Homogenisation of a passive tracer concentration in an isolated domain

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Introduction

Consider a compressible fluid flow taking place in the domain of interest Ω. The latter is time-independent and its boundary, Γ, is impermeable. In other words, the domain of interest is isolated from its environment. The fluid density and velocity at time t and location $\mathbf{x}$ are denoted $\rho(t,\mathbf{x})$ and $\mathbf{v}(t,\mathbf{x})$, respectively. These variables satisfy the continuity equation:

$$\frac{\partial\rho}{\partial t} + \nabla\bullet(\mathbf{v}\rho) = 0 . \tag{1}$$

The impermeability condition of the domain boundary reads

$$\left[\mathbf{v}\bullet\mathbf{n}\right]_{\mathbf{x}\in\Omega} = 0 . \tag{2}$$

Now assume that a passive tracer[2] is dissolved in the fluid under consideration. The concentration $C(t,\mathbf{x})$ of this tracer, which is defined as a mass fraction (which is a dimensionless variable), obeys the following advection-diffusion equation

$$\frac{\partial}{\partial t}(\rho C) = -\nabla\bullet(\underbrace{\mathbf{v}\rho C-\rho\mathbf{K}\bullet\nabla C}_{\text{tracer flux}}) . \tag{3}$$

In this equation, $\mathbf{v}\rho C$ represents the advective part of the tracer flux, which is associated with (resolved) macroscopic transport processes. Here, the impact at the macroscopic scales of unresolved (small-scale) processes is parameterised by having recourse to the most general form of Fick's Law (1855), yielding the so-called diffusive flux $-\rho\mathbf{K}\bullet\nabla C$. In the latter expression, $\mathbf{K}$ is the diffusivity tensor.

For solving tracer equation (3), initial and boundary conditions must be specified. No specific constraint is imposed on the former, i.e.

$$C(0,\mathbf{x}) = C_0(\mathbf{x}) , \tag{4}$$

where $C_0(\mathbf{x})$ is any suitable function of the position defined in the domain of interest. As the domain boundary is impermeable, no tracer flux is allowed to cross the surface Γ, requiring

$$\left[(\mathbf{v}\rho C-\rho\mathbf{K}\bullet\nabla C)\bullet\mathbf{n}\right]_{\mathbf{x}\in\Gamma} = 0 . \tag{5}$$

Combining (2) and (5) yields

$$\left[(-\rho\mathbf{K}\bullet\nabla C)\bullet\mathbf{n}\right]_{\mathbf{x}\in\Gamma} = 0 . \tag{6}$$

Therefore, there is neither an advective tracer flux nor a diffusive one crossing the domain boundary.

To obtain the tracer concentration, one must solve partial differential equation (3) under the initial and boundary conditions (4) and (6), assuming that the density and velocity fields satisfy relations (1) and (2). Clearly, deriving a general analytical solution thereof is impossible. However, by having recourse to integral methods, one may derive properties of the solution without knowing it explicitly. In particular, it will be seen that it is desirable that

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[1] Benjamin Dewals provided formation that helped prepare the third version of this working note.

[2] A tracer is termed passive if it is neither produced nor destroyed by (local) reactive phenomena, whose nature may be nuclear, chemical or biological.

the diffusivity tensor be symmetric. In addition, if the diffusivity tensor is positive definite, it will be demonstrated that the tracer concentration will homogenise in all circumstances. Finally, properties of the local concentration extrema will also be established.

Evolution of the total tracer mass

Since the domain of interest is isolated from its environment and the tracer under study is of a passive nature, the amount of fluid and tracer contained in the domain of interest should remain constant. It is, however, necessary to make sure that the model used herein satisfies this constraint.

