

Two-Zone Model of Shear Dispersion in a Channel Using Centre Manifolds

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Abstract

To achieve better precision in describing contaminant dispersion in channels some authors resort to dividing a channel into two zones, fast and slow, leading to a pair of coupled evolution equations for cross-sectionally averaged concentrations in the zones. We construct a two-zone model whose accuracy is guaranteed by the centre manifold theory. The model leads to the evolution equations that differ from existing models. We also formulate modified initial conditions for the model to obtain closer correlation between the manifold solution and real solution. Effectiveness of the modified initial conditions is demonstrated numerically by a comparison between the manifold solution and direct numerical simulations of the original advection-diffusion equations.

1 Introduction

The problem of the long-term evolution of contaminant in shear flows has attracted attention since the work of Taylor [1, 2]. He argued that cross-sectional diffusion smooths out the concentration of a contaminant across a channel to an almost uniform state. The nearly uniform concentration, across the channel, then varies slowly along the channel as a result of the interaction between advection and diffusion. The long-term dynamics of the contaminant can be effectively described in terms of the cross-sectional average concentration C for which Taylor derived the advection-diffusion model

$$\partial_t C = -U \partial_x C + D \partial_x^2 C .$$

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The work of Taylor was followed by extensive research on dispersion in shear flows (Aris [3], Gill and Sankarasubramanian [4], Smith [5], Frankel and Brenner [6], Balakotaiah and Chang [7] and others).

In order to achieve better accuracy some authors use two-layer models. Chatwin [8] considered the mainstream layer and the viscous layer. For the linear velocity profile he estimated the role of the viscous layer on turbulent dispersion. Thacker [9] showed that for a flow with two equal layers, each of which is well-mixed and has negligible horizontal diffusivity, the bulk concentration satisfies a telegraph equation. He found its exact solution and also briefly discussed the case when the diffusion is present. Smith [10, 11] has studied a delay-diffusion description that is equivalent to the two-layer model, and also used a telegraph equation to obtain solutions for the non-diffusive case. He showed how the layers should be chosen in order to get satisfactory results. Chikwendu [12] and Chikwendu and Ojiakor [13] constructed a two-zone model where the flow is divided into a fast section (surface section for an open channel) with approximately uniform velocity and a slow (bottom) section where the velocity rapidly changes due to friction. The contaminant concentration is averaged over the fast zone and slow zone separately, and the dynamics is described in terms of the average concentrations. An important element of such models is the adopted approximations for the diffusional exchange between the zones. Chikwendu assumed that the diffusional exchange is described by Newton's law, that is, the contaminant flux is proportional to the difference in the concentrations in the zones. This assumption along with the heuristic way of introducing the model coefficients renders the model rather approximate.

In the present paper we construct the two-layer model using a different approach—based on the centre manifold theory—which allows us to avoid the use of heuristic coefficients and guarantees exponentially fast convergence of the model solution to the actual solution. Our preliminary results are reported in [14], and now we generalize and continue this research by constructing the initial conditions for the model and comparing the model solution with the solution of the original equations. This comparison is crucial: firstly, it proves the correctness of the model itself and, secondly, demonstrates the effectiveness of the initial conditions.

Previously Mercer and Roberts [15] applied the centre manifold theory to a *one-layer* problem and deduced the Taylor-type asymptotic equations. Watt and Roberts [16, 17] attempted to design *zonal* models using techniques closely connected to the centre manifold

approach.

Before constructing the new model we describe their results in detail to show why further efforts are needed to develop an accurate two-zone model of contaminant dispersion in channels.

2 Dispersion in channels using centre manifolds

We start with basic ideas of the centre manifold approach. Consider a dynamical system

$$\dot{x} = Ax + f(x, y, \sigma), \quad \dot{y} = By + g(x, y, \sigma), \quad (2.1)$$

where the overdot denotes d/dt , σ is a set of parameters, x and y are generally multidimensional variables, and f and g are nonlinear functions. It is assumed that the eigenvalues of the $m \times m$ matrix A all have zero real part, and the eigenvalues of the $n \times n$ matrix B all have strictly negative real part. Near the origin $(x, y, \sigma) = (0, 0, 0)$ the *linear* dynamics dominate and the modes y are driven exponentially quickly to 0 due to the equations $\dot{y} = By$. These modes are thus ignored when considering the linear long-term evolution, and the dynamics are approximately described just by $\dot{x} = Ax$. Then centre manifold theory asserts that this linear picture is only modified by the nonlinear terms f and g : the modes $y(t)$ go exponentially quickly to a manifold $y = h(x, \sigma)$, called the centre manifold; and thereafter the long-term evolution of the system is described by the low-dimensional system $\dot{x} = Ax + f(x, h, \sigma)$. A more detailed discussion of centre manifold theory is given by Carr [18].

We now show, following Mercer and Roberts [15], how this mathematical theory can be employed to model the dispersion in a channel. The paper of Mercer and Roberts is concerned with a one-zone model, however we will use its principal components for constructing the zonal model.

The concentration c of the contaminant obeys the advection-diffusion equation

$$\partial_t c + u(y)\partial_x c = \partial_y[D(y)\partial_y c], \quad -\infty < x < \infty, \quad 0 < y < h, \quad (2.2)$$

where $u(y)$ is the downstream velocity of the flow, and D is the diffusion coefficient. For definiteness take $u(y) = U(3/2)(1 - y^2/h^2)$, where U is the constant average downstream

velocity. In our model formulated in Section 3 we use a constant diffusion coefficient to simplify mathematical analysis. This assumption is by no means crucial and varying diffusion coefficients can also be considered within the same approach. Now we discuss the model of Mercer and Roberts who adopted a parabolic profile, $D(y) = D_{max}(1 - y^2/h^2)$.

