

On diffusive timescales¹

Eric Deleersnijder, 25 July 2020

Abstract. We assess the strengths and weaknesses of the classical diffusive timescale, i.e. the ratio of the square of the size of the domain to a characteristic value of the diffusivity (e.g. the domain-averaged diffusivity). On the basis of existing analytical solutions of one-dimensional diffusive problems, slightly different timescales are suggested, which, unfortunately, offer no decisive advantages. Things are seen to be even more intricate when dealing with a one-dimensional advection-diffusion problem. Clearly, asking for more than an order of magnitude is futile.

Introduction

When investigating transport problems involving diffusive processes, one is often led to estimate a timescale related to such phenomena. The usual formulation of it is as follows

$$\text{diffusion timescale} \approx \frac{(\text{length scale})^2}{\text{typical diffusivity}} \quad (1)$$

In spite of the word of caution issued by Deleersnijder (2019), it is generally believed that evaluating the relevant length scale and typical diffusivity is straightforward. As will be seen, this is not always so.

In this working note, we will revisit some of the analytical solutions of Deleersnijder (2007, 2014) in order to build relevant diffusion timescales and, in the process, show that seemingly correct diffusive timescale estimates may vary by up to one order of magnitude.

Vertical diffusion in a water column model

Consider a water column whose horizontal cross-sectional area is S . If z is the vertical coordinate (increasing upwards), the lower (resp. upper) boundary of the water column is located at $z = -h$ (resp. $z = 0$) so that the height of the water column is h (Figure 1). The domain of interest contains a non-reactive tracer whose concentration is assumed to be horizontally homogeneous. The Boussinesq approximation is assumed to hold valid. Constant ρ is the reference density of the fluid mixture under study. Accordingly, at time t , the mass of tracer present in the domain of interest reads

$$M(t) = \rho S \int_{-h}^0 C(t,z) dz \quad , \quad (2)$$

where $C(t,z)$ is the concentration of the tracer under study, which is defined as a mass fraction and, hence, is a dimensionless variable.

The abovementioned concentration obeys one-dimensional diffusion equation

¹ This working note is a tentative answer to a question posed by Dr Lisa V. Lucas in April 2020.

$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial z} \left(\kappa \frac{\partial C}{\partial z} \right) . \quad (3)$$

For the sake of simplicity, the (positive definite) vertical diffusivity κ is assumed to be a function of only the vertical coordinate z and, hence, is time-independent. The upper and lower boundaries are impermeable:

$$\left[\kappa \frac{\partial C}{\partial z} \right]_{z=-h} = 0 = \left[\kappa \frac{\partial C}{\partial z} \right]_{z=0} . \quad (4)$$

The initial condition reads

$$C(0, z) = C^0(z) . \quad (5)$$

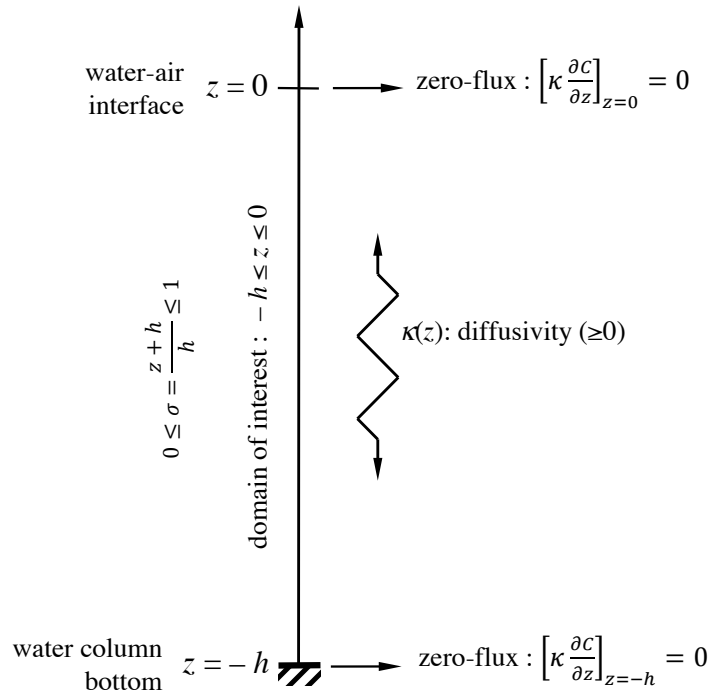


Figure 1. Illustration of the geometry and boundary conditions of the water column model under consideration. The height of the domain is denoted h . The bottom ($z = -h$) and surface ($z = 0$) boundaries are impermeable: there is no diffusive flux through them.

