On the impermeability conditions of a motionless surface

Eric Deleersnijder, 12 November 2017

Abstract. *The fluxes due to advection and turbulent diffusion of every constituent of a fluid mixture are recalled. The impermeability condition of a surface to a given constituent is established. If the surface under consideration is completely impermeable, then both the advective flux and the diffusive one of every constituent that cross this surface are zero. This is illustrated by studying the solution of a reactive (with first-order decay) transport equation in a semi-infinite domain, which is obtained by means of the method of mirror images. The shortcomings of this model are shown not to be critical. The analytical solution is displayed, illustrating the impact of the key parameters of the model.*

Mass fluxes

Consider a fluid mixture consisting of $N+1$ constituents, whose concentrations are denoted $C_n(t,\mathbf{x})$ $(n=0,1,...N)$. The concentrations are defined as mass fractions, implying that they are dimensionless functions satisfying the following constraint:

$$\sum_{n=0}^{N} C_n(t,\mathbf{x}) = 1 \quad . \tag{1}$$

Let $\rho(t,\mathbf{x})$ represent the density[1] of the mixture ($\mathrm{kg\,m^{-3}}$). Then, the mass flux of the *n*-th constituent ($\mathrm{kg\,m^{-2}\,s^{-1}}$) reads

$$\boldsymbol{\phi}_n = \rho C_n \mathbf{v} - \rho \kappa_t \nabla C_n \quad , \tag{2}$$

where $\kappa_t(t,\mathbf{x})$ is the relevant eddy diffusivity and $\mathbf{v}(t,\mathbf{x})$ is the barycentric velocity[2] of the mixture. Obviously, the mass flux of the mixture is

$$\boldsymbol{\Phi} = \sum_{n=0}^{N} \boldsymbol{\phi}_n = \rho \underbrace{\left(\sum_{n=0}^{N} C_n\right)}_{=1,\text{ see (1)}} \mathbf{v} - \rho\kappa_t \nabla \underbrace{\left(\sum_{n=0}^{N} C_n\right)}_{=1,\text{ see (1)}} = \rho \mathbf{v} \tag{3}$$

Now consider motionless surface Γ, which is delineated by thought. Let unit vector $\mathbf{n}$ be normal to this surface. The mass of the *n*-th constituent crossing surface element $\delta\Gamma$ per unit time ($\mathrm{kg\,s^{-1}}$) is

$$\boldsymbol{\phi}_n \bullet \mathbf{n}\,\delta\Gamma \sim \left(\rho C_n \mathbf{v} - \rho\kappa_t \nabla C_n\right) \bullet \mathbf{n}\,\delta\Gamma \quad , \quad \delta\Gamma \to 0 \quad . \tag{4}$$

It is then readily understood that the mass of the mixture crossing the same surface element per unit time is

$$\boldsymbol{\Phi} \bullet \mathbf{n}\,\delta\Gamma \sim \sum_{n=0}^{N} \boldsymbol{\phi}_n \bullet \mathbf{n}\,\delta\Gamma \sim \rho\mathbf{v} \bullet \mathbf{n}\,\delta\Gamma \quad , \quad \delta\Gamma \to 0 \quad . \tag{5}$$

[1] If the Boussinesq approximation is used, density $\rho(t,\mathbf{x})$ must be replaced by its constant, reference value ρ_*.

[2] de Groot S.R. and P. Mazur, 1962, *Non-Equilibrium Thermodynamics*, North-Holland, Amsterdam, 510 pages

Impermeability conditions

If surface Γ is impermeable to the n-th constituent[3], then there is no flux of this constituent through it, yielding the related impermeability condition

$$[\boldsymbol{\phi}_n \bullet \mathbf{n}]_{\mathbf{x}\in\Gamma} = \left[\left(\rho C_n \mathbf{v} - \rho\kappa_t \nabla C_n\right)\bullet \mathbf{n}\right]_{\mathbf{x}\in\Gamma} = 0 \quad . \tag{6}$$

If the surface under consideration is impermeable to all the constituents, then the mass flux of the mixture crossing it is zero:

$$[\boldsymbol{\Phi} \bullet \mathbf{n}]_{\mathbf{x}\in\Gamma} = \left[\sum_{n=0}^{N} \boldsymbol{\phi}_n \bullet \mathbf{n}\right]_{\mathbf{x}\in\Gamma} = [\rho \mathbf{v} \bullet \mathbf{n}]_{\mathbf{x}\in\Gamma} = 0 \quad . \tag{7}$$

