

Mathematical Physics of Water Systems

Exam

code: 195400900, year: 2012/13

date: Friday 19 April 2012, time: 13:45-17:15, location: OH-116

- This exam consists of 14 numbered items, worth a total of 28 points.
- It is *not* allowed to use the syllabus, textbooks or personal notes.
- The use of a pocket calculator is allowed.
- Write your answers in either English or Dutch.
- After the exam, this paper must be handed in along with your answers.
- Time: 3.5 hours. Good luck!

Advection and diffusion of a pollutant (8p)

In an elongated basin of length L , the concentration of a certain pollutant simultaneously experiences advection by a background current as well as diffusion due to mixing processes. At both boundaries, the concentration is artificially kept to nonzero values. The concentration $c(x, t)$, a function of space x (in m) and time t (in s), thus obeys the following differential problem:

$$\frac{\partial c}{\partial t} + \gamma \frac{\partial c}{\partial x} = \delta \frac{\partial^2 c}{\partial x^2}, \quad c(0, t) = C, \quad c(L, t) = 2C, \quad c(x, 0) = c_{\text{init}}(x). \quad (1)$$

The parameters γ , δ and C are all positive. The initial profile has three parts:

$$c_{\text{init}}(x) = \underbrace{C \left[1 + \frac{x}{L} \right]}_{(i)} + \underbrace{C \sin \left(\frac{\pi x}{L} \right)}_{(ii)} + \underbrace{C \sin \left(\frac{5\pi x}{L} \right)}_{(iii)}. \quad (2)$$

- (1p) **1.** Determine whether the PDE in Eq.(1) is *hyperbolic*, *parabolic* or *elliptic*. How does this property depend on the value of γ ?
- (2p) **2.** In four plots, sketch the three contributions in Eq.(2) as well as c_{init} itself.
- The problem posed by Eqs.(1) and (2) allows for equilibrium solutions that turn out to depend on the so-called Péclet number $\text{Pe} = \gamma L / \delta$. See Fig.1.
- (1p) **3.** What is the physical meaning of small or large values of the Péclet number?
- (3p) **4.** Derive an expression for the equilibrium profile $c_{\text{eq}}(x)$ in terms of Pe .
Hint: derive an ODE for $f_{\text{eq}} = \frac{dc_{\text{eq}}}{dx}$, solve it and translate back to c_{eq} .
- (1p) **5.** Explain which of the two c_{eq} -profiles in Fig.1 corresponds to large Pe -values.

Diffusion only: analytical solution (9p)

Assuming that advection is absent ($\gamma = 0$), the solution can be written as

$$c(x, t) = C \left[1 + \frac{x}{L} \right] + A_1(t) \sin \left(\frac{\pi x}{L} \right) + A_2(t) \sin \left(\frac{5\pi x}{L} \right), \quad (3)$$

with two new unknowns: the time-dependent amplitudes $A_1(t)$ and $A_2(t)$. It can be shown that each of these quantities satisfies a *differential problem*. For example, by combining Eqs.(1) and (3), it follows that $A_1(t)$ satisfies the following ODE:

$$\frac{dA_1}{dt} + \left[\frac{\delta \pi^2}{L^2} \right] A_1 = 0. \quad (4)$$

- (1p) **6.** What type of behaviour is reflected by Eq.(4)?
- (5p) **7.** Derive and solve the *two differential problems* for $A_1(t)$ and $A_2(t)$.
- (2p) **8.** Explain the difference in behaviour between $A_1(t)$ and $A_2(t)$. Do this in terms of e-folding time scales and the underlying diffusion process.
- (1p) **9.** Is the total amount of pollutant in the domain constant over time? Explain.

items 10-14 on next pages >

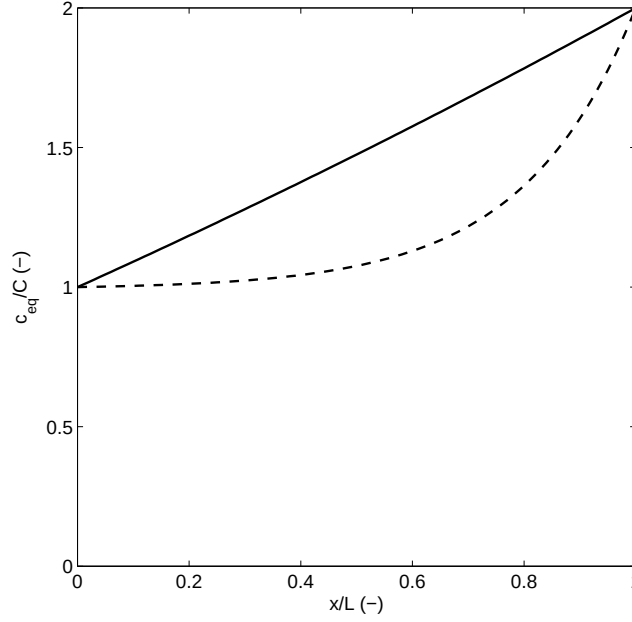


Figure 1: Two examples of equilibrium profiles $c_{\text{eq}}(x)$: one for a small value and one for a large value of the Péclet number.

