Lagrangian modelling of multi-dimensional advection-diffusion with space-varying diffusivities

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Introduction

Most numerical methods for simulating advection-diffusion processes can be split into three categories: Eulerian, Lagrangian and mixed Eulerian-Lagrangian methods. For the problems that involve sharp concentration front Eulerian method is susceptible to excessive numerical dispersion and artificial oscillations. The examples of these problems are advection-dominated problems, problems with delta-like initial concentration and the problems with non-diagonal space-varying diffusivity. Lagrangian methods provide an accurate and efficient solution to advection dominated problems by essentially eliminating the effects of numerical dispersion and artificial oscillations. The random walk methods requires relatively little computer storage as compared with the Eulerian methods. However, the lack of a fixed grid or fixed coordinate in Lagrangian method may lead to numerical instability and computational difficulties.Another source of numerical error is a the interpolation of flow variables in arbitrary particle location that can lead to local mass balance error and solution anomalies. The choice of methods depends on the problem under consideration. Sometimes, it is not easy to classify the problem and decide which method should be applied. The mixed Eulerian-Lagrangianmethods attempt to combine the advantages of Lagrangian and Eulerian methods.

Random walk model (in Ito sense)

The concentration of the tracer can be found from the **advection-diffusion equation**:

$$\boxed{\begin{aligned}&\frac{\partial C}{\partial t} = -\nabla \bullet (\mathbf{u}C - \mathbf{K}\bullet\nabla C)\\ &C(0,\mathbf{x}) = \delta(\mathbf{x}-\mathbf{x}_0)\end{aligned}}$$

The advection-diffusion equation can be interpreted as a Fokker-Planck equation (or forward Kolmogorov equation) and the system of the SDEs (Stochastic Differential Equations) can be derived. This stochastic system is usually called **the random walk model** (in Ito sense):

$$\boxed{\begin{aligned}&d\mathbf{X}(t) = (\mathbf{u} + \nabla\bullet\mathbf{K})dt + \sqrt{2}\mathbf{V}d\mathbf{W}(t)\\ &\mathbf{X}(0) = \mathbf{x}_0\end{aligned}}$$

This random walk model can be used to model the track of an individual particle of the pollutant. The concentration function is now the probability density function of the stochastic process **X**. By running the random walk model many times we obtain the different locations $\mathbf{X}^i$, $i=1,\ldots,N$ of pollutant particles. One can find the concentration by using the standard method of non-parametric statistics, called **kernel estimator**

$$\boxed{C(t,\mathbf{x}) = \frac{1}{N\lambda^d}\sum_{n=1}^{N} K\left(\frac{\mathbf{X}^{(n)}(T)-\mathbf{x}}{\lambda}\right)}$$

Here λ is a bandwidth, d is a dimension of a model and K is a kernel function.

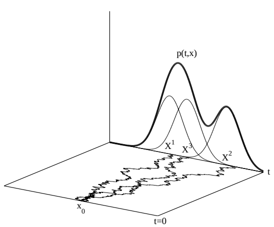


Figure 1. Kernel estimator
One can think of the kernel estimator as spreading of a "probability mass" of size 1/N associated with each data point about its neighborhood. Combining contributions from each data point means that in regions with many observations the density has a relatively large value and opposite in regions with only few observations.

Test case 1: Iso- and diapycnal diffusion

It is common knowledge that large-scale diffusion processes in the ocean occur mostly along isopycnal surfaces, i.e. surfaces of equal density. There is also some diapycnal diffusion. The latter is associated with a diffusion flux orthogonal to isopycnal surfaces. The diapycnal and isopycnal diffusion fluxes are commonly parameterized â la Fourier-Fick, a formulation involving a diffusion tensor that is not diagonal (Redi (1982)).

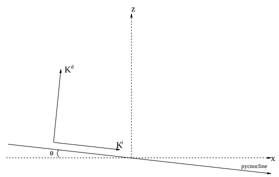


Figure 2. Iso- and diapycnal diffusion
If homogeneity can be assumed along one horizontal coordinates, a two-dimensional problem is to be dealt with. For a large-scale ocean model the formulation of diffusion model resorts to two diffusivity coefficients, K^i and K^d, which are isopycnal and diapycnal diffusivities, respectively. Let θ denotes the angle between the horizontal and the isopycnal direction.

We consider a multi-dimensional model and suppose that the advective processes can be neglected. In the ocean, the slope of the isopycnal surfaces is usually small. For numerical experiments, the following values can be used (Mathieu and Deleersnijder (1998)) $\theta \approx 10^{-3}$.

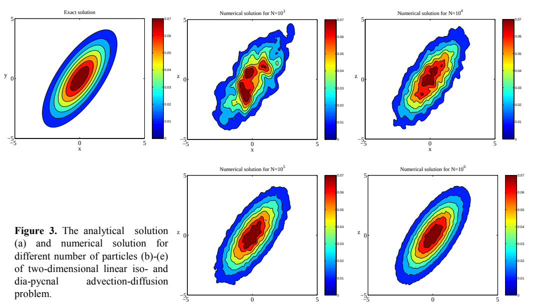


Figure 3. The analytical solution (a) and numerical solution for different number of particles (b)-(e) of two-dimensional linear iso- and dia-pycnal advection-diffusion problem.