Thus, for a **completely impermeable surface**, both the advective flux and the diffusive one of every constituent are zero. The zero diffusive flux boundary conditions read

$$[-\rho\kappa_t \nabla C_n \bullet \mathbf{n}]_{\mathbf{x}\in\Gamma} = 0 \quad , \qquad n = 0,1,\ldots N \tag{8}$$

Concentration in a semi-infinite domain

The domain of interest is defined by inequalities

$$-\infty < x,y < \infty \quad , \quad 0 \le z \le \infty \quad . \tag{9}$$

Surface Γ is defined by $z=0$ and is assumed to be completely impermeable.

The velocity is $\mathbf{v} = U\mathbf{e}_x$, where U is a positive constant. The eddy coefficient K is also constant. Under the Boussinesq approximation, the concentration $C(t,\mathbf{x})$ of a constituent exhibiting a first-order decay (with a constant decay rate) reads

$$\frac{\partial C}{\partial t} + U\frac{\partial C}{\partial x} = -\frac{C}{\tau} + K\left(\frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial y^2} + \frac{\partial^2 C}{\partial z^2}\right) \quad , \tag{10}$$

where constant τ is the mean life[4] of the tracer under consideration. At the initial instant (t=0), the tracer concentration is zero and a mass M of the tracer under study is abruptly injected into the domain at point $\mathbf{x} = L\mathbf{e}_z$. The corresponding initial condition is

$$C(0^+,\mathbf{x}) = \frac{M}{\rho_\bullet}\delta(\mathbf{x} - L\mathbf{e}_z) \quad , \tag{11}$$

where δ denotes the Dirac delta function. The mixture velocity obviously is parallel to impermeable surface Γ, implying that no advective flux crosses this surface. There is no diffusive flux of the tracer under study through this surface either:

$$\left[-K\frac{\partial C}{\partial x}\right]_{z=0} = 0 \quad . \tag{12}$$

If the domain were infinite, i.e. if the domain were not limited by impermeable surface Γ, the concentration would be

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[3] A physical interface can be permeable to some of the constituents of a fluid mixture and impermeable to the others. For instance, when evaporation and precipitation are negligible, the sea surface can be regarded as impermeable to pure water and permeable to a range of gases, such as oxygen, carbon dioxide, (stratospheric ozone-depleting) chlorofluorocarbons, etc.

[4] The corresponding half-life is $\tau_{1/2} = (\log 2)\tau \approx 0.7\,\tau$.

$$C_+(t,\mathbf{x}) = \frac{M\ e^{-t/\tau}}{\rho_\bullet (4\pi K t)^{3/2}} \exp\left[-\frac{(x-Ut)^2+y^2+(z-L)^2}{4Kt}\right] \tag{13}$$

In other words, $C_+(t,\mathbf{x})$ satisfies governing equation (10) and initial condition (11), but not boundary condition (12). The solution to differential problem (10)-(20) can be obtained by having recourse to the method of mirror images (Figure 1). This consists in assuming for an instant that the domain of interest is infinite and injecting abruptly a mass M of tracer at $\mathbf{x}=-L\mathbf{e}_z$. The corresponding solution reads

$$C(t,\mathbf{x}) = C_+(t,\mathbf{x}) + C_-(t,\mathbf{x}) \tag{14}$$

with

$$C_\pm(t,\mathbf{x}) = \frac{M\ e^{-t/\tau}}{\rho_\bullet (4\pi K t)^{3/2}} \exp\left[-\frac{(x-Ut)^2+y^2+(z\mp L)^2}{4Kt}\right] . \tag{16}$$

Function (14) is symmetric with respect to surface $z=0$, implying that it satisfies boundary condition (12). This is easily verified:

$$\left[-K\frac{\partial C}{\partial x}\right]_{z=0} = (-K)\frac{M\ e^{-t/\tau}}{\rho_\bullet (4\pi K t)^{3/2}} \exp\left[-\frac{(x-Ut)^2+y^2+L^2}{4Kt}\right] \times\left(-\frac{1}{4Kt}\right)\underbrace{\left[2(z-L)+2(z+L)\right]_{z=0}}_{=0} = 0 \tag{15}$$