On the boundaries the concentration flux equals zero:

$$D\partial_y c|_{y=0} = D\partial_y c|_{y=h} = 0.$$

We neglect longitudinal diffusion since, in the final analysis, its influence on the dynamics is small compared to the advection. Non-dimensionalize the problem using h as a spatial scale and h^2/D_{max} as a time scale and take the Fourier transformation of (2.2):

$$\partial_t \hat{c} = L\hat{c} - ik(3/2)P(1 - y^2)\hat{c}, \quad (2.3)$$

where $\hat{c}(k, t)$ denotes Fourier transform $1/(2\pi) \int_{-\infty}^{\infty} \exp(-ikx)c dx$, $P = Uh/D_{max}$ is the Peclet number, and $L\hat{c} = \partial_y[(1 - y^2)\partial_y \hat{c}]$. We are interested in solutions which vary slowly in x ; therefore, the wave number k is considered a small parameter. The linear operator L represents the cross-stream diffusion and has a discrete spectrum of eigenvalues $\lambda_l = -l(l + 1)$ corresponding to eigenfunctions $P_l(y)$ being the l th Legendre polynomials. The linear dynamics $\partial_t \hat{c} = L\hat{c}$ has one neutral mode, corresponding to the one zero eigenvalue of L , and an infinite number of discrete decaying modes corresponding to the negative eigenvalues. The neutral mode represents a spatially uniform distribution to which the concentration is driven by the diffusion after spatial non-uniformities, represented by the decaying modes, are smoothed out. Adjoin to (2.3) the equation $\partial_t k = 0$ in order to formally treat the wave number k as a variable and the term $k\hat{c}$ as a “nonlinear” term. The system (2.3) evolves exponentially quickly to a low-dimensional state dominated by the neutral mode $P_0(y)$. The system then evolves slowly being permanently affected by the small nonlinear perturbation. According to centre manifold theory we assume that the concentration field is dependent only on this neutral mode and how it evolves:

$$\hat{c} = V(\hat{C}, y) \quad \text{such that} \quad \partial_t \hat{C} = G(\hat{C}), \quad (2.4)$$

where $\hat{C}(k, t)$ is defined to be the cross-stream average of \hat{c} and is therefore a measure of the “amplitude” of the neutral mode. Substituting (2.4) into (2.3) gives the following PDE to be

satisfied by V and G :

$$LV = \frac{\partial V}{\partial \hat{C}} G + ikuV. \quad (2.5)$$

Due to the linearity in c of the original problem, we assume an asymptotic expansion for V and G which is also linear in \hat{C} , that is

$$V \sim \sum_{n=0}^{\infty} v_n(y)(ik)^n \hat{C}, \quad G \sim \sum_{n=1}^{\infty} g_n(ik)^n \hat{C}. \quad (2.6)$$

Substituting (2.6) into (2.5) and collecting terms of the same order in (ik) , we obtain the hierarchy of equations

$$Lv_n = \sum_{m=1}^n v_{n-m} g_m + u(y)v_{n-1}, \quad (2.7)$$

where quantities with negative subscripts are taken to be zero. By the definition of \hat{C} as the cross-stream average of \hat{c} we take the cross-stream average of the asymptotic expansion for V in (2.6) to deduce the subsidiary conditions

$$\bar{v}_0 = 1, \quad \bar{v}_n = 0, \quad n > 0, \quad (2.8)$$

where $\bar{v} = \int_0^1 v dy$ is the cross-stream average. The g_n 's are found by taking the cross-stream average of (2.7) and using the conditions (2.8):

$$g_n = -\overline{u(y)v_{n-1}}. \quad (2.9)$$

Proceeding with the computations we find $v_0 = 1$, $g_1 = -P$, $v_1 = (y^2/4 - 1/12)P$, $g_2 = (1/30)P^2$, etc.. Then the transformed average concentration evolves according to an approximate equation

$$\partial_t \hat{C} \sim g_1(ik)\hat{C} + g_2(ik)^2\hat{C} = -ikP\hat{C} + (ik)^2 \frac{1}{30}P^2\hat{C},$$

from which by taking the inverse transform we recover the Taylor model

$$\partial_t C = -P\partial_x C + \frac{1}{30}P^2\partial_x^2 C.$$

An advantage of the presented approach in comparison to the work of Taylor is that the centre manifold theory guarantees that all solutions are described exponentially quickly by this model.

Using an extension of the above technique, Watt and Roberts [17] developed an invariant manifold model of the contaminant dispersion, based on two modes — the neutral mode, $Q_0(y) = 1$, and the slowest decaying mode, $Q_2(y) = 3y^2 - 1$. After passing to new variables as shown below this model effectively becomes a two-zone model. In the absence of any downstream variations, the solution to (2.2) is

$$c = \sum_{l=0}^{\infty} c_l Q_l(y) e^{\lambda_l t}. \quad (2.10)$$

Taking into account only the first two modes in (2.10) one approximates the dynamics by $c = c_0 Q_0(y) + c_2 Q_2(y) e^{-6t}$ with $Q_0 = 1$ and $Q_2 = 3y^2 - 1$. Thus, the model describes the solution in terms of the amplitudes, $C_0(t) = c_0$ and $C_2(t) = c_2 e^{-6t}$, of these modes. Analogously, when downstream variation is present, the dynamics is described with good accuracy in terms of the amplitudes of the two leading modes. Up to the second order in $\partial/\partial x$, the amplitudes, C_0 and C_2 , were shown to obey the system

$$\begin{aligned} \partial_t C_0 &= -P \partial_x C_0 + (2/5) P \partial_x C_2, \\ \partial_t C_2 &= -6C_2 + (1/2) P \partial_x C_0 - (5/7) P \partial_x C_2 + (18/1715) P^2 \partial_x^2 C_2. \end{aligned} \quad (2.11)$$

By introducing new variables $\alpha(x, t)$ and $\beta(x, t)$ such that

$$C_0 = \alpha + \beta, \quad C_2 = \alpha(5 + 3\sqrt{30})/14 + \beta(5 - 3\sqrt{30})/14$$

the model (2.11) was transformed into a form revealing that the variables α and β may be attributed the sense of concentrations in slow and fast zones respectively. Indeed, in terms of the new variables, the concentration field is

$$c \approx \left[1 + \frac{5 + \sqrt{30}}{14} (3y^2 - 1) \right] \alpha + \left[1 + \frac{5 - \sqrt{30}}{14} (3y^2 - 1) \right] \beta.$$

