

**Fluid flow in porous media:  
continuum modelling  
based upon microscopic considerations**

Ian Murdoch

*Department of Mathematics  
University of Strathclyde  
Glasgow, Scotland  
aim@maths.strath.ac.uk*

Continuum concepts, fields, and relations in the macroscopic modelling of fluid motion within porous media are related to molecular considerations using weighting function methodology and without reference to statistical mechanics. The boundary of a porous body is delineated at any scale and porosity shown to involve two scales : the scale  $\varepsilon_1$  at which pore structure is examined and REV scale  $\varepsilon_2$ . Forms of mass conservation and linear momentum balance for fluid are derived at both scales. Darcy's law is established by  $\varepsilon_2$  scale averaging of  $\varepsilon_1$  scale flow of a Navier-Stokes fluid through a rigid porous body it saturates via a sequence of clear modelling assumptions and simplifications.

*Key words: molecular considerations, weighting function methodology, scale-dependent fields, microscopic-macroscopic links*

## 1. Introduction

In order that fluid is able to flow through a solid body it is necessary that

- (i) there is space available 'within' the body to accommodate such fluid, and
- (ii) the space in which the fluid can reside must be connected in order that the fluid can move *through* the body.

Available space is termed 'pore space', a measure of which is the so-called **porosity**, while connectivity is linked with the notion of **permeability**. Consider an insect attempting to crawl through a rectangular block of porous material from the centre of one face and to exit through another face. This may or may not be possible. It could be that no connected route between the point of entry and the other destination face exists, or that the insect is unable to squeeze through available 'gaps' *en route*. The former snag indicates that permeability may be in some sense direction-dependent, while the latter problem indicates that both porosity and permeability are scale-dependent.

To make precise the notion of porosity it is necessary to delineate the 'boundary' of the body. Common experience indicates that the notion of a boundary is scale-dependent: most objects have surfaces which reveal more and more topographical features when viewed by magnifying glasses of greater and greater resolving power. To introduce scale-dependence it is necessary to take a perspective outside that of Continuum Mechanics, since from the continuum viewpoint the region occupied by a body is the *support*<sup>1)</sup> of the mass density function  $\rho$  which is a primitive quantity from this viewpoint. (Of course, the boundary of this region is taken to be the boundary of the body.)

Consider the molecules of the body and model these as point masses. (To each such point mass is attributed the mass of the molecule it represents, and

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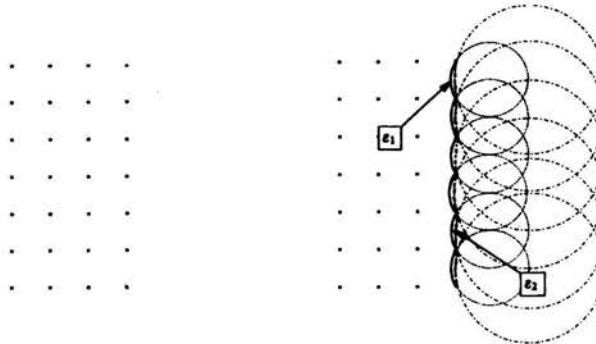
<sup>1)</sup>The *support* of  $\rho$  is the set of points at which  $\rho$  takes non-zero (and hence positive) values.

its location at any instant is taken to be the mass centre of this molecule.) Let  $\text{Ext}_\varepsilon(t)$  denote the set which consists of the union of the interiors of all spheres of radius  $\varepsilon$  which do not contain *any* molecular mass centres at instant  $t$ . Then the **geometric region occupied by the body at scale  $\varepsilon$**  at instant  $t$  is

$$R_\varepsilon^g(t) := \mathcal{E} - \text{Ext}_\varepsilon(t), \quad (1.1)$$

where  $\mathcal{E}$  denotes Euclidean space.