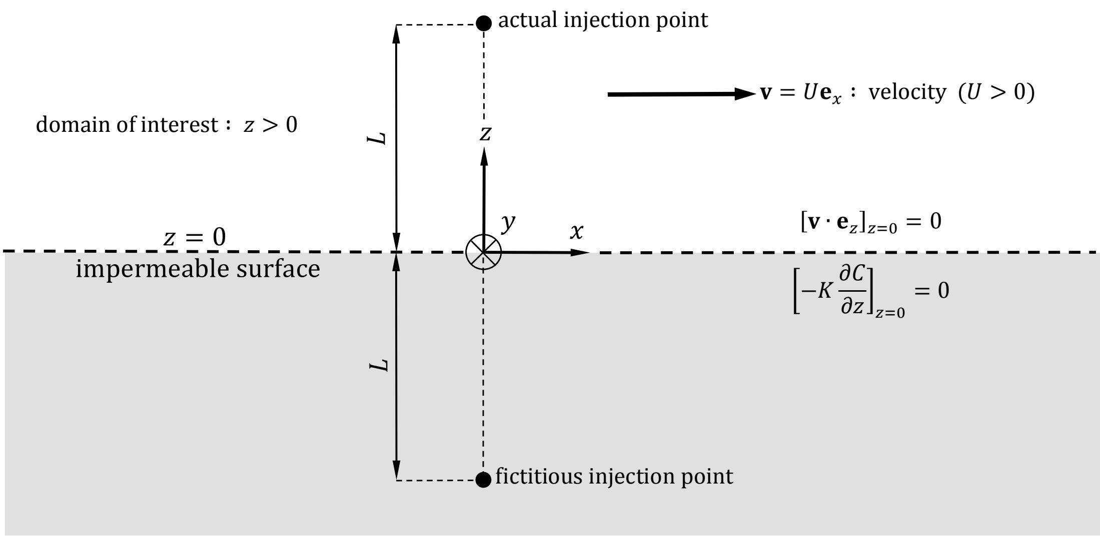

Figure 1. Illustration of the geometry of the domain of interest (z>0) showing the point where mass M of tracer is abruptly injected at t=0 and the fictitious injection point associated with the method of mirror images. Surface z=0 is completely impermeable, implying that the advective and diffusive mass fluxes crossing it are both prescribed to be zero.

Expression (14) satisfies governing equation (10), initial condition (11) and impermeability condition (12). Therefore, it is the solution of the differential problem under consideration.

Using integral

$$\int_0^\infty e^{-a\varsigma^2}\, d\varsigma = \sqrt{\frac{\pi}{4a}} \ , \quad a > 0 \ , \tag{17}$$

it may be seen that the mass of tracer present in the domain of interest is

$$m(t) \ = \ \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_0^{\infty} \rho_\bullet C(t,\mathbf{x})\, dz\, dy\, dz \ = \ M\, e^{-t/\tau} \quad . \tag{18}$$

At the initial instant, the mass of tracer is equal to the mass injected abruptly injected into the domain, i.e. $m(0) = M$. This is reassuring as to the well foundedness of solution (14). The mass of tracer present in the domain decays exponentially with timescale τ . This property is independent of advective and diffusive transport processes. This is because the first-order decay process affecting the fate of the tracer under consideration proceeds at the same (constant) rate at any time and location.

The rate of decay of the tracer considered herein is τ^{-1} . If he latter is zero, i.e. $\tau \to \infty$ ("infinitely slow" decay or "infinite mean life"), then the tracer actually is passive or inert, implying that its total mass is conserved: (18) transforms to $m(t) = M$. This result is in accordance with elementary physical intuition.

Pathology of the model

Concentration (14) is a dimensionless function intended to be a mass fraction. Hence, it should be smaller than or equal to unity at any time and location. In the vicinity of injection point $\mathbf{x} = Z\,\mathbf{e}_z$ and for sufficiently small values of the time, this condition is not satisfied. This is because the initial condition is an unrealistic one: a finite mass of tracer cannot be concentrated in an arbitrarily small volume. To make things worse, the mixture velocity cannot be assumed to be a constant in the vicinity of the injection for small values of time. In this region, the mixture velocity is likely to be dominated by that of the particles of the newly injected tracer.