Observe that the variable α predominantly describes the contaminant in the slow zone near the sides of the channel and β predominantly describes that in the fast zone in the channel centre. However, this approach does not create a sharp division between the zones. The transformed equations for this model are

$$\partial_t \alpha = -\frac{7}{108} (\gamma_+ \alpha + \gamma_- \beta) - u_\alpha P \partial_x \alpha + \frac{1}{245} P^2 (\gamma_+ \partial_x^2 \alpha + \gamma_- \partial_x^2 \beta),$$

$$\partial_t \beta = \frac{7}{108}(\gamma_+ \alpha + \gamma_- \beta) - u_\beta P \partial_x \beta - \frac{1}{245} P^2 (\gamma_+ \partial_x^2 \alpha + \gamma_- \partial_x^2 \beta),$$

where $\gamma_\pm \approx 1.6769, -0.8945$, $u_\alpha \approx 0.3877$, $u_\beta \approx 1.3266$. Observe that the slow zone α has a relatively low effective velocity of $0.3877P$ while the fast zone β has a relatively high velocity of $1.3266P$.

Another approach to constructing a zonal model (with $D = \text{const}$) was applied in the work of Watt and Roberts [16]. They postulated a model of the form

$$\begin{aligned} \partial_t C_1 &= a(C_2 - C_1) - s_1 \partial_x C_1 + d_1 \partial_x^2 C_1, \\ \partial_t C_2 &= b(C_1 - C_2) - s_2 \partial_x C_2 + d_2 \partial_x^2 C_2, \end{aligned} \tag{2.12}$$

where the advection and diffusion matrices are *a priori* assumed to be diagonal, that is the x -derivative of C_2 is absent in the evolution equation for C_1 and vice versa. Since the system (2.12) conserves the value of $bC_1 + aC_2$, the ratio of the widths of the effective zones is $b : a$. Upon assuming that the zonal concentrations C_1 and C_2 are functions of the ‘‘cross-channel’’ average $C = (bC_1 + aC_2)/(a + b)$, it was shown that, to the second order in $\partial/\partial x$, the evolution on the centre manifold of the zonal model is described by the generalized advection-diffusion equation

$$\partial_t C = -\bar{u} \partial_x C + \bar{d} \partial_x^2 C + \dots,$$

where the coefficients are known functions of a, b, s_1, s_2, d_1 and d_2 , such as

$$\bar{u} = \frac{bs_1 + as_2}{a + b}, \quad \bar{d} = \frac{ab(s_1 - s_2)^2}{(a + b)^3} + \frac{bd_1 + ad_2}{a + b}.$$

This model was matched to the centre manifold model of the channel dispersion obtained in [15]. As there are six degrees of freedom in the zonal model, those being the as yet undetermined parameters a, b, s_1, s_2, d_1 , and d_2 , one establishes an agreement between the model (2.12) and the dispersion model up to sixth order in $\partial/\partial x$. The values of the parameters of this model are presented in Table 1 of the next section.

These analyses of the zonal models show that the invariant manifold approach, although rigorous, produces overlapping zones and thus does not encompass zones in a clear sense. The matched centre manifold approach involves only a finite number of terms and matches the rigorous one-zone theory up to a certain order in $\partial/\partial x$; consequently, this approach is not quite exact. Below we construct an exact model based on distinct zones, which is free from these disadvantages.

3 Two-zone model

Consider the shear flow in an open channel of constant depth h . As in the earlier studies, we neglect the longitudinal diffusion in view of the dominant role of the shear dispersion. Under this assumption the concentration c of the contaminant is described by the advection-diffusion equation

$$\partial_t c + u(y)\partial_x c = D\partial_y^2 c, \quad (3.1)$$

where $u(y) = U(3/2)(1 - y^2/h^2)$ is the velocity of the fluid, and D is the constant coefficient of diffusion. These profiles of $u(y)$ and $D(y)$ are chosen as typical specific examples—other profiles can be easily analyzed. On the surface $y = 0$ and the bottom $y = h$ the zero-flux condition holds:

$$\partial_y c|_{y=0} = \partial_y c|_{y=h} = 0. \quad (3.2)$$

Choosing h as a spatial scale and h^2/D as a time scale we set (3.1) to the non-dimensional form

$$\partial_t c + (3/2)P(1 - y^2)\partial_x c = \partial_y^2 c, \quad (3.3)$$

where $P = Uh/D$ is a Peclet number. The boundary condition (3.2) becomes

$$\partial_y c|_{y=0} = \partial_y c|_{y=1} = 0. \quad (3.4)$$

Divide the channel into a fast zone $0 < y < \alpha$ and a slow zone $\alpha < y < 1$ and denote the concentration in the fast zone as c_1 and that in the slow zone as c_2 and the cross-zone average concentrations as $C_1(x, t)$ and $C_2(x, t)$ respectively:

$$C_1 = \frac{1}{\alpha} \int_0^\alpha c_1 dy, \quad C_2 = \frac{1}{1-\alpha} \int_\alpha^1 c_2 dy. \quad (3.5)$$

Across the boundary between the zones we impose the usual condition of continuity of the contaminant flux

$$\partial_y c_1|_{y=\alpha} = \partial_y c_2|_{y=\alpha}, \quad (3.6)$$

and, which is a non-trivial point of our approach, an artificial condition

$$(1 - \gamma)(\partial_y c_1 + \partial_y c_2)|_{y=\alpha} = \gamma(c_1 - c_2)|_{y=\alpha}. \quad (3.7)$$

The condition (3.7) is arranged so that: at $\gamma = 0$ the equations (3.6) and (3.7) combined give the “insulating” condition $\partial_y c_1|_{y=\alpha} = \partial_y c_2|_{y=\alpha} = 0$; whereas at $\gamma = 1$, $c_1(\alpha, t) = c_2(\alpha, t)$

which, together with (3.6), ensures sufficient continuity to recover physically applicable equations. We represent the solution to our problem as an asymptotic series in small γ and then evaluate at $\gamma = 1$ to address the real situation.