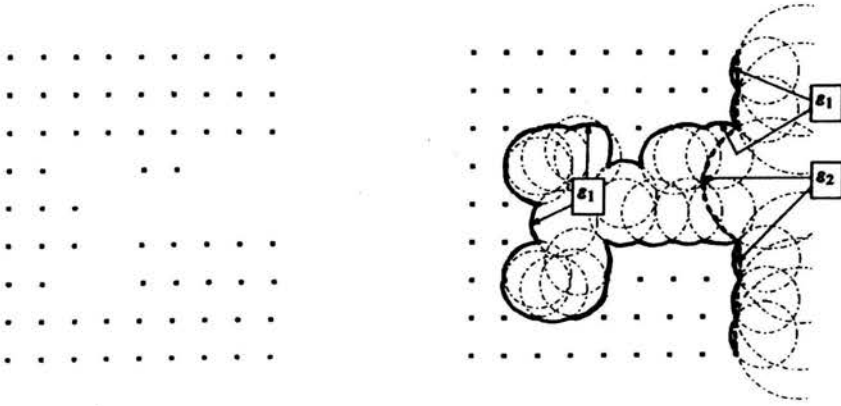
$\text{Ext}_\varepsilon$  may be visualised in terms of spherical balloons of radius  $\varepsilon$  being brought from a location remote from the body ever 'closer' to the body. When such a balloon encounters a molecular mass centre on its boundary for the first time, 'lock' this boundary point and constrain the sphere only to rotate about this point. In such rotation the sphere will encounter, in general,<sup>2)</sup> a second molecule. Again lock the sphere onto this second molecule so that it may now only rotate about an axis which contains the two molecular mass centres. In such rotation the sphere will in general encounter a third molecule and then be anchored completely. In the context of porous bodies it may also be possible to inflate spherical balloons which can lock onto three molecules in the foregoing fashion, have no molecules within, yet be unable to be moved to locations remote from the body. The totality of the interiors of all such 'boundary-anchored' spheres, together with those of spheres which contain *no* molecules, constitute  $\text{Ext}_\varepsilon$ . Figures 1 depict the geometric boundaries of a perfect crystal lattice are depicted at two scales,  $\varepsilon_1$  and  $\varepsilon_2$ .



Figures 1: The geometric boundaries to a perfect crystal lattice are depicted at two scales,  $\varepsilon_1$  and  $\varepsilon_2$ .

<sup>2)</sup>If this does not happen  $R_\varepsilon^g$  contains the molecule as an isolated point.

fissure in a crystal lattice and its geometric boundaries at two scales. The foregoing has drawn attention to the scale-dependence of the mass density field  $\rho$  employed in Continuum Mechanics via consideration of the manifestly scale-dependent nature of the boundary of a solid body. A natural question arises as to how the geometrical boundary of such a body at a given scale may be related to a scale-dependent definition of  $\rho$ . In what follows this is accomplished by relating  $\rho$  and other continuum fields to local, scale-dependent, spatial averages of molecular quantities in which molecules are (somewhat simplistically) modelled as interacting point masses (which will also be termed 'particles'). Such a procedure enables the basic concepts of Continuum Mechanics (see, for example, Truesdell & Noll [1], Eringen [2], Gurtin [3], Chadwick [4]) to be understood more clearly than by an *a priori* adoption of continuum modelling.



Figures 2: The geometric boundaries to a crack/fissure in a crystal lattice are depicted at two scales,  $\epsilon_1$  and  $\epsilon_2$ .

## 2. Kinematics and mass conservation

### 2.1. *Material systems, mass and momentum densities via weighting functions, and local mass conservation*

A **material system** (or ‘**body**’)  $\mathcal{M}$  is considered to be composed of a fixed, identifiable, set of ( $N$ , say) interacting point masses. These point masses model the molecules of which  $\mathcal{M}$  is composed. In considering fluid flow through a porous body, there are two relevant material systems: the set of porous body molecules, and the set of fluid molecules. (Another associated material system is the set of all fluid *and* porous body molecules.) Labelling the point masses of  $\mathcal{M}$  as  $P_i$  ( $i = 1, 2, \dots, N$ ), the mass, location, and velocity at instant  $t$  of  $P_i$  are denoted by  $m_i$ ,  $\mathbf{x}_i(t)$ , and  $\mathbf{v}_i(t)$ , respectively.

