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Some aspects of modelling pollutant transport in fluid flow

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Abstract

Modelling the dispersal of pollution by a fluid stream presents several interesting mathematical challenges. In this paper, the case where the fluid flows slowly and steadily between two parallel plates is considered. The forward time problem is investigated.

Introduction

Pollutant dispersion is the mechanism by which a pollutant, either as solid particles or dissolved in the fluid is spread through the medium. Advection (or convection) refers to the process by which the pollutant is physically transported by the fluid's velocity profile. The dispersion depends on the rates of molecular diffusion or mechanical processes such as turbulence.

In this paper, we will be focusing on one aspect of a research project that has been undertaken by the author, namely the forward and inverse modelling of the one–dimensional advection-dispersion model. The model being considered here is applied to fluid flow with velocity distribution $u(y)$ between two horizontal plates of infinite lateral extent, a distance d apart.

It is supposed that, at time $t = 0$, an amount Q kg m^{-1} (mass per unit width) of pollutant is emplaced in the region $0 \le x \le \Delta$ between the plates, giving an initial concentration $F_0 = Q/d\Delta$ in that region, with concentration $F = 0$ elsewhere [see Figure 1(a)].

Our problem can then be modelled with the following partial differential equation:

$$\frac{\partial F}{\partial t} + u(y)\frac{\partial F}{\partial x} = D\frac{\partial^2 F}{\partial x^2} \qquad (1)$$

subject to the initial condition:

$$F(x, y, 0) = F_0\left[H(x) - H(x - \Delta)\right]$$

where H is the Heaviside function, $F(x, y, t)$ is the volumetric density of the pollutant, D is the overall dispersion coefficient, $u(y)$ is the speed of the fluid, while F_0 and Δ are the initial density and axial length (along x-axis) of the pollutant region respectively. Figure 1(b) shows the situation a short time later.

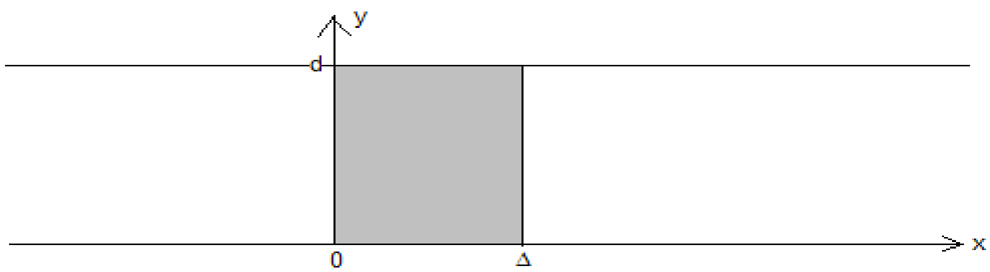

Figure 1(a) - Schematic of a configuration before the dispersion and advection begins.

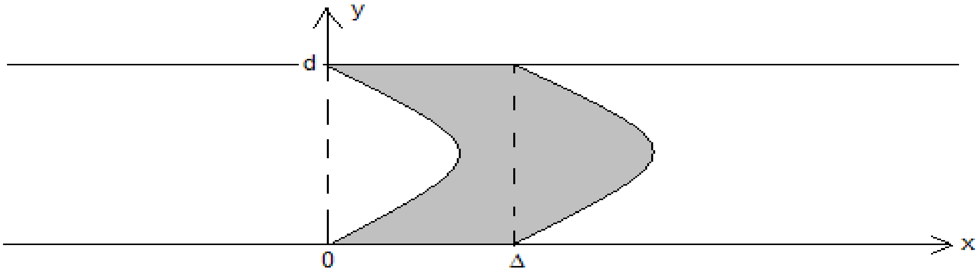

Figure 1(b) - Schematic of a configuration a short time ($t < \Delta/u_{\max}$) after dispersion and advection begins.

Forward Time Problem

We assume that the flow has a small Reynolds number and therefore that the speed of the fluid has a parabolic profile which takes the form (Currie, 1993):

$$u(y) = \frac{4u_{\max}}{d^2} y(d-y) \qquad (2)$$

where d is the height of the pollutation region, $u_{\max}$ is the maximum speed of the fluid (located at the centre for laminar flows).

The solution $F(x, y, t)$ to the above problem is obtained by first applying an appropriate transformation (Logan, 1998):

$$F(x,y,t) = w(x,y,t)\exp\left\{\frac{2xu(y) - t\,[u(y)]^2}{4D}\right\} \qquad (3)$$

The purpose is to eliminate the advective term in Equation (1).