Take the Fourier transform of the advection-diffusion equation (3.3) with respect to x , with $\hat{\cdot}$'s denoting the transformed quantities and k denoting the downstream wave number, to get

$$\partial_t \hat{c} = \partial_y^2 \hat{c} - ik(3/2)P(1 - y^2)\hat{c}. \quad (3.8)$$

The boundary conditions (3.4), (3.6) and (3.7) remain symbolically the same, that is c_i should be simply changed to \hat{c}_i . To describe the long-term dynamics we need be interested only in solutions which vary slowly in x . In Fourier space this corresponds to small wave numbers, k , so k becomes a small perturbation parameter. Now using a standard trick [18] adjoin the trivial dynamical equations

$$\partial_t k = \partial_t \gamma = 0, \quad (3.9)$$

so that terms involving k and γ , such as $k\hat{c}$ and $\gamma\partial_y\hat{c}$, are viewed as nonlinear. Then there exists a subspace of fixed points: $k = \gamma = 0$ and $\hat{c}_1 = \text{const}$ and $\hat{c}_2 = \text{const}$. Due to the cross-stream diffusion in each zone, about each of these fixed points the linear dynamics are those of exponential decay except for k , γ and the constant mode in each zone; the non-dimensional time scale of the decay being

$$T = \left(\frac{2 \max\{\alpha, 1 - \alpha\}}{\pi} \right)^2.$$

Thus centre manifold theory [18] guarantees a four dimensional centre manifold exists parametrized by a measure of the concentration in the two zones, the longitudinal wavenumber k , and the artificial parameter γ :

$$\hat{c}_1 = V_1(\hat{C}_1, \hat{C}_2, k, \gamma, y), \quad \hat{c}_2 = V_2(\hat{C}_1, \hat{C}_2, k, \gamma, y), \quad (3.10)$$

where $\hat{C}_1(k, t)$ and $\hat{C}_2(k, t)$ are the Fourier transforms of the cross-zone averages C_1 and C_2 . On the centre manifold the solutions then evolve according to

$$\partial_t \hat{C}_1 = G_1(\hat{C}_1, \hat{C}_2, k, \gamma), \quad \partial_t \hat{C}_2 = G_2(\hat{C}_1, \hat{C}_2, k, \gamma). \quad (3.11)$$

Theory also asserts that provided k and γ are small enough, then the solutions of the original equations exponentially quickly approach solutions of (3.11) on the centre manifold.

Thus the model (3.11) completely describes the evolution of the system on time scales longer than T . Lastly, theory asserts that simply by substituting (3.10) and (3.11) into the governing equations and solving to some order in k and γ we will obtain a model accurate to the same order.

Substituting (3.10) and (3.11) into (3.8) we obtain

$$\begin{aligned}\partial_y^2 V_1 &= \frac{\partial V_1}{\partial \hat{C}_1} G_1 + \frac{\partial V_1}{\partial \hat{C}_2} G_2 + ik(3/2)P(1-y^2)V_1, \\ \partial_y^2 V_2 &= \frac{\partial V_2}{\partial \hat{C}_1} G_1 + \frac{\partial V_2}{\partial \hat{C}_2} G_2 + ik(3/2)P(1-y^2)V_2.\end{aligned}\tag{3.12}$$

We seek asymptotic solutions to (3.12) with internal boundary conditions (3.6) and (3.7) following procedures described in Coulet and Spiegel [19] and Roberts [20]. As the problem is linear in the concentration c , we assume linear asymptotic expansions in \hat{C}_1 and \hat{C}_2 :

$$\begin{aligned}V_1 &\sim \sum_{n=0}^{\infty} p_1^{(n)}(y)(ik)^n \hat{C}_1 + \sum_{n=0}^{\infty} p_2^{(n)}(y)(ik)^n \hat{C}_2, \\ V_2 &\sim \sum_{n=0}^{\infty} q_1^{(n)}(y)(ik)^n \hat{C}_1 + \sum_{n=0}^{\infty} q_2^{(n)}(y)(ik)^n \hat{C}_2;\end{aligned}\tag{3.13}$$

and

$$\begin{aligned}G_1 &\sim \sum_{n=0}^{\infty} g_1^{(n)}(ik)^n \hat{C}_1 + \sum_{n=0}^{\infty} g_2^{(n)}(ik)^n \hat{C}_2, \\ G_2 &\sim \sum_{n=0}^{\infty} f_1^{(n)}(ik)^n \hat{C}_1 + \sum_{n=0}^{\infty} f_2^{(n)}(ik)^n \hat{C}_2.\end{aligned}\tag{3.14}$$

Substituting (3.13) and (3.14) into (3.12) we collect terms with \hat{C}_1 and \hat{C}_2 and like powers of ik and set the resulting expressions to zero. The latter is based on the fact that the concentrations are independent functions of their arguments and the wave number k .

$$\begin{aligned}\frac{d^2 p_1^{(n)}}{dy^2} &= \sum_{m=0}^n p_1^{(n-m)} g_1^{(m)} + \sum_{m=0}^n p_2^{(n-m)} f_1^{(m)} + (3/2)P(1-y^2)p_1^{(n-1)}, \\ \frac{d^2 p_2^{(n)}}{dy^2} &= \sum_{m=0}^n p_1^{(n-m)} g_2^{(m)} + \sum_{m=0}^n p_2^{(n-m)} f_2^{(m)} + (3/2)P(1-y^2)p_2^{(n-1)}, \\ \frac{d^2 q_1^{(n)}}{dy^2} &= \sum_{m=0}^n q_1^{(n-m)} g_1^{(m)} + \sum_{m=0}^n q_2^{(n-m)} f_1^{(m)} + (3/2)P(1-y^2)q_1^{(n-1)}, \\ \frac{d^2 q_2^{(n)}}{dy^2} &= \sum_{m=0}^n q_1^{(n-m)} g_2^{(m)} + \sum_{m=0}^n q_2^{(n-m)} f_2^{(m)} + (3/2)P(1-y^2)q_2^{(n-1)}.\end{aligned}\tag{3.15}$$