The depth-averaged concentration is denoted by means of an overbar:

$$[\bar{C}(t), \bar{C}^0] = \frac{1}{h} \int_{-h}^0 [C(t, z), C^0(z)] dz . \quad (6)$$

Integrating (3) over the domain and using boundary conditions (4), it is readily seen that the mean concentration is time-independent,

$$\bar{C}(t) = \bar{C}^0 , \quad (7)$$

implying that the tracer mass present in the domain is constant, i.e.

$$M(t) = \rho Sh \bar{C}^0 = M(0) . \quad (8)$$

The following integral relation is readily established

$$\frac{d}{dt} \int_{-h}^0 (\hat{C})^2 dz = -2 \int_{-h}^0 \kappa \left(\frac{\partial \hat{C}}{\partial z} \right)^2 dz \leq 0 , \quad (9)$$

where $\hat{C}(t, z) = C(t, z) - \bar{C}$ is the deviation of the concentration with respect to its depth mean. Thus, its L^2 -norm will decrease monotonically in such a way that

$$\lim_{t \rightarrow \infty} C(t, z) = \bar{C}^0 . \quad (10)$$

In other words, the tracer concentration progressively homogenises as time passes.

Analytical solutions

To derive the general expression of the analytical solution of the problem at hand, it is convenient to first introduce a dimensionless vertical coordinate,

$$\sigma = \frac{z+h}{h} , \quad (11)$$

which is zero at the bottom of the water column and is equal to unity at the top of it. Then, the diffusivity may be rewritten as follows

$$\kappa(\sigma) = K \kappa'(\sigma) , \quad (12)$$

with

$$K = \int_0^1 \kappa(\sigma) d\sigma = \bar{\kappa} , \quad (13)$$

and

$$\int_0^1 \kappa'(\sigma) d\sigma = 1 . \quad (14)$$

Clearly, characteristic diffusivity K (m^2/s) is the depth-averaged value of the diffusivity ($\bar{\kappa}$), whilst the depth-mean of dimensionless function κ' is equal to unity.

The concentration is of the form

$$C(t, z) = \underbrace{\frac{M}{\rho Sh}}_{=\bar{C}} \left[1 + \sum_{n=1}^{\infty} a_n e^{-\gamma_n t} \psi_n(\sigma) \right] \quad (15)$$

with $\gamma_n = \bar{\kappa} \lambda_n / h^2$; λ_n and ψ_n denote the n -th eigenvalue and eigenfunction of the following Sturm-Liouville problem²

$$\frac{d}{d\sigma} \left[\kappa'(\sigma) \frac{d\psi_n}{d\sigma} \right] = -\lambda_n \psi_n , \quad (16)$$

² Strictly speaking, this eigenvalue problem also has a zero-th order eigenvalue and eigenfunction, i.e. $\lambda_0 = 0$ and $\psi_0(\sigma) = 1$. They are associated with the first term in the right-hand side of (15).

$$\left[\kappa'(\sigma) \frac{d\psi_n}{d\sigma} \right]_{\sigma=0} = 0 = \left[\kappa'(\sigma) \frac{d\psi_n}{d\sigma} \right]_{\sigma=1} . \quad (17)$$

According to Sturm-Liouville's theory, the eigenfunctions have zero mean

$$\int_0^1 \psi_n(\sigma) d\sigma = 0 \quad (18)$$

and are orthogonal

$$\int_0^1 \psi_m \psi_n d\sigma = 0 \text{ if } m \neq n . \quad (19)$$

It is convenient to normalise them so that

$$\int_0^1 \psi_n^2 d\sigma = 1 . \quad (20)$$

The eigenvalues satisfy

$$0 < \lambda_1 < \lambda_2 < \dots < \lambda_n < \lambda_{n+1} < \dots \quad (21)$$