After we substitute expression (3) into Equation (1), we obtain a diffusion equation for $w(x, y, t)$:

$$\frac{\partial w}{\partial t} = D\frac{\partial^2 w}{\partial x^2} \qquad (4)$$

Using the Green's function method, $w(x, y, t)$ has the following form (Logan, 1998):

$$w(x,y,t) = \int_0^\infty \frac{w(v,y,0)}{\sqrt{4\pi Dt}}\exp\left\{\frac{-(x-v)^2}{4Dt}\right\} dv$$

where $w(x,y,0) = F_0[H(x) - H(x-\Delta)]\exp\left\{\frac{-2xu(y)}{4D}\right\}$ is the initial condition for $w(x, y, t)$ and $F_0 = Q/d\Delta$. After we substitute the fundamental solution for $w(x, y, t)$ into the expression for $F(x, y, t)$ and use the properties of the Heaviside function, we obtain:

$$F(x,y,t) = \frac{Q}{d\Delta\sqrt{4\pi Dt}} \int_0^\Delta \exp\left\{\frac{-(x - u(y)t - v)^2}{4Dt}\right\} dv \qquad (5)$$

We want to investigate this function for the flow in the conduit in question. One of the ways of achieving this is through non-dimensionalisation. Applying an appropriate scaling, as detailed below, (5) is transformed into (6). (Note that the starred quantities are dimensionless.)

$$x = d x^* \quad ; \quad \Delta = d \Delta^* \quad ; \quad t = \frac{d}{u_{\max}} t^* \quad ;$$

$$D = u_{\max} d D^* \quad ; \quad F = \frac{Q}{d^2} F^* \quad ; \quad v = d v^* \quad ; \quad y = d y^*$$

$$F^* = \frac{1}{\Delta^* \sqrt{4 \pi D^* t^*}} \int_0^{\Delta^*} \exp\left\{ \frac{-\left(x^* - 4\left(y^* - y^{*2}\right)t^* - v^*\right)^2}{4 D^* t^*} \right\} dv^* \qquad (6)$$

Now, we shall show some plots of (6) for the case $\Delta^* = 1$; $D^* = 1$. This means that the axial length of the pollutant region is the same as the width of the conduit. The integral in Equation (6) is evaluated using the Trapezium Rule. In particular, we shall focus on the following scenarios, plotted in Figures 3 – 7.

Some observations and conclusions can be made based on the plots given in Figures 3 – 8, noting that, for the parameters chosen as above, $F^*(x^*, y^*, t^*) = H(x^*) - H(x^* - \Delta^*)$.

1. The density values fall quickly from the value $F^* = 1$ at $t^* = 0$ to those shown for at $t^* = 5$. The latter non-dimensionalised time translates into the time taken for the initial front edge of the fluid to travel a distance $5d$.

2. The density profiles for $x^* = 0.5$, 1 and 2 have their minima at the centre of the conduit ($y^* = 0.5$). Because the fluid flow has a parabolic velocity profile, the maximum speed of the fluid is at the centre, and so the pollutant at the centre gets carried along and dispersed more quickly than at the edges.

3. As time gets large, the density of the pollutant tends to zero. This is because the bulk of the pollutant is already advected and diffused by the fluid.

4. At a position ahead of the initial pollutant region (e.g. at $x^* = 2$), we see that, at a given time, the minimum F values are greater than at points in the initial pollutant regime (e.g. at the points where $x^* = 0.5$ and $x^* = 1$). However, we note that the density at the edges is lower than at points in the initial pollutant region. We note that at the density values throughout the cross-section at $x^* = 2$ are initially zero and rise in value before they fall.

5. At $y^* = 0.5$, i.e. at the centre of the conduit, we observe that the density profile flattens out and decreases in overall value as time progresses. This illustrates the manner in which the fluid spreads and smears the pollutant as it pushes through the conduit.

6. The density profile at the edges, as depicted in Figures 7 and 8 are the same, which reflects the consistency of the model insofar as the flow pattern is symmetric about $y^* = 0.5$.

Conclusion

Pollutant dispersion is a topic which presents several interesting mathematical challenges. The one-dimensional advection-diffusion model forms the principal basis for the forward modelling of pollutant transport mechanisms. There are various approaches to this problem, some drawn from statistics, but the methodology developed here is deterministic in nature. Recent developments in this field have involved a combination of statistics and differential equations to tackle such problems. Such ties are evident in recent publications involving the probability density function, which is used to solve a class of differential equations known as stochastic PDEs.