The hierarchy of equations (3.15) is supplemented by boundary conditions straightforwardly obtained using (3.4), (3.6) and (3.7), and subsidiary conditions obtained by taking cross-zone averages of (3.13):

$$\begin{aligned} \frac{1}{\alpha} \int_0^\alpha p_1^{(0)}(y) dy &= 1, & \int_0^\alpha p_1^{(n)}(y) dy &= 0 \quad (n > 0); \\ \frac{1}{1-\alpha} \int_\alpha^1 q_2^{(0)}(y) dy &= 1, & \int_\alpha^1 q_2^{(n)}(y) dy &= 0 \quad (n > 0); \\ \int_0^\alpha p_2^{(n)}(y) dy &= 0, & \int_\alpha^1 q_1^{(n)}(y) dy &= 0 \quad (n \geq 0). \end{aligned} \tag{3.16}$$

We solved (3.15)–(3.16) using REDUCE to perform all the computer algebra. The result showed rapid convergence for $\gamma = 1$.

In principle we can find the unknown coefficients $g_1^{(n)}$, $g_2^{(n)}$, $f_1^{(n)}$ and $f_2^{(n)}$ and unknown functions $p_1^{(n)}(y)$, $p_2^{(n)}(y)$, $q_1^{(n)}(y)$ and $q_2^{(n)}(y)$ for any n . Performing the inverse Fourier transformation and taking into account only the terms up to the second order in $\partial/\partial x$, we obtained for $\alpha = 0.55$:

$$\begin{aligned} \partial_t C_1 &= -4.441C_1 + 4.441C_2 - 1.397P\partial_x C_1 + 0.0478P\partial_x C_2 \\ &\quad + 9.68 \times 10^{-4}P^2\partial_x^2 C_1 - 1.85 \times 10^{-3}P^2\partial_x^2 C_2, \\ \partial_t C_2 &= 5.428C_1 - 5.428C_2 - 0.0461P\partial_x C_1 - 0.527P\partial_x C_2 \\ &\quad - 1.78 \times 10^{-3}P^2\partial_x^2 C_1 + 3.34 \times 10^{-3}P^2\partial_x^2 C_2. \end{aligned} \tag{3.17}$$

The dynamical system (3.17) is more complicated than just two reaction-advection-diffusion equations expressing the advection and down-stream diffusion in each zone and the cross-stream diffusional exchange between the zones (“reaction”). In each equation we also have first and second x -derivatives of the concentration in the other zone. Calculations showed that at no α does the advection matrix (as well as the diffusion matrix) assume strictly diagonal form. Fig. 1 shows that the coefficients $f_1^{(1)}$ and $g_2^{(1)}$ considered as functions of α do not cross zero simultaneously. However, at $\alpha = 0.55$ the non-diagonal terms are both quite small (for this specific velocity profile).

In (3.17) the coefficient of the term $\partial_x C_1$ in the first equation and the coefficient of the term $\partial_x C_2$ in the second equation are regarded as effective velocities of the advection in the fast and slow zones respectively. These coefficients are close to the cross-zone average

Fast zone.

	C_1	C_2	$\partial_x C_1$	$\partial_x C_2$	$\partial_x^2 C_1$	$\partial_x^2 C_2$
centre manifold	- 4.441	4.441	-1.397	0.0478	9.68×10^{-4}	-1.85×10^{-3}
matched centre manifold	-4.567	4.567	-1.383	0	5.04×10^{-4}	0
heuristic	-3.636	3.636		0		0

Slow zone.

	C_1	C_2	$\partial_x C_1$	$\partial_x C_2$	$\partial_x^2 C_1$	$\partial_x^2 C_2$
centre manifold	5.428	-5.428	-0.0461	-0.527	-1.78×10^{-3}	3.34×10^{-3}
matched centre manifold	5.657	-5.657	0	-0.528	0	2.24×10^{-3}
heuristic	4.444	-4.444	0		0	

Table 1: The coefficients for the three zonal models.

velocities: $3/(2\alpha) \int_0^\alpha (1-y^2) dx \approx 1.349$ in the fast zone and $3/(2(1-\alpha)) \int_\alpha^1 (1-y^2) dx \approx 0.574$ in the slow zone. It is interesting to compare the coefficients entering (3.17) with those in other models where a sharp boundary between the zones exists, namely the matched centre manifold model and the heuristic model. The data are presented in Table 1. Note that within the heuristic approach [13] the coefficients of the advective and diffusion terms were calculated using a different (logarithmic) velocity profile. For this reason we leave the respective cells in the table empty. The other coefficients for the heuristic model were calculated using equations (2.4a), (2.4b) and (3.13) of [13]. In the absence of the x -variations those give, in dimensional form, $\partial_t c_1 = \frac{2D}{\alpha h^2} (c_2 - c_1)$, $\partial_t c_2 = \frac{2D}{(1-\alpha)h^2} (c_1 - c_2)$. As our time scale is chosen to be h^2/D , then, non-dimensionally, $\partial_t c_1 = \frac{2}{\alpha} (c_2 - c_1)$, $\partial_t c_2 = \frac{2}{(1-\alpha)} (c_1 - c_2)$. Now substituting $\alpha = 0.55$ we obtain the values presented in the table. Observe that both centre manifold based models give close results up to first-order terms in $\partial/\partial x$. The difference in the values of the coefficients at the second-order terms are larger: about 50% and 30% for the fast and slow zones respectively. This is explained by the incomplete nature of the matched centre manifold theory. Comparing to the heuristic model, we notice a substantial difference, about 25%, already in the values of the coefficients of the zeroth order.