Advection and diffusion: numerical solution (4p)

Let us return to the general case including advection ($\gamma > 0$). The problem posed by Eq.(1) can also be solved numerically, e.g. using the technique of finite differences. To this end, we define $x_j = j \Delta x$ with index j and space step Δx , such that $x_M = L$ for some integer M . Likewise, we define $t_k = k \Delta t$ with time step Δt . The quantity $c_{j,k}$ refers to the numerical solution at $x = x_j$ and $t = t_k$.

Let us now consider the following discretisations of the derivatives in Eq.(1):

Forward Euler for the time derivative,

Upwind for the first-order space derivative,

Central Space for the second-order space derivative.

The resulting numerical scheme can be written as

$$c_{j,k+1} = pc_{j-1,k} + qc_{j,k} + rc_{j+1,k}, \quad (5)$$

with constants p , q and r to be determined below (see item 11). The scheme in Eq.(5) can be used to calculate the solution everywhere in the numerical domain, except at the boundaries where the BC in Eq.(1) are readily imposed.

- (1p) **10.** Sketch the numerical space-time domain, showing the *numerical stencil* and the meanings of Δx , Δt and M .
- (3p) **11.** Express the quantities p , q and r in Eq.(5) in terms of only the Courant number $\mathcal{C}$ and the diffusion number $\mathcal{D}$.

turn page for items 12-14 >

Alternative numerical scheme (4p)

In fact, many numerical schemes exist. As an alternative scheme to the one in Eq.(5), let us consider:

$$\begin{aligned} \left[-\frac{\gamma\Delta t}{2\Delta x} - \frac{\delta\Delta t}{[\Delta x]^2} \right] c_{j-1,k+1} + \left[1 + \frac{2\delta\Delta t}{[\Delta x]^2} \right] c_{j,k+1} \\ + \left[\frac{\gamma\Delta t}{2\Delta x} - \frac{\delta\Delta t}{[\Delta x]^2} \right] c_{j+1,k+1} = c_{j,k}. \end{aligned} \quad (6)$$

Also this scheme is based on discretisations of the derivatives in Eq.(1). However, they are unknown (see item 12):

unknown discretisation of the time derivative,

unknown discretisation of the first-order space derivative,

unknown discretisation of the second-order space derivative.

- (3p) **12.** From Eq.(6), draw the *numerical stencil* and find out which discretisations were actually used to arrive at Eq.(6).
- (1p) **13.** Eq.(6) is *one* relationship involving *three* unknowns. Briefly explain how you would implement this kind of scheme in practise.

Complex numbers (2p)

Finally, we consider complex numbers. Of central importance is the so-called complex exponential, in terms of a (dimensionless) coordinate s defined as

$$\exp(is) = \cos s + i \sin s. \quad (7)$$

- (2p) **14.** By using the above definition of the complex exponential, show that

$$\frac{d}{ds}[\exp(is)] = i \exp(is) \quad (8)$$

Note: Do not use the chain rule here. This item is meant to show that the differentiation rule also works for exponentials with an imaginary argument!

end of exam <

Answers

Item 1 (1p)

The PDE is *parabolic* [1/3], because with $a = \pm\delta$ and $b = c = 0$ we get a vanishing discriminant $\text{Discr} = b^2 - 4ac = 0$ [1/3]. This property is independent of the value of the advection velocity γ [1/3].

Item 2 (2p)

The plots should display the following:

- (i) a linearly sloping profile from a value C at $x = 0$ to $2C$ at $x = L$ [1/2].
- (ii) a single sinusoidal hump of amplitude C , covering the spatial domain [1/2].
- (iii) a sequence of smaller sinusoidal humps (three peaks and two troughs), covering the spatial domain [1/2].
 - a correct superposition of the three parts above (note: no penalty if the wrong contributions are correctly added) [1/2].

Subtract [1/2] if the axes are not correctly labeled.

Item 3 (1p)

Low values of Pe implies a diffusion-dominated situation (relative to advection) [1/2]. High values of Pe implies an advection-dominated situation (relative to diffusion) [1/2].

Item 4 (4p)

Equilibrium profile requires solving the problem in Eq.(1) with

$$\frac{dc}{dt} = 0, \quad [1/3] \quad (9)$$

boundary conditions as imposed and disregarding the initial profile. We thus get the following equilibrium condition:

$$\gamma \frac{dc}{dx} = \delta \frac{d^2c}{dx^2}. \quad [1/3] \quad (10)$$

Upon defining $f_{\text{eq}} = \frac{dc}{dx}$, this translates to

$$\frac{df_{\text{eq}}}{dx} = \frac{\gamma}{\delta} f_{\text{eq}}, \quad [1/3] \quad (11)$$

which is a simple growth equation for f_{eq} as a function of x . The solution reads:

$$f_{\text{eq}}(x) = B \exp(\gamma x / \delta), \quad [1/3] \quad (12)$$

for some integration constant B . Transforming back to c_{eq} requires one integration, leading to

$$c_{\text{eq}}(x) = B_1 \exp(\gamma x / \delta) + B_2, \quad [1/3] \quad (13)$$

for arbitrary constants B_1 and B_2 . Their values follow from imposing the BC:

$$c_{\text{eq}}(0) = B_1 + B_2 = C, \quad c_{\text{eq}}(L) = B_1 \exp(\text{Pe}) + B_2, \quad [\mathbf{1/3}] \quad (14)$$

which gives after substitution/elimination

$$B_1 = \frac{C}{\exp(\text{Pe}) - 1}, \quad B_2 = \frac{C[\exp(\text{Pe}) - 2]}{\exp(\text{Pe}) - 1}. \quad [\mathbf{1/3}] \quad (15)$$