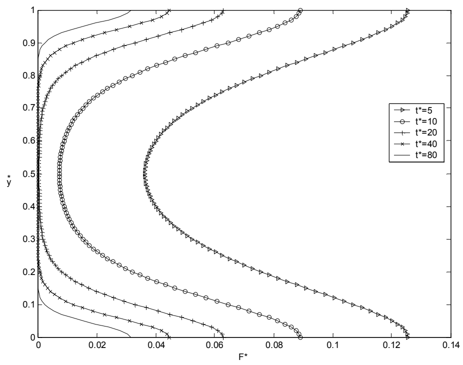

Figure 3 - Plot of non-dimensionalised density, F^* vs non-dimensionalised cross-sectional width y^* for $x^* = 0.5$.

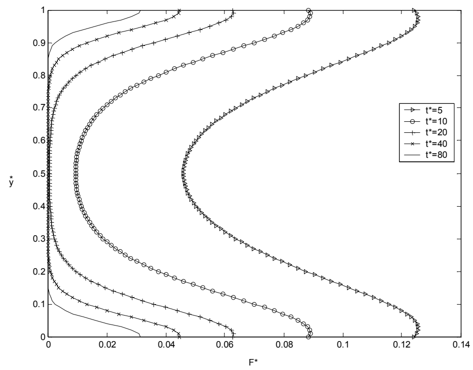

Figure 4 - Plot of non-dimensionalised density, F^* vs non-dimensionalised cross-sectional width y^* for $x^* = 1$.

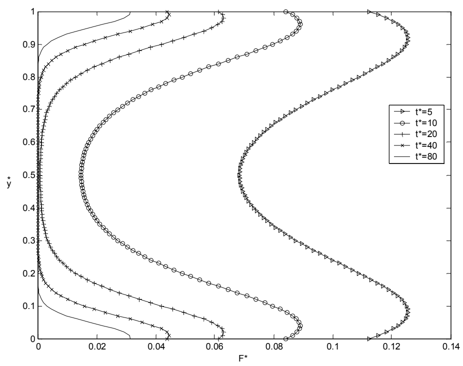

Figure 5 - Plot of non-dimensionalised density, F^* vs non-dimensionalised cross-sectional width y^* for $x^* = 2$.

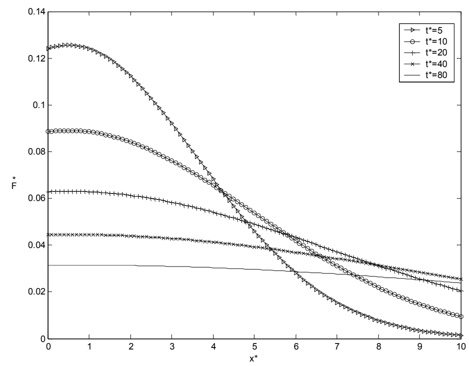

Figure 6 - Plot of non-dimensionalised density, F^* vs non-dimensionalised axial length x^* at $y^* = 0$.

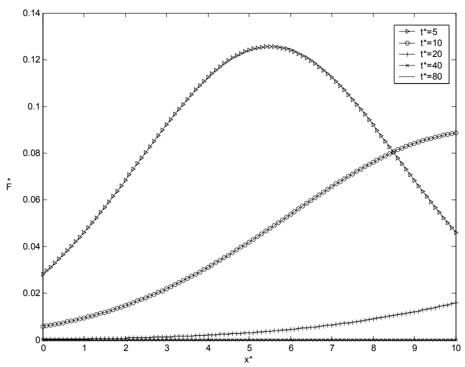

Figure 7 - Plot of non-dimensionalised density, F^* vs non-dimensionalised axial length x^* at $y^* = 0.5$.

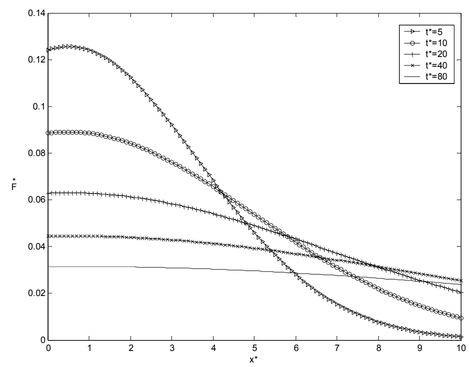

Figure 8 - Plot of non-dimensionalised density, F^* vs non-dimensionalised axial length x^* at $y^* = 1$.

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