Also recall that for the matched centre manifold model the value of α is a consequence of the model, not a prescribed value. However, as the advection matrices in this model are

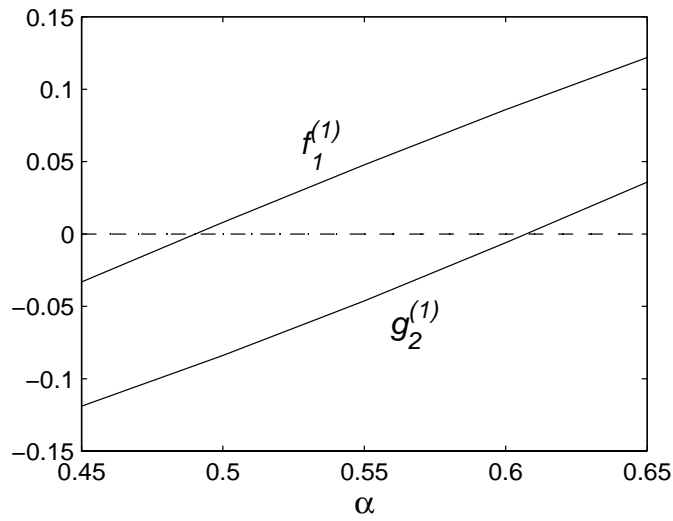


Figure 1: The coefficients of advective terms versus α , the fraction of the channel allocated to the fast zone.

stipulated to have a diagonal form (that is the advection-diffusion equation for each zone contains the first x -derivative of the concentration in this particular zone only), we must expect that the value of α should be close to 0.55 at which the full model is nearly diagonal. As was mentioned in Section 2, the ratio of the zone widths in the matched centre manifold model equals b/a . Therefore the fast zone occupies a fraction $b/(a+b)$ of the channel. See from the table and (2.12) that $a = 5.657$, $b = 4.567$, consequently $\alpha = b/(a+b) = 0.5533$ which is indeed close to 0.55.

4 Initial conditions for the centre manifold model

Given an initial concentration field $c^0(x, y)$, the challenge is to deduce the appropriate *initial* values of the fields C_1 and C_2 for the centre manifold model (3.17) in order to ensure long term agreement between the model and the physical system. Surprisingly, it is not simply a matter of evaluating the cross-zone averages (3.5) although they are a first approximation.

To illustrate the essence of the problem consider a simple example from [21]. The dynamical system $\dot{x} = -xy$, $\dot{y} = -y + x^2 - 2y^2$ can be readily shown to have a centre manifold, $y = x^2$, parametrically described as $x = s$, $y = s^2$, on which $\dot{s} = -s^3$. We aim to find out a starting point on the centre manifold, s_0 , that should be used in order to best match

the long term behaviour of the solution which is initially at some point (x_0, y_0) not on the manifold. Conveniently this dynamical system has exact solutions. As was demonstrated [21], the evolution of the system along a particular trajectory is expressed by the formulae $x = [1/x_0^2 + 2(t+\tau) - \tau \exp(-t)/x_0^2]^{-1/2} + O(\psi^2)$, where $\tau = (y_0/x_0^2 - 1) \exp(y_0/x_0^2 - 1)$ and ψ is the constant that labels the trajectory (i.e., the equations for the trajectories can be written in the form $\psi(x, y) = \text{const}$). The values ψ and τ both reflect how far from the manifold the system was initially; on the centre manifold $\psi = 0$ and $\tau = 0$. The quickly decaying term $\exp(-t)$ has no long-term effect, but the term τ has. However, if we choose the initial point on the centre manifold to be not x_0 but s_0 such that $1/s_0^2 = 1/x_0^2 + 2\tau$ then the trajectory on the manifold will be (upon neglecting the exponential transient) $x = [1/s_0^2 + 2t]^{-1/2}$. This is precisely the evolution along the real trajectory. Our task is to find the value s_0 . Substituting the expression for τ into the expression for s_0 and decomposing into Taylor series in small parameter $y_0 - x_0^2$ we deduce $s_0 = x_0 - x_0(y_0 - x_0^2) + O(\psi^2)$. This choice of initial condition for the model results in exponentially quick agreement with the actual solution.

We carry out similar manipulations in our case of the system with infinite number of degrees of freedom representing the dispersion of the contaminant in a channel. We determine two sorts of projection vectors z , one for each zone: z^1 is approximately the fast zone average; whereas z^2 is approximately the slow zone average.

The first step is to define an appropriate inner product on the space of functions describing the vertical structure: let

$$\langle z, n \rangle = \int_0^1 z^\dagger n \, dy, \quad (4.1)$$

where \dagger denotes the complex conjugate (and later the adjoint). In this inner product determine the adjoint of the right-hand side of equation (3.8) and its boundary conditions *linearized* about the centre manifold. Because the problem is linear in c , the operator is

$$J = \frac{\partial^2}{\partial y^2} - ikPu.$$

Thus in the inner product (4.1) the adjoint is

$$J^\dagger z = \frac{\partial^2 z}{\partial y^2} + ikPuz, \quad (4.2)$$

with boundary conditions

$$\frac{\partial z^j}{\partial y} = 0 \quad \text{on } y = 0, 1, \quad (4.3)$$

$$\frac{\partial z^1}{\partial y} = \frac{\partial z^2}{\partial y} \quad \text{on } y = \alpha, \quad (4.4)$$

$$(1 - \gamma) \left(\frac{\partial z^1}{\partial y} + \frac{\partial z^2}{\partial y} \right) = \gamma(z^1 - z^2) \quad \text{on } y = \alpha. \quad (4.5)$$

