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Improved mathematical and numerical modelling of dispersion of a solute from a continuous source

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We present a refinement of a model due to Mondal and Mazumder [7] for dispersion of fine particles in an oscillatory turbulent flow. The model is based on the time-dependent advection-diffusion equation posed on a semi-infinite strip, and whose solution represents the concentration of particles over time and down-stream distances.

The problem is solved by first mapping to a finite domain and then using a monotone finite difference method on a tensor product, piecewise uniform mesh. The numerical results obtained for the related steady-state problem, and are compared with experimental data.

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1 Introduction

This paper is concerned with a mathematical model for the dispersion of fine particles in an advection-dominated flow, and its numerical resolution. In presenting it, our goals are three-fold:

1. To present an improvement of the model in [7];
2. To outline how a layer adapted piecewise uniform (“Shishkin”) mesh may be applied when solving this model, and further, to motivate the use of a parameter-robust method for this applied problem;
3. To obtain better agreement between the model’s predictions and experimental data than that was achieved in related studies.

It is important to understand the basic mechanism of dispersion processes of passive contaminants in a stream or in the atmosphere from a continuous source; in particular it gives an insight to control the pollution level in the environment. It is shown in [7] how the spreading of injected particles is influenced by the combined action of oscillatory flow (with or without a non-zero mean), settling velocity, and

vertically varying eddy diffusivity over the rough-surface for all time periods. The introduced particles are represented as a single point discontinuity at the in-flow boundary. In addition, a transformation is used to map the unbounded region to a bounded one. A finite difference method on a uniform grid is then used to solve the model numerically.

In §2 we present a mathematical model that is a modification of one described in [7]. The concentration of the particles introduced into the flow as a continuous source term and it is represented mathematically as a two-dimensional Dirac delta function, leading to an interior layer in the solution. Furthermore, we take the diffusivity term has been a combination of molecular diffusivity and turbulence eddy diffusivity (the earlier study neglected molecular diffusivity, leading to problems with the representation of the boundary conditions at the free surface).

In §3.1 we describe the transformation from the semi-infinite to a finite domain that has been used in related studies [4, 6, 7]. In §3.2 we give a simple example that demonstrates how the transformation effects the development of the interior layer, and so the choice of numerical procedure.

As stated, we wish to validate the model by comparison with a suitable set of experimental results. One such, widely cited study is [9]. However, those experiments are for a situation that is not as general as the model presented here allows; it corresponds to the steady case. Therefore, the numerical method described in §3.3 is only concerned with the solution of a two-dimensional (in space) advection-diffusion problem. We use a standard finite-difference discretization on a fitted piecewise uniform mesh of Shishkin type. The comparison between the experimental data and the numerical results are given in §4. We conclude with some observations, and an outline for future work.

2 The model

Figure 1 gives a simple diagram of the coordinate system, representing a body of water in an infinitely long stream of finite depth. Expressed in dimensionless variables (see [7]), the rough stream bed is at $z = z_0 > 0$, and the free surface is at $z = 1$. The flow is assumed to be steady two dimensional flow, and is advection dominated, in the positive x -direction. The flow is turbulent, and the effects of this turbulence is represented in the model by an eddy diffusivity term that varies only with the vertical coordinate, z .

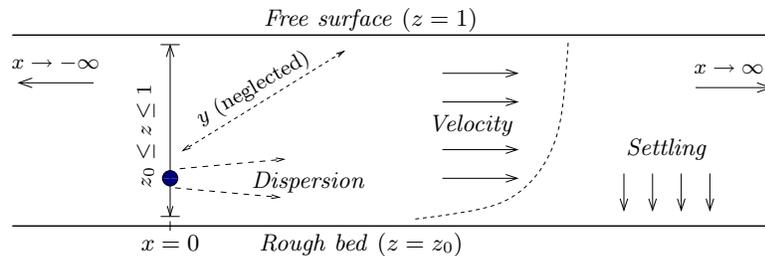


Fig. 1. Sketch of the coordinate system

Particles are introduced into the stream at the point $x = 0, z = z_p$, their concentration represented in the source term as a distribution (Dirac delta). The equation is

$$\frac{\partial C}{\partial t} + u(z)\frac{\partial C}{\partial x} - \omega_s \frac{\partial C}{\partial z} = k_x(z)\frac{\partial^2 C}{\partial x^2} + \frac{\partial}{\partial z}\left(k_z(z)\frac{\partial C}{\partial z}\right) + f(x, z), \quad (1a)$$

on $(-\infty, \infty) \times (z_0, 1) \times (0, T]$, and subject to boundary and initial conditions

$$C(\pm\infty, z, t) = 0, \quad \left[k_z(z)\frac{\partial C}{\partial z} + \omega_s C\right]_{z=z_0,1} = 0, \quad C(x, z, 0) = 0, \quad (1b)$$

where z_0 is the boundary roughness height, ω_s is the settling velocity, and $f(x, z) = \delta(x)\delta(z - z_p)$, i.e., point source at $(x, z) = (0, z_p)$. Here the problem has been expressed in terms of dimensionless variables. That is, where D is the depth of the carrier fluid and where u_* is the friction velocity (taken as reference velocity), we take

$$x = \frac{x^*}{D}, \quad z = \frac{z^*}{D}, \quad t = \frac{t^* u_*}{D}, \quad u = \frac{u^*}{u_*}, \quad \omega_s = \frac{\omega_s^*}{u_*}.$$

