On the structure of a compartment model for tracer transport

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It is seen how to build a compartment model for predicting or understanding tracer transport that shares some of the properties of the corresponding continuous model.

Continuous tracer transport model

Let t and $\mathbf{x}$ denote time and the position vector. Under the Boussinesq approximation, in the domain of interest Ω limited by the surface Γ, the concentration $C(t,\mathbf{x})$ of a tracer obeys the following equation

$$\frac{\partial C}{\partial t} = q - \nabla \bullet (\mathbf{u}C - \mathbf{K} \bullet \nabla C) \ , \tag{1}$$

where $\mathbf{u}$ is the velocity field, which is divergence-free, i.e.

$$\nabla \bullet \mathbf{u} = 0 \ ; \tag{2}$$

the diffusivity tensor $\mathbf{K}$ is symmetric and positive definite (Deleersnijder et al. 2001, Deleersnijder 2003); q is the source/sink term, i.e. the rate of production/destruction of the tracer, which is zero if the tracer is passive — or inert.

The mean tracer concentration is defined to be

$$\overline{C}(t) = \frac{1}{\Omega} \int_{\Omega} C(t,\mathbf{x}) \, d\Omega \ , \tag{3}$$

while the variance of the concentration is

$$\sigma^2(t) = \frac{1}{\Omega} \int_{\Omega} [C(t,\mathbf{x}) - \overline{C}(t)]^2 \, d\Omega \ . \tag{4}$$

The flux that enters the domain through the boundary Γ is

$$\Phi = -\int_{\Gamma} (\mathbf{u}C - \mathbf{K} \bullet \nabla C) \bullet \mathbf{n} \, d\Gamma \ , \tag{5}$$

where $\mathbf{n}$ is the outward unit normal to Γ. If the domain boundary is impermeable, then the relations $\mathbf{u} \bullet \mathbf{n} = 0$ and $(\mathbf{K} \bullet \nabla C) \bullet \mathbf{n} = 0$ hold true at any point of Γ, implying that $\Phi = 0$. On the other hand, the mean rate of production/destruction will be denoted

$$\overline{q} = \int_{\Omega} q \, d\Omega \ . \tag{6}$$

The following properties are readily seen to hold valid:

Property 1: The mean tracer concentration satisfies the following relation

$$\frac{d\overline{C}}{dt} = \overline{q} + \frac{\Phi}{\Omega} \ . \tag{7}$$

This relation is obtained by integrating (1) over the domain of interest and by taking into account (3), (5) and (6).

Property 2: For a passive tracer in an isolated domain, the mean tracer concentrations is a constant, i.e.

$$\overline{C}(t) = \overline{C}(0) . \tag{8}$$

For the tracer under consideration, $\overline{q} = 0$ and $\Phi = 0$. Substituting these relations into (7) immediately leads to (8).

Property 3: For a passive tracer in an isolated domain, the variance of the concentration decreases monotonically until the tracer concentration is equal at any time and position to $\overline{C}(0)$. *This is because*

$$\frac{d\sigma^2}{dt} = -\frac{2}{\Omega}\int_{\Omega} \nabla C \bullet \mathbf{K} \bullet \nabla C \, d\Omega . \tag{9}$$

Clearly, advective transport has no impact on the homogenisation of the tracer concentration; only diffusive processes do.

To establish this relation, it is first necessary to introduce the deviation of the concentration with respect to its domain-averaged value,

$$\hat{C}(t) = C(t) - \overline{C}(t) . \tag{10}$$

Combining (1)-(2), (8) and (10) yields

$$\frac{\partial \hat{C}}{\partial t} = -\nabla \bullet (\mathbf{u}\hat{C} - \mathbf{K} \bullet \nabla \hat{C}) . \tag{11}$$

Then, multiplying (11) by $\hat{C}(t)$, one has after some manipulations

$$\frac{\partial \hat{C}^2}{\partial t} = -\nabla \bullet (\mathbf{u}\hat{C}^2 - 2\hat{C}\mathbf{K} \bullet \nabla C) - 2\nabla C \bullet \mathbf{K} \bullet \nabla C . \tag{12}$$