Except for the perturbing advection term, $ikPu$, the operator J is self-adjoint. Defining the dual operator $R = \frac{\partial}{\partial t} + J^\dagger$ we now solve (see [21])

$$Rz^j - \sum_{k=1}^2 \langle Rz^j, e^k \rangle^\dagger z^k = 0, \quad (4.6)$$

together with the orthogonality condition

$$\langle z^j, e^k \rangle = \delta_{jk}, \quad (4.7)$$

where $e^k = \frac{\partial V}{\partial C_k}$ are ‘‘tangent vectors’’ to the centre manifold. Equations (4.6)–(4.7) are solved iteratively using a REDUCE algebra program presented in the Appendix. We start with the approximation corresponding to cross-zone averaging:

$$z^1 \approx \begin{cases} \frac{1}{\alpha}, & 0 < y < \alpha, \\ 0, & \alpha < y < 1; \end{cases} \quad (4.8)$$

$$z^2 \approx \begin{cases} 0, & 0 < y < \alpha, \\ \frac{1}{1-\alpha}, & \alpha < y < 1. \end{cases} \quad (4.9)$$

Then corrections are sought to drive the residuals of the dual equation (4.6) to zero along with the residual of the orthogonality condition (4.7). For the case of $\alpha = 0.55$ we find

$$\begin{aligned} z^1 &= 2.159 - 5.720y^2 + 4.705y^4 - 1.548y^6 + o(y^6) \\ &+ ikP[-0.010 + 0.174y^2 - 0.482y^4 + 0.494y^6 + o(y^6)] + O(k^2). \end{aligned} \quad (4.10)$$

$$\begin{aligned} z^2 &= -0.417 + 6.991y^2 - 5.750y^4 + 1.892y^6 + o(y^6) \\ &+ ikP[0.020 - 0.333y^2 + 0.867y^4 - 0.786y^6 + o(y^6)] + O(k^2). \end{aligned} \quad (4.11)$$

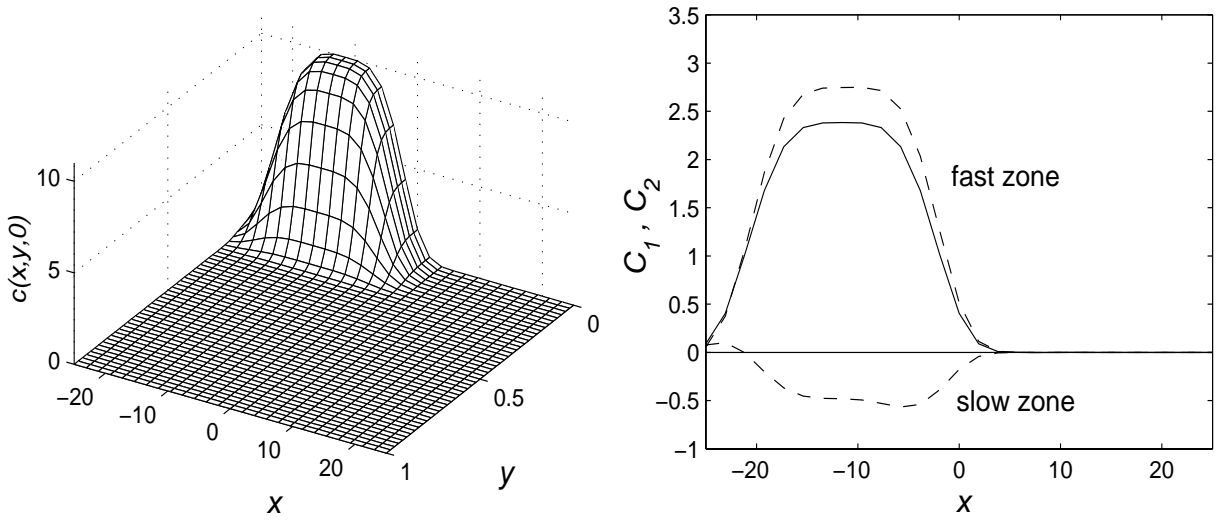


Figure 2: Left: the initial field. Right: the corrected (dashed line) and uncorrected (solid line) initial conditions.

Confining ourselves to the terms up to the sixth order we deduce the corrected initial conditions:

$$\begin{aligned}
 C_1(x, 0) \approx & \int_0^1 (2.159 - 5.720y^2 + 4.705y^4 - 1.548y^6)c(x, y, 0) dy \\
 & + P \int_0^1 (-0.010 + 0.174y^2 - 0.482y^4 + 0.494y^6) \frac{\partial c(x, y, 0)}{\partial x} dy.
 \end{aligned} \tag{4.12}$$

$$\begin{aligned}
 C_2(x, 0) \approx & \int_0^1 (-0.417 + 6.991y^2 - 5.750y^4 + 1.892y^6)c(x, y, 0) dy \\
 & + P \int_0^1 (0.020 - 0.333y^2 + 0.867y^4 - 0.786y^6) \frac{\partial c(x, y, 0)}{\partial x} dy.
 \end{aligned} \tag{4.13}$$

To present numerical examples we consider different localized instantaneous sources of the contaminant. The boundary between the zones is assumed to locate on the level corresponding to the nearly diagonal form of the advection matrix, specifically (see the previous section) $y = \alpha = 0.55$. The length of the segment along the channel is 50, time step 0.005, the number of points across the channel 47 and along the channel 27. The original model (3.3), (3.4) and the low-dimensional model (3.17) are calculated using the Crank-Nicolson finite-difference scheme with the help of the IMSL package to resolve discretized equations.

In Fig. 2–4 we present the numerical results for the flow with $P = 60$. Initially the contaminant is concentrated in the fast zone with the maximum of the concentration located

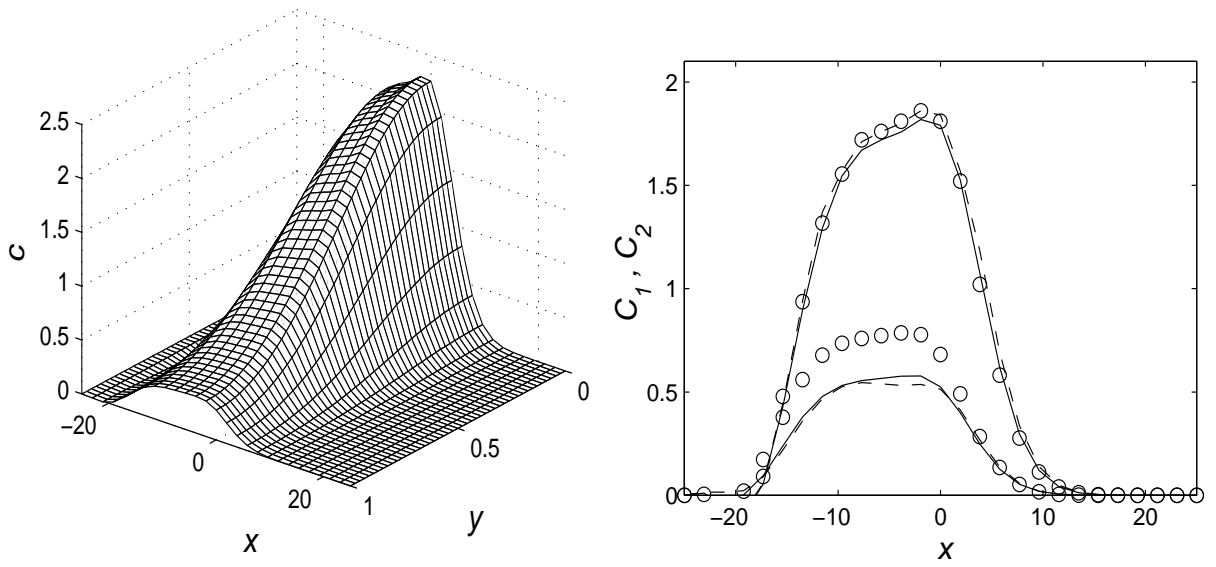


Figure 3: $t = 0.09$. Left: the concentration field. Right: the comparison between the original model (solid line) and the centre manifold model for the corrected (dashed line) and uncorrected (circles) initial conditions.

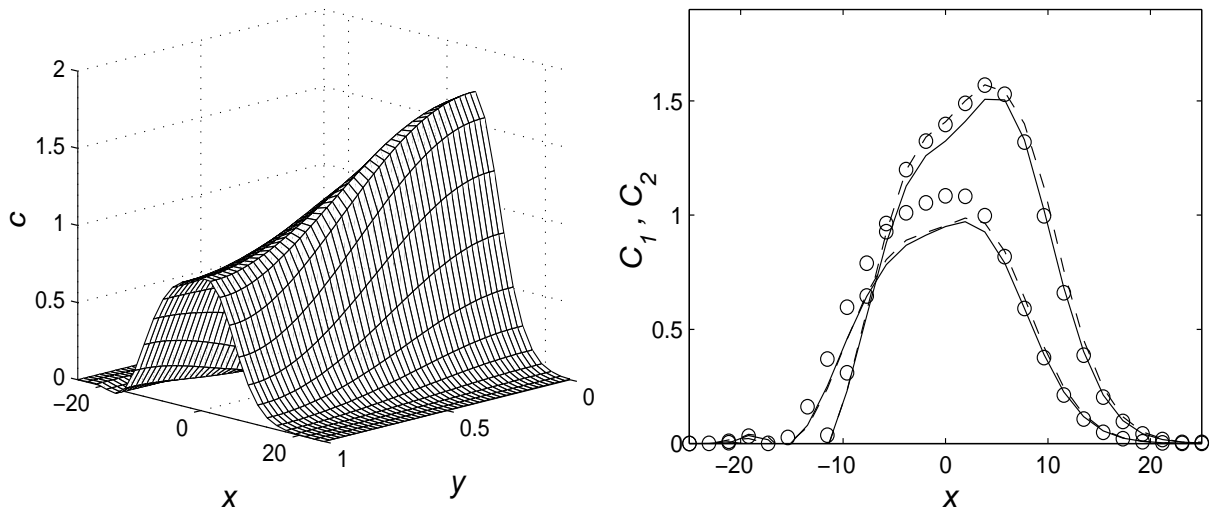


Figure 4: $t = 0.18$. Left: the concentration field. Right: the comparison between the models with the same line codes as for Fig. 3–4.

at the surface, $y = 0$:

$$c(x, y, 0) = 10 \exp[-(0.1(x + 11.5))^4 - (7y)^4].$$

Interestingly, the corrected initial concentration profile for the slow zone (Fig. 2, right) is negative! However, the physically irrelevant negative concentration exists only for a short period required for the solution to approach the original model. The corrected initial condition leads to better agreement with the original model (Fig. 3–4). Similarly to the one-zone model [15] the solution originated from the uncorrected initial condition sustains a shift along the channel with respect to the original solution. This shift, most discernible for the slow zone, is due to the fact that during a short period of time the contaminant is not yet spread across the zone and drifts predominantly near the surface where the flow is faster. The uncorrected initial condition implies, however, that the contaminant is already evenly distributed over the zone and, as governed by the dynamical equations, moves downstream at a lower speed (which approximately equals the zonal average speed as we showed in the previous section). This shift is a long-term effect which cannot be eliminated without correcting the initial conditions. At the same time we observe that the difference in magnitude between the slow-zone results for the corrected and uncorrected initial conditions is more noticeable than the along-channel shift. Using the corrected initial conditions seems to have small effect in the fast zone.

The situation with corrected initial conditions for the given model and centre manifold models in general is unusual from the point of view that initial conditions are *external* to differential equations. We see in our problem of dispersion in channels that the *corrected* initial conditions explicitly contain information from the differential equation, namely the Peclet number.

5 Conclusions

A two-zone model of contaminant dispersion in a channel is constructed with the use of centre manifold theory. For certainty the vertical profile of flow velocity is assumed parabolic; however other profiles can be readily analyzed in a similar way. The model uses a clear mathematical criterion to determine fractions of a channel occupied by zones and ensures,

on the ground of centre manifold theory, accurate approximation of real concentrations.

A mathematical transformation is proposed for initial concentration profiles to convert them into special initial conditions that provide the fastest approach to a real solution by a manifold solution. The transformed initial conditions differ from cross-zone averaged concentrations and incorporate some information about a flow. The effectiveness of the initial conditions is demonstrated numerically by a comparison between a model and simulations of original advection-diffusion equations.

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