**Mass and momentum density fields**, which represent local spatial averages of mass and momentum, can be defined in terms of a scalar-valued, non-negative **weighting function**  $w$  whose domain is the space  $\mathcal{V}$  of all displacements in Euclidean space  $\mathcal{E}$ . Specifically, at any location  $\mathbf{x}$  (a geometrical point) and instant  $t$ ,

$$\rho_w(\mathbf{x}, t) := \sum_{i=1}^N m_i w(\mathbf{x}_i(t) - \mathbf{x}) \quad (2.1)$$

and

$$\mathbf{p}_w(\mathbf{x}, t) := \sum_{i=1}^N m_i \mathbf{v}_i(t) w(\mathbf{x}_i(t) - \mathbf{x}). \quad (2.2)$$

Here  $\mathbf{x}_i(t) - \mathbf{x}$  denotes the displacement of  $\mathbf{x}_i(t)$  from field point  $\mathbf{x}$ . In order that  $\rho_w$  and  $\mathbf{p}_w$  represent spatial averages it is necessary that  $w$  have physical dimension  $(\text{length})^{-3}$ . Further, to reflect *local* spatial averages,  $w$  should accord greater ‘weight’ to particles near  $\mathbf{x}$  than particles far from  $\mathbf{x}$ . That the integral over all space  $\mathcal{E}$  of  $\rho_w$  ( $\mathbf{p}_w$ ) should equal the total mass (momentum)

of  $\mathcal{M}$  imposes the *normalisation condition*<sup>3)</sup>

$$\int_{\mathcal{V}} w = 1. \tag{2.3}$$

*Exercise 2.1.* Show that (2.3) implies that

$$\int_{\mathcal{V}} \rho_w = \text{total mass of system } \mathcal{M}. \quad (*)$$

Show further that if  $\mathcal{M}$  consists of a single molecule then (\*) implies relation (2.3).

Of course, (2.3) requires that  $w$  be integrable. More generally, any spatial continuity or smoothness possessed by  $w$  will be inherited by  $\rho_w$  and  $\mathbf{p}_w$ . If a Cartesian co-ordinate system in which  $\mathbf{e}_1, \mathbf{e}_2$  and  $\mathbf{e}_3$  are the distinguished orthonormal basis vectors, then for any  $\mathbf{u} \in \mathcal{V}$  we define  $\hat{w} : \mathbb{R}^3 \rightarrow \mathbb{R}$  by

$$w(\mathbf{u}) = w(u_1 \mathbf{e}_1 + u_2 \mathbf{e}_2 + u_3 \mathbf{e}_3) =: \hat{w}(u_1, u_2, u_3). \tag{2.4}$$

The spatial derivative, or gradient,  $\nabla w$  of  $w$  is defined by

$$\nabla w := \hat{w}_{,k} \mathbf{e}_k = \text{grad } \hat{w}. \tag{2.5}$$

Differentiating (2.1) with respect to  $t$ , holding  $\mathbf{x}$  fixed, yields

$$\frac{\partial \rho_w}{\partial t} = \sum_{i=1}^N m_i \frac{\partial w}{\partial t} = \sum_{i=1}^N m_i \nabla w \cdot \dot{\mathbf{x}}_i = \sum_{i=1}^N m_i \nabla w \cdot \mathbf{v}_i. \tag{2.6}$$

(The second equality follows from the Chain Rule.) However,

$$\begin{aligned} \text{div } \mathbf{p}_w &= \sum_{i=1}^N m_i \text{div}(w\mathbf{v}_i) = \sum_{i=1}^N m_i \{w \text{div } \mathbf{v}_i - \nabla w \cdot \mathbf{v}_i\} \\ &= - \sum_{i=1}^N m_i \nabla w \cdot \mathbf{v}_i, \end{aligned} \tag{2.7}$$

since  $m_i$  and  $\mathbf{v}_i$  are independent of field variable  $\mathbf{x}$ . (The minus sign occurs because differentiation throughout is with respect to  $\mathbf{x}$ . Specifically, noting