Integrating (12) over the domain of interest, using the divergence theorem one obtains

$$\begin{aligned} \Omega\frac{d\sigma^2}{dt} &= -\int_{\Gamma} (\mathbf{u}\hat{C}^2 - 2\hat{C}\mathbf{K} \bullet \nabla C) \bullet \mathbf{n} \, d\Gamma - 2\int_{\Omega} \nabla C \bullet \mathbf{K} \bullet \nabla C \, d\Omega \\ &= -\int_{\Gamma} [\hat{C}^2 \underbrace{\mathbf{u} \bullet \mathbf{n}}_{=0} - 2\hat{C}\underbrace{(\mathbf{K} \bullet \nabla C) \bullet \mathbf{n}}_{=0}] \, d\Gamma - 2\int_{\Omega} \nabla C \bullet \mathbf{K} \bullet \nabla C \, d\Omega \end{aligned} . \tag{13}$$

The surface integral is zero, because the domain is isolated, so that (13) simplifies to (9). As the diffusivity tensor is positive definite, the right-hand side member of (9) is negative until the concentration gradient is zero at any location in the domain of interest. If so, the concentration is equal to a constant, and, by virtue of (8), the latter must be equal to $\overline{C}(0)$.

Property 4: For a passive tracer in an isolated domain, if the initial concentration is constant, then it must remain constant.

If $q = 0$ and if $C(0,\mathbf{x}) = C_0$, where C_0 is a constant, then substituting $C(t,\mathbf{x}) = C_0$ into (1) yields $-(\nabla \bullet \mathbf{u}C_0) = 0$, which is identically satisfied by virtue of (2). As there is no flux through every part of the boundary of the domain, $C(t,\mathbf{x}) = C_0$ is the solution of the problem dealt with.

Compartment model

To derive a compartment model, first divide the domain of interest into *N* subdomains:

$$\Omega = \Omega_1 \cup \Omega_2 \cup ..\Omega_N \ . \tag{14}$$

Let $\Gamma_{i,j} = \Gamma_{j,i}$ denote the interface between subdomain Ω_i and Ω_j. Clearly, if the latter are not contiguous, the area of $\Gamma_{i,j}$ is zero. Similarly, the interface separating the subdomain Ω_i from the domain environment is denoted $\Gamma_{i,e}$. The unit vector that is normal to $\Gamma_{i,j}$ and is pointing from Ω_i to Ω_j is $\mathbf{n}_{i,j}$, with $\mathbf{n}_{i,j} = -\mathbf{n}_{j,i}$. The average over the subdomain Ω_i of the tracer concentration and the production/destruction term are

$$C_i(t) = \frac{1}{\Omega_i} \int_{\Omega_i} C(t,\mathbf{x})\, d\Omega_i \tag{15}$$

and

$$q_i(t) = \frac{1}{\Omega_i} \int_{\Omega_i} q(t,\mathbf{x})\, d\Omega_i \ . \tag{16}$$

Then, integrating (1) over subdomain Ω_i yields

$$\begin{aligned} \Omega_i \frac{dC_i}{dt} = \Omega_i q_i &- \sum_{\substack{j=1 \\ j\neq i}}^{N} \overbrace{\int_{\Gamma i,j} (\mathbf{u}C - \mathbf{K} \bullet \nabla C) \bullet \mathbf{n}_{i,j}\, d\Gamma_{i,j}}^{\phi_{i,j}} \\ &- \underbrace{\int_{\Gamma i,e} (\mathbf{u}C - \mathbf{K} \bullet \nabla C) \bullet \mathbf{n}_{i,e}\, d\Gamma_{i,e}}_{\phi_{i,e}} \end{aligned} \tag{17}$$

with $\phi_{i,j} = -\phi_{j,i}$ and $\phi_{i,e} = \phi_{e,i}$.