We use the standard “log-law” as the steady velocity distribution $u(z)$ with an additional term, the wake function $W(z)$ which is required to incorporate the effects of wakes generated below the free surface. The combination of “log-law” and wake function is called the “log-wake law” and it is used for fully developed homogeneous turbulent flow. In our present study, we have not taken account the effect of inhomogeneous turbulent fluctuations, so the velocity distribution is

$$u(z) = \frac{1}{\kappa} \ln\left(\frac{z}{z_0}\right) + W(z),$$

where κ is the von-Kármán constant and z_0 is the equivalent bed roughness. The wake function $W(z)$ is taken as that of Coles [1]:

$$W(z) = \frac{2\Pi}{\kappa} \sin^2\left(\frac{\pi}{2}z\right),$$

where Π is the wake-strength parameter.

When the Reynolds decomposition is performed on the laminar advection-diffusion equation by decomposing the velocity ($u = \bar{u} + u'$) and concentration ($C = \bar{C} + C'$) into the sum of their mean and fluctuating parts, the term $\partial(\overline{u'C'})/\partial x_j$ represents the transport of concentration C due to turbulent fluctuations. Because the molecular diffusivity (k_{md}) is usually a very small quantity, $\overline{u'C'} \gg k_{\text{md}}\partial C/\partial x_j$, the effects for molecular diffusion is often negligible compared to the effects of turbulence, and so omitted from the model (e.g., as in [12, 3]). However, in this model the molecular diffusion is an important mechanism for mixing of the concentration to the flow at the smallest scales, and so we take the diffusivity profile as

$$k_x(z) = k_{\text{md}} + k_{\text{ed}}(z),$$

where $k_{\text{ed}}(z)$ is the eddy-diffusivity as proposed by Nezu and Rodi [8]:

$$k_{\text{ed}}(z) = \kappa(1-z) \left[\frac{1}{z} + \Pi\pi \sin(\pi z) \right]^{-1}.$$

Since our problem is posed in a fully developed homogeneous turbulent flow, we take $k_x(z) = k_z(z)$, and neglect the cross-stream diffusion terms.

Note that, since $k_z(1) = 0$, if the settling velocity $\omega_s = 0$ and k_{md} neglected, then boundary condition at the free surface carries no physical significance, and the mathematical problem is ill-posed.

3 Numerical solution of the model

To compute an accurate numerical solution to model given above, several issues need to be addressed. Firstly, the problem is posed on a semi-infinite domain. Numerical solutions are only possible on finite domains, so the domain must either be truncated or transformed. Here we take the latter approach, discussed in §3.1, since it has proved successful in related studies. Then the layer(s) present in the solution must be resolved; a suitable method is described in §3.3.

3.1 Transformation of the domain

In [7], a tanh-transformation from the domain $(x, z) \in (-\infty, \infty) \times [z_0, 1]$ to $(\zeta, z) \in (-1, 1) \times [z_0, 1]$ is made using

$$x = \frac{1}{2a} \log \left(\frac{1 + \zeta}{1 - \zeta} \right),$$

where a is a “stretching” factor, usually chosen based on computational experience. Following the transformation the model becomes

$$\begin{aligned} & \frac{\partial C}{\partial t} + u(z)a(1 - \zeta^2) \frac{\partial C}{\partial \zeta} - \omega_s \frac{\partial C}{\partial z} \\ & = a^2 k_\zeta(z)(1 - \zeta^2) \left[(1 - \zeta^2) \frac{\partial^2 C}{\partial \zeta^2} - 2\zeta \frac{\partial C}{\partial \zeta} \right] \\ & \quad + \frac{\partial}{\partial z} \left(k_z(z) \frac{\partial C}{\partial z} \right) + \delta(\zeta) \delta(z - z_p), \end{aligned} \quad (2a)$$

$$C(\pm 1, z, t) = 0, \quad \left[k_z(z) \frac{\partial C}{\partial z} + \omega_s C \right]_{z=z_0, 1} = 0, \quad C(\zeta, z, 0) = 0. \quad (2b)$$

Remark 1. Although the full model as presented here is time-dependent, for the remainder of this paper we consider only the analogous steady problem. This is because we wish to compare our numerical results with experimental data. Since a reliable and well-tested set is available in the literature [9] for the steady case, we have opted to restrict our attention to that. We note that the issues concerning transformation from the semi-infinite domain to a finite one, and resolution of the interior layer, still feature.