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<sup>3)</sup>Integration over all displacements in  $\mathcal{V}$  is intended. All subsequent integrals will omit ‘dummy’ variables: the nature of an integral will be evident from the domain of integration.

that with  $\mathbf{u} := \mathbf{x}_i - \mathbf{x}$ ,  $\nabla w := \nabla_{\mathbf{u}} w = \text{grad } \hat{w} = -\nabla_{\mathbf{x}} \hat{w} = -\nabla_{\mathbf{x}} w$ .) From (2.6) and (2.7),

$$\frac{\partial \rho_w}{\partial t} + \text{div } \mathbf{p}_w = 0. \quad (2.8)$$

Wherever and whenever  $\rho_w(\mathbf{x}, t) \neq 0$  the **velocity** field

$$\mathbf{v}_w := (\rho_w)^{-1} \mathbf{p}_w. \quad (2.9)$$

Accordingly the mass density and velocity fields satisfy the so-called ‘continuity equation’

$$\frac{\partial \rho_w}{\partial t} + \text{div} \{ \rho_w \mathbf{v}_w \} = 0, \quad (2.10)$$

also known as the local (or ‘point’) form of mass conservation. If (2.10) is integrated over a region  $\mathcal{R}$  then the result is expressible in the form

$$\frac{\partial}{\partial t} \left\{ \int_{\mathcal{R}} \rho_w \right\} = - \int_{\partial \mathcal{R}} \rho_w \mathbf{v}_w \cdot \mathbf{n}, \quad (2.11)$$

where  $\mathbf{n}$  denotes the outward unit normal to the boundary  $\partial \mathcal{R}$  of  $\mathcal{R}$ . Of course, in obtaining (2.11) use has been made of the divergence theorem. In standard works on Continuum Mechanics the density and velocity fields  $\rho$  and  $\mathbf{v}$  are assumed to satisfy (2.11) (with  $\rho_w = \rho$  and  $\mathbf{v}_w = \mathbf{v}$ ) which is taken to be a statement of mass conservation. Continuity of  $\rho$  and  $\mathbf{v}$ , together with the arbitrary nature of  $\mathcal{R}$ , then enables (2.10) to be *deduced*. The weighting function approach has delivered (2.10) directly, and fields  $\rho_w$  and  $\mathbf{v}_w$  have precise, scale-dependent, interpretations.

*Exercise 2.2.* Show that  $\int_{\mathcal{R}} \rho_w$  represents a mass which lies between the mass of molecules within  $\mathcal{R}_\epsilon^-$  and the mass of molecules within  $\mathcal{R}_\epsilon^+$ , where

$$\mathcal{R}_\epsilon^- := \{ \mathbf{x} \in \mathcal{E} : \mathbf{x} \in \mathcal{R}_\epsilon \text{ and } d(\mathbf{x}, \partial \mathcal{R}_\epsilon) \leq \epsilon \}$$

and

$$\mathcal{R}_\epsilon^+ := \{ \mathbf{x} \in \mathcal{E} : \mathbf{x} \notin \mathcal{R}_\epsilon \text{ but } d(\mathbf{x}, \partial \mathcal{R}_\epsilon) \leq \epsilon \}.$$

[An analogous result holds for the components of momentum density.  $d(\mathbf{x}, \partial \mathcal{R}_\epsilon)$  denotes the smallest distance between  $\mathbf{x}$  and points on  $\partial \mathcal{R}_\epsilon$ .]

*Remark 2.1.* Relation (2.10) is *formal*: the physical interpretations of  $\rho_w$  and  $\mathbf{v}_w$  depend upon the specific form of  $w$ . The simplest choice, for a given



length scale  $\varepsilon$ , is that which delivers  $\rho_w(\mathbf{x}, t)$  as the total mass (at instant  $t$ ) of those particles which lie within or on the boundary of a sphere of radius  $\varepsilon$ , centred at  $\mathbf{x}$ , divided by the volume of this sphere. In such case, for any  $\mathbf{u} \in \mathcal{V}$ ,

$$\begin{aligned} w_\varepsilon(\mathbf{u}) &= V_\varepsilon^{-1} \quad \text{if } \|\mathbf{u}\| \leq \varepsilon \\ w_\varepsilon(\mathbf{u}) &= 0 \quad \text{if } \|\mathbf{u}\| > \varepsilon, \end{aligned} \tag{2.12}$$

where

$$V_\varepsilon := 4\pi\varepsilon^3/3, \tag{2.13}$$

and subscript  $\varepsilon$  has been introduced to emphasise the specific scale-dependence.