In a compartment model, only the subdomain-averaged concentrations are available. Therefore, the surface integrals in the right-hand side member of (17) cannot be evaluated exactly and, hence, must be approximated. It seems natural to work out parameterisations involving both an advective and a diffusive contribution, i.e.

$$\phi_{i,j} \approx \underbrace{\Gamma_{i,j}\, u_{i,j}\, \frac{C_i + C_j}{2}}_{\text{advective flux}} + \underbrace{\left(-\Gamma_{i,j}\, k_{i,j}\, \frac{C_j - C_i}{l_{i,j}} \right)}_{\text{diffusive flux}} , \tag{18}$$

where the velocity $u_{i,j}$, the diffusivity $k_{i,j}$ and the distance $l_{i,j}$ must satisfy

$$u_{i,j} = -u_{j,i} \ , \tag{19}$$

$$k_{i,j} = k_{j,i} > 0 \tag{20}$$

and

$$l_{i,j} = l_{j,i} > 0 \ . \tag{21}$$

Similar expressions apply if j is replaced by e, i.e. for the fluxes between the subdomain under consideration and the environment of the domain of interest. For the sake of simplicity, introduce the following "fluxes" (which are expressed in $m^3\, s^{-1}$)

$$U_{i,j} = \Gamma_{i,j}\, u_{i,j} \tag{22}$$

and

$$V_{i,j} = \frac{\Gamma_{i,j}\, k_{i,j}}{l_{i,j}} \ . \tag{23}$$

Clearly, these fluxes are such that

$$U_{i,j} = -U_{j,i} \tag{24}$$

and

$$V_{i,j} = V_{j,i} > 0 \ . \tag{25}$$

Using all of the above definitions and parameterisations, the equation governing the evolution of the concentration in each compartment is

$$\Omega_i \frac{dC_i}{dt} = \Omega_i q_i - \underbrace{\sum_{\substack{j=1 \\ j\neq i}}^{N} U_{i,j} \frac{C_i + C_j}{2}}_{\text{advective flux budget}} - \underbrace{\sum_{\substack{j=1 \\ j\neq i}}^{N} \left[-V_{i,j}(C_j - C_i)\right]}_{\text{diffusive flux budget}} + \phi_{e,i} \tag{26}$$

Upon defining the velocity $u_{i,j}$ in such a way that

$$\Gamma_{i,j}\, u_{i,j} = \int_{\Gamma_{i,j}} \mathbf{u} \bullet \mathbf{n}_{i,j}\, d\Gamma_{i,j} \ , \tag{27}$$

it is readily seen that

$$\sum_{\substack{j=1 \\ j\neq i}}^{N} U_{i,j} + U_{i,e} = 0 \ , \tag{28}$$

which is the counterpart to the continuity equation (2).

In the compartment representation, the domain-averaged concentration and the variance of the concentration are

$$\bar{C}(t) = \frac{1}{\Omega} \sum_{i=1}^{N} \Omega_i\, C_i(t) \tag{29}$$

and

$$\sigma^2(t) = \frac{1}{\Omega} \sum_{i=1}^{N} \Omega_i \left[C_i(t) - \overline{C}(t)\right]^2 \ , \tag{30}$$

respectively.

Properties of the compartment model solution

It will be seen that all of the properties established above in the continuous representation have a counterpart in the compartment model.

Property 1: The mean tracer concentration satisfies the following relation

$$\frac{d\overline{C}}{dt} = \frac{1}{\Omega} \sum_{i=1}^{N} \left(\Omega_i q_i + \phi_{e,i}\right) \ . \tag{31}$$

This relation may be established by combining (24), (25), (26) and (29).

Property 2: For a passive tracer in an isolated domain, the mean tracer concentration is a constant.

This result is easily obtained by setting $q_i = 0$ and $\phi_{e,i} = 0$ in (31).

Property 3: For a passive tracer in an isolated domain, the variance of the concentration decreases monotonically until the tracer concentration is equal at any time and position to $\overline{C}(0)$. *This is because*

$$\frac{d\sigma^2}{dt} = -\frac{1}{\Omega} \sum_{i=1}^{N} \sum_{j=1}^{N} V_{i,j} (C_j - C_i)^2 \ . \tag{32}$$

In other words, the advective part of the fluxes does not contribute to homogenisation of the concentration; only the diffusive part does.