3.2 A simple example

To consider how one might construct a suitable mesh for this problem, and to consider the effect of the transformation parameter, we present the following simple example: omit the $\partial C/\partial t$ term in (2a) above, and take $u \equiv 1$, $\omega_s = 0$, and constant viscosity $\varepsilon \approx k_\zeta(z_p) = k_z(z_p)$:

$$-\varepsilon a^2(1 - \zeta^2) \left[(1 - \zeta^2) \frac{\partial^2 C}{\partial \zeta^2} - 2\zeta \frac{\partial C}{\partial \zeta} \right] - \varepsilon \frac{\partial^2 C}{\partial z^2} + a(1 - \zeta^2) \frac{\partial C}{\partial \zeta} = \delta(\zeta)\delta(z - z_p), \quad (3)$$

and the boundary conditions as in (2b) above.

In Figure 2 we show the cross-section at $z = z_p$ of the computed solution, restricting to a small region around $\zeta = 0$ where the interior layer is most obvious. The given results are for $\varepsilon = 10^{-4}$, and cases $a = 10, 1$ and 0.1 . As one would expect, taking relatively large values of a expands the layer in the computational domain, while for smaller values of a the layer is sharper.

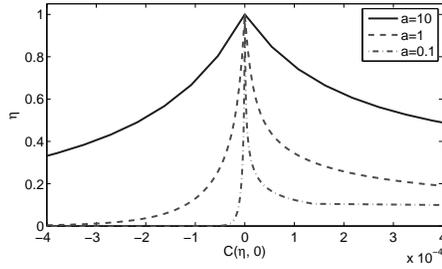


Fig. 2. Solution to (3) with $\varepsilon = 10^{-4}$ and $a = 10, 1$ and 0.1

In choosing a for a particular problem, we would like to take it as large as possible, so that the layer is easily resolved. However, taking a very large value of a will result in the region away from the layer is squeezed into the boundary. In practise, one usually is seeking values of the solution at certain points, so a should be small enough so that these are included in the computational domain. Thus we note that even when the problem data is fixed, one may be interested in solutions for different values of a . *Therefore, the use of a parameter uniform method is desirable.*

3.3 The numerical method

To simplify notation, we restate the steady problem succinctly as

$$-\varepsilon_1(\zeta, z) \frac{\partial^2 C}{\partial \zeta^2} - \varepsilon_2(\zeta, z) \frac{\partial^2 C}{\partial z^2} + \beta_1(\zeta, z) \frac{\partial C}{\partial \zeta} + \beta_2(\zeta, z) \frac{\partial C}{\partial z} = \delta(\zeta)\delta(z - z_p), \quad (4)$$

where ε and β are continuous column vectors. Taking (for now) arbitrary meshes $\omega_\zeta : 0 = \zeta_0 < \zeta_1 < \dots < \zeta_M = 1$, and $\omega_z : 0 = z_0 < z_1 < \dots < z_N = 1$ in the ζ - and z -directions, one may form the tensor-product mesh $\omega := \omega_\zeta \times \omega_z$. We denote the mesh widths as $\Delta\zeta_i = \zeta_i - \zeta_{i-1}$ and $\Delta z_i = z_i - z_{i-1}$, and the approximation for

$C(\zeta, z)$ at (ζ_i, z_j) as $C_{i,j}$. Derivatives with respect to ζ are discretized using standard second order finite difference:

$$D_\zeta^2 C_{i,j} := \frac{2}{\Delta\zeta_i + \Delta\zeta_{i+1}} \left(\frac{C_{i+1,j} - C_{i,j}}{\Delta\zeta_{i+1}} - \frac{C_{i,j} - C_{i-1,j}}{\Delta\zeta_i} \right),$$

and first-order upwinded finite difference:

$$D_\zeta^1 C_{i,j} := \left(\frac{C_{i,j} - C_{i-1,j}}{\Delta\zeta_i} \right).$$

The discretizations of the derivatives with respect to z are analogous, though with a suitable down-winding operator for $\partial C/\partial z$. The discrete problem is

$$\begin{aligned} \left(-\varepsilon_1(\zeta_i, z_j) D_\zeta^2 - \varepsilon_2(\zeta_i, z_j) D_z^2 + \beta_1(\zeta_i, z_j) D_\zeta^1 + \beta_2(\zeta_i, z_j) D_z^1 \right) C_{i,j} = \\ \delta(\zeta_i) \delta(z_j - z_p) \quad \text{for } i = 1, \dots, M-1, j = 1, \dots, N-1. \end{aligned}$$

With a suitable implementation of the boundary conditions, this is easily solved.

We wish to construct a piecewise uniform, Shishkin-type mesh that will resolve the interior layer; in particular we want the mesh to be refined around the injection point $(0, z_p)$. Define $\sigma_z = \varepsilon_2(0, z_p)/\beta_2(0, z_p)$, and set $\tau_z = \sigma_z \ln N$. If $\tau_z \geq 2(1 - z_0)/N$, take ω_z to be the uniform mesh of N intervals on $[z_p, 1]$. Otherwise proceed as follows. Construct two meshes: ω_z^A is the uniform mesh with $N/2$ intervals on $[z_0, 1]$ and ω_z^B is the uniform mesh with $N/2$ intervals on $[z_p - \tau_z/2, z_p + \tau_z/2]$. Then take ω_z to be the union of $\omega_z^A \setminus [z_p - \tau_z/2, z_p + \tau_z/2]$ and ω_z^B . The mesh ω_ζ is constructed in an analogous fashion.

Remark 2. This construction varies slightly from the usual Shishkin mesh, which selects appropriate transition points at which to switch between a course and fine piecewise uniform mesh. In this case, since the injection point may be close to one of the boundaries, the construction given here is easier to implement, and ensures uniform mesh widths in the regions away from the injection point.

4 Numerical Results

We compare our numerical results for the steady problem (i.e., (2a–2b) but with the time derivative omitted) with experimental results of [9]. A heat source was treated as the passive tracers and the wind flow maintained in such a way that the flow yielded an approximate logarithmic velocity profile $u^* = u_* \log(z^*/z_0^*)/\kappa$ with roughness height $z_0^* = 0.12$ mm and $\kappa = 0.38$. We take the molecular viscosity to be $k_{\text{md}} = 10^{-6}$. The wake-strength parameter is taken as $\Pi = 0.09$, see [11]. The heat source was situated at 60mm above the zero plane of the surface and the depth of the carrier fluid was $D = 540$ mm, giving the non-dimensional height of the source as $z_p = 60/540$.

The vertical and downstream distances were normalized by the heat source height z_p and the concentration C has been normalized as $C^n = C$ by a temperature scale of the form: $\Theta^* = F/(z_p u(z_p))$, where F is the constant flux of contaminant through a plane normal to the flow.

Measurements of the concentration are available from [9] at four down-stream locations: $x = 0.2778, 0.8333, 1.6667,$ and 3.3333 . These are shown, left to right, as circles in Figure 3 below. The closest down-stream station is our main interest of location where the interior layer is much more stronger than the other three locations. That diagram also shows the model's predictions at each of these four down-stream locations. For the first location, we took $a = 0.02$ (chosen by inspection to resolve the portion of the later of interest). When the problem is reformulated as in (4) this leads to values of $\varepsilon_1(0, z_p)$ and $\varepsilon_2(0, z_p)$ required to form the mesh described in Section 3.3 as 0.0062 and 0.0390, respectively. Clearly excellent agreement can be observed between the data concentration measurements and the predictions when the fitted mesh described above is employed. We also give the predictions obtained using a uniform mesh. As was observed in [7], that approach overestimates the width of the layer, and underestimate the strength of the concentration.

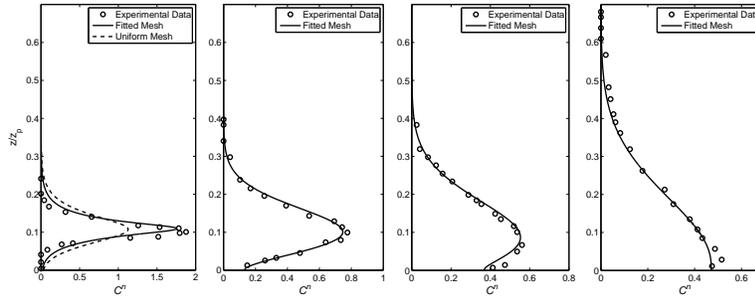


Fig. 3. Comparisons at the four down-stream locations

For the remaining three down-stream distances we took $a = 0.4$ and give the results just for a fitted mesh; the results for a uniform mesh are very similar. Again excellent agreement is found between measurements and numerical results, though at these distances the layer is not as strong.

5 Conclusions and observations

We have provided an improved model for dispersion of settling particles in an advection-driven flow, shown how to employ a piecewise uniform, Shishkin-type mesh, and found excellent agreement between the experimental measurements and the numerical results.

The use of a Shishkin meshes for singularly perturbed problems has been widely studied; see e.g., [5, 10, 2]. The majority of studies are concerned with obtaining uniform convergence results for model problems; this study adds to the smaller number dealing with models that can validated against experimental data. Much further work is required, however, to provide a mathematical justification for the approach for this specific problem.

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