The mass of fluid contained in the domain of interest is

$$m_f(t) \;=\; \int_\Omega \rho(t,\mathbf{x})\,d\Omega \;. \tag{7}$$

Then, by using continuity equation (1) and boundary condition (2), it is easily seen that the time derivative of this mass is zero:

$$\frac{dm_f}{dt} \;=\; \underbrace{\int_\Omega \frac{\partial\rho}{\partial t}\,d\Omega \;=\; -\int_\Omega \nabla\bullet(\mathbf{v}\rho)\,d\Omega}_{\text{by virtue of (1)}} \;=\; \int_\Gamma \underbrace{(\mathbf{v}\rho)\bullet\mathbf{n}}_{\substack{=0\\ \text{see (2)}}}\,d\Gamma \;=\; 0\;. \tag{8}$$

Thus, the mass of fluid present in the domain is conserved indeed.

A similar reasoning may be applied to the tracer under consideration. The mass of tracer contained in the domain of interest is

$$m(t) \;=\; \int_\Omega \rho(t,\mathbf{x})C(t,\mathbf{x})\,d\Omega \;. \tag{9}$$

Taking advantage of evolution equation (3) and boundary condition (5), the time-derivative of the total tracer mass may be transformed as follows:

$$\begin{aligned}\frac{dm}{dt} \;&=\; \underbrace{\int_\Omega \frac{\partial}{\partial t}(\rho C)\,d\Omega \;=\; -\int_\Omega (\mathbf{v}\rho C-\rho\mathbf{K}\bullet\nabla C)\,d\Omega}_{\text{by virtue of (3)}}\\ &=\; \int_\Gamma \underbrace{(\mathbf{v}\rho C-\rho\mathbf{K}\bullet\nabla C)\bullet\mathbf{n}}_{\substack{=0\\ \text{by virtue of (5)}}}\,d\Gamma \;=\; 0\end{aligned} \tag{10}$$

As expected, the amount of tracer contained in the domain of interest remains constant as time progresses.

It is convenient to define the mean tracer concentration as the density-weighted average over the domain of the tracer concentration:

$$\overline{C}(t) \;=\; \frac{\displaystyle\int_\Omega \rho(t,\mathbf{x})C(t,\mathbf{x})\,d\Omega}{\displaystyle\int_\Omega \rho(t,\mathbf{x})\,d\Omega}\;. \tag{11}$$

The latter is equal to the ratio of the tracer mass to the fluid mass, i.e. $\overline{C}(t)=m(t)/m_f(t)$. Then, as these masses are time-independent, the mean tracer concentration is a constant too, which obviously is equal to the mean of the initial concentration,

$$\overline{C}_0 = \frac{\int\limits_{\Omega} \rho(0,\mathbf{x})\, C(0,\mathbf{x})\; d\Omega}{\int\limits_{\Omega} \rho(0,\mathbf{x})\; d\Omega} \; . \tag{12}$$

Splitting of the diffusivity tensor

Any tensor may be split into its anti-symmetric and symmetric parts. Applying this concept to the diffusivity tensor yields $\mathbf{K} = \mathbf{K}_a + \mathbf{K}_s$, where $\mathbf{K}_a = (\mathbf{K} - \mathbf{K}^T)/2$ and $\mathbf{K}_s = (\mathbf{K} + \mathbf{K}^T)/2$ are the anti-symmetric and symmetric parts of the tensor under consideration assuming that $\mathbf{K}^T$ denotes the transpose[3] of $\mathbf{K}$. Then, the diffusive flux may be regarded as the sum of two contributions, i.e. $-\rho\mathbf{K}\bullet\nabla C = -\rho\mathbf{K}_a\bullet\nabla C - \rho\mathbf{K}_s\bullet\nabla C$. The impact on the tracer budget of the anti-symmetric part of the diffusivity tensor is worth examining in detail.