Finally, coefficients a_n are

$$a_n = \int_0^1 C^0(\sigma) \psi_n(\sigma) d\sigma . \quad (22)$$

Solution (15) is the sum of the time-independent depth-averaged concentration and exponentially-decreasing modes. The higher the order of the mode, the faster the decay. Thus, the mode exhibiting the slowest rate of decay is the first one ($n=1$), which is why it seems quite natural to assume that the relevant diffusive timescale must be associated with it: it represents the timescale for the adjustment of the transient solution to the steady-state one. Accordingly, this timescale is

$$T \approx \frac{1}{\gamma_1} = \frac{(h/\sqrt{\lambda_1})^2}{\bar{\kappa}} \approx \frac{(L_v)^2}{\bar{\kappa}} \quad (23)$$

A simple inspection of (1) and (23) reveals that these formulas are of the same type, as they should be. We can safely assume that the typical value of the diffusivity is its depth mean. Then, the relevant length scale is not the height of the water column. Instead, it is the ratio of the water column depth to the square root of the $n=1$ eigenvalue of the above Sturm-Liouville problem. In other words, the length scale is $L_v \approx h/\sqrt{\lambda_1}$.

The rms difference between concentration (15) and its depth-mean value reads

$$\varepsilon(t) = \sqrt{\int_0^1 [C - \bar{C}^0]^2 d\sigma} = \sqrt{\sum_{n=1}^{\infty} a_n^2 e^{-2\gamma_n t}} . \quad (24)$$

This expression admits asymptotic expansion

$$\varepsilon(t) \sim |a_1| e^{-\gamma_1 t} , \quad \gamma_1 t \rightarrow \infty , \quad (25)$$

which confirms that $1/\gamma_1$ is a relevant timescale.

Obviously, determining *a priori* timescale (23) is uneasy in practice. This is all the more so since the diffusivity generally varies in time. However, we will examine below the solutions

associated with a few, (hopefully) well-chosen diffusivity profiles, allowing us to suggest a rule that seems to be rather easy to apply for most practical purposes.

A diffusive timescale easy to estimate

Several vertical diffusivity profiles are worth considering. The simplest of them is a constant, leading to $\kappa'(\sigma) = 1$. Then, to account for the presence of the upper and lower boundaries, a parabolic profile may be deemed to be appropriate, yielding $\kappa'(\sigma) = 6\sigma(1-\sigma)$. In the vicinity of the seabed, the diffusivity increases as a linear function of the distance to the boundary, which is consistent with the existence of the logarithmic layer. Though the bottom is generally regarded as a solid boundary, the ocean-atmosphere interface is a freely-moving boundary. To take into account the difference in the nature of the lower and upper boundaries, another diffusivity profile may also be worth studying, namely $\kappa'(\sigma) = 3\sigma(1-\sigma/2)$. This diffusivity profile is maximum at the surface. The corresponding eigenvalues, diffusive timescales and eigenfunctions are listed in Table 1, and are illustrated in Figures 2-4.

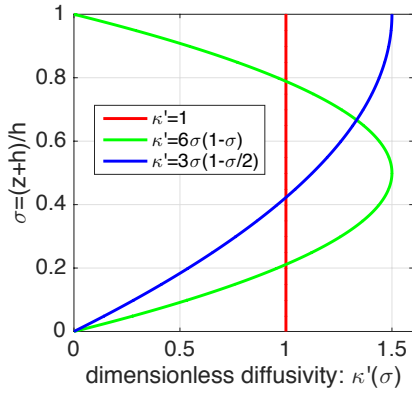


Figure 2. Dimensionless diffusivity profiles $\kappa' = \kappa / K$ considered herein.

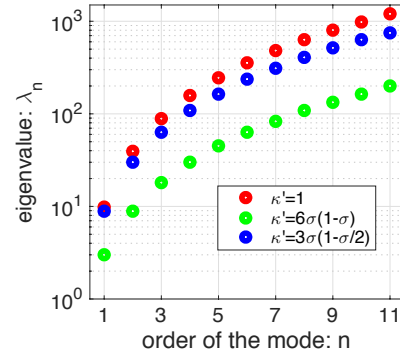


Figure 3. Eigenvalues of Sturm-Liouville problem (16)-(17).

