8

Multiscale Dispersion in 2 Dimensions

8.1 Introduction

In Chapter 7, we have developed the 2 dimensional solute transport model and estimated the dispersion coefficients in both longitudinal and transverse directions using the stochastic inverse method (SIM), which is based on the maximum likelihood method. We have seen that transverse dispersion coefficient relative to longitudinal dispersion coefficient increases as σ^2 increases when the flow length is confined to 1.0. In this chapter, we extend the SSTM2d into a partially dimensional form as we did for 1 dimension, so that we can explore the larger scale behaviours of the model. However, the experimental data on transverse dispersion is scarce in laboratory and field scales limiting our ability to validate the multiscale dispersion model. In this chapter, we briefly outline the dimensionless form of SSTM2d and illustrate the numerical solution for a particular value of flow length. We also estimate the dispersion coefficients using the SIM for the same flow length.

8.2 Basic Equations

As in the one dimensional case, we define dimensionless distances to start with:

$$z_x = \frac{x}{L_x}, \qquad 0 \le z_x \le 1,$$

and

$$z_y = \frac{y}{L_y}, \qquad 0 \le z_y \le 1.$$

We also define dimensionless concentration with respect to the maximum concentration, C_0 :

$$\Gamma(x,y,t) = \frac{C(x,y,t)}{C_0}, \qquad 0 \le \Gamma \le 1.$$

As in Chapter 6, we derive the following partial derivatives:

$$\frac{\partial C}{\partial x} = \frac{C_0}{L_x}\frac{\partial \Gamma}{\partial z_x}; \quad \frac{\partial^2 C}{\partial x^2} = \frac{C_0}{L_x^2}\frac{\partial^2 \Gamma}{\partial z_x^2}; \quad \frac{\partial C}{\partial y} = \frac{C_0}{L_y}\frac{\partial \Gamma}{\partial z_y}; \text{ and } \frac{\partial^2 C}{\partial y^2} = \frac{C_0}{L_y^2}\frac{\partial^2 \Gamma}{\partial z_y^2}.$$

As we have developed the SSTM2d for [0,1] domains in both x and y directions (see Chapter 6), we define the cosine and sine of the angle as follows,

$$\cos\theta = \frac{z_x}{\sqrt{z_x^2 + z_y^2}}, \text{and}$$

$$\sin\theta = \frac{z_y}{\sqrt{z_x^2 + z_y^2}}.$$

We can also express the partial derivatives of the mean velocities in both x and y directions in terms of dimensionless space variables:

$$\frac{\partial \bar{v}_x}{\partial x} = \frac{\partial \bar{v}_x}{\partial z_x}\frac{\partial z_x}{\partial x} = \frac{1}{L_x}\frac{\partial \bar{v}_x}{\partial z_x};$$

$$\frac{\partial^2 \bar{v}_x}{\partial x^2} = \frac{\partial}{\partial z_x}\left(\frac{\partial \bar{v}_x}{\partial x}\right)\frac{\partial z_x}{\partial x} = \frac{1}{L_x}\frac{\partial}{\partial z_x}\left(\frac{1}{L_x}\frac{\partial \bar{v}_x}{\partial z_x}\right) = \frac{1}{L_x^2}\frac{\partial^2 \bar{v}_x}{\partial z_x^2};$$

$$\frac{\partial \bar{v}_y}{\partial y} = \frac{1}{L_y}\frac{\partial \bar{v}_y}{\partial z_y}; \text{and,}$$

$$\frac{\partial^2 \bar{v}_y}{\partial y^2} = \frac{1}{L_y^2}\frac{\partial^2 \bar{v}_y}{\partial z_y^2}.$$

Similarly, we can express the derivatives related to solute concentration in terms of dimensionless variables:

$$\frac{\partial C}{\partial t} = C_0\frac{\partial \Gamma}{\partial t};$$

$$\frac{\partial^2 C}{\partial x^2} = \frac{C_0}{L_x^2}\frac{\partial^2 \Gamma}{\partial z_x^2}; \text{ and,}$$

$$\frac{\partial^2 C}{\partial y^2} = \frac{C_0}{L_y^2}\frac{\partial^2 \Gamma}{\partial z_y^2}.$$