To establish this relation, one has to first define the deviation of the concentration with respect to its domain-averaged value:

$$\hat{C}_i(t) = C_i(t) - \overline{C}(t) \ , \tag{33}$$

where $\overline{C}(t) = \overline{C}(0)$, as the domain is isolated and the tracer is passive. Then, combining (26), (28) and (33), the equation governing the tracer concentration in each compartment may be transformed to

$$\Omega_i \frac{d\hat{C}_i}{dt} = - \sum_{\substack{j=1 \\ j \neq i}}^{N} U_{i,j} \frac{\hat{C}_i + \hat{C}_j}{2} - \sum_{\substack{j=1 \\ j \neq i}}^{N} \left[-V_{i,j} (\hat{C}_j - \hat{C}_i) \right] . \tag{34}$$

Multiplying (34) by $\hat{C}_i(t)$, using definition (30), one obtains after some calculations

$$\Omega \frac{d\sigma^2}{dt} = - \sum_{i=1}^{N} \sum_{\substack{j=1 \\ j \neq i}}^{N} U_{i,j} (\hat{C}_i + \hat{C}_j) \hat{C}_i + 2 \sum_{i=1}^{N} \sum_{\substack{j=1 \\ j \neq i}}^{N} V_{i,j} (\hat{C}_j - \hat{C}_i) \hat{C}_i \ . \tag{35}$$

The first term in the right-hand side of (35) may be seen to be zero:

$$\sum_{i=1}^{N} \sum_{\substack{j=1 \\ j \neq i}}^{N} U_{i,j} (\hat{C}_i + \hat{C}_j) \hat{C}_i = \underbrace{\sum_{i=1}^{N} \sum_{\substack{j=1 \\ j \neq i}}^{N} U_{i,j} (\hat{C}_i)^2}_{=0} + \sum_{i=1}^{N} \sum_{\substack{j=1 \\ j \neq i}}^{N} U_{i,j} \hat{C}_j \hat{C}_i$$

$$= \sum_{i=1}^{N} \sum_{\substack{j=1 \\ j \neq i}}^{N} \frac{\overbrace{U_{i,j} + U_{j,i}}^{=0}}{2} \hat{C}_j \hat{C}_i = 0 \tag{36}$$

Next, using (25), the last sum of (35) may be transformed as follows

$$2 \sum_{i=1}^{N} \sum_{\substack{j=1 \\ j \neq i}}^{N} V_{i,j} (\hat{C}_j - \hat{C}_i) \hat{C}_i$$

$$= 2 \sum_{i=1}^{N} \sum_{j=1}^{N} V_{i,j} (\hat{C}_j - \hat{C}_i)(\hat{C}_i - \hat{C}_j) + 2 \sum_{i=1}^{N} \sum_{j=1}^{N} V_{i,j} (\hat{C}_j - \hat{C}_i) \hat{C}_j \tag{37}$$

$$= -2 \sum_{i=1}^{N} \sum_{j=1}^{N} V_{i,j} (\hat{C}_j - \hat{C}_i)^2 - 2 \sum_{i=1}^{N} \sum_{j=1}^{N} V_{i,j} (\hat{C}_j - \hat{C}_i) \hat{C}_i$$

eventually yielding

$$2\sum_{i=1}^{N}\sum_{\substack{j=1\\ j\neq i}}^{N} V_{i,j}(\hat{C}_j-\hat{C}_i)\hat{C}_i \;=\; -\sum_{i=1}^{N}\sum_{j=1}^{N} V_{i,j}(\hat{C}_j-\hat{C}_i)^2 \;=\; -\sum_{i=1}^{N}\sum_{j=1}^{N} V_{i,j}(C_j-C_i)^2 \;. \qquad (38)$$

Finally, combining (35), (36) and (38) leads to (32). QED.

Property 4: For a passive tracer in an isolated domain, if the initial concentration is constant, then it must remain constant.