For such choice of  $w$ ,

- (i)  $\mathbf{p}_w(\mathbf{x}, t)$  represents the total momentum associated with particles which lie, at instant  $t$ , less than or equal to a distance of  $\varepsilon$  from  $\mathbf{x}$  divided by  $V_\varepsilon$ , and (see (2.9))
- (ii)  $\mathbf{v}_w(\mathbf{x}, t)$  represents the velocity of the mass centre of the foregoing particles.

There is a snag, however:  $w_\varepsilon$  is not continuous (and hence is not differentiable) for displacements  $\mathbf{u}$  with  $\|\mathbf{u}\| = \varepsilon$ . However, the ‘jump’ may be ‘mollified’ in such a way that the foregoing interpretations change insignificantly, and the mollified version of  $w$  has derivatives of all orders. To see this let  $\phi$  denote any smooth, real-valued, monotonic function defined on  $[0, 1]$  for which  $\phi(0) = 1, \phi(1) = 0, \phi'(0) = 0$  and  $\phi'(1) = 0$ . (The derivatives are intended in the one-sided sense.) Writing

$$u := \|\mathbf{u}\|, \tag{2.14}$$

define

$$\left. \begin{aligned} w_{\varepsilon,h}(u) &= \frac{1}{\alpha} & \text{if } u < \varepsilon, \\ w_{\varepsilon,h}(u) &= \frac{\phi(\lambda)}{\alpha} & \text{if } u = \varepsilon + \lambda h \quad (0 \leq \lambda \leq 1), \\ \text{and } w_{\varepsilon,h}(u) &= 0 & \text{if } u > \varepsilon + h, \end{aligned} \right\} \tag{2.15}$$

where  $h > 0$  and  $\alpha$  is a constant determined by the normalisation condition (2.3). This condition requires that

$$4\pi \int_0^\infty w_{\varepsilon,h}(u)u^2 du = 1. \tag{2.16}$$

Since  $0 \leq \phi(\lambda) \leq 1$  it follows from (2.15) and (2.16) that

$$\frac{\alpha}{V_\varepsilon} = 1 + O\left(\frac{h}{\varepsilon}\right) \quad \text{as } h \rightarrow 0. \quad (2.17)$$

Accordingly, by making  $h$  arbitrarily small, it is possible to approximate  $w_\varepsilon$  given in (2.12) and (2.13) by  $w_{\varepsilon,h}$  as accurately as may be desired. Said differently, for a given choice  $\varepsilon$  of length scale, the field values for  $\rho_w, \mathbf{p}_w$  and  $\mathbf{v}_w$  obtained by choosing  $w = w_\varepsilon$  in definitions (2.1), (2.2) and (2.9) may be approximated to any degree of accuracy by selecting a mollifying function  $\phi$  (which may have any degree of smoothness up to class  $C^\infty$ ), choosing  $h$  suitably small,<sup>4)</sup> and replacing  $w_\varepsilon$  by  $w_{\varepsilon,h}$ . The resulting fields  $\rho_{\varepsilon,h}, \mathbf{p}_{\varepsilon,h}$  and  $\mathbf{v}_{\varepsilon,h}$  will inherit the degree of spatial smoothness possessed by  $\phi$ . Motivated by the foregoing remarks, in what follows dependence upon  $h$  will be suppressed.