We recall the SSTM2d in x and y co-ordinates,

$$dC = -CdI_{0,x} - \frac{\partial C}{\partial x}dI_{1,x} - \frac{\partial^2 C}{\partial x^2}dI_{2,x} - CdI_{0,y} - \frac{\partial C}{\partial y}dI_{1,y} - \frac{\partial^2 C}{\partial y^2}dI_{2,y};$$

$$\text{where} \quad dI_{0,x} = \left(\frac{\partial \bar{v}_x}{\partial x} + \frac{h_x}{2}\frac{\partial^2 \bar{v}_x}{\partial x^2}\right)dt + \sigma\sum_{j=1}^{m}\sqrt{\lambda_{xj}\lambda_{yj}}P_{0j}db_j(t);$$

$$dI_{1,x} = \left(\bar{v}_x + h_x\frac{\partial \bar{v}_x}{\partial x}\right)dt + \sigma\sum_{j=1}^{m}\sqrt{\lambda_{xj}\lambda_{yj}}P_{1j}db_j(t);$$

$$dI_{2,x} = \left(\frac{h_x}{2} \bar{v}_x \right) dt + \sigma \sum_{j=1}^{m} \sqrt{\lambda_{xj} \lambda_{yj}} P_{2j} db_j(t);$$

$$dI_{0,y} = \left(\frac{\partial \bar{v}_y}{\partial y} + \frac{h_y}{2} \frac{\partial^2 \bar{v}_y}{\partial y^2} \right) dt + \sigma \sum_{j=1}^{m} \sqrt{\lambda_{xj} \lambda_{yj}} Q_{0j} db_j(t);$$

$$dI_{1,y} = \left(\bar{v}_y + h_y \frac{\partial \bar{v}_y}{\partial y} \right) dt + \sigma \sum_{j=1}^{m} \sqrt{\lambda_{xj} \lambda_{yj}} Q_{1j} db_j(t); \text{and,}$$

$$dI_{2,y} = \left(\frac{h_y}{2} \bar{v}_y \right) dt + \sigma \sum_{j=1}^{m} \sqrt{\lambda_{xj} \lambda_{yj}} Q_{2j} db_j(t).$$

Because $\lambda_{xj}, \lambda_{yj}, h_x, h_y, P_{0j}, P_{1j}, P_{2j}, Q_{0j}, Q_{1j}$, and Q_{2j} are calculated for the domain [0, 1], we use the same values and functions but we use the following symbols: $\lambda_{z_x j}, \lambda_{z_y j}, h_{z_x}, h_{z_y}, P_{0j}, P_{1j}, P_{2j}, Q_{0j}, Q_{1j}$, and Q_{2j}. Now we calculate $d\Gamma$ based on the transformed partially dimensional governing equation:

$$d\Gamma = -\Gamma dI_{0,z_x} - \frac{1}{L_x} \frac{\partial \Gamma}{\partial z_x} dI_{1,z_x} - \frac{1}{L_x^2} \frac{\partial^2 \Gamma}{\partial z_x^2} dI_{2,z_x} - \Gamma dI_{0,z_y} - \frac{1}{L_y} \frac{\partial \Gamma}{\partial z_y} dI_{1,z_y} - \frac{1}{L_y^2} \frac{\partial^2 \Gamma}{\partial z_y^2} dI_{2,z_y}; \qquad (8.2.1)$$

where $dI_{0,z_x} = \left(\frac{1}{L_x} \frac{\partial \bar{v}_x}{\partial z_x} + \frac{h_{z_x}}{2} \frac{1}{L_x^2} \frac{\partial^2 \bar{v}_x}{\partial z_x^2} \right) dt + \sigma \sum_{j=1}^{m} \sqrt{\lambda_{z_x j} \lambda_{z_y j}} P_{0j} db_j(t);$

$$dI_{1,z_x} = \left(\bar{v}_x + h_{z_x} \frac{1}{L_x} \frac{\partial \bar{v}_x}{\partial z_x} \right) dt + \sigma \sum_{j=1}^{m} \sqrt{\lambda_{z_x j} \lambda_{z_y j}} P_{1j} db_j(t);$$

$$dI_{2,z_x} = \left(\frac{h_{z_x}}{2} \bar{v}_x \right) dt + \sigma \sum_{j=1}^{m} \sqrt{\lambda_{z_x j} \lambda_{z_y j}} P_{2j} db_j(t);$$

$$dI_{0,z_y} = \left(\frac{1}{L_y} \frac{\partial \bar{v}_y}{\partial z_y} + \frac{h_{z_y}}{2} \frac{1}{L_y^2} \frac{\partial^2 \bar{v}_y}{\partial z_y^2} \right) dt + \sigma \sum_{j=1}^{m} \sqrt{\lambda_{z_x j} \lambda_{z_y j}} Q_{0j} db_j(t);$$

$$\partial I_{1,z_y} = \left(\bar{v}_y + h_{z_y} \frac{1}{L_y} \frac{\partial \bar{v}_y}{\partial z_y} \right) \partial t + \sigma \sum_{j=1}^{m} \sqrt{\lambda_{z_x j} \lambda_{z_y j}} Q_{1j} db_j(t); \text{ and,}$$

$$dI_{2,z_y} = \left(\frac{h_{z_y}}{2} \bar{v}_y \right) dt + \sigma \sum_{j=1}^{m} \sqrt{\lambda_{z_x j} \lambda_{z_y j}} Q_{2j} db_j(t).$$

The above equations constitute the multiscale SSTM2d and we developed the numerical solutions when the flow length along the main flow direction is 100 m and the flow length in the direction perpendicular to the main direction is 25 m.