The dot product of an anti-symmetric tensor and a vector may always be transformed to a vector product. Accordingly, there exists a vector **a** satisfying[4]

$$-\rho\mathbf{K}_a\bullet\nabla C \;=\; \mathbf{a}\times\nabla C \; . \tag{13}$$

The divergence of this vector needs be evaluated, leading to

$$\nabla\bullet(-\rho\mathbf{K}_a\bullet\nabla C) \;=\; \nabla\bullet(\mathbf{a}\times\nabla C) \;=\; (\nabla\times\mathbf{a})\bullet\nabla C \;-\; \mathbf{a}\bullet(\underbrace{\nabla\times\nabla C}_{=0}) \;=\; (\nabla\times\mathbf{a})\bullet\nabla C \, . \tag{14}$$

Clearly, $\nabla\times\mathbf{a}$ is a vector that is divergence-free, suggesting that the equivalent velocity

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[3] Let the components of the diffusivity tensor be written as follows

$$\mathbf{K} = \begin{pmatrix} K_{11} & K_{12} & K_{13} \\ K_{21} & K_{22} & K_{23} \\ K_{31} & K_{32} & K_{33} \end{pmatrix} .$$

Then, the transpose of **K**, and its anti-symmetric and symmetric part read

$$\mathbf{K}^T = \begin{pmatrix} K_{11} & K_{21} & K_{31} \\ K_{12} & K_{22} & K_{32} \\ K_{13} & K_{23} & K_{33} \end{pmatrix} ,$$

$$\mathbf{K}_a = \begin{pmatrix} 0 & (K_{12}-K_{21})/2 & (K_{13}-K_{31})/2 \\ (K_{21}-K_{12})/2 & 0 & (K_{23}-K_{32})/2 \\ (K_{31}-K_{13})/2 & (K_{32}-K_{23})/2 & 0 \end{pmatrix} ,$$

$$\mathbf{K}_s = \begin{pmatrix} K_{11} & (K_{12}+K_{21})/2 & (K_{13}+K_{31})/2 \\ (K_{21}+K_{12})/2 & K_{22} & (K_{23}+K_{32})/2 \\ (K_{31}+K_{13})/2 & (K_{32}+K_{23})/2 & K_{33} \end{pmatrix} .$$

[4] After some tedious calculations, the components of vector **a** may be seen to be

$$\mathbf{a} = \frac{\rho}{2}\begin{pmatrix} K_{23}-K_{32} \\ K_{31}-K_{13} \\ K_{12}-K_{21} \end{pmatrix} .$$

$$\mathbf{u} \;=\; \mathbf{v} \;+\; \frac{\nabla \times \mathbf{a}}{\rho} \tag{15}$$

be introduced. Next, by substituting (13)-(15) into the continuity and tracer budget equations (1) and (3), one readily obtains

$$\frac{\partial\rho}{\partial t} \;+\; \nabla\bullet(\mathbf{u}\rho) \;=\; 0 \tag{16}$$

and

$$\frac{\partial}{\partial t}(\rho C) \;=\; -\nabla\bullet(\mathbf{u}\rho C - \rho\mathbf{K}_s\bullet\nabla C)\ . \tag{17}$$

As a consequence, the tracer flux associated with the anti-symmetric part of the diffusivity tensor plays a role that may be viewed as equivalent to advective transport.

Homogenisation of the tracer concentration

A measure of the heterogeneity of the tracer distribution is needed. An expression conducive to fruitful results is the variance of the tracer concentration,

$$\sigma^2(t) \;=\; \frac{1}{m}\int_{\Omega} \rho(t,\mathbf{x})[\hat{C}(t,\mathbf{x})]^2\, d\Omega\ , \tag{18}$$

where $\hat{C}(t,\mathbf{x}) = C(t,\mathbf{x}) - \overline{C}_0$ is the deviation of the concentration with respect to its domain-averaged value as defined in (11); the smaller the variance, the more homogeneous the tracer concentration. Clearly, the lower limit to the value of the aforementioned variance is zero, which corresponds to a situation in which the concentration is equal to $\overline{C}_0$ at any location.

