Introductory Examples of Homogenization Method

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In this introductory chapter we shall use several one-dimensional examples to demonstrate the homogenization theory for deriving effective equations. To illustrate the importance of scales we show in Secs. 1.1 and 1.2 that, for waves in a space-wise periodic medium, different relations among length scales lead to different effective equations, representing different physics. In the last section, an example of multiple time scales is demonstrated through the celebrated theory of Taylor (1953, 1954) on shear-enhanced diffusion in a pipe flow.

1.1. Long Waves in a Layered Elastic Medium

Let us start with an example where the material inhomogeneity and the physical process are characterized by two very different length scales. Consider the longitudinal vibrations or wave propagation in an elastic rod, governed by the following partial differential equation,

$$\frac{\partial}{\partial x}\left(E\frac{\partial v}{\partial x}\right) = \rho\frac{\partial^2 v}{\partial t^2}\,, \tag{1.1.1}$$

where v, E, and ρ denote, respectively, the longitudinal displacement, Young's modulus of elasticity, and the mass per unit length. We assume that the material properties E and ρ are spatially periodic with the period ℓ. As a short-hand expression, we shall say that E and ρ are ℓ-periodic in x.

If ω is the characteristic frequency, then the characteristic length of the elastic waves can be estimated by

$$\frac{2\pi}{k} = \sqrt{\frac{E_o}{\rho_o}}\frac{1}{\omega}\,, \tag{1.1.2}$$

where k is the wavenumber and E_o and ρ_o are the characteristic values of $E(x)$ and $\rho(x)$, respectively. There are at least two possible scenarios: (i) $k\ell \ll 1$, and (ii) $k\ell = \mathcal{O}(1)$.

We consider here the first case of long waves and designate the wavelength as the macroscale $\ell' = 2\pi/k$ so that

$$\epsilon \equiv \frac{\ell}{\ell'} \ll 1\,. \tag{1.1.3}$$

If one is primarily interested in the averaged variation over a scale of a wavelength, can the details on the microscale be bypassed and an equation obtained for the global behavior on the scale of ℓ'?

Let us introduce the following normalization,

$$v = v_o v^\dagger\,, \quad x = \ell x^\dagger\,, \quad t = \frac{t^\dagger}{\omega}\,, \quad E = E_o E^\dagger\,, \quad \rho = \rho_o \rho^\dagger\,, \tag{1.1.4}$$

where dimensionless quantities are distinguished by $\{\cdot\}^\dagger$ and u_0, E_0, and ρ_0 are the characteristic scales of u, E, and ρ, respectively. Note that x is normalized by the microlength ℓ. In dimensionless variables, Eq. (1.1.1) becomes

$$\frac{\partial}{\partial x^\dagger}\left(E^\dagger \frac{\partial v^\dagger}{\partial x^\dagger}\right) = \left(\frac{\ell^2}{E_o/\rho_o\omega^2}\right)\rho^\dagger \frac{\partial^2 v^\dagger}{\partial {t^\dagger}^2} = \epsilon^2 \rho^\dagger \frac{\partial^2 v^\dagger}{\partial {t^\dagger}^2}\,. \tag{1.1.5}$$

Clearly inertia is much smaller than the stress force on the microscale. For exhibiting the physical origin of each term, it is often convenient to keep the equations in dimensional form, but to indicate the relative weight of each term by the ordering parameter ϵ, with the normalizing scales defined. From here on we shall omit the daggers and simply write Eq. (1.1.5) as

$$\frac{\partial}{\partial x}\left(E \frac{\partial v}{\partial x}\right) = \epsilon^2 \rho \frac{\partial^2 v}{\partial t^2}\,. \tag{1.1.6}$$

Using the fact that there exist two characteristic lengths, let us employ the perturbation method of multiple scales by introducing the fast and slow variables x and $x' = \epsilon x$. The unknown displacement is now expanded in the form of a power series in ϵ:

$$v = v_0 + \epsilon v_1 + \epsilon^2 v_2 + \cdots\,, \tag{1.1.7}$$

where $v_i, i = 0, 1, 2, \ldots$ are functions of both x and x'. The original derivative then becomes, according to the chain rule,

$$\frac{\partial}{\partial x} \to \frac{\partial}{\partial x} + \epsilon \frac{\partial}{\partial x'}\,.$$

It follows from Eq. (1.1.6) that

$$\left(\frac{\partial}{\partial x}+\epsilon\frac{\partial}{\partial x'}\right)\left[E\left(\frac{\partial}{\partial x}+\epsilon\frac{\partial}{\partial x'}\right)(v_0+\epsilon v_1+\epsilon^2 v_2+\cdots)\right]$$
$$=\epsilon^2\rho\frac{\partial^2}{\partial t^2}(v_0+\epsilon v_1+\epsilon^2 v_2+\cdots)\,.$$

Equating the coefficient of each power of ϵ to zero leads to a sequence of perturbation equations. At the order $\mathcal{O}(\epsilon^0)$, we get,

$$\frac{\partial}{\partial x}\left(E\frac{\partial v_0}{\partial x}\right)=0\,, \tag{1.1.8}$$

which governs the microscale variation of v_0. Because the microstructure is assumed to be periodic on the ℓ-scale, v_0 should be likewise periodic. The general solution to the homogeneous equation (1.1.8) is

$$v_0=A_1(x')\int_{x_0}^{x}\frac{dx}{E(x,x')}+A_2(x')\,,$$

where x_0 is an arbitrary starting point and $A_1(x')$ and $A_2(x')$ are integration constants. To ensure periodicity over the distance ℓ (i.e., $v_0(x_0)=v_0(x_0+\ell)$), $A_1(x')$ must vanish, implying that the leading-order displacement depends only on the macroscale, i.e.,

$$v_0=v_0(x')=A_2(x')\,. \tag{1.1.9}$$

Therefore, v_0 must represent the ℓ-average of v with an error of $\mathcal{O}(\epsilon)$. At the leading order, variations within a few spatial periods ($\mathcal{O}(\ell)$) are insignificant.