The final solution thus reads

$$c_{\text{eq}}(x) = C \frac{[\exp(\gamma x / \delta) + \exp(\text{Pe}) - 2]}{\exp(\text{Pe}) - 1}. \quad [\mathbf{2/3}] \quad (16)$$

Item 5 (1p)

The dashed curve $[\mathbf{1/2}]$. This strongly skewed profile is obtained for large Pe-values, as it reflects the strong advection of the values at the left-boundary $[\mathbf{1/2}]$.

Item 6 (1p)

Relaxation or exponential decay $[\mathbf{1}]$.

Item 7 (5p)

Substituting the trial solution in the PDE (without advection) requires the following derivatives

$$\frac{\partial c}{\partial t} = \frac{dA_1}{dt} \sin\left(\frac{\pi x}{L}\right) + \frac{dA_2}{dt} \sin\left(\frac{5\pi x}{L}\right), \quad [\mathbf{1/2}] \quad (17)$$

$$\frac{\partial^2 c}{\partial x^2} = -\left(\frac{\pi^2}{L^2}\right) A_1 \sin\left(\frac{\pi x}{L}\right) - \left(\frac{25\pi^2}{L^2}\right) A_2 \sin\left(\frac{5\pi x}{L}\right). \quad [\mathbf{1/2}] \quad (18)$$

Substituting these expressions in the PDE yields, after suitably collecting terms, the following result

$$\left[\frac{dA_1}{dt} + \left(\frac{\delta\pi^2}{L^2}\right) A_1 \right] \sin\left(\frac{\pi x}{L}\right) + \left[\frac{dA_2}{dt} + \left(\frac{25\delta\pi^2}{L^2}\right) A_2 \right] \sin\left(\frac{5\pi x}{L}\right) = 0, \quad [\mathbf{1}] \quad (19)$$

which must hold for any x . This implies that each of the terms in square brackets must vanish $[\mathbf{1}]$. From the initial profile in Eq.(2), it follows that the ICs read $A_1(0) = C$ and $A_2(0) = C$, which along with the differential equations above completes the formulation of the required differential problems $[\mathbf{1}]$. The solutions read

$$A_1(t) = C \exp\left(-\frac{\delta\pi^2}{L^2} t\right), \quad [\mathbf{1/2}] \quad (20)$$

$$A_2(t) = C \exp\left(-\frac{25\delta\pi^2}{L^2} t\right). \quad [\mathbf{1/2}] \quad (21)$$

Item 8 (2p)

The exponential decay of A_1 occurs much slower (larger e-folding time scale) than the exponential decay of A_2 (smaller e-folding time scale). [1] This is because of the weaker slopes of the single sine hump, which — compared to the 5 humps — have a much weaker diffusive flux (which is proportional to the slope). [1]

Item 9 (1p)

No [1/2].

Because of the Dirichlet conditions, the flux over the boundaries is not controlled. In this example, the total amount happens to decrease over time as the positive humps (most of them) and negative humps (a smaller number) all disappear [1/2].

Item 10 (1p)

Numerical domain should have the correct axes [1/4], show the stencil [1/4] and explain the meanings of Δx [1/8], Δt [1/8] and M [1/4].

Item 11 (3p)

By applying the correct discretisations [1/3][1/3][1/3], one obtains after some rearrangements [1/2], the following expressions [1/2][1/2][1/2]

$$p = \mathcal{D} + \mathcal{C}, \quad q = 1 - 2\mathcal{D} - \mathcal{C}, \quad r = \mathcal{D}. \quad (22)$$

Item 12 (3p)

Correct numerical stencil [3/4] We have the following discretisations:

Backward Euler for the time derivative [3/4],

Central Space for the first-order space derivative [3/4],

Central Space for the second-order space derivative [3/4].

Item 13 (1p)

This implicit method requires simultaneously considering all equations, along with the boundary conditions. This gives a set of $(M - 1)$ coupled linear equations with $(M - 1)$ unknowns, one equation for each interior point [1].

Item 14 (2p)

From the definition it follows that

$$\begin{aligned} \frac{d}{ds} \exp(is) &= \frac{d}{ds} (\cos s + i \sin s) && [1/2] \\ &= -\sin s + i \cos s && [1/2] \\ &= i^2 \sin s + i \cos s = i[i \sin s + \cos s] && [1/2] \\ &= i \exp(is). && [1/2] \end{aligned} \quad (23)$$