It is readily seen that the evolution of $\hat{C}(t,\mathbf{x})$ is governed by the following partial differential problem:

$$\frac{\partial}{\partial t}(\rho\hat{C}) \;=\; -\nabla\bullet(\mathbf{v}\rho\hat{C} - \rho\mathbf{K}\bullet\nabla\hat{C})\ , \tag{19}$$

$$\Big[(-\rho\mathbf{K}\bullet\nabla\hat{C})\bullet\mathbf{n}\Big]_{\mathbf{x}\in\Gamma} \;=\; 0\ , \tag{20}$$

$$\hat{C}(0,\mathbf{x}) \;=\; C_0(\mathbf{x}) \;-\; \overline{C}_0\ . \tag{21}$$

Using the continuity equation (1), the convective form of (19) is readily obtained

$$\rho D_t\hat{C} \;=\; \nabla\bullet(\rho\mathbf{K}\bullet\nabla\hat{C})\ , \tag{22}$$

where $D_t = \partial/\partial t + \mathbf{v}\bullet\nabla$ denotes the material derivative operator[5]. Multiplying (22) by $\hat{C}$ leads to

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[5] Deriving the convective form from the conservative one or *vice versa* may be achieved by resorting to the continuity equation (1) as follows:

$$\begin{aligned}\frac{\partial}{\partial t}(\rho\psi) + \nabla\bullet(\mathbf{v}\rho\psi) &= \frac{\partial\rho}{\partial t}\psi + \rho\frac{\partial\psi}{\partial t} + \nabla\bullet(\mathbf{v}\rho)\psi + \rho\mathbf{v}\bullet\nabla\psi \\ &= \underbrace{\left[\frac{\partial\rho}{\partial t} + \nabla\bullet(\mathbf{v}\rho)\right]}_{\substack{=0\\ \text{see (1)}}}\psi + \rho\underbrace{\left(\frac{\partial\psi}{\partial t} + \mathbf{v}\bullet\nabla\psi\right)}_{\substack{=\,D_t\psi\,=\,\text{material}\\ \text{derivative of }\psi}} = \rho D_t\psi\end{aligned}$$

where $\psi(t,\mathbf{x})$ is any variable whose evolution is governed by and advective-diffusion-reaction equation — or “reactive transport” equation for short.

$$\rho\hat{C}\,D_t\hat{C} \;=\; \frac{\rho}{2}D_t\hat{C}^2 \;=\; \hat{C}\nabla\bullet(\rho\mathbf{K}\bullet\nabla\hat{C}) \;=\; \nabla\bullet(\hat{C}\rho\mathbf{K}\bullet\nabla\hat{C}) \;-\; \rho\nabla\hat{C}\bullet\mathbf{K}\bullet\nabla\hat{C}\ . \tag{23}$$

Then, by having recourse again to the continuity equation (1), the conservative form of (23) is derived, i.e.

$$\frac{\partial}{\partial t}(\rho\hat{C}^2) \;=\; -\nabla\bullet(\mathbf{v}\rho\hat{C}^2 - 2\hat{C}\rho\mathbf{K}\bullet\nabla\hat{C}) \;-\; 2\rho\nabla\hat{C}\bullet\mathbf{K}\bullet\nabla\hat{C}\ . \tag{24}$$

Next, integrating (24) over the domain of interest, using the definition (18) of the variance of the tracer concentration and employing the divergence theorem yields

$$\frac{d\sigma^2}{dt} \;=\; -\frac{1}{m}\int_{\Gamma}\underbrace{(\mathbf{v}\rho\hat{C}^2 - 2\hat{C}\rho\mathbf{K}\bullet\nabla\hat{C})\bullet\mathbf{n}}_{\substack{=0\\ \text{see (2) and (20)}}}\,d\Gamma \;-\; \frac{2}{m}\int_{\Omega}\rho\nabla\hat{C}\bullet\mathbf{K}\bullet\nabla\hat{C}\,d\Gamma\ . \tag{25}$$

Thus, the variance of the tracer concentration obeys

$$\frac{d\sigma^2}{dt} \;=\; -\frac{2}{m}\int_{\Omega}\rho\nabla\hat{C}\bullet\mathbf{K}\bullet\nabla\hat{C}\,d\Gamma\ . \tag{26}$$

Bearing in mind that $\mathbf{K} = \mathbf{K}_a + \mathbf{K}_s$ and using (13) allows one to manipulate the integrand in the right-hand side member of (26) as follows:

$$\begin{aligned}\rho\nabla\hat{C}\bullet\mathbf{K}\bullet\nabla\hat{C} \;&=\; \rho\nabla\hat{C}\bullet(\mathbf{K}_a+\mathbf{K}_s)\bullet\nabla\hat{C}\\ &=\; \rho\nabla\hat{C}\bullet\mathbf{K}_a\bullet\nabla\hat{C} \;+\; \rho\nabla\hat{C}\bullet\mathbf{K}_s\bullet\nabla\hat{C}\\ &=\; -\underbrace{\nabla\hat{C}\bullet(\mathbf{a}\times\nabla\hat{C})}_{=0} \;+\; \rho\nabla\hat{C}\bullet\mathbf{K}_s\bullet\nabla\hat{C} \;=\; \rho\nabla\hat{C}\bullet\mathbf{K}_s\bullet\nabla\hat{C}\end{aligned} \tag{27}$$

By substituting (27) into (26), one obtains

$$\frac{d\sigma^2}{dt} \;=\; -\frac{2}{m}\int_{\Omega}\rho\nabla\hat{C}\bullet\mathbf{K}\bullet\nabla\hat{C}\,d\Gamma \;=\; -\frac{2}{m}\int_{\Omega}\rho\nabla\hat{C}\bullet\mathbf{K}_s\bullet\nabla\hat{C}\,d\Gamma\ . \tag{28}$$

In the previous section, it has been seen that the tracer flux associated with the anti-symmetric part of the diffusivity tensor, $\mathbf{K}_a$, may be regarded as an advective flux. Furthermore relation (28) indicates that $\mathbf{K}_a$ has no impact on the evolution of the variance of the tracer concentration. As a consequence, it is highly desirable that the diffusivity tensor be symmetric.

If the diffusivity tensor is positive definite[6], the variance of the tracer will decrease monotonically until the tracer concentration is everywhere equal to its domain-averaged value $\bar{C}_0$, i.e.

$$\lim_{t\to\infty} C(t,\mathbf{x}) = \bar{C}_0\ . \tag{29}$$

It must be underscored that this result has been arrived at whithout any explicit knowledge of the solution of the tracer transport study under consideration. Instead, it is solely by manipulating integral quantities that (29) was established, pointing to the power of integral methods.

The results obtained so far may be summarised as follows:

1. *The anti-symmetric part of the diffusivity tensor leads to a tracer flux whose impact on the tracer budget is similar to that of the (macroscopic) advection*

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[6] The diffusivity tensor is positive definite if and only if $\mathbf{y}\bullet\mathbf{K}\bullet\mathbf{y} > 0$ for any vector $\mathbf{y} \neq 0$.

flux;

2. *The anti-symmetric part of the diffusivity tensor plays no role in the homogenisation of the tracer concentration;*
3. *If the diffusivity tensor is positive definite, the variance of the tracer concentration decreases monotonically until the concentration is homogeneous.*

Therefore, as the tracer flux due to unresolved (small-scale) processes is generally thought to reduce concentration contrasts, it is highly desirable that **the diffusvity tensor, K, be symmetric and positive definite**. From this point onwards, these constraints will be assumed to be satisfied.

Evolution of extrema

A maximum is a point where the tracer concentration is zero and all second derivatives are not positive. Thus, for the concentration maximum located at $\mathbf{x} = \mathbf{r}(t)$, the tracer concentration satisfies

$$\left[\nabla C\right]_{\mathbf{x}=\mathbf{r}(t)} = 0 \tag{30}$$

and

$$\left[\frac{\partial^2 C}{\partial x_i^2}\right]_{\mathbf{x}=\mathbf{r}(t)} \leq 0 \ , \quad i = 1,2 \ldots N \ , \tag{31}$$

where N is the number of space dimensions relevant to the flow under study. The rate of change of the concentration measured by an observer whose position is $\mathbf{r}(t)$ is

$$\frac{d}{dt} C[t,\mathbf{r}(t)] = \left[\frac{\partial C}{\partial t} + \frac{d\mathbf{r}}{dt} \bullet \nabla C\right]_{\mathbf{x}=\mathbf{r}(t)} . \tag{32}$$

Then, combining this relation with the tracer budget equation (3) and using the continuity equation, one obtains after some manipulations

$$\frac{d}{dt} C[t,\mathbf{r}(t)] = \underbrace{\left[\left(-\mathbf{v} + \frac{d\mathbf{r}}{dt} + \frac{1}{\rho} \nabla \bullet (\rho \mathbf{K})\right) \bullet \nabla C\right]_{\mathbf{x}=\mathbf{r}(t)}}_{=0 \ , \ \text{see (30)}} + \mathbf{K} : (\nabla\nabla C) = \mathbf{K} : (\nabla\nabla C) \ , \tag{33}$$

with

$$\mathbf{K} : (\nabla\nabla C) = \sum_{i=1}^{N} \sum_{j=1}^{N} K_{ij} \frac{\partial^2 C}{\partial x_i \, \partial x_j} . \tag{34}$$

Expression (34) takes a simpler form in the principal axes. If the associated coordinates are denoted ξ_i (i=1,2...*N*), then (34) simplifies to

$$\mathbf{K} : (\nabla\nabla C) = \sum_{k=1}^{N} \tilde{K}_{kk} \frac{\partial^2 C}{\partial \xi_k^2} , \tag{35}$$

where $\tilde{K}_{kk}$ are the principal components of the diffusivity tensor, which are all positive ($\tilde{K}_{kk} > 0$) since **K** is positive definite. Since (31) implies

$$\left[\frac{\partial^2 C}{\partial \xi_k^2}\right]_{\mathbf{x}=\mathbf{r}(t)} \leq 0 , \quad k = 1,2 \ldots N \ , \tag{36}$$

expression (35) is smaller than or equal to zero. Therefore, $C[t,\mathbf{r}(t)]$ does not increase:

$$\frac{d}{dt}C[t,\mathbf{r}(t)] \;\le\; 0 \;. \tag{37}$$

Following a similar line of reasoning, it is readily seen that the tracer concentration related to a local minimum does not decrease.

The findings of this section can be summarised as follows: **the tracer concentration at a local maximum (minimum) does not increase (decrease)**. This is another property of the transport phenomena causing the tracer concentration to become progressively homogeneous.

Final remarks

If the largest unresolved scales are much smaller than the smallest macroscopic scales, then it is unlikely that there exist preferred directions for the flux due to unresolved-scale processes. Accordingly, the diffusivity tensor should be isotropic:

$$\mathbf{K} \;=\; K\mathbf{I}\,, \tag{38}$$

where **I** is the identity tensor, i.e. $\mathbf{I} = \mathrm{diag}(1,1,...)$. Then, the parameterisation of the diffusive flux simplifies to

$$-\rho\mathbf{K}\bullet\nabla C \;=\; -\,\rho K\underbrace{\mathbf{I}\bullet\nabla C}_{=\nabla C} \;=\; -\,\rho K\nabla C\;, \tag{39}$$

where the diffusivity K must be positive (>0) at any time and position for the corresponding (isotropic) diffusivity tensor to be positive definite.

The Boussinesq approximation has not been invoked herein. However, for a flow in which this approximation is seen to hold valid, then the density ρ must be regarded as a constant. Obviously, all the results arrived at here remain valid under the Boussinesq approximation.

Reference

Fick A., 1855, Ueber Diffusion, *Annalen der Physik*, 170, 59-86