At the next order $\mathcal{O}(\epsilon)$, the perturbation equation governing v_1 is

$$\frac{\partial}{\partial x}\left[E\left(\frac{\partial v_1}{\partial x}+\frac{\partial v_0}{\partial x'}\right)\right]=0\,. \tag{1.1.10}$$

As a boundary condition, v_1 must also be ℓ-periodic. Equation (1.1.10) is a linear inhomogeneous equation for v_1, which may be represented formally by

$$v_1=S(x,x')\frac{\partial v_0}{\partial x'}\,, \tag{1.1.11}$$

so that

$$\frac{\partial}{\partial x}\left[E\left(1+\frac{\partial S}{\partial x}\right)\right]=0\,, \tag{1.1.12}$$

where S is ℓ-periodic in x. The solution of the above problem is determined up to an additive constant. To ensure that v_0 represents the wavelength-average with an error of $\mathcal{O}(\epsilon^2)$, we add the condition that

$$\langle S \rangle = \frac{1}{\ell}\int_{x_0}^{x_0+\ell} S\,dx = 0\,, \tag{1.1.13}$$

where angle brackets signify the wavelength-average. Successive integrations of Eq. (1.1.12) yield

$$\frac{\partial S}{\partial x} = \frac{\mathcal{E}}{E} - 1\,, \tag{1.1.14}$$

and

$$S = S_0 - \int_{x_0}^{x} \frac{E-\mathcal{E}}{E}dx\,, \tag{1.1.15}$$

where $\mathcal{E}(x')$ and $S_0(x')$ are constants of integration. Since v_1 must be ℓ-periodic, it is necessary that $S(x_0) = S(x_0+\ell)$, i.e.,

$$S_0 = S_0 - \ell + \mathcal{E}\int_{x_0}^{x_0+\ell}\frac{dx}{E}\,,$$

therefore

$$\mathcal{E} = \left(\frac{1}{\ell}\int_{x_0}^{x_0+\ell}\frac{dx}{E}\right)^{-1}, \quad \text{or} \quad \frac{1}{\mathcal{E}} = \frac{1}{\ell}\int_{x_0}^{x_0+\ell}\frac{dx}{E}\,. \tag{1.1.16}$$

Thus $\mathcal{E}$ is the harmonic mean of E over the period ℓ. $S(x_0)$ can be fixed by applying the auxiliary condition (Eq. (1.1.13)),

$$S(x_0) = \left\langle \int_{x_0}^{x}\frac{E-\mathcal{E}}{E}dx\right\rangle = \frac{1}{\ell}\int_{x_0}^{x_0+\ell}dx\int_{x_0}^{x}\frac{E-\mathcal{E}}{E}d\bar{x}\,. \tag{1.1.17}$$

Next we proceed to the perturbation equation at the order $\mathcal{O}(\epsilon^2)$:

$$\frac{\partial}{\partial x}\left(E\frac{\partial v_2}{\partial x}\right) + \frac{\partial}{\partial x'}\left(E\frac{\partial v_0}{\partial x'}\right) + \frac{\partial}{\partial x}\left(E\frac{\partial v_1}{\partial x'}\right) + \frac{\partial}{\partial x'}\left(E\frac{\partial v_1}{\partial x}\right) = \rho\frac{\partial^2 v_0}{\partial t^2}\,, \tag{1.1.18}$$

which is again an inhomogeneous equation for v_2, similar to Eq. (1.1.10) for v_1. Furthermore, v_2 is ℓ-periodic. Since from Eqs. (1.1.11) and (1.1.14),

$$\frac{\partial v_1}{\partial x} = -\frac{\partial v_0}{\partial x'} + \frac{\mathcal{E}}{E}\frac{\partial v_0}{\partial x'}\,, \tag{1.1.19}$$

it follows that

$$\frac{\partial}{\partial x'}\left(E\frac{\partial v_1}{\partial x}\right)+\frac{\partial}{\partial x'}\left(E\frac{\partial v_0}{\partial x'}\right)=\frac{\partial}{\partial x'}\left(\mathcal{E}\frac{\partial v_0}{\partial x'}\right).$$

With this result Eq. (1.1.18) may be rewritten as

$$\frac{\partial}{\partial x}\left(E\frac{\partial v_2}{\partial x}\right)+\frac{\partial}{\partial x'}\left(\mathcal{E}\frac{\partial v_0}{\partial x'}\right)+\frac{\partial}{\partial x}\left(E\frac{\partial v_1}{\partial x'}\right)=\rho\frac{\partial^2 v_0}{\partial t^2}.$$

By taking the wavelength-average of the preceding equation and invoking periodicity, we get

$$\frac{\partial}{\partial x'}\left(\mathcal{E}\frac{\partial v_0}{\partial x'}\right)=\langle\rho\rangle\frac{\partial^2 v_0}{\partial t^2}, \tag{1.1.20}$$

where

$$\langle\rho\rangle=\frac{1}{\ell}\int_{x_0}^{x_0+\ell}\rho\,dx. \tag{1.1.21}$$

Equation (1.1.20) governs the macroscale variation of the mean displacement. While the effective Young's modulus is the harmonic mean of E, the effective density is the arithmetic mean of ρ. Subject to further boundary conditions on the macroscale, v_0 can be solved.

Once v_0 is found, the fluctuation about the mean, v_1, can be found from Eq. (1.1.11).

The procedure described above is typical of the *method of homogenization.* A boundary-value problem is solved for each typical period (cell) at each order. At the leading order the cell problem is homogeneous and the solution is indeterminate. At higher orders the problems are inhomogeneous; their solvability imposes constraints on the lower order solution. It is one of the constraints (*solvability conditions*) that leads to the averaged equation governing the global behavior of the lowest order. As an important byproduct, the effective constitutive coefficient is also derived in terms of the known material property on the microscale.

So far the elastic coefficient E has been treated as a continuous function of x. For laminated materials E is discontinuous. Thus within each ℓ-period we must add the jump conditions representing, respectively, the continuity of displacement and stress:

$$[v]_\xi=0\,,\quad \left[E\frac{\partial v}{\partial x}\right]_\xi=0\,, \tag{1.1.22}$$

where $[F]_\xi = F|_{\xi+} - F|_{\xi-}$ denotes the discontinuity of F at $x=\xi$ within each ℓ-period. In the perturbation analysis, one must add the following jump conditions at successive orders:

$$
\begin{aligned}
&[v_0]_\xi = 0\,, \quad \left[E\frac{\partial v_0}{\partial x}\right]_\xi = 0\,,\\
&[v_1]_\xi = 0\,, \quad \left[E\left(\frac{\partial v_1}{\partial x} + \frac{\partial v_0}{\partial x'}\right)\right]_\xi = 0\,,\\
&[v_2]_\xi = 0\,, \quad \left[E\left(\frac{\partial v_2}{\partial x} + \frac{\partial v_1}{\partial x'}\right)\right]_\xi = 0\,,\\
&\qquad\vdots
\end{aligned}
\tag{1.1.23}
$$

It can be shown that the results (Eq. (1.1.20)) with Eqs. (1.1.16) and (1.1.21) are the same as if E were continuous. This conclusion can be reached alternatively by employing the theory of generalized functions (see Bakhvalov and Panasenko, 1989).