## 2.2. The region occupied by a material system at a given scale

From the continuum viewpoint, consequent upon any choice of weighting function  $w$ , the **region**  $R_w(t)$  **occupied by the body at instant**  $t$  is the region in which matter is 'detected' by the corresponding density function  $\rho_w$ . That is,

$$R_w(t) := \{\mathbf{x} \in \mathcal{E} : \rho_w(\mathbf{x}, t) > 0\}. \quad (2.18)$$

Choice  $w = w_\varepsilon$  results in this region being

$$R_\varepsilon(t) = \bigcup_{i=1}^N S_\varepsilon(\mathbf{x}_i(t)), \quad (2.19)$$

where, for any point  $\mathbf{y} \in \mathcal{E}$ ,  $S_\varepsilon(\mathbf{y})$  denotes that closed ball of radius  $\varepsilon$  centred at  $\mathbf{y}$ . That is,

$$S_\varepsilon(\mathbf{y}) := \{\mathbf{z} \in \mathcal{E} : \|\mathbf{z} - \mathbf{y}\| \leq \varepsilon\}. \quad (2.20)$$

*Exercise 2.3.* Show that

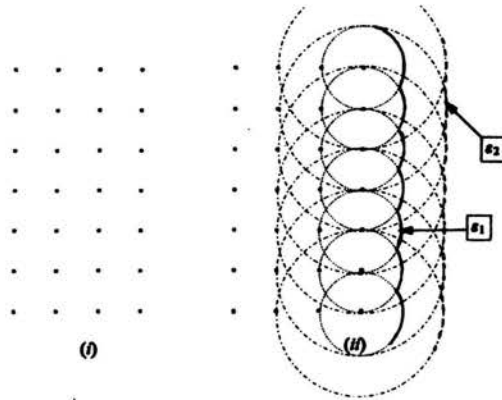
$$R_{\varepsilon_1}(t) \subset R_{\varepsilon_2}(t) \quad \text{if } \varepsilon_2 > \varepsilon_1. \quad (2.21)$$

<sup>4)</sup>In condensed phases, nearest-neighbour separations of molecular mass centres exceed  $1 = 10^{-10}$  m. Any choice  $h \ll 1$  will thus be suitable.

The boundary of the body at instant  $t$  for choice  $w$  is the boundary  $\partial R_w(t)$  of  $R_w(t)$ . Choice  $w = w_\epsilon$  results in the boundary at scale  $\epsilon$  and instant  $t$  being  $\partial R_\epsilon(t)$ . Accordingly, from (2.19) and (2.20), a point  $\mathbf{x}$  lies on  $\partial R_\epsilon(t)$  if, and only if,

- (i) there is at least one molecule of the body distant  $\epsilon$  from  $\mathbf{x}$ , and
- (ii) all molecules of the body are distant at least  $\epsilon$  from  $\mathbf{x}$ .

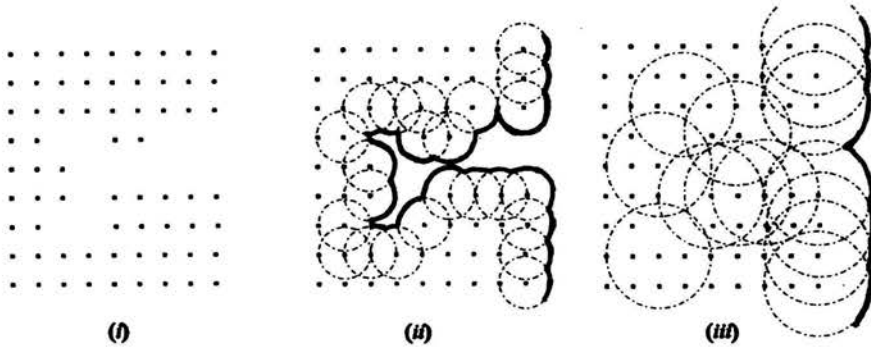
*Remark 2.2.* If  $\epsilon$  is less than the order of nearest-neighbour molecular separations then the body will appear to be riddled with holes or even to be a disjoint collection of spheres, each one centred at a molecular mass centre. For example, in an infinite cubic lattice with nearest-neighbour separation  $\epsilon_0$ , then  $\epsilon = \epsilon_0$  yields no boundary,  $\epsilon = 4\epsilon_0/5$  results in an infinite number of unconnected holes, each one of which contains the mid-point of a lattice cell, and  $\epsilon = \frac{\epsilon_0}{3}$  results in a disjoint collection of isolated spheres. (Convince yourself of these situations!) Of course, selecting scales smaller than  $\epsilon_0$  is physically inappropriate, since quantum considerations become relevant: that is, the corpuscular modelling here adopted becomes inappropriate at such scales.



