large-scale source

$$S(y) = \cos\left(\frac{2\pi}{L_y}y\right). \tag{18}$$

Because the source is only a function of y, half of the source is performed after the $x-$advection substep

$$\vartheta^{n+1/2} = \vartheta^{n+1/2} + \frac{\Delta t}{2}S(y). \tag{19}$$

The other half of the source could be applied in the same fashion, after the $y-$advection substep

$$\vartheta^{n+1} = \vartheta^{n+1} + \frac{\Delta t}{2}S(y). \tag{20}$$

In principle (20) is a brutal way to apply the source since source term is not invariant in y. To apply the source more accurately, we note that in the "y-advection"+"half-source" substeps, we are solving

$$\vartheta_t + v(x)\vartheta_y = \cos\left(\frac{2\pi}{L_y}y\right), \tag{21}$$

which can be easily integrated along the characteristics $y = y_0 + v\Delta t/2$, to give

$$\vartheta(x, y, t + \Delta t) = \vartheta(x, y, \Delta t) + \frac{\sin\left[k_1(y_0 + v\Delta t/2)\right] - \sin k_1 y_0}{k_1 v}. \tag{22}$$

where $k_1 \stackrel{\text{def}}{=} \frac{2\pi}{L_y}$. We anticipate loss of accuracy for in regions where $v \approx 0$. To avoid this inaccuracies, we identify these points numerically, and use the exact value in limit $\Delta t \to 0$. This limit can be calculated using the L'Hospital rule, simply expanding about $v = 0$, to obtain

$$\frac{\sin\left[k_1(y_0 + v\Delta t/2)\right] - \sin k_1 y_0}{k_1 v} \to \frac{\Delta t}{2}\cos k_1 y_0 \qquad \text{as} \qquad v \to 0. \tag{23}$$

In summary, the algorithm for this forced advection-diffusion problem on a lattice, every iteration is composed by the following substeps:

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1. $x-$advection

2. half source

3. $y-$advection + half source

4. diffusion

Of course, one could break the diffusion step in two substeps, to be performed after the advection. In practice, there is no significant difference, and we opt to use the single step difusion above for computational efficiency.

2.2 Did Einstein get it right?

For this simple model the $x-$averaged equation is

$$\bar{\vartheta}_t = \cos k_1 y + D\partial_y^2 \bar{\vartheta} \,, \tag{24}$$

In statistical steady state, averaging either in time or over ensembles, we obtain

$$D\partial_y^2 \langle \bar{\vartheta} \rangle = -\cos k_1 y \,, \tag{25}$$

$\langle \rangle$ denotes either time or ensemble average. Thus,

$$\langle \bar{\vartheta} \rangle = \frac{\cos k_1 y}{Dk_1^2} \,. \tag{26}$$

For this simple model, we can calculate the effective diffusivity D exactly (Einstein, 1905)

$$D = \frac{\langle (\Delta x)^2 \rangle}{2\Delta t} \,, \tag{27}$$

where $\langle (\Delta x)^2 \rangle$ is the mean-square displacement. Intrinsic in the derivation of (27) is the scale separation between the flow that performs the advection and the large-scale gradient. In the generalized RW model, we have

$$\langle (\Delta x)^2 \rangle = \langle u_n^2 (\Delta t)^2 \rangle = \frac{u_{rms}^2 (\Delta t)^2}{4} \,, \tag{28}$$

and therefore

$$D = \frac{u_{rms}^2 \Delta t}{4} \,. \tag{29}$$

Figure 2.4 shows a comparison between theory, using Einstein's effective difusivity (29), and numerical calculation on the lattice model. With scale separation, there is spectacular agreement between theory and numerics (see Figure 2.4 left). Even the $x-$averaged concentration of snapshots is reasonably consistent with the theoretical prediction. Without scale separation, there is still reasonable consistency, but the spread about the time-mean is much larger.

2.3 Tracer variance spectrum

2.4 Dependence on molecular diffusivity

3 Approximate Methods for Effective Diffusivity

These methods have the form

$$K = A^2 \kappa \,, \tag{30}$$

where K is an approximation to the true diffusivity D, κ is the molecular diffusivity, and A^2 is an amplification factor.
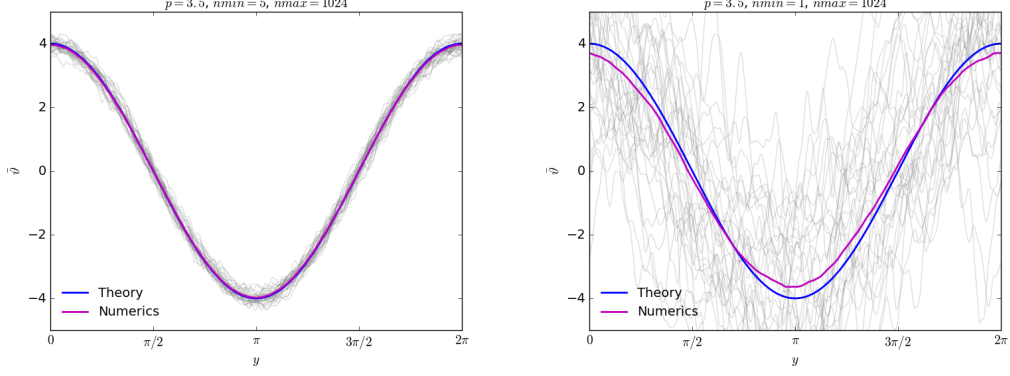
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Figure 2: $x-$averaged tracer concentration simulated with $N_x = N_y = 1024$, $L_x = L_y = 2\pi$, $n_{min} = 5$ (left) and $n_{min} = 1$(right), $n_{max} = 1024$, and $p = 1024$. The magenta line represents time-averaged and the thin gray lines represent snapshots. The blue line is the theoretical prediction.

3.1 A variance budget approach: Osborn-Cox

Osborn-Cox employs a tracer variance budget approach to estimate the effective diffusivity. Multiplying (8) and $x-$averaging, we obtain

$$\frac{\mathrm{d}}{\mathrm{d}t}\frac{\overline{\vartheta'^2}}{2} + \partial_y\left(\overline{v'\frac{\vartheta'^2}{2}}\right) + \overline{v'\vartheta'}\partial_y\bar{\vartheta} = -\kappa\overline{|\nabla\vartheta'|^2} + \kappa\partial_y^2\frac{\overline{\vartheta'^2}}{2}\,. \tag{31}$$

With the eddy diffusivity hypothesis, i.e.,

$$\overline{v'\vartheta'} = -K_{oc}\partial_y\bar{\vartheta}\,, \tag{32}$$

we have, in statistical steady state,

$$-\partial_y\left(\overline{v'\frac{\vartheta'^2}{2}}\right) - K_{oc}(\partial_y\bar{\vartheta})^2 = -\kappa\overline{|\nabla\vartheta'|^2} + \kappa\partial_y^2\frac{\overline{\vartheta'^2}}{2}\,. \tag{33}$$

The Osborn-Cox approach ignores the first term on the left and the last term on the right of (33), so that the Osborn-Cox eddy diffusivity is

$$K_{oc} = \frac{\overline{|\nabla\vartheta'|^2}}{\bar{\vartheta}_y^2}\kappa\,. \tag{34}$$

3.2 Monitoring the lengthening of tracer contours: Nakamura

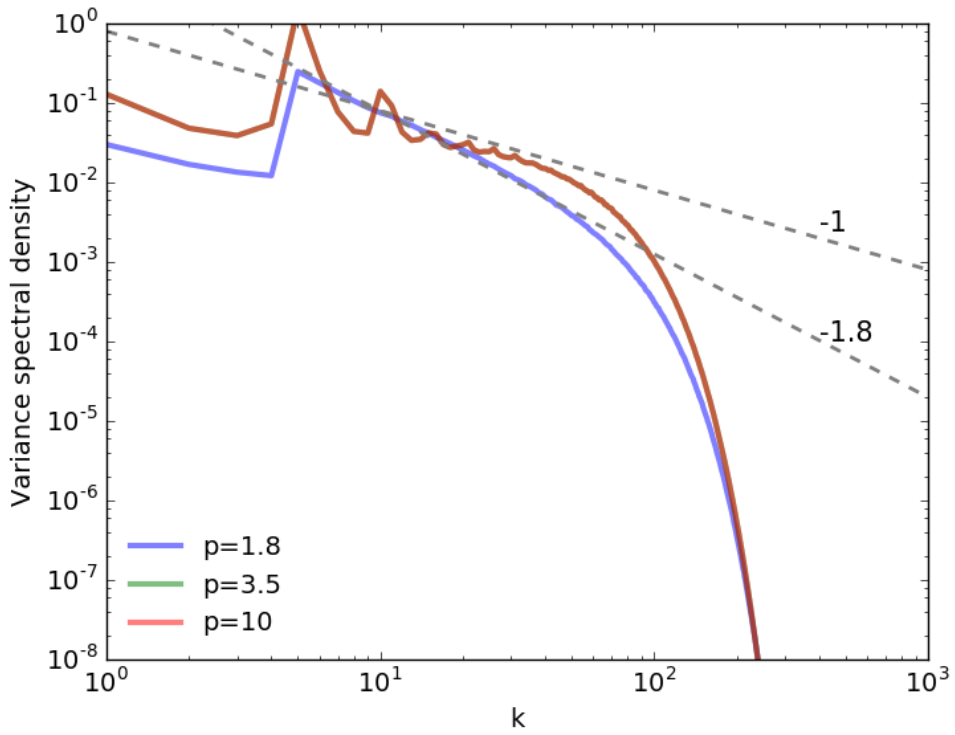$$K_N = \frac{L^2}{L_{min}^2}\kappa\,. \tag{35}$$

Figure 3: Trace variance spectra as a function of $x-$wavenumber for two runs with $p = 1.8$, $p = 3.5$, $p = 10$, $\kappa = 1.e - 3$, $u_{rms} = 1$, n_{min}=5. The $x-$average trace concentration has been removed before calculating the spectrum.
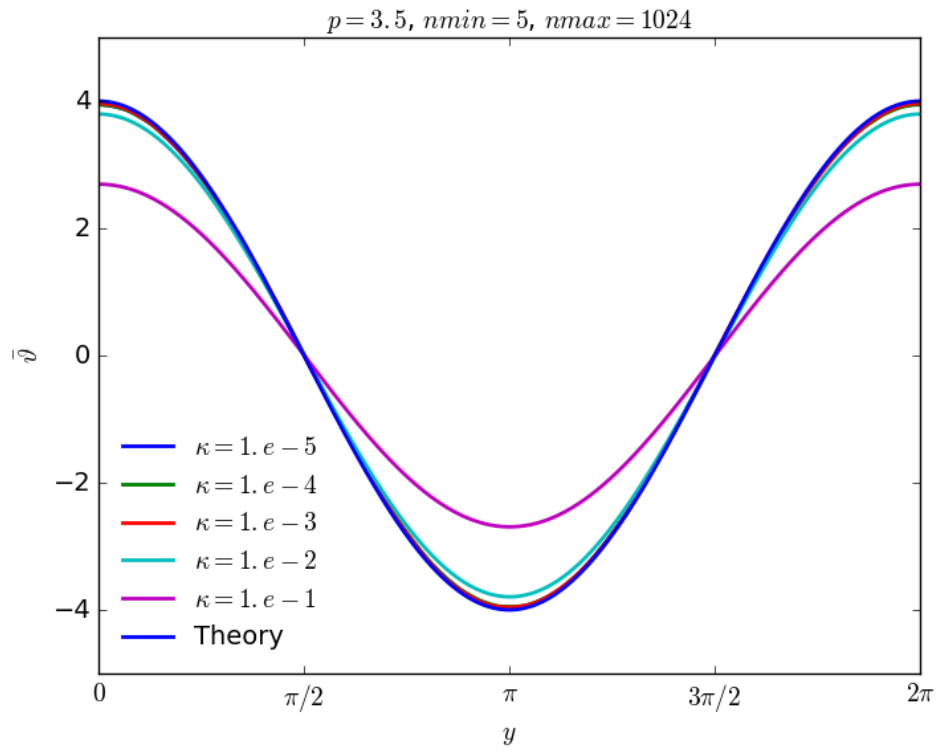
Figure 4: Dependence of $x-$averaged tracer concentration on the numerical value of the molecular diffusivity. As expected, the $x-$averaged tracer concentration is nearly independent unless the molecular diffusivity is too large.