Demonstrating that this property holds true is readily achieved by invoking the same arguments as in the continuous representation: a constant concentration is a solution of (26) since, in this case, (26) simplifies to the continuity equation (28), which is thus identically satisfied.

Upwind approximation of the advective flux

In the developments above, the advective part of the flux from the *i*-th compartment to the *j*-th compartment is approximated by the expression $U_{i,j}(C_i+C_j)/2$, which is inspired by the so-called space-centred finite volume numerical scheme. One may also adopt the counterpart of the first-order upwind scheme. Accordingly, the advective flux would be $U_{i,j}C_i$ if $U_{i,j}>0$, and $U_{i,j}C_j$ otherwise. In other words, the tracer concentration involved in this approach is that of the upstream compartment. Since property (24) stipulates that $U_{i,j}=-U_{j,i}$, the new version of the advective fluw may be rewritten as follows

$$\frac{U_{i,j}+|U_{i,j}|}{2}C_i+\frac{U_{j,i}+|U_{ij,i}|}{2}C_j \;=\; U_{i,j}\frac{C_i+C_j}{2}-\frac{|U_{i,j}|}{2}(C_j-C_i)\;. \qquad (39)$$

With the upwind expression of the advective flux (39), the mass budget equation (26) transforms to

$$\Omega_i\frac{dC_i}{dt} \;=\; \Omega_i q_i \;-\; \underbrace{\sum_{\substack{j=1\\ j\neq i}}^{N} U_{i,j}\frac{C_i+C_j}{2}}_{\text{advective flux budget}} \;-\; \underbrace{\sum_{\substack{j=1\\ j\neq i}}^{N}\left[-\tilde{V}_{i,j}(C_j-C_i)\right]}_{\text{diffusive flux budget}} \;+\; \phi_{e,i} \qquad (40)$$

with

$$\tilde{V}_{i,j} \;=\; V_{i,j}+\frac{|U_{i,j}|}{2} \qquad (41)$$

and

$$\tilde{V}_{i,j} \;=\; \tilde{V}_{j,i} \;>\; 0\;. \qquad (42)$$

Clearly, the coefficient $\tilde{V}_{i,j}$ satisfies a property similar to (25). Therefore, it is legitimate to view the flux $-\tilde{V}_{i,j}(C_j-C_i)$ as a modified version of the diffusive flux. Thus, having recourse to the upwind approximation of the advective flux amounts to modifying only the diffusive part of the budget equation (26) by enhancing the diffusive flux.This is because

$$\tilde{V}_{i,j} \;\geq\; V_{i,j}\;. \qquad (43)$$

The solution of the upwind compartment model obviously satisfies properties 1, 2 and 4. However, it does not satisfy property 3. Indeed, the variance of the tracer concentration now obeys

$$\frac{d\sigma^2}{dt} = -\frac{1}{\Omega}\sum_{i=1}^{N}\sum_{j=1}^{N}\tilde{V}_{i,j}(C_j - C_i)^2 \quad . \tag{44}$$

In view of (43), the decay of the variance is likely to be quicker and, more importantly, the variance will not be conserved if there is not explicit diffusion ($V_{i,j} = 0$), since, in this case, (44) leads to

$$\frac{d\sigma^2}{dt} = -\frac{1}{\Omega}\sum_{i=1}^{N}\sum_{j=1}^{N}\frac{|U_{i,j}|}{2}(C_j - C_i)^2 \quad . \tag{45}$$

With the upwind scheme, advection impacts the variance of the concentration, which may be regarded as undesirable.

These results are in line with the well-known features of the first order upwind numerical scheme, which is known to encompass a rather large spurious diffusivity.

References

Deleersnijder E., J.-M. Campin and E.J.M. Delhez, 2001, The concept of age in marine modelling: I. Theory and preliminary model results, *Journal of Marine Systems*, 28, 229-267

Deleersnijder E., 2003, Some aspects of turbulence closure schemes for marine models, Lecture for the course CT5312, Delft University of Technology, available on the web from http://www.climate.be/users/ericd/doc/TurbulenceClosure.pdf

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