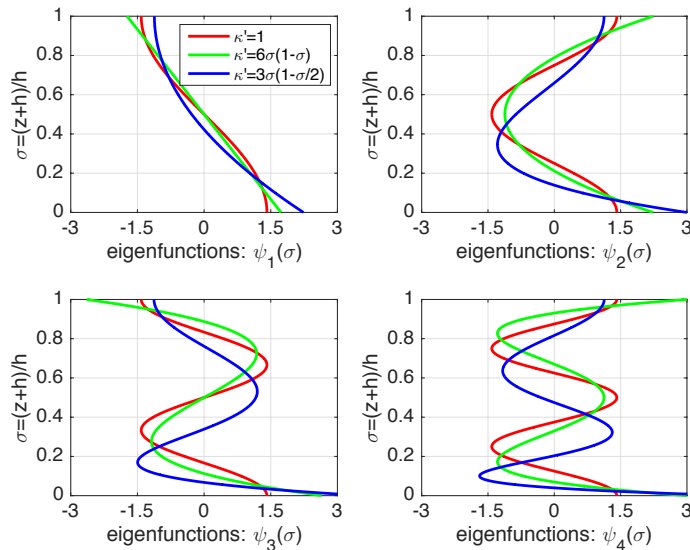


Figure 4. The first four eigenfunctions of Sturm-Liouville problem (16)-(17) for the diffusivity profiles under consideration.

Table 1. The eigenvalues λ_n and eigenfunctions $\psi_n(\sigma)$ for the diffusivity profiles considered in this study. The order of the mode is identified by integer index n , with $n=1,2,\dots$. The symbol P_n represents the n -th order Legendre polynomial. The vertical length scale to be taken into account for estimating the diffusive timescale according to formula (23) is $L_v = h / \sqrt{\lambda_1}$.

$\kappa'(\sigma) = 1$	$\kappa'(\sigma) = 6\sigma(1-\sigma)$	$\kappa'(\sigma) = 3\sigma(1-\sigma/2)$
$\lambda_n = n^2\pi^2$	$\lambda_n = \frac{3}{2}n(n+1)$	$\lambda_n = 3n(2n+1)$
$\frac{T}{h^2/\bar{\kappa}} \approx \frac{1}{\pi^2} \approx 0.10$ $L_v = h/\pi \approx 0.32h$	$\frac{T}{h^2/\bar{\kappa}} \approx \frac{1}{3} \approx 0.33$ $L_v = h/\sqrt{3} \approx 0.58h$	$\frac{T}{h^2/\bar{\kappa}} \approx \frac{1}{9} \approx 0.11$ $L_v = h/3 \approx 0.33h$
$\psi_n = \sqrt{2} \cos(n\pi\sigma)$	$\psi_n = (-1)^n \sqrt{2n+1} P_n(-1+2\sigma)$	$\psi_n = \sqrt{4n+1} P_{2n}(1-\sigma)$