Test case 2: Settling and diffusion model

In the next test case we apply the random walk scheme for the model with space-varyir diffusivity in the presence of boundaries. This model has been introduced and investigate in Deleersnijder et al. (2006a,b).

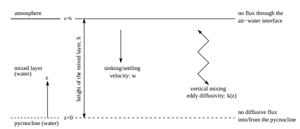


Figure 4. Sinking-diffusion model: illustration of its geometry, parameters and boundary conditions. Source: Deleersnijder et al. (2006a)

The parabolic diffusivity profile

$$\boxed{k(z) = 6z(1-z)}$$

was chosen. This choice is consistent with the diffusion processes in the upper mixed laye The diffusivity profile k(z) tends to zero as the bottom of the mixed layer us approache and the maximum of the diffusivity should not occur at surface For this diffusivity profi and zero velocity the analytical solution is known

$$\boxed{C(t,z) = 1 + \sum_{n=1}^{\infty}(2n+1)P_n(2z-1)P_n(2z_0-1)e^{-6n(n+1)t}}$$

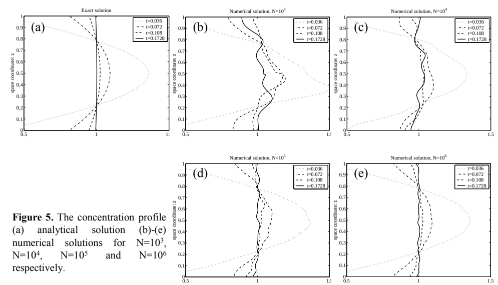
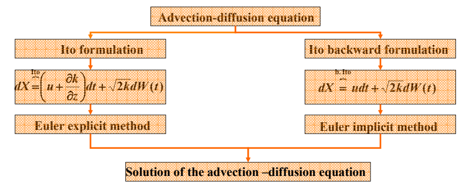


Figure 5. The concentration profile (a) analytical solution (b)-(e) numerical solutions for $N=10^3$, $N=10^4$, $N=10^5$ and $N=10^6$ respectively.

Backward Ito random walk model

The standard random walk methods are only applied when the flow velocities and diffusivity are sufficiently smooth functions. In practice, there are some regions where the rapid but continuous change in diffusivity may be represented by a discontinuity. The random walk model based on backward Ito calculus can be used for these problems. This model was proposed by LaBolle et. al. (2000).



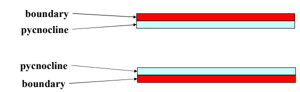
In general, the analytical solution of the advection-diffusion problem cannot be found; however, the residence time of a tracer can be obtained. The residence time of a water or tracer parcel in a control domain is usually defined as the time taken by this parcel to leave the domain of interest. For the sinking-diffusion the residence time can be found from the following expression (Deleersnijder et al. (2006a))

$$\boxed{\theta(z) = \frac{z}{w} + \frac{1}{w}\int_z^h \exp\left[-w\int_z^{\xi}\frac{d\zeta}{k(\zeta)}\right]d\xi}$$

Now we assume that the boundary of interest is $z=\delta$, rather than $z = 0$. δ is positive or negative according to whether the boundary is located in the mixed layer or the pycnocline, respectively. The corresponding residence time is hereinafter denoted $\tau(z, \delta)$. Assume that the eddy diffusivity is a positive constant λ, in the mixed layer and zero in the pycnocline. Deleersnijder et al. (2006b) show that the residence time may exhibit a discontinuity at the interval between the mixed layer ($0 < z < h$) and pycnocline ($z < 0$), for the eddy diffusivity is zero in the latter and positive in the former. Because the dimensionless variables are introduced only one parameter should take into account: $Pe=(wh)/\lambda$

$$\boxed{\tau(z,0^+) = z - \frac{e^{-Pe(1-z)} - e^{-Pe}}{Pe}}$$

$$\boxed{\tau(z,0^-) = z + \frac{1 - e^{-Pe(1-z)}}{Pe}}$$



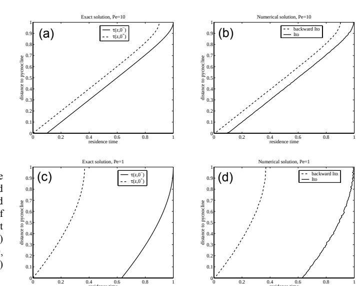


Figure 6. The profile of the residence times $\tau(z, 0^-)$ and $\tau(z, 0^+)$ in the surface mixed layer for various values of the Peclet number. (a) exact solution, Pe=10, (b) numerical solution, Pe=10, (c) exact solution, Pe=1, (d) numerical solution, Pe=1

Conclusions

The random walk model for the simulation of diffusion processes with space-varying diffusivity is introduced and analyzed. This Lagrangian model is applied to several test problems and results show that this random walk model may be a good alternative to commonly-used Eulerian models. The random walk model based on backward Ito calculus can be used for problems with rapid change in diffusivity.

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