As a special case, let each ℓ period be composed of two distinct layers, within which Young's moduli and thicknesses are, respectively, (E_1, E_2) and $(1-\theta\ell, \theta\ell)$. From Eq. (1.1.16)

$$
\mathcal{E} = \left\langle \frac{1}{E} \right\rangle^{-1} = \left(\frac{1-\theta}{E_1} + \frac{\theta}{E_2} \right)^{-1} = \frac{E_1 E_2}{(1-\theta)E_2 + \theta E_1}\,, \tag{1.1.24}
$$

i.e., $\mathcal{E}$ is the harmonic mean of E_1 and E_2.

In particular, if θ or $1-\theta$ is not too small compared to unity, then

$$
\mathcal{E} \sim \frac{E_2}{\theta} \quad \text{if} \quad E_1 \gg E_2; \qquad \mathcal{E} \sim \frac{E_1}{(1-\theta)} \quad \text{if} \quad E_1 \ll E_2\,.
$$

1.2. Short Waves in a Weakly Stratified Elastic Medium

We now consider the case where $k\ell = \mathcal{O}(1)$ for a scenario that gives rise to contrasting scales and calls for homogenization. In many dynamical problems, contrasting space and time scales arise as a result of resonance, even when the material inhomogeneity is weak. As an example let us consider the slow evolution of waves through a slightly periodic medium, by taking Eq. (1.1.1) with

$$
\rho = \text{constant}\,, \quad E = E_o(1 + \epsilon D \cos Kx)\,, \tag{1.2.1}
$$

where D is of order unity, i.e.,

$$
E_0 \frac{\partial}{\partial x}\left[(1 + \epsilon D \cos Kx)\frac{\partial v}{\partial x}\right] = \rho \frac{\partial^2 v}{\partial t^2}\,. \tag{1.2.2}
$$

We now assume that the spatial period of inhomogeneity $\ell \equiv 2\pi/K$ and the elastic wavelength $2\pi/k = \sqrt{E_o/\rho}/\omega$ are comparable. As a consequence, wave reflection can be significant.

Let us first try a naive expansion, $v = v_0 + \epsilon v_1 + \cdots$. The crudest solution is easily found to be

$$v_0 = \frac{A}{2} e^{ikx - i\omega t} + \text{c.c.}\,, \tag{1.2.3}$$

where c.c. signifies the complex conjugate of the preceding term, and

$$\frac{2\pi}{k} \equiv \sqrt{\frac{E_o}{\rho}}\frac{1}{\omega}\,. \tag{1.2.4}$$

At the next order the governing equation is

$$\begin{aligned} &\frac{\partial}{\partial x}\left(E_o \frac{\partial v_1}{\partial x}\right) - \rho \frac{\partial^2 v_1}{\partial t^2} \\ &\quad = -\frac{E_o D}{2}\frac{\partial}{\partial x}\left[\left(e^{iKx} + e^{-iKx}\right)\frac{\partial v_0}{\partial x}\right] \\ &\quad = -\frac{E_o D}{2}\frac{\partial}{\partial x}\left[\left(e^{iKx} + e^{-iKx}\right)\left(\frac{ikA}{2}e^{ikx - i\omega t} - \frac{ikA^\dagger}{2}e^{-ikx + i\omega t}\right)\right], \end{aligned} \tag{1.2.5}$$

where $A^\dagger$ denotes the complex conjugate of A. For general K, v_1 can be found in terms of the harmonics $\exp(\pm i(K \pm k) \pm \omega t)$. Higher order improvements can be proceeded straightforwardly. However, when

$$K = 2k + \delta\,, \quad \delta \ll k\,, \tag{1.2.6}$$

some of the forcing terms on the right-hand side will be close to a natural mode $\exp(\pm i(kx + \omega t))$. Resonance of the reflected waves must be expected. The relation $K = 2k$ (cf. Eq. (1.2.6)) is the well-known condition for Bragg resonance. Let us consider the response to forcing of reflected waves

$$E_o \frac{\partial^2 v_1}{\partial x^2} - \rho \frac{\partial^2 v_1}{\partial t^2} = R e^{i\phi_o} e^{i\delta x} + \text{c.c.}$$

with

$$R = -\frac{E_0 D k^2 A^\dagger}{4} \quad \text{and} \quad \phi_o = kx + \omega t\,,$$

where c.c. denotes the complex conjugate of the preceding term. Combining homogeneous and inhomogeneous solutions and requiring that $v_1(0, t) = 0$, we get

$$v_1 = \frac{R e^{i\phi_o}\left(1 - e^{i\delta x}\right)}{E_o((k+\delta)^2 - k^2)} + \text{c.c.}\,.$$

Clearly if $\delta = \mathcal{O}(\epsilon)$, $\epsilon v_1 \sim \mathcal{O}(\epsilon/\delta)$ and is not small compared to v_0 when $\epsilon x = \mathcal{O}(1)$. Furthermore as x increases, v_1 grows as ϵx. This implies that the reflected waves are resonated and are no longer much smaller than the incident waves in the distance $\epsilon x = \mathcal{O}(1)$. The naive expansion is no longer useful.