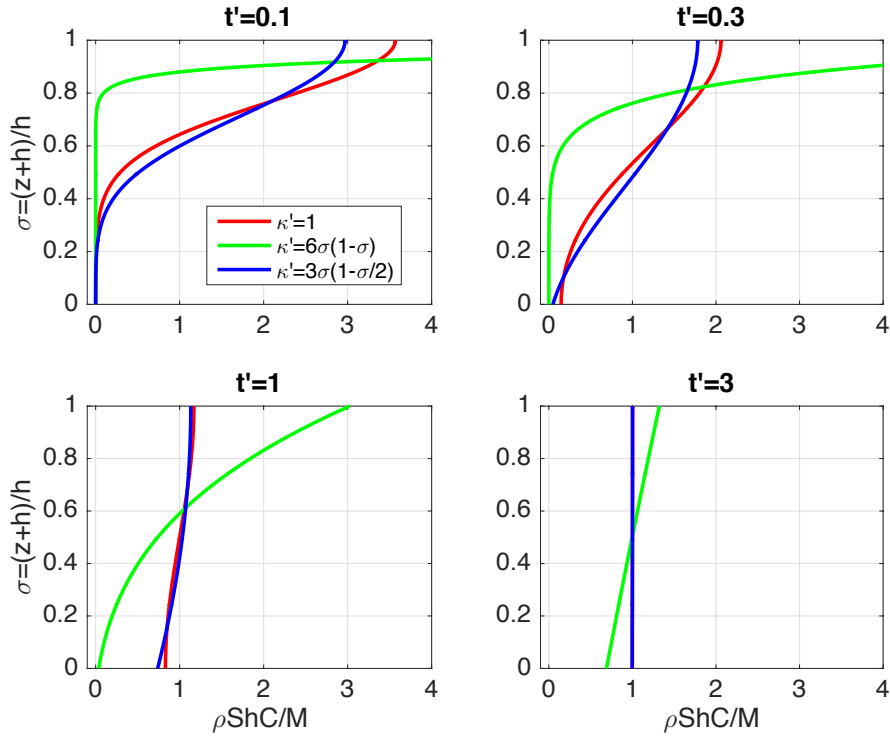


Figure 5. Normalized concentration profiles at various instants, with $t' = t/T$ and $T = h^2 / (4\bar{\kappa})$.

Of the three diffusivity profiles considered above, the most realistic one probably is $\kappa'(\sigma) = 6\sigma(1-\sigma)$. The associated vertical length scale, in the sense of expression (23), is $h/\sqrt{3} \approx 0.58h$. The vertical length scales related to the other two diffusivity profiles are

somewhat smaller. Therefore, it is suggested that, for all practical purposes, the vertical length scale be taken to be

$$L_v \approx \frac{h}{2} \Rightarrow T \approx \frac{h^2}{4\bar{\kappa}} \quad (26)$$

Figure 5 displays concentration profiles at various instants. The concentration corresponding to diffusivity $\kappa'(\sigma) = 6\sigma(1-\sigma)$ tends to the steady-profile slower than the other solutions, which would suggest that the adjustment timescale (26) is insufficiently relevant — as opposed to what has been said above. In fact, this is because the diffusivity is zero at both ends of the water column, which does not force the concentration gradient to be zero on the boundaries, thereby reducing the rate at which the concentration tends to its steady-state limit. In other words, diffusive timescale (26) is in agreement with (23), but things are more complex than this simple estimate suggests. This is confirmed by Figure 6.

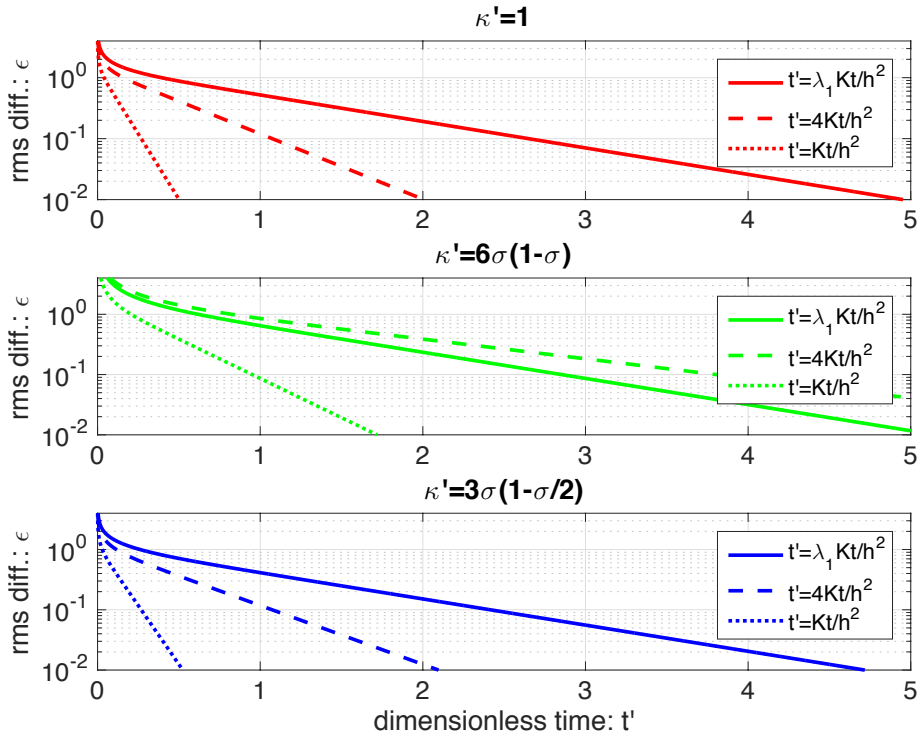


Figure 6. Time evolution of rms difference (24) for the three diffusivity profiles considered herein.

Discussion

The efforts made above to build a diffusive timescale that would be more relevant than commonly used expression $h^2 / \bar{\kappa}$ are largely fruitless. Admittedly, formula (26) is not without merit, but there is probably no decisive argument in its favour, partly because the boundary conditions also play a role in the adjustment toward the steady-state concentration profile. Things get even more complicated when diffusion is not the only transport process

taken into account. This is illustrated by the one-dimensional advection-diffusion problem dealt with below.

In the domain $0 \leq x \leq L$, we consider a one-dimensional advection-diffusion problem with constant velocity U and diffusivity K . We use dimensionless variables defined in such a way that the characteristic time is advective timescale $T_a = L/U$ and the length scale is L . Then, the Peclet number is, as usual, the ratio of diffusive timescale $T_d = L^2/K$ to the advective one, i.e.

$$Pe = \frac{T_d}{T_a} = \frac{L^2/K}{L/U} = \frac{UL}{K} . \quad (27)$$

For simplicity, we impose Dirichlet boundary conditions (zero concentration) at both ends of the domain. Then, the partial differential problem to be solved reads

$$\frac{\partial C}{\partial t} = -\frac{\partial C}{\partial x} + \frac{1}{Pe} \frac{\partial^2 C}{\partial x^2} , \quad (28)$$

$$C(t,0) = 0 = C(t,1) , \quad (29)$$

$$C(0,x) = C^0(x) . \quad (30)$$

The solution of (28)-(30) is of the form

$$C(t,x) = \exp\left(\frac{Pe x}{2}\right) \tilde{C}(t,x) , \quad (31)$$

where $\tilde{C}(t,x)$ satisfies

$$\frac{\partial \tilde{C}}{\partial t} = -\frac{Pe}{4} \tilde{C} + \frac{1}{Pe} \frac{\partial^2 \tilde{C}}{\partial x^2} , \quad (32)$$

$$\tilde{C}(t,0) = 0 = \tilde{C}(t,1) , \quad (33)$$

$$\tilde{C}(0,x) = \exp\left(-\frac{Pe x}{2}\right) C^0(x) . \quad (34)$$

This leads to

$$\tilde{C}(t,x) = \sum_{n=1}^{\infty} a_n e^{-\gamma_n t} \sin(k_n x) , \quad (35)$$

with

$$k_n = \pi n , \quad (36)$$

$$\gamma_n = \frac{Pe}{4} + \frac{\pi^2 n^2}{Pe} , \quad (37)$$

$$a_n = \frac{\int_0^1 \exp\left(-\frac{Pe x}{2}\right) C^0(x) \sin(k_n x) dx}{\int_0^1 \sin^2(k_n x) dx} = 2 \int_0^1 \exp\left(-\frac{Pe x}{2}\right) C^0(x) \sin(k_n x) dx . \quad (38)$$

As time progresses, the concentration tends to zero,

$$\lim_{t \rightarrow \infty} C(t, x) = 0 \quad (39)$$

and the associated adjustment timescale is that related with the first mode ($n = 1$) in (35), i.e.

$$T = \frac{T_a}{\gamma_1} = \frac{4T_d}{4\pi^2 + (T_d/T_a)^2} = \frac{4T_d}{4\pi^2 + Pe^2} \quad (40)$$

For an advection-dominated problem ($T_a \ll T_d$), this timescale behaves as follows:

$$T \sim \frac{4T_a^2}{T_d} - \frac{16\pi^2 T_a^4}{T_d^3}, \quad \frac{T_a}{T_d} \rightarrow 0 \quad (41)$$

In contrast, if diffusion proceeds much faster than advection ($T_d/T_a \ll 1$), we obtain

$$T \sim \frac{T_d}{\pi^2} - \frac{T_d^3}{4\pi^4 T_a^2}, \quad \frac{T_d}{T_a} \rightarrow 0 \quad (42)$$

Conclusion

All of the developments above suggest that building a diffusive timescale that would be both accurate and valid in most cases is hardly possible. The only thing one can hope for is an order of magnitude. Demanding more than that is most probably futile.

References

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