Figures 3: (i) represents the perfect crystal lattice of Figures 1 and (ii) depicts the boundary  $\partial R_\epsilon$  at two scales,  $\epsilon_1$  and  $\epsilon_2$ .

*Remark 2.3.* Figures 4 illustrate the manner in which surface features depend upon  $\epsilon$ . A crack whose characteristic dimensions are only marginally above the scale  $\epsilon_0$  of nearest neighbour molecular separations is manifest at scale  $\epsilon = \epsilon_0$  but cannot be distinguished at scale  $2\epsilon_0$ . See Figures 2 for geometric

boundaries of the same crack at two scales  $\varepsilon_1$  and  $\varepsilon_2$ .



Figures 4: (i) depicts the crack/fissure in a crystal lattice as in Figures 2, (ii) shows the boundary  $\partial R_\varepsilon$  at a scale  $\varepsilon = \varepsilon_0$ , where  $\varepsilon_0$  is the nearest-neighbour separation and (iii) indicates the boundary  $\partial R_\varepsilon$  at scale  $\varepsilon = 2\varepsilon_0$ .

*Remark 2.4.* The regions  $\mathcal{R}_\varepsilon^g$  and  $\mathcal{R}_\varepsilon$  are, of course, related. Specifically,

$$R_\varepsilon^g(t) = \{ \mathbf{x} \in R_\varepsilon(t) : d(\mathbf{x}, \partial R_\varepsilon(t)) \geq \varepsilon \}. \tag{2.22}$$

(Here  $d(\mathbf{x}, \partial R_\varepsilon(t))$  denotes the distance of  $\mathbf{x}$  to the nearest point on boundary  $\partial R_\varepsilon(t)$ .) Boundaries  $\partial R_\varepsilon$  and  $\partial R_\varepsilon^g$  are defined uniquely in terms of molecular locations, but *neither* is to be identified precisely with the boundary actually *perceived* by an observer whose limiting observational scale is  $\varepsilon$ . Indeed, such an observer is incapable of detecting the cusps in these surfaces, and will have the impression of a surface, smoother than either, each point of which lies within  $\varepsilon$  of  $\partial R_\varepsilon^g$ .

*Remark 2.5.* In modelling fluid flow through porous bodies we are in general interested only in gross features of mass transport of fluid rather than local flows within pores. From the foregoing discussion of scales this means that the continuum model will reflect  $\varepsilon$ -scale spatial averaging in which  $\varepsilon$  is much greater than pore size and structural dimension of the porous body: say  $\varepsilon \sim \varepsilon_2$ . Of course, a much smaller value of  $\varepsilon$  is necessary to delineate the pore structure, say  $\varepsilon \sim \varepsilon_1$ . We will return to this matter later to show how an  $\varepsilon_2$ -scale continuum balance of linear momentum can be derived from continuum modelling at scale  $\varepsilon_1$ . In the event that incompressible liquid with density  $\rho_0$  fills up (or ‘saturates’) all pore space at scale  $\varepsilon_1$ , then  $\rho_w$  computed with scale

$\varepsilon = \varepsilon_1$  will coincide with  $\rho_0$  almost everywhere in the pores. However,  $\rho_w$  computed with scale  $\varepsilon = \varepsilon_2$  will be significantly less than  $\rho_0$ . This is because  $\rho_w(\mathbf{x}, t)$  is computed as the sum of liquid molecular masses within a sphere that includes the porous body as well as liquid. Denoting the two densities by  $\rho_{\varepsilon_1}$  and  $\rho_{\varepsilon_2}$ , the quