Chapter 11
Reduced Models for PDE Problems

In previous chapters, we have considered methods for solving problems in partial differential equations: the method of characteristics in Chap. 2, similarity solutions in Chap. 5, and Fourier series in Chap. 8. Now we pursue another approach that can be applied to problems where we want to obtain certain properties of the solution, but do not need an explicit representation of the entire solution. We will see that in some cases, this leads to substantially shorter calculations.

The approach of *reduced models* is to reformulate a problem into a simpler form that preserves the properties of interest, but decouples them from the calculation of other details of the solution's behaviour. We will describe the *method of moments*, which produces reduced models that can describe the evolution of some quantities for the solution averaged over the domain.[1]

11.1 The Method of Moments

For a solution $\rho(x, t)$ of a PDE problem on a domain D, we can define the *moment integrals*,

$$M_n(t) \equiv \int_D x^n \rho(x, t)\, dx \qquad n = 0, 1, 2, \ldots \tag{11.1}$$

If ρ represents a density, then the $n = 0$ integral corresponds to the total mass. For some problems, we can determine a simple set of equations governing the evolution of the moment integrals (without explicitly finding the solution $\rho(x, t)$) and then use those results to infer information about the behaviour of the solution to the problem.

[1] We have already encountered *reduced dimension models* in Chap. 8, where we developed a methodology for solving PDEs on slender two-dimensional domains by replacing them with ODE problems for an asymptotic solution applying on most of the domain.

T. Witelski and M. Bowen, *Methods of Mathematical Modelling*,
Springer Undergraduate Mathematics Series, DOI 10.1007/978-3-319-23042-9_11

We illustrate this approach for the heat equation on $-\infty < x < \infty$

$$\frac{\partial \rho}{\partial t} = \frac{\partial^2 \rho}{\partial x^2}, \tag{11.2a}$$

with far-field boundary conditions $u \to 0$ as $|x| \to \infty$ and initial condition

$$\rho(x, t = 0) = f(x), \tag{11.2b}$$

where $f \to 0$ rapidly as $|x| \to \infty$.

Consider the zeroth moment (mass) integral,

$$M_0(t) = \int_{-\infty}^{\infty} \rho(x, t)\, dx.$$

In order to obtain an equation to describe the evolution of $M_0(t)$, we calculate its rate of change with respect to time

$$\frac{dM_0}{dt} = \frac{d}{dt} \int_{-\infty}^{\infty} \rho\, dx = \int_{-\infty}^{\infty} \frac{\partial \rho}{\partial t}\, dx,$$

where we have interchanged the order of differentiation (with respect to time) and integration (over space). Using the PDE (11.2a) to replace the time derivative with the second order spatial derivative and then integrating yields

$$\frac{dM_0}{dt} = \int_{-\infty}^{\infty} \frac{\partial^2 \rho}{\partial x^2}\, dx = \left.\frac{\partial \rho}{\partial x}\right|_{-\infty}^{\infty} = 0 - 0 = 0,$$

where we have used that $\rho_x \to 0$ as $|x| \to \infty$ for smooth $\rho \to$ constant (specifically $\rho \to 0$) in evaluating the boundary terms. Consequently, we have

$$\frac{dM_0}{dt} = 0,$$

so that the total mass is constant in the problem and its value for problem (11.2a, 11.2b) is determined by its initial value at $t = 0$,

$$M_0(0) = \int_{-\infty}^{\infty} f(x)\, dx. \tag{11.3}$$

We can proceed similarly for the first moment, $M_1(t) = \int_{-\infty}^{\infty} x\rho\,dx$, for which we find

$$\frac{dM_1}{dt} = \frac{d}{dt}\int_{-\infty}^{\infty} x\rho\,dx = \int_{-\infty}^{\infty} x\frac{\partial\rho}{\partial t}\,dx = \int_{-\infty}^{\infty} x\frac{\partial^2\rho}{\partial x^2}\,dx.$$

Making use of integration by parts and employing further assumptions about the decay of the solution as $|x| \to \infty$ being sufficiently rapid to eliminate boundary terms from integration by parts, we obtain

$$\frac{dM_1}{dt} = x\frac{\partial\rho}{\partial x}\bigg|_{-\infty}^{\infty} - \int_{-\infty}^{\infty}\frac{\partial\rho}{\partial x}\,dx = 0.$$

Therefore, M_1 is also a constant, also set by the initial conditions as

$$M_1(0) = \int_{-\infty}^{\infty} xf(x)\,dx. \tag{11.4}$$

Having these moments allow us to evaluate the centre of mass (the average value of position weighted by the density), defined by the ratio of the first moment to the mass,

$$\bar{x}(t) = \frac{M_1}{M_0} = \frac{\int xf\,dx}{\int f\,dx}. \tag{11.5}$$

Investigating the evolution of $\bar{x}$ can provide an understanding of whether the solution is generally moving in some direction or remaining in a fixed location; in this case, $\bar{x}$ remains fixed at its initial position as both M_0 and M_1 are constants.

Proceeding to the second moment, we find

$$\begin{aligned}\frac{dM_2}{dt} &= \int_{-\infty}^{\infty} x^2\frac{\partial\rho}{\partial t}\,dx = \int_{-\infty}^{\infty} x^2\frac{\partial^2\rho}{\partial x^2}\,dx\\ &= x^2\frac{\partial\rho}{\partial x}\bigg|_{-\infty}^{\infty} - \int 2x\frac{\partial\rho}{\partial x}\,dx\\ &= -2\left(x\rho\bigg|_{-\infty}^{\infty} - \int_{-\infty}^{\infty}\rho\,dx\right),\end{aligned}$$

where the boundary conditions have been used to successively eliminate the boundary terms from the two applications of integration by parts. Consequently, the rate of change of the second moment is given in terms of the mass M_0,

$$\frac{dM_2}{dt} = 2M_0. \tag{11.6}$$

For the heat equation, we have already shown that the mass is constant and so the second moment increases at a constant rate. We can therefore express M_2 in terms of the initial conditions as

$$M_2(t) = 2t \int_{-\infty}^{\infty} f\, dx + \int_{-\infty}^{\infty} x^2 f\, dx. \tag{11.7}$$

The *variance* is defined as the second moment of ρ with respect to the centre of mass and yields a fundamental measure of the spreading of the solution

$$\begin{aligned} V(t) &= \int_{-\infty}^{\infty} (x-\bar{x})^2 \rho\, dx \\ &= \int_{-\infty}^{\infty} x^2 \rho\, dx - 2\bar{x} \int_{-\infty}^{\infty} x\rho\, dx + \bar{x}^2 \int_{-\infty}^{\infty} \rho\, dx \\ &= M_2 - 2\bar{x} M_1 + \bar{x}^2 M_0 \\ &= M_2 - 2\frac{M_1^2}{M_0} + \frac{M_1^2}{M_0^2} M_0 \\ &= M_2 - \frac{M_1^2}{M_0}. \end{aligned}$$

The variance is also used to define the standard deviation in terms of its square-root, $\sigma = \sqrt{|V|}$, yielding

$$\sigma^2(t) = \left| M_2 - \frac{M_1^2}{M_0} \right|. \tag{11.8}$$

While the terminology used above comes from probability and statistics, the definitions are direct analogues of the formulas for the moment of inertia ($V \to I$) and radius of gyration ($\sigma \to R$) used in mechanics for describing the motion of objects [40, 67].

A somewhat more direct approach for constructing moment equations is to directly the integrate the product of the weight function with the PDE over the domain,

$$\int_D x^n (\text{PDE})\, dx.$$

Consider for example the following problem for the wave equation on the finite domain, $0 \le x \le 1$,

$$\frac{\partial^2 \rho}{\partial t^2} = \frac{\partial^2 \rho}{\partial x^2} \tag{11.9a}$$

subject to boundary conditions

$$\left.\frac{\partial \rho}{\partial x}\right|_{x=0} = e^t, \qquad \left.\frac{\partial \rho}{\partial x}\right|_{x=1} = 12t^2, \tag{11.9b}$$

and initial conditions

$$\rho(x,0) = 1 \qquad \left.\frac{\partial \rho}{\partial t}\right|_{t=0} = \cos(3\pi x). \tag{11.9c}$$

Integrating (11.9a) over the domain and the applying boundary conditions yields an ODE for the zeroth moment,

$$\int_0^1 (\rho_{tt} = \rho_{xx})\, dx \quad \Longrightarrow \quad \frac{d^2 M_0}{dt^2} = \left.\frac{\partial \rho}{\partial x}\right|_{x=0}^{x=1} \quad \Longrightarrow \quad \frac{d^2 M_0}{dt^2} = 12t^2 - e^t.$$

Integrating the initial conditions for ρ generates initial conditions for M_0, $M_0(0) = 1$ and $M_0'(0) = 0$ and consequently yields $M_0(t) = t^4 + t + 2 - e^t$.

In general, the method of moments is considered to be successful when it produces a finite, closed set of ODEs that can used to describe selected solution properties. If the moment equations depend on an indefinite number of further moments or other properties of ρ, then the system is not closed. In such cases, the system may be approximated through the use of problem-specific *closure relations*, as used in the modelling of turbulent fluid flows. While this method has been described here as an analytical approach, similar analysis is used to reduce PDE problems to simpler systems of equations that can be evaluated computationally in numerical methods such as *Galerkin projection methods*.

We now go on to consider two classic applied mathematics problems that have different relations to the method of moments.

11.2 Turing Instability and Pattern Formation

In this section, we present an example of how to analyse the development of patterns in PDE models, as occur in important systems in mathematical biology and other applications. The problem considered will also show that predictions from reduced models can sometimes be misleading and must be considered with caution.

We have observed that solutions of the heat equation will generically exhibit diffusive spreading (as implied by $\sigma(t)$ increasing with time from (11.8) and similarity solutions having $x = O(\sqrt{t})$ from Sect. 5.5). Consider the problem for the heat equation on a finite domain with no-flux boundary conditions,

$$\frac{\partial \rho}{\partial t} = \frac{\partial^2 \rho}{\partial x^2}, \qquad 0 \le x \le \pi,$$

$$\left.\frac{\partial \rho}{\partial x}\right|_{x=0} = 0, \qquad \left.\frac{\partial \rho}{\partial x}\right|_{x=\pi} = 0,$$

with a given initial condition

$$\rho(x, 0) = f(x).$$

The mass of the solution will be conserved for all times. Further, it can be shown that for $t \to \infty$, the solution will approach the average value set by the initial condition

$$\rho(x, t \to \infty) \to \bar{f} \qquad \text{where} \quad \bar{f} = \frac{1}{\pi}\int_0^{\pi} f(x)\, dx.$$

Similarly, adding diffusive effects to a transport equation can generally be expected to cause the solution to both spread and smooth out. Likewise, if diffusion is incorporated into a model for chemical reaction kinetics to yield a partial differential equation, as in

$$\frac{dc}{dt} = -c \qquad \Longrightarrow \qquad \frac{\partial c}{\partial t} = \frac{\partial^2 c}{\partial x^2} - c,$$

then it can be shown that the spatial variation in the initial condition $c(x, 0)$ will eventually level-out as the solution approaches the solution of the original ODE, $c(x, t) \to c(t)$ (see Exercise 11.3).

However, the work of Alan Turing (1912–1954) showed that this intuition is not always a good guide for more complicated systems. In the context of developmental biology [100], he showed that the addition of diffusive effects to a system of reactions could enhance spatial structure rather than suppressing it.

To illustrate this effect, let us consider a simple system involving two chemicals, P and Q, that interact and are also supplied into or drained out of the system according to

$$P + Q \to 2P \qquad P \to \text{(drain)} \qquad Q \to 2Q \qquad \text{(source)} \to Q.$$

These two substances may diffuse at different rates, so we will describe their spatial evolution using diffusion terms with different coefficients. Hence, consider the nondimensionalized governing equations,

$$\frac{\partial p}{\partial t} = 2pq - 4 + \frac{\partial^2 p}{\partial x^2}, \qquad \frac{\partial q}{\partial t} = -2pq + q + 3 + D\frac{\partial^2 q}{\partial x^2} \tag{11.10a}$$

where $D \geq 1$ is the ratio of diffusion coefficients giving the relative spreading rate of Q compared to P. Let the domain be $0 \leq x \leq \pi$, with no-flux boundary conditions,

$$\frac{\partial p}{\partial x} = 0 \quad \text{and} \quad \frac{\partial q}{\partial x} = 0 \qquad \text{at } x = 0 \text{ and } x = \pi \tag{11.10b}$$

and initial conditions at $t = 0$,

$$p(x, 0) = p_0(x), \qquad q(x, 0) = q_0(x). \tag{11.10c}$$

This is a simple example of a *reaction-diffusion system*. Research on similar systems has shown that they can produce surprisingly complicated results, so the general approach to studying reaction-diffusion problems is to start with the simplest possible solutions and build up an understanding from there.

Seeking time-independent steady states reduces the PDEs for $p(x, t)$, $q(x, t)$ to two coupled nonlinear ODEs for $\bar{p}(x)$, $\bar{q}(x)$, which can still be difficult to solve. Hence, we further constrain our search and obtain spatially uniform (constant) solutions, p_*, q_* from the algebraic relations

$$0 = 2p_*q_* - 4, \qquad 0 = -2p_*q_* + q_* + 3, \tag{11.11}$$

which yield the equilibrium solution $p_* = 2$, $q_* = 1$. To explore the stability of this state to small perturbations, let

$$p = p_* + \varepsilon\tilde{p}(x, t), \qquad q = q_* + \varepsilon\tilde{q}(x, t) \tag{11.12}$$

with $\varepsilon \to 0$. Treating these expression as perturbation expansions, we substitute into (11.10a). At leading order we recover the steady-state equations (11.11), while at $O(\varepsilon)$ we get the linearised version of (11.10a),

$$\frac{\partial \tilde{p}}{\partial t} = 2\tilde{p} + 4\tilde{q} + \frac{\partial^2 \tilde{p}}{\partial x^2}, \qquad \frac{\partial \tilde{q}}{\partial t} = -2\tilde{p} - 3\tilde{q} + D\frac{\partial^2 \tilde{q}}{\partial x^2}. \tag{11.13}$$

Applying the method of moments to this system, we can determine the evolution of the mean values of $\tilde{p}$ and $\tilde{q}$ from the zeroth moment integrals,

$$P_0(t) = \frac{1}{\pi}\int_0^\pi \tilde{p}(x, t)\, dx, \qquad Q_0(t) = \frac{1}{\pi}\int_0^\pi \tilde{q}(x, t)\, dx.$$

Integrating (11.13) over the domain and applying the boundary conditions yields the coupled ODEs,

$$\frac{dP_0}{dt} = 2P_0 + 4Q_0, \qquad \frac{dQ_0}{dt} = -2P_0 - 3Q_0. \tag{11.14}$$

Note that (11.14) corresponds to (11.13) restricted to spatially uniform solutions. A phase plane analysis of this system shows that $(P_0, Q_0) = (0, 0)$ is the only equilibrium point and has eigenvalues $\lambda = (-1 \pm i\sqrt{7})/2$, so it is a stable spiral point. Hence all solutions of (11.14) will converge to $(P_0, Q_0) = (0, 0)$ as $t \to \infty$. While this correctly predicts the evolution of the means of the perturbations $\tilde{p}$ and $\tilde{q}$, further analysis is needed to describe their spatial structure.

The process of reducing a nonlinear problem, like (11.10a), to a linear problem, (11.13), by focusing on the evolution of solutions starting near an equilibrium state is a classic example of linear stability analysis. We applied this approach to ODEs in Chap. 1; this is also one of the most general approaches to exploring the behaviour of nonlinear PDEs [26].

To complete the analysis, we make use of the linearity of system (11.13) to obtain solutions as linear superpositions of eigenmodes, $\tilde{p} = \sum_k \tilde{p}_k(x, t)$, and apply separation of variables to express the eigenmodes as products $\tilde{p}_k(x, t) = f_k(x)g_k(t)$ [44]. Requiring each eigenmode to satisfy the boundary conditions (11.10b) yields

$$\begin{pmatrix} p_k(x,t) \\ q_k(x,t) \end{pmatrix} = \begin{pmatrix} a_k \\ b_k \end{pmatrix} \cos(kx) e^{\lambda_k t}, \tag{11.15}$$

where a_k, b_k, λ_k are constants depending on the wavenumber $k = 0, 1, 2, \ldots$. Substituting each independent mode into (11.13) and eliminating common factors, we arrive at the matrix eigenvalue problem

$$\lambda_k \begin{pmatrix} a_k \\ b_k \end{pmatrix} = \begin{pmatrix} 2 - k^2 & 4 \\ -2 & -3 - k^2 D \end{pmatrix} \begin{pmatrix} a_k \\ b_k \end{pmatrix}. \tag{11.16}$$

For $k = 0$, this is the eigenvalue problem that would be obtained from the stability analysis of the ODE system (11.14). More generally, for $k \geq 0$, we can determine the stability of the eigenmodes from solving the characteristic polynomial for λ_k

$$(\lambda_k + k^2 - 2)(\lambda_k + k^2 D + 3) + 8 = 0. \tag{11.17}$$

The relation between the spatial wavenumber and the real part of the dominant eigenvalue, $\sigma(k) = \mathrm{Re}(\lambda_k^+)$ is often called the *dispersion relation* and concisely conveys the PDE stability results with respect to all admissible types of perturbations, as represented by the eigenmodes with different values of k.

For the case where Q diffuses much more rapidly than P ($D \gg 1$) it can be shown that $\mathrm{Re}(\lambda_k^+)$ can become positive and hence some eigenmodes will grow in amplitude; this is known as a *Turing instability*. The growth rates for system (11.13) when $D = 100$ are plotted in Fig. 11.1, where it can be seen that $k = 1$ is selected as the dominant growing mode (the only integer-valued k with a positive growth rate). Consequently, this mode will eventually dominate the dynamics of the system and produce a pattern

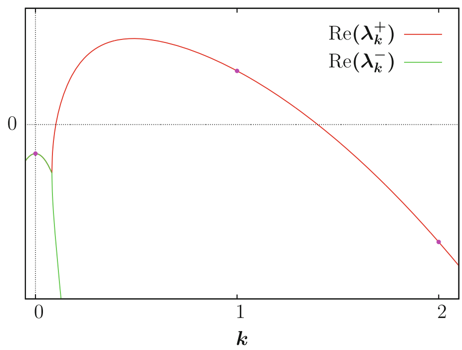

Fig. 11.1 The dispersion relation showing growth rates of eigenmodes (11.15) with $k = 0, 1, 2, \ldots$ of the linearised system (11.13) with $D = 100$

resembling $\cos(x)$ unless the initial conditions (11.10c) have no contribution from the $k = 1$ unstable mode, i.e. $\int_0^\pi (p_0, q_0) \cos(x)\, dx = (0, 0)$. We note that the influence of the parameter D (giving the relative rates of diffusion) dramatically changes the stability of the equilibrium solution for different wavenumbers: a stable spiral for $k = 0$, a saddle point for $k = 1$, and stable node for $k = 2, 3, \ldots$.

For different choices of system parameters, there may be a band of unstable wavenumbers, $k \in \{1, 2, \ldots, k_c\}$ with $\sigma(k) > 0$, that will all grow until nonlinear coupling effects take over to determine the further dynamics of the solution. Systems having $\sigma(k) \geq 0$ below some critical wavenumber, $0 \leq k \leq k_c$, are often called *long-wave unstable* since they involve spatial variations involving only the longest wavelength eigenmodes. The Turing instability has been used in many studies as a model for biological pattern formation, such as the spots and stripes on animal coats [26, 42, 74].

We note that in attempting to use the method of moments for this problem, we considered the zeroth moments of the perturbations in the linearised system (11.13) rather than in the original nonlinear system. There would have been a difficulty in integrating (11.10a) directly, as it might not be immediately clear how to analyse the integral of the nonlinear term, $\int_0^\pi pq\, dx$. In the next section, we will see how this type of issue can be dealt with in the context of a different system.

11.3 Taylor Dispersion and Enhanced Diffusion

We now describe a classic model from fluid dynamics that illustrates the effectiveness of reduction via the moment-type approach.

If a substance (called the *solute*) is released into a channel containing a flowing stream of fluid, the substance will spread out as it is carried downstream by the flow. Part of this behaviour is due to standard "molecular diffusion" effects, but spatial variations in the flow velocity also contribute since the different transport speeds will broaden the area of distribution of the solute.

This problem was studied by G.I. Taylor (1886–1975), who explained how the full transport problem for the solute could be reduced to a one-dimensional model. Taylor's model showed that convective effects can increase the effect of diffusion; this has come to be known as *Taylor dispersion* and has been applied to describe the spread of pollutants in rivers, drugs in blood flow as well as in many other settings. Taylor's original paper [98] was presented in his unique and very physically intuitive style; it is deceptively short and challenging to follow. Here we present a derivation of Taylor's result that is very similar to the approach given by Leal [61, Sect. 3H] (also see [20]).

Consider a dimensional transport problem for the concentration of a solute $\mathsf{C}(\mathsf{X}, \mathsf{Y}, \mathsf{T})$, given by the advection-diffusion equation

$$\frac{\partial \mathsf{C}}{\partial \mathsf{T}} + \nabla \cdot (\mathsf{C}\mathbf{U}) = \mathsf{D}\nabla^2 \mathsf{C}, \tag{11.18a}$$

where $\mathbf{U}(\mathsf{X}, \mathsf{Y}, \mathsf{T})$ is the fluid velocity field and D is the constant of molecular diffusion. We choose the domain to be a two-dimensional long slender channel, $-\infty < X < \infty$, $-\mathrm{H} \le \mathsf{Y} \le \mathrm{H}$, and let the velocity field take the classic *Poiseuille flow* parabolic profile

$$\mathbf{U} = \mathrm{U}_0 \left(1 - \frac{\mathsf{Y}^2}{\mathrm{H}^2}\right) \hat{\mathbf{i}} \qquad -\mathrm{H} \le \mathsf{Y} \le \mathrm{H}, \tag{11.18b}$$

where U_0 is the maximum speed of the flow (see Fig. 11.2 for a schematic of the problem). We assume that there is no flux of the solute out of the sides of the domain, $\hat{\mathbf{n}} \cdot \nabla C = 0$, which for the uniform width channel, simplifies to

$$\left.\frac{\partial \mathsf{C}}{\partial \mathsf{Y}}\right|_{\mathsf{Y}=\pm \mathrm{H}} = 0. \tag{11.18c}$$

While in most common situations, diffusion occurs at the same rate in every direction (so-called *isotropic* behaviour), to help distinguish different effects, we label the diffusion coefficients in the direction of and transverse to the imposed flow as D_x

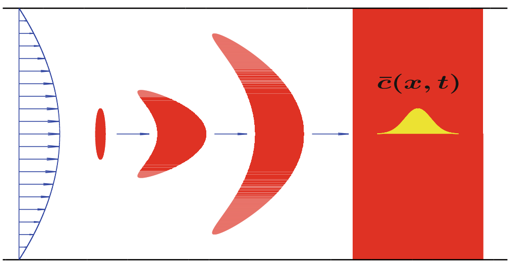

Fig. 11.2 Schematic behaviour of solute dispersion (*green* contours) in a long channel starting from a small release area due to a velocity field (*red*)

and D_y respectively. In this *anisotropic* context, the transport equation (11.18a) takes the form

$$\partial_{\mathsf{T}}\mathsf{C} + \nabla \cdot (\mathsf{C}\mathbf{V}) = 0, \qquad \mathbf{V} = \mathbf{U} - \mathbf{D}\nabla\mathsf{C},$$

where $\mathbf{D}$ is a diffusion coefficient matrix, $\mathbf{D} = \begin{pmatrix} \mathrm{D}_x & 0 \\ 0 & \mathrm{D}_y \end{pmatrix}$. For the isotropic case, where $\mathrm{D}_x = \mathrm{D}_y = \mathrm{D}$, this equation reduces to (11.18a).

We nondimensionalize by taking

$$\mathsf{C} = \mathrm{C}_0 c, \qquad \mathsf{X} = \mathrm{L}x, \qquad \mathsf{Y} = \mathrm{H}y, \qquad \mathsf{T} = (\mathrm{L}/\mathrm{U}_0)t,$$

where C_0 is a concentration scale that could be set by the initial conditions and L is a typical length scale along the channel. Consequently, the scaled problem on $-\infty < x < \infty$, $-1 \le y \le 1$ becomes

$$\frac{\partial c}{\partial t} + (1 - y^2)\frac{\partial c}{\partial x} = \frac{1}{\mathrm{Pe}_x}\frac{\partial^2 c}{\partial x^2} + \frac{1}{\mathrm{Pe}_y}\frac{\partial^2 c}{\partial y^2}, \tag{11.19}$$

with boundary conditions $\partial_y c|_{y=\pm 1} = 0$. The Peclet numbers,

$$\mathrm{Pe}_x = \frac{\mathrm{U}_0\mathrm{L}}{D_x}, \qquad \mathrm{Pe}_y = \frac{\mathrm{U}_0\mathrm{H}^2}{D_y\mathrm{L}},$$

give the relative importance of the convective flow along the channel versus diffusive effects in the x and y directions respectively. As the flow carries the solute along the channel, the concentration will disperse across the full width of the channel. Taylor showed that the average concentration across the channel at each x position could be estimated from a reduced model.

We note that the concentration can be separated into the average across the channel and deviation from the average

$$c(x, y, t) = \bar{c}(x, t) + \tilde{c}(x, y, t), \tag{11.20a}$$

where the average $\bar{c}$ is defined by

$$\bar{c}(x, t) \equiv \frac{1}{2}\int_{-1}^{1} c(x, y, t)\, dy. \tag{11.20b}$$

A consequence of this definition of $\bar{c}$ is that the deviation $\tilde{c}$ has zero-mean, i.e.

$$\int_{-1}^{1} \tilde{c}(x, y, t)\, dy = 0. \tag{11.20c}$$

Similarly, we can separate the flow, $u(y) = 1 - y^2$, into mean flow and deviation from the mean,

$$u(y) = \bar{u} + \tilde{u}(y), \tag{11.21a}$$

$$\bar{u} = \frac{1}{2}\int_{-1}^{1} 1 - y^2\, dy = \frac{2}{3}, \qquad \tilde{u}(y) = \frac{1}{3} - y^2. \tag{11.21b}$$

The PDE (11.19) can now be expanded as

$$\frac{\partial \bar{c}}{\partial t} + \frac{\partial \tilde{c}}{\partial t} + \bar{u}\frac{\partial \bar{c}}{\partial x} + \tilde{u}\frac{\partial \bar{c}}{\partial x} + \bar{u}\frac{\partial \tilde{c}}{\partial x} + \tilde{u}\frac{\partial \tilde{c}}{\partial x}$$
$$= \frac{1}{\mathrm{Pe}_x}\frac{\partial^2 \bar{c}}{\partial x^2} + \frac{1}{\mathrm{Pe}_x}\frac{\partial^2 \tilde{c}}{\partial x^2} + \frac{1}{\mathrm{Pe}_y}\frac{\partial^2 \tilde{c}}{\partial y^2}. \tag{11.22}$$

This equation can be integrated term by term across the width of the channel,

$$\frac{1}{2}\int_{-1}^{1} (11.2)\, dy,$$

to give an evolution equation for $\bar{c}(x, t)$. The integrals of the deviations vanish, thus

$$\int_{-1}^{1} \tilde{c}_t\, dy = \bar{u}\int_{-1}^{1} \tilde{c}_x\, dy = \bar{c}\int_{-1}^{1} \tilde{u}\, dy = 0.$$

The boundary conditions on c yield corresponding no-flux boundary conditions on $\tilde{c}$ and hence the integral of the last term in the PDE also vanishes,

$$\left.\frac{\partial \tilde{c}}{\partial y}\right|_{y=\pm 1} = 0 \qquad \Longrightarrow \qquad \int_{-1}^{1} \frac{\partial^2 \tilde{c}}{\partial y^2}\, dy = \left.\frac{\partial \tilde{c}}{\partial y}\right|_{-1}^{1} = 0. \tag{11.23}$$

The remaining terms determine the evolution of the mean concentration,

$$\frac{\partial \bar{c}}{\partial t} + \bar{u}\frac{\partial \bar{c}}{\partial x} + \frac{1}{2}\int_{-1}^{1} \tilde{u}\frac{\partial \tilde{c}}{\partial x}\, dy = \frac{1}{\mathrm{Pe}_x}\frac{\partial^2 \bar{c}}{\partial x^2}. \tag{11.24}$$

In the absence of the integral term, this would be a linear advection-diffusion equation for $\bar{c}(x, t)$. While the integral involves only perturbation terms, it is not valid to neglect it since while the mean of each deviation factor is zero, the average of a product is generally not equal to the product of the averages. Consequently, additional analysis on the properties of $\tilde{c}$ is needed.

Subtracting the averaged Eq. (11.24) from the full problem (11.22) we obtain an equation for $\tilde{c}(x, y, t)$,

$$\frac{\partial \tilde{c}}{\partial t} + \tilde{u}\frac{\partial \bar{c}}{\partial x} + \bar{u}\frac{\partial \tilde{c}}{\partial x} + \tilde{u}\frac{\partial \tilde{c}}{\partial x} - \frac{1}{2}\int_{-1}^{1} \tilde{u}\frac{\partial \tilde{c}}{\partial x}\,dy = \frac{1}{\mathrm{Pe}_x}\frac{\partial^2 \tilde{c}}{\partial x^2} + \frac{1}{\mathrm{Pe}_y}\frac{\partial^2 \tilde{c}}{\partial y^2}. \quad (11.25)$$

Taylor's approach can then be expressed in terms of two assumptions: (i) the deviation is generally smaller than the mean, $\tilde{c} \ll \bar{c}$, and (ii) the channel can be assumed to be slender (similarly to problems in Chap. 8) and the y-derivative terms will dominate the corresponding x-derivatives, $\partial_y \gg \partial_x$. The leading order dominant balance of the largest terms from the left and right sides of (11.25) then yields

$$\left(\tfrac{1}{3} - y^2\right)\frac{\partial \bar{c}}{\partial x} = \frac{1}{\mathrm{Pe}_y}\frac{\partial^2 \tilde{c}}{\partial y^2}. \quad (11.26)$$

Since $\bar{c}$ does not depend on y, we can integrate this equation once with respect to y to get

$$\frac{\partial \tilde{c}}{\partial y} = \mathrm{Pe}_y \frac{\partial \bar{c}}{\partial x}\left(\tfrac{1}{3}y - \tfrac{1}{3}y^3 + A_1(x, t)\right).$$

Applying the no-flux boundary conditions (11.23) at $y = \pm 1$ determines the function of integration to be $A_1(x, t) \equiv 0$, so we can proceed by integrating again to yield

$$\tilde{c} = \mathrm{Pe}_y \frac{\partial \bar{c}}{\partial x}\left(\frac{1}{6}y^2 - \frac{1}{12}y^4 + A_2(x, t)\right),$$

where A_2 is a second function of integration. By definition, the perturbation must have zero mean, namely, $\int_{-1}^{1} \tilde{c}\,dy = 0$. Applying this condition determines $A_2 \equiv -7/180$ and hence we conclude that

$$\tilde{c} = \mathrm{Pe}_y \frac{\partial \bar{c}}{\partial x}\left(\frac{1}{6}y^2 - \frac{1}{12}y^4 - \frac{7}{180}\right). \quad (11.27)$$

We can now use this to calculate the integral term from (11.24),

$$\frac{1}{2}\int_{-1}^{1} \tilde{u}\frac{\partial \tilde{c}}{\partial x}\,dy = -\frac{8\mathrm{Pe}_y}{945}\frac{\partial^2 \bar{c}}{\partial x^2}.$$

Consequently, we can complete our model equation for the evolution of the average density across the channel (11.24) as

$$\frac{\partial \bar{c}}{\partial t} + \bar{u}\frac{\partial \bar{c}}{\partial x} = \alpha \frac{\partial^2 \bar{c}}{\partial x^2} \qquad \alpha = \frac{1}{\mathrm{Pe}_x}\left(1 + \frac{8}{945}\frac{\mathrm{U}_0^2\mathrm{H}^2}{\mathrm{D}_x\mathrm{D}_y}\right), \tag{11.28}$$

where α is called the *Taylor enhanced diffusion coefficient*.

In comparison with the original two-dimensional problem (11.19), we have obtained a reduced model. Equation (11.28) is a one-dimensional linear convection-diffusion equation. Considering the left side of the model, we can identify a convective derivative with constant speed $\bar{u}$ and in fact, making a change of variables with this wave speed, $\bar{c}(x, t) = F(x - \bar{u}t, t)$, yields the classical diffusion equation for F,

$$\frac{\partial F}{\partial t} = \alpha \frac{\partial^2 F}{\partial z^2}. \tag{11.29}$$

As we have seen in Chap. 5, this can be solved using similarity solutions, the one appropriate for a point source (consistent with initial conditions describing release of solute at a single location) is $F(z, t) = M_0 \exp(-z^2/(4\alpha t))/\sqrt{4\pi\alpha t}$ and hence we can predict the large-time behaviour as

$$\bar{c}(x, t) \sim \frac{M_0}{\sqrt{4\pi\alpha t}} \exp\left(-\frac{(x - \bar{u}t)^2}{4\alpha t}\right), \tag{11.30}$$

where M_0 is the mass of solute (determined from the initial conditions).

11.4 Further Directions

In this chapter, we have sought to present approaches for obtaining information about the behaviour of solutions of PDEs that do not rely as heavily on perturbation methods as some of the previous chapters. The derivation of the Taylor dispersion results can be made more rigorous in terms of an asymptotic analysis similar to that used in Chap. 8 (see Fowler [37, pp. 222–223] and [58]).

11.5 Exercises

11.1 In Chap. 5 we derived the Gaussian self-similar solution of the heat equation $\rho_r = \rho_{xx}$. The most general form of this solution is

$$\rho(x, t) = \frac{C_1}{\sqrt{4\pi(t + C_2)}} \exp\left(-\frac{(x - C_3)^2}{4(t + C_2)}\right),$$

which contains three arbitrary constants. Evaluate the M_0, M_1, M_2 moment integrals for this solution and determine C_1, C_2, C_3 in terms of the results for (11.2a, 11.2b). This can be shown to select the $t \to \infty$ asymptotic solution of the initial value problem for the heat equation [108].

11.2 Consider the convection-diffusion-reaction equation

$$\frac{\partial \rho}{\partial t} + 2\frac{\partial \rho}{\partial x} = 3\frac{\partial^2 \rho}{\partial x^2} + 4\rho$$

subject to the following conditions:

(a) On the domain $-\infty < x < \infty$ with initial condition $\rho(x, 0) = e^{-x^2}$ and boundary conditions $\rho \to 0$ as $|x| \to \infty$. Define the moment integrals as

$$M_n(t) = \int_{-\infty}^{\infty} x^n \rho(x, t)\, dx.$$

Find $M_0(t)$, $M_1(t)$, $M_2(t)$.

(b) For the same equation on a semi-infinite domain, $0 \le x < \infty$, with initial condition $\rho(x, 0) = e^{-x}$ and boundary conditions

$$\rho(0, t) = 1, \qquad \rho(x \to \infty, t) = 0.$$

Define the moment integrals as

$$M_n(t) = \int_{0}^{\infty} x^n \rho(x, t)\, dx.$$

Write the differential equations and initial conditions for dM_0/dt and dM_1/dt. Write what additional information you would need in order to solve for $M_0(t)$ and $M_1(t)$.

11.3 Consider the reaction-diffusion equation

$$\frac{\partial \rho}{\partial t} = \frac{\partial^2 \rho}{\partial x^2} - \rho,$$

on $0 \le x \le \pi$ with no-flux boundary conditions,

$$\left.\frac{\partial \rho}{\partial x}\right|_{x=0} = 0, \qquad \left.\frac{\partial \rho}{\partial x}\right|_{x=\pi} = 0,$$

and the initial condition, $\rho(x, 0) = f(x)$.

(a) Derive the problem for the evolution of the mass $M_0(t)$, but show that the equations for the higher moments are not closed.
(b) Show that separation of variables can be used to write the solution in the form

$$\rho(x,t) = \sum_{k=0}^{\infty} a_k e^{-\lambda_k t} \cos(kx).$$

Determine the coefficients a_k in terms of the initial condition. Show that

$$\rho(x,t) \sim \frac{M_0(t)}{\pi} \quad \text{as} \quad t \to \infty.$$

(c) If the domain is changed to be $-\infty < x < \infty$, and the first three moment integrals of $f(x)$ converge, the exact solution can be written as

$$\rho(x,t) = \frac{e^{-t}}{\sqrt{4\pi t}} \int_{-\infty}^{\infty} f(x-y) e^{-y^2/(4t)}\, dy.$$

Using results on integrals of the Gaussian and basic properties of double integrals, show that moments of this formula for the exact solution reproduce the results for M_0, M_1, M_2 that can be obtained from using the PDE alone.

11.4 The *Von Foerster/McKendrick model* describes the evolution of populations where age-distribution of individuals is of interest (called an *age-structured population model*). Consider a population described by a density function $\rho(a,t)$ of individuals with ages $a \geq 0$ [74]. Let the density for $0 < a < \infty$ evolve according to the transport equation

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho}{\partial a} = -2\rho \tag{11.31}$$

with $\rho(a \to \infty) \to 0$ (describing that no-one lives forever).

(a) Suppose that the new births at any time are proportional to the total population size,

$$\rho(0,t) = \beta \int_0^{\infty} \rho(a,t)\, da.$$

Show that the model can be reduced to a single ODE for the total population, $M_0(t) = \int_0^{\infty} \rho(a,t)\, da$.
(b) One possible refinement of the birth condition could be to account for the fact that reproductive activity of individuals tends to decrease with increasing age. Consider the revised birth condition

$$\rho(0,t) = \int_0^\infty e^{-3a}\rho(a,t)\,da.$$

Cushing [28] describes an approach that can reduce age-structured models to ODE systems in terms of weighted moment integrals. Show that the model with this birth condition can be reduced to a system of two ODEs for

$$M_0(t) = \int_0^\infty \rho\,da, \qquad M_1(t) = \int_0^\infty e^{-3a}\rho\,da.$$

11.5 In Chap. 5 a similarity solution of the porous medium equation was derived using the same approach that was used for the heat equation. To see how the method of moments applies to nonlinear equations, consider

$$\frac{\partial \rho}{\partial t} = \frac{\partial}{\partial x}\left(\rho^3 \frac{\partial \rho}{\partial x}\right),$$

with $\rho \to 0$ for $|x| \to \infty$ and initial condition $\rho(x,0) = f(x) \geq 0$ on $-\infty < x < \infty$.

(a) Show that M_0, M_1 are constant for this problem.
(b) Show that while the moment model is not closed for M_2, $M_2(t)$ is a strictly increasing function.

11.6 While describing the spreading of the solute in the transverse direction depends on the presence of diffusion, justify the curved shape of the solute contours sketched in Fig. 11.2 using the method of characteristics for the PDE

$$\frac{\partial c}{\partial t} + (1-y^2)\frac{\partial c}{\partial x} = 0$$

starting from the initial conditions

$$c(x,y,t=0) = \begin{cases} \frac{1}{4} - (x^2+y^2) & x^2+y^2 \leq \frac{1}{4} \\ 0 & \text{elsewhere} \end{cases}$$

Hint: Recall Exercise 2.8.

11.7 Examine how the Taylor dispersion derivation changes for different velocity fields:

(a) for the uniform "plug flow" $\mathbf{U} = \mathrm{U}_0\hat{\mathbf{I}}$,
(b) for linear shear flow $\mathbf{U} = \mathrm{U}_0(1 - \mathrm{Y}/\mathrm{H})\hat{\mathbf{I}}$,

11.8 Derive the Taylor diffusion model for laminar axisymmetric flow in a circular pipe of radius $\mathsf{R} = \mathrm{R}_0$:

$$\frac{\partial \mathsf{C}}{\partial \mathsf{T}} + \mathsf{U}_0\left(1 - \frac{\mathsf{R}^2}{\mathrm{R}_0^2}\right)\frac{\partial \mathsf{C}}{\partial \mathsf{X}} = \mathrm{D}_x \frac{\partial^2 \mathsf{C}}{\partial \mathsf{X}^2} + \frac{\mathrm{D}_r}{\mathsf{R}}\frac{\partial}{\partial \mathsf{R}}\left(\mathsf{R}\frac{\partial \mathsf{C}}{\partial \mathsf{R}}\right)$$

with no flux boundary conditions at the pipe wall.

11.9 The key detail obtained in the derivation of the Taylor diffusion model (11.28) was the coefficient 8/945. The corresponding correction factor in Exercise 11.8 or for other geometries will be different constants. For the problem of two-dimensional laminar flows (11.19), some books and articles may give the "magic number" 2/105 instead. Show that this result does not clash with 8/945 given in the derivation above. Hint: Consider a different choice for the scaling of the flow velocity.