However imperfect the present model may be, it leads to a differential problem that is relatively easy to solve. In addition, the tracer concentration quickly becomes much smaller than unity, thereby causing the abovementioned inconsistencies of the present model to vanish. In other words, the weakness of the present model quickly disappears as time progresses. This flaw is not a critical one, which is why this kind of model is likely to remain in use in the long term.

Graphical representation

To represent solution (14) graphically, it is convenient to use a suitably-normalised form of the concentration and relevant dimensionless independent variables (Figure 2):

$$C'(t',\mathbf{x}') \ = \ C'_+(t',\mathbf{x}') \ + \ C'_-(t',\mathbf{x}') \ \ , \tag{19}$$

with

$$C'_{\pm} \;=\; \frac{\rho_{\bullet} K^3}{MU^3} C_{\pm} \quad , \tag{20}$$

and

$$t' = \frac{t}{K/U^2} \quad , \quad \mathbf{x}' = \frac{\mathbf{x}}{K/U} \quad . \tag{21}$$

This yields

$$C'_{\pm}(t',\mathbf{x}') \;=\; \frac{e^{-t'/Je}}{(4\pi t')^{3/2}} \exp\left[-\frac{(x'-t')^2 + (y')^2 + (z' \mp Pe)^2}{4t'} \right] \tag{22}$$

where $Pe = UL/K$ is the Peclet number, whilst $Je = U^2 \tau / K$ is the Jenkins number[5]. The latter may be viewed as a Peclet number for which the length scale is $U\tau$, i.e. the distance travelled at velocity U during the mean life of the decaying tracer. The Jenkins number is a measure of the importance of the first-order decay process: when Je is large (small), then the first-order decay is much slower (faster) than the transport processes.

Unsurprisingly, (19) satisfies the following integral constraint

$$\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{0}^{\infty} C'(t,\mathbf{x}')\, dz'\, dy'\, dz' \;=\; e^{-t'/Je} \quad , \tag{23}$$

which is the dimensionless counterpart of (18).

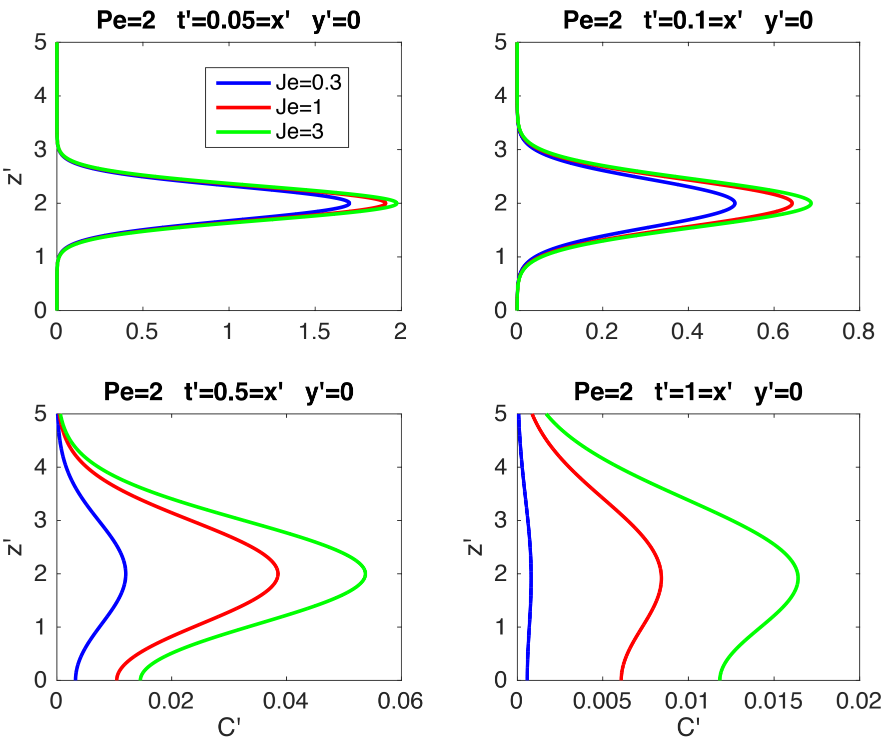

Figure 2. Illustration of normalised solution (19).

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[5] Mouchet A. and E. Deleersnijder, 2008, The leaky funnel model, a metaphor of the ventilation of the World Ocean as simulated by an OGCM, *Tellus*, 60A, 761-774