To get a solution uniformly valid for all x, we focus on the neighborhood of resonance. Since the spatial scale of resonance is characterized by $\epsilon x = \mathcal{O}(1)$ we introduce fast and slow variables in space

$$x \quad \text{and} \quad x' = \epsilon x \,. \tag{1.2.7}$$

Let the detuning from exact resonance be small, i.e., the incident wave frequency is $\omega + \epsilon\omega'$, where $\epsilon\omega'$ is the frequency detuning. This amounts to a very slow variation in time. Therefore two time variables are needed,

$$t \quad \text{and} \quad t' = \epsilon t \,. \tag{1.2.8}$$

The following multiple-scale expansion is then proposed,

$$v = v_0(x, x'; t, t') + \epsilon v_1(x, x'; t, t') + \cdots \,. \tag{1.2.9}$$

After making the changes

$$\frac{\partial}{\partial x} \to \frac{\partial}{\partial x} + \epsilon \frac{\partial}{\partial x'} \,, \quad \frac{\partial}{\partial t} \to \frac{\partial}{\partial t} + \epsilon \frac{\partial}{\partial t'} \,, \tag{1.2.10}$$

and substituting Eqs. (1.2.9) and (1.2.10) into Eq. (1.2.2), we get

$$\frac{\partial}{\partial x}\left(E_o \frac{\partial v_0}{\partial x}\right) - \rho \frac{\partial^2 v_0}{\partial t^2} = 0 \tag{1.2.11}$$

at $\mathcal{O}(\epsilon^0) = \mathcal{O}(1)$. Anticipating strong but finite reflection, we take the solution to be

$$v_0 = \frac{A}{2} e^{ikx - i\omega t} + \text{c.c.} + \frac{B}{2} e^{-ikx - i\omega t} + \text{c.c.} \,, \tag{1.2.12}$$

where $A(x', t')$ and $B(x', t')$ vary slowly in space and time. At the order $O(\epsilon)$ we have

$$\frac{\partial}{\partial x}\left(E_o \frac{\partial v_1}{\partial x}\right) - \rho \frac{\partial^2 v_1}{\partial t^2}$$

$$= -2E_o \frac{\partial^2 v_0}{\partial x \partial x'} + 2\rho \frac{\partial^2 v_0}{\partial t \partial t'} - \frac{E_o D}{2} \frac{\partial}{\partial x}\left[(e^{2ikx} + e^{-2ikx}) \frac{\partial v_0}{\partial x}\right]$$

$$
\begin{aligned}
&= -E_o\left[\frac{\partial A}{\partial x'}(ik)e^{ikx-i\omega t} + \text{c.c.} + \frac{\partial B}{\partial x'}(-ik)e^{-ikx-i\omega t} + \text{c.c.}\right] \\
&\quad + \rho\left[\frac{\partial A}{\partial t'}(-i\omega)e^{ikx-i\omega t} + \text{c.c.} + \frac{\partial B}{\partial t'}(-i\omega)e^{-ikx-i\omega t} + \text{c.c.}\right] \\
&\quad - \frac{E_o D}{4}\frac{\partial}{\partial x}\left\{(e^{2ikx} + \text{c.c.})\frac{\partial}{\partial x}[Ae^{ikx-i\omega t} + \text{c.c.} + Be^{-ikx-i\omega t} + \text{c.c.}]\right\}.
\end{aligned}
\tag{1.2.13}
$$

The last line can be reduced to

$$
\begin{aligned}
&-\frac{E_o D}{4}(k^2 Be^{ikx-i\omega t} + \text{c.c.} + k^2 Ae^{-ikx-i\omega t} + \text{c.c.} \\
&\qquad - 3k^2 Ae^{3ikx-i\omega t} + \text{c.c.} - 3k^2 Be^{-3ikx-i\omega t} + \text{c.c.})\,.
\end{aligned}
$$

To avoid unbounded resonance of v_1, i.e., to ensure the solvability of v_1, we equate to zero the coefficients of terms $e^{\pm i(kx-\omega t)}$ and $e^{\pm i(kx+\omega t)}$ on the right-hand side of Eq. (1.2.13). The following equations are then obtained:

$$
\frac{\partial A}{\partial t'} + C\frac{\partial A}{\partial x'} = \frac{ikCD}{4}B\,, \tag{1.2.14}
$$

$$
\frac{\partial B}{\partial t'} - C\frac{\partial B}{\partial x'} = \frac{ikCD}{4}A\,, \tag{1.2.15}
$$

where $\sqrt{E_o/\rho} = C = \omega/k$ denotes the phase speed. These equations govern the macroscale variation of the envelopes of the incident and reflected waves, and can be combined to give the Klein–Gordon equation

$$
\frac{\partial^2 A}{\partial t'^2} - C^2\frac{\partial^2 A}{\partial x'^2} + \Omega_0^2 A = 0\,, \quad \text{where } \Omega_0 = \frac{kCD}{4}\,. \tag{1.2.16}
$$

If the domain is infinite, the following is a simple solution

$$
A = A_0 e^{i(Kx'-\Omega t')}\,. \tag{1.2.17}
$$

The corresponding right-going wave

$$
v_+ = \frac{A_0}{2}\exp\left[i((k+\epsilon K)x - (\omega+\epsilon\Omega)t)\right] \tag{1.2.18}
$$

is slightly detuned from (k,ω). Substituting Eq. (1.2.17) into Eq. (1.2.16) we get

$$
K = \pm\frac{1}{C}\sqrt{\frac{\Omega^2}{\Omega_0^2} - 1}. \tag{1.2.19}
$$

In the ranges $\Omega > \Omega_0$ and $\Omega < -\Omega_0$, K is real; the envelope is a propagating wave. The relations between K and Ω are two branches of hyperbola, and hence nonlinear. The envelope is a dispersive wave whose wave speed varies with the wavelength. In the range $-\Omega_0 < \Omega < \Omega_0$, K is pure imaginary. Propagation is forbidden; the envelope must decay exponentially in space. Hence the range $[-\Omega_0, \Omega_0]$ is called the *bandgap*.

With suitable boundary conditions on the macroscale, interesting physics can be deduced for the slow variation of wave envelopes, and hence the global behavior of wave motion.

The use of multiple scales to study the slow modulation of nearly sinusoidal waves is very common in the wave dynamics literature, but is usually known as the WKB or geometrical optics approximation instead of the homogenization theory (see e.g., Nayfeh, 1981; Mei, 1985, 1989; Mei *et al.*, 2005).

1.3. Dispersion of Passive Solute in Pipe Flow

How does one predict the transport of dissolved chemicals in a blood vessel, the spreading of pollutants in a pipe or a river, in shallow estuaries, or in the ever-moving atmosphere? For dilute concentration one can in principle find the fluid motion first and then the convective diffusion of the solute concentration next. In general the computational task can be quite demanding. In some cases, such as in a pipe or channel flow, the velocity of the two- or three-dimensional flow is essentially in one direction, with transverse variations. Since mixing tends to homogenize the solute concentration in the transverse direction, why do not we focus attention on the macroscale spreading in the longitudinal direction by averaging over the microscale in the transverse direction?