8.3 A Sample of Realisations of Multiscale SSTM2d

For the illustrative purposes, we plot three realisations of concentration when C_0 =1.0 at (x=0; and y=0) when time is 20 days for two different σ^2 values, 0.01 and 0.1. These are shown in Figures 8.1 and 8.2.

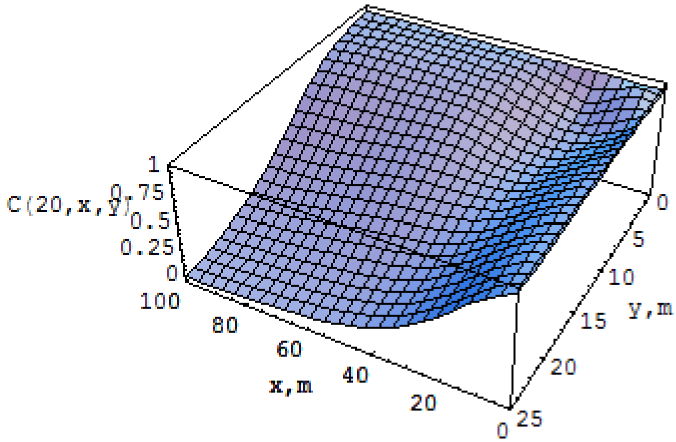

Figure 8.1. A concentration realisation when time is 20 days for σ^2 =0.01. Mean velocity in x direction is 0.5 m/day and, in y direction is 0.0.

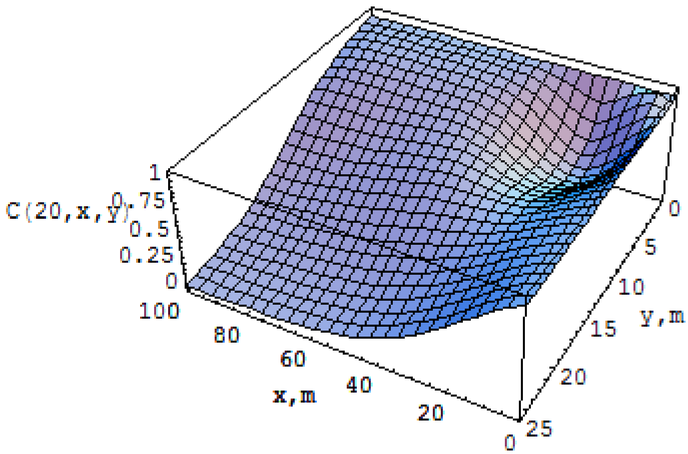

Figure 8.2. A concentration realisation when time is 20 days for σ^2 =0.1. (Same conditions as in Figure 8.1.)

8.4 Estimation of Dispersion Coefficients

We use the same methodology as in Chapter 7 with a slight modification to the advection-dispersion stochastic partial differential equation (SPDE) to make it dimensionless.

The SPDE becomes,

$$\frac{\partial \Gamma}{\partial t} = \left\{ \frac{D_L}{L_x^2} \frac{\partial^2 \Gamma}{\partial z_x^2} + \frac{D_T}{L_y^2} \frac{\partial^2 \Gamma}{\partial z_y^2} \right\} - \frac{\overline{v}_x}{L_x} \frac{\partial \Gamma}{\partial z_x} + \xi(z,t). \tag{8.4.1}$$

We can use the SIM to estimate the parameters but to obtain the dispersion coefficients, we note the following relations:

$$D_L = \left[\text{estimated} \left(\frac{D_L}{L_x^2} \right) \right] \times L_x^2 \text{;and}$$

$$D_T = \left[\text{estimated} \left(\frac{D_T}{L_y^2} \right) \right] \times L_y^2 .$$

Based on 60 realisations for each value of σ^2, Table 8.1 shows the estimated mean dispersion coefficients for the same boundary and initial conditions.

σ^2	D_L	D_T
0.01	5.445969667	0.259079583
0.1	6.853118	1.043493717

Table 8.1. The estimated mean dispersion coefficients for two different σ^2 values (b=0.1).

8.5 Summary

In this brief chapter, we have given sufficient details of development of the multiscale SSTM2d and a sample of its realisations. We also have adopted SIM to estimate dispersion coefficients in both longitudinal and lateral directions. The computational experiments we have done with the SSTM2d show realistic solutions under variety of boundary and initial conditions, even for larger scales such 10000 m. However, it is not important to illustrate the results, as we have discussed the one dimensional SSTM in detail in Chapter 6. If there are reliable dispersivity data in different scales, both in longitudinal and transverse directions, then one can develop much more meaningful relations between longitudinal and lateral dispersivities based on a properly validated model.