It was discovered half a century ago for pipe flows by Taylor (1953, 1954) that the cross-sectionally averaged concentration of a dye cloud is not simply convected by the mean velocity and diffused by molecular or eddy viscosity. Instead, the velocity shear across the pipe tends to augment the effective diffusion in the direction of flow; the enhanced diffusion is now known as *Taylor dispersion*. This theory and its extensions are now the scientific foundation of nearly all studies on the transport of contaminants in the environment, and on the exchange of oxygen or carbon dioxide between blood-carrying arteries or capillaries and surrounding tissues. For the one-dimensional pipe flow Taylor's original analysis was quite heuristic. A more formal procedure called the method of moments was introduced later by

Aris (1960) who also studied the case of pulsating flows in a pipe. Here we demonstrate the use of the homogenization theory by multiple scales.

1.3.1. *Scale Estimates*

Consider the laminar flow in a long pipe with radius a. Let x axis be the axis of the pipe, and r be the radial distance from the axis. Due to a spatially constant pressure gradient the profile of fluid velocity is given by

$$u = U_s(r) + \mathcal{R}e[U_w(r)e^{-i\omega t}], \tag{1.3.1}$$

where $\mathcal{R}e(F)$ denotes the real part of the complex quantity F. The concentration of the solute is governed by the convection–diffusion equation

$$\frac{\partial C}{\partial t} + \frac{\partial (uC)}{\partial x} = D\left[\frac{\partial^2 C}{\partial x^2} + \frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial C}{\partial r}\right)\right], \quad 0 < r < a, \tag{1.3.2}$$

where D is the molecular diffusivity. We shall be interested in the transport over a distance L (macroscale) much greater than the radius a (microscale). Let us first assume the pipe radius to be so small that lateral diffusion is completed within a few periods, i.e.,

$$\frac{2\pi}{\omega} \sim \frac{a^2}{D}, \tag{1.3.3}$$

and choose the following normalizations,

$$x = Lx^\dagger, \quad r = ar^\dagger, \quad u = U_o u^\dagger, \quad t = \frac{a^2}{D}t^\dagger, \tag{1.3.4}$$

where U_o is the scale of u, which can be the center line velocity in either the steady flow or the oscillatory flow. Equation (1.3.2) is then normalized to

$$\frac{\partial C}{\partial t^\dagger} + \frac{U_o a}{D}\frac{a}{L}\frac{\partial (u^\dagger C)}{\partial x^\dagger} = \frac{a^2}{L^2}\frac{\partial^2 C}{\partial {x^\dagger}^2} + \frac{1}{r^\dagger}\frac{\partial}{\partial r^\dagger}\left(r^\dagger\frac{\partial C}{\partial r^\dagger}\right). \tag{1.3.5}$$

Let

$$Pe = \frac{U_o a}{D}, \quad \epsilon = \frac{a}{L} \tag{1.3.6}$$

be defined as the Péclet number and the aspect ratio, respectively. We shall next assume for generality that $Pe = \mathcal{O}(1)$ but $\epsilon \ll 1$. Equation (1.3.5) becomes,

$$\frac{\partial C}{\partial t^\dagger} + \epsilon Pe\frac{\partial (u^\dagger C)}{\partial x^\dagger} = \epsilon^2\frac{\partial^2 C}{\partial {x^\dagger}^2} + \frac{1}{r^\dagger}\frac{\partial}{\partial r^\dagger}\left(r^\dagger\frac{\partial C}{\partial r^\dagger}\right). \tag{1.3.7}$$

Again let us return to physical variables with dimensions and insert the order symbol ϵ to indicate the relative magnitude of each term,

$$\frac{\partial C}{\partial t} + \epsilon \frac{\partial (uC)}{\partial x} = \epsilon^2 D \frac{\partial^2 C}{\partial x^2} + \frac{D}{r}\frac{\partial}{\partial r}\left(r \frac{\partial C}{\partial r}\right). \tag{1.3.8}$$

1.3.2. *Multiple-Scale Analysis*

Associated with two sharply different length scales a and L, there are three sharply distinct time scales whose ratios are:

$$\left(\frac{1}{\omega} \sim \frac{a^2}{D}\right) : \frac{L}{U_o} : \frac{L^2}{D} = \frac{a^2}{D}\left(1 : \frac{1}{\epsilon} : \frac{1}{\epsilon^2}\right). \tag{1.3.9}$$

Let us introduce the multiple time coordinates

$$t\,,\ t' = \epsilon t\,,\ t'' = \epsilon^2 t\,, \tag{1.3.10}$$

and assume

$$C = C_0 + \epsilon C_1 + \epsilon^2 C_2 + \cdots\,, \tag{1.3.11}$$

where $C_i = C_i(x, r, t, t', t'')$. The original time derivative becomes, according to the chain rule:

$$\frac{\partial}{\partial t} \to \frac{\partial}{\partial t} + \epsilon \frac{\partial}{\partial t'} + \epsilon^2 \frac{\partial}{\partial t''}\,. \tag{1.3.12}$$

A sequence of perturbation problems is obtained. At the leading order of $\mathcal{O}(\epsilon^0)$, C_0 is governed by

$$\frac{\partial C_0}{\partial t} = \frac{D}{r}\frac{\partial}{\partial r}\left(r \frac{\partial C_0}{\partial r}\right) \tag{1.3.13}$$

with the boundary conditions:

$$\frac{\partial C_0}{\partial r} = 0\,, \quad r = 0, a\,. \tag{1.3.14}$$

Here x is just a parameter. For any given initial $C_0(x, r, 0, 0, 0)$ nonuniform in r, the general solution at $\mathcal{O}(1)$ is

$$C_0 = C_{00}(x, t', t'') + \sum_{n=1}^{\infty} C_{0n}(x) e^{-(k_n)^2 t} J_0(k_n r)\,,$$

where k_n is the nth root of $J_0'(ka) = 0$, with J_0 being the Bessel function of first kind and order zero. The series terms die out exponentially fast with t and are insignificant for $t' \geq \mathcal{O}(1)$. Limiting ourselves to the behavior long after the time for transverse diffusion to complete or periodicity to be achieved, i.e., after $t \sim \mathcal{O}(1/\omega) \sim \mathcal{O}(a^2/D)$, we shall omit the series part and take the solution to be

$$C_0 = C_0(x, t', t'')\,, \tag{1.3.15}$$

which amounts to replacing Eq. (1.3.13) by

$$0 = \frac{D}{r}\frac{\partial}{\partial r}\left(r\frac{\partial C_0}{\partial r}\right). \tag{1.3.16}$$

Thus C_0 is the nontrivial solution to the homogeneous boundary value problem governed by Eqs. (1.3.16) and (1.3.14).

At $\mathcal{O}(\epsilon)$, C_1 is governed by:

$$\frac{\partial C_0}{\partial t'} + \frac{\partial C_1}{\partial t} + \frac{\partial (uC_0)}{\partial x} = \frac{D}{r}\frac{\partial}{\partial r}\left(r\frac{\partial C_1}{\partial r}\right) \tag{1.3.17}$$

with the boundary conditions

$$\frac{\partial C_1}{\partial r} = 0\,, \quad r = 0, a\,. \tag{1.3.18}$$

At $\mathcal{O}(\epsilon^2)$, C_2 must satisfy

$$\frac{\partial C_0}{\partial t''} + \frac{\partial C_1}{\partial t'} + \frac{\partial C_2}{\partial t} + \frac{\partial (uC_1)}{\partial x} = D\frac{\partial^2 C_0}{\partial x^2} + \frac{D}{r}\frac{\partial}{\partial r}\left(r\frac{\partial C_2}{\partial r}\right) \tag{1.3.19}$$

with

$$\frac{\partial C_2}{\partial r} = 0\,, \quad r = 0, a\,. \tag{1.3.20}$$

Let the known velocity be the sum of the steady and oscillatory parts,

$$u = U_s(r) + \mathcal{R}e(U_w(r)\, e^{-i\omega t})\,, \tag{1.3.21}$$

then at $\mathcal{O}(\epsilon)$,

$$\frac{\partial C_0}{\partial t'} + \frac{\partial C_1}{\partial t} + \left\{U_s + \mathcal{R}e\left[U_w(r)e^{-i\omega t}\right]\right\}\frac{\partial C_0}{\partial x} = \frac{D}{r}\frac{\partial}{\partial r}\left(r\frac{\partial C_1}{\partial r}\right). \tag{1.3.22}$$

In both Eqs. (1.3.13) and (1.3.17), we shall be interested in the time-harmonic response after the initial transient relative to the shortest time scale. Denoting the time(period)-average by overline, i.e.,

$$\bar{f} = \frac{\omega}{2\pi}\int_t^{t+2\pi/\omega} f\, dt\,,$$

and taking the time-average of Eqs. (1.3.22) and (1.3.18), we get

$$\frac{\partial C_0}{\partial t'} + U_s \frac{\partial C_0}{\partial x} = \frac{D}{r}\frac{\partial}{\partial r}\left(r\frac{\partial \overline{C}_1}{\partial r}\right) \tag{1.3.23}$$

with

$$\frac{\partial \overline{C}_1}{\partial r} = 0\,, \quad r = 0, a\,. \tag{1.3.24}$$

Thus $\overline{C}_1$ is governed by an inhomogeneous but steady boundary value problem. Denoting the area-average of f by $\langle f\rangle$, i.e.,

$$\langle f\rangle = \frac{1}{\pi a^2}\int_0^a 2\pi r f\, dr\,,$$

we obtain from Eq. (1.3.23)

$$\frac{\partial C_0}{\partial t'} + \langle U_s\rangle \frac{\partial C_0}{\partial x} = 0\,. \tag{1.3.25}$$

Mathematically, Eq. (1.3.25) is the solvability condition for the inhomogeneous boundary value problem for $\overline{C}_1$. Physically, over the time scale $t' = \mathcal{O}(1)$, or $t = \mathcal{O}(1/\epsilon)$, the solute is simply convected by the mean flow.

Let us subtract Eq. (1.3.25) from Eq. (1.3.22) to get

$$\frac{\partial C_1}{\partial t} + \left\{\widetilde{U}_s + \mathcal{R}e\big[U_w e^{-i\omega t}\big]\right\}\frac{\partial C_0}{\partial x} = \frac{D}{r}\frac{\partial}{\partial r}\left(r\frac{\partial C_1}{\partial r}\right), \tag{1.3.26}$$

where

$$\widetilde{U}_s = U_s(r) - \langle U_s(r)\rangle \tag{1.3.27}$$

is the velocity deviation from its area-average. Thus the fluctuation C_1 satisfies an inhomogeneous diffusion equation. In view of linearity the solution can be formally expressed as

$$C_1 = \frac{\partial C_0}{\partial x}\{B_s(r) + \mathcal{R}e[B_w(r)e^{-i\omega t}]\}\,, \tag{1.3.28}$$

and substituted in Eqs. (1.3.26) and (1.3.18), leading to two cell problems for B_s and B_w. The cell problem for the steady part B_s is governed by:

$$\frac{D}{r}\frac{d}{dr}\left(r\frac{dB_s}{dr}\right) = \widetilde{U}_s(r)\,, \tag{1.3.29}$$

and the boundary conditions

$$\frac{dB_s}{dr} = 0\,, \quad r = 0, a\,. \tag{1.3.30}$$

For the oscillatory part B_w we have instead,

$$\frac{D}{r}\frac{d}{dr}\left(r\frac{dB_w}{dr}\right) + i\omega B_w = U_w(r) \tag{1.3.31}$$

with

$$\frac{dB_w}{dr} = 0\,, \quad r = 0, a\,. \tag{1.3.32}$$

These two cell problems are solved explicitly in later sections for the circular pipe. For any other cross-section, numerical solution is not difficult.

After solving for $B_s(r)$ and $B_w(r)$, we go to $\mathcal{O}(\epsilon^2)$, i.e., Eq. (1.3.19), and get

$$\begin{aligned}&\frac{\partial C_0}{\partial t''} + \frac{\partial C_1}{\partial t'} + \frac{\partial C_2}{\partial t}\\ &\quad + \{\langle U_s\rangle + \widetilde{U}_s + \mathcal{R}e[U_w e^{-i\omega t}]\}\{B_s + \mathcal{R}e[B_w(r)e^{-i\omega t}]\}\frac{\partial^2 C_0}{\partial x^2}\\ &\quad = D\frac{\partial^2 C_0}{\partial x^2} + \frac{D}{r}\frac{\partial}{\partial r}\left(r\frac{\partial C_2}{\partial r}\right).\end{aligned} \tag{1.3.33}$$

From Eqs. (1.3.28) and (1.3.25) we find

$$\frac{\partial C_1}{\partial t'} = -\frac{\partial^2 C_0}{\partial x^2}\langle U_s\rangle\{B_s(r) + \mathcal{R}e[B_w(r)e^{-i\omega t}]\}\,. \tag{1.3.34}$$

It follows from Eq. (1.3.33) that

$$\begin{aligned}&\frac{\partial C_0}{\partial t''} + \frac{\partial C_2}{\partial t} + \{\widetilde{U}_s + \mathcal{R}e[U_w e^{-i\Omega t}]\}\{B_s + \mathcal{R}e[B_w e^{-i\omega t}]\}\frac{\partial^2 C_0}{\partial x^2}\\ &\quad = D\frac{\partial^2 C_0}{\partial x^2} + \frac{D}{r}\frac{\partial}{\partial r}\left(r\frac{\partial C_2}{\partial r}\right).\end{aligned} \tag{1.3.35}$$

By taking the time-average over a period,[1] we get a differential equation for $\overline{C}_2$

$$\frac{\partial C_0}{\partial t''} + \left\{\widetilde{U}_s B_s + \frac{1}{2}\mathcal{R}e[U_w B_w^*]\right\}\frac{\partial^2 C_0}{\partial x^2} = D\frac{\partial^2 C_0}{\partial x^2} + \frac{D}{r}\frac{\partial}{\partial r}\left(r\frac{\partial \overline{C}_2}{\partial r}\right) \tag{1.3.36}$$

with B_w^* denoting the complex conjugate of B_w, and the boundary conditions

$$\frac{\partial \overline{C}_2}{\partial r} = 0\,, \quad r = 0, a\,. \tag{1.3.37}$$

[1]There is a handy formula for the period-average of a quadratic product of two simple harmonic functions. If $a = \mathcal{R}e[a_o e^{-i\omega t}]$ and $b = \mathcal{R}e[b_o e^{-i\omega t}]$, then $\overline{ab} = (1/2)\mathcal{R}e\{a_o b_o^*\} = (1/2)\mathcal{R}e\{a_o^* b_o\}$.

Note that $\overline{C}_2$ is governed by an inhomogeneous steady boundary-value problem. Finally the area-average of Eq. (1.3.36) across the pipe gives

$$\frac{\partial C_0}{\partial t''} = (D + \mathcal{D})\frac{\partial^2 C_0}{\partial x^2}, \tag{1.3.38}$$

where

$$\mathcal{D} = -\left\{\langle \tilde{U}_s B_s \rangle + \frac{1}{2}\mathcal{R}e\langle U_w B_w^* \rangle\right\}. \tag{1.3.39}$$

Mathematically Eq. (1.3.36) is the solvability condition for the inhomogeneous problem of $\overline{C}_2$ on the microscale. Physically, over the time scale $t'' = \mathcal{O}(1)$, or $t = \mathcal{O}(1/\epsilon^2)$, the solvent also undergoes longitudinal diffusion where the effective diffusivity is the sum of the molecular diffusivity D and the dispersivity $\mathcal{D}$ which owes its existence to transverse shear.

To combine the effects of convection and diffusion over the long time scale, we add Eq. (1.3.25) to $\epsilon \times$ Eq. (1.3.38) to get:

$$\left(\frac{\partial}{\partial t'} + \epsilon\frac{\partial}{\partial t''}\right) C_0 + \langle U_s \rangle \frac{\partial C_0}{\partial x} = \epsilon(D + \mathcal{D})\frac{\partial^2 C_0}{\partial x^2}\,. \tag{1.3.40}$$

Now the artifice of two times is no longer needed and can be removed so that

$$\frac{\partial C_0}{\partial t} + \langle U_s \rangle \frac{\partial C_0}{\partial x} = (D + \mathcal{D})\frac{\partial^2 C_0}{\partial x^2}\,, \tag{1.3.41}$$

which is a one-dimensional convective diffusion equation describing the averaged behavior of a two-dimensional phenomenon.

The expression of the dispersion coefficient will be worked out in the next subsections for steady and oscillatory flows separately by solving for B_s and B_w. Even without their explicit solutions, it can be shown that $\mathcal{D}$ must be positive. We demonstrate below that $\langle \widetilde{U}_s B_s \rangle < 0$. Note by definition that

$$\langle \widetilde{U}_s B_s \rangle = \frac{2\pi}{\pi a^2}\int_0^a r\widetilde{U}_s B_s\, dr\,.$$

Using Eq. (1.3.29) and omitting the factor D/a^2, the right-hand side may be written as

$$\begin{aligned}
\int_0^a B_s \frac{d}{dr}\left(r\frac{dB_s}{dr}\right) dr &= \int_0^a \frac{d}{dr}\left(rB_s\frac{dB_s}{dr}\right) dr - \int_0^a r\left(\frac{dB_s}{dr}\right)^2 dr \\
&= \left[rB_s\frac{dB_s}{dr}\right]_0^a - \int_0^a r\left(\frac{dB_s}{dr}\right)^2 dr \\
&= -\int_0^a r\left(\frac{dB_s}{dr}\right)^2 dr < 0\,,
\end{aligned}$$

by partial integration and by virtue of the boundary conditions (Eq. (1.3.30)). Hence

$$\langle \widetilde{U}_s B_s \rangle < 0 \tag{1.3.42}$$

which implies that the steady part of the dispersion coefficient is positive. By a similar reasoning it is easy to demonstrate that

$$\frac{1}{2}\mathcal{R}e\langle U_w {B^*}_w \rangle < 0\,, \tag{1.3.43}$$

and hence $\mathcal{D}$ is positive-definite.

We leave it as an exercise to show that the dispersion coefficient for a pipe of any cross-section is always positive.

1.3.3. *Dispersion Coefficient for Steady Flow*

Let us work out the details for the special case of a steady flow.

With $U_w = 0$, the steady velocity profile is parabolic

$$U_s(r) = \frac{2\langle U_s \rangle}{a^2}(a^2 - r^2)\,, \tag{1.3.44}$$

where $\langle U_s \rangle$ is the cross-sectional average, which is related to the steady part of the applied pressure gradient by

$$\langle U_s \rangle = -\frac{a^2}{8\rho\nu}\frac{\partial p_s}{\partial x}\,. \tag{1.3.45}$$

The equation for B_s is

$$\frac{D}{r}\frac{d}{dr}\left(r\frac{dB_s}{dr}\right) = \frac{2\langle U_s \rangle}{a^2}\left(\frac{a^2}{2} - r^2\right). \tag{1.3.46}$$

It follows by integration that

$$B_s = \frac{\langle U_s \rangle}{2a^2 D}\left(\frac{a^2 r^2}{2} - \frac{r^4}{4}\right) + B_o\,. \tag{1.3.47}$$

For uniqueness we can impose the condition that

$$\langle B_s \rangle = 2\int_0^a r B_s dr = 0\,, \tag{1.3.48}$$

yielding,

$$B_o = -\frac{\langle U_s \rangle a^2}{12D}\,, \tag{1.3.49}$$

so that

$$B_s = \frac{\langle U_s \rangle}{2a^2 D}\left(\frac{a^2 r^2}{2} - \frac{r^4}{4} - \frac{a^4}{6}\right). \tag{1.3.50}$$

Further integration gives

$$\mathcal{D}_s = -\langle \widetilde{U}_s B_s \rangle = \frac{\langle U_s \rangle^2 a^2}{48D} = \frac{Pe^2 D}{48}, \tag{1.3.51}$$

which was first obtained by Taylor (1953) using a different reasoning. The greater the Péclet number, $Pe = \langle U_s a \rangle / D$, the more dominant is dispersion over molecular diffusion.

1.3.4. *Dispersion Coefficient for Oscillatory Flow*

Let the oscillatory part of the applied pressure gradient be

$$-\frac{1}{\rho}\frac{\partial p_w}{\partial x} = Q\,\mathcal{R}e[e^{-i\omega t}], \tag{1.3.52}$$

where Q is the amplitude of the pressure gradient. It is straightforward to show that the velocity profile is

$$U_w(r) = \frac{iQ}{\omega}\left[1 - \frac{J_0(\alpha r)}{J_0(\alpha a)}\right], \tag{1.3.53}$$

where

$$\alpha = \sqrt{\frac{i\omega}{\nu}} = \frac{1+i}{\delta}, \quad \text{with } \delta = \sqrt{\frac{2\omega}{\nu}} \tag{1.3.54}$$

being the Stokes boundary layer thickness of momentum. Bessel functions with a complex argument can be expressed in terms of Kelvin functions.

The cell problem for B_w is then governed by

$$\frac{D}{r}\frac{d}{dr}\left(r\frac{dB_w}{dr}\right) + i\omega B_w = U_w(r) = \frac{iQ}{\omega}\left[1 - \frac{J_0(\alpha r)}{J_0(\alpha a)}\right]. \tag{1.3.55}$$

Let us write

$$B_w = \frac{Q}{\omega^2} + B'_w, \tag{1.3.56}$$

so that

$$\frac{D}{r}\frac{d}{dr}\left(r\frac{dB'_w}{dr}\right) + i\omega B'_w = -\frac{iQ}{\omega}\frac{J_0(\alpha r)}{J_0(\alpha a)}. \tag{1.3.57}$$

B'_w can be decomposed into a homogeneous and an inhomogeneous part. The homogeneous part is

$$AJ_o(\beta r), \quad \text{where } \beta = \sqrt{\frac{i\omega}{D}},$$

and A is a constant yet to be determined. The inhomogeneous part can be readily shown to be

$$-\frac{iQ}{\omega D}\frac{1}{\beta^2-\alpha^2}\frac{J_0(\alpha r)}{J_0(\alpha a)}\,.$$

Hence

$$B_w = AJ_0(\beta r) + \frac{Q}{\omega^2}\left[1 - \frac{\beta^2}{\beta^2-\alpha^2}\frac{J_0(\alpha r)}{J_0(\alpha a)}\right]. \qquad (1.3.58)$$

Applying the no-flux condition on the pipe wall $r = a$, we easily find A,

$$A = \frac{\beta}{\alpha}\frac{J_1(\alpha a)}{J_1(\beta a)} \qquad (1.3.59)$$

and obtain

$$B_w = \frac{Q}{\omega^2}\left\{1 + \frac{\beta^2}{\beta^2-\alpha^2}\frac{(\alpha/\beta)J_1(\alpha a)J_0(\beta r) - J_0(\alpha r)J_1(\beta a)}{J_0(\alpha a)J_1(\beta a)}\right\}. \qquad (1.3.60)$$

We leave it as an exercise to derive the dispersion coefficient. Indeed, one can show that the dispersion coefficient in a pure oscillatory flow is

$$\mathcal{D}_w = \frac{Q^2}{\omega^3}\mathcal{R}e\left\{\frac{A^*[\alpha J_0(\beta^* a)J_1(\alpha a) - \beta^* J_0(\alpha a)J_1(\beta^* a)]}{(\omega a/\nu)(\nu^2/D^2)|J_0(\alpha a)|^2}\right\}. \qquad (1.3.61)$$

This result was first found by Aris (1960),[2] and is the form given by Ng (2006) who also studied the effects of chemical reactions of the pipe wall (Ng, 2000, 2004). The theoretical result has been confirmed in laboratory experiments by Joshi *et al.* (1983).

Further extensions have been made by Hydon and Pedley (1993) to dispersion in a tube with elastic wall which is of interest to transport in blood flow.

1.4. Typical Procedure of Homogenization Analysis

The elementary examples in this chapter demonstrate the basic ideas of the homogenization theory which can be extended to many problems with a sharp contrast between micro- and macroscales. Developed

[2]See also Watson (1983).

mostly for periodic microstructures, the typical steps can be summarized as follows

(i) Identify the micro- and macroscales.
(ii) Introduce multiple-scale variables and expansions and deduce boundary-value problems for a typical period at successive orders. The leading-order ($\mathcal{O}(\epsilon^0)$) problem is homogeneous; either the solution itself or the coefficient of the homogeneous solution is indeterminate and independent of the microscale coordinates.
(iii) At the next order $\mathcal{O}(\epsilon)$, the inhomogeneous microscale problem is forced by the leading-order solution. Solve a canonical microscale problem for unit forcing.
(iv) Taking the average of the inhomogeneous microscale problem at the order $\mathcal{O}(\epsilon^2)$, one gets the equation governing the macroscale behavior of the leading order unknown. The constitutive coefficients in the macroscale equation are obtained from the solution of the canonical cell problem.

We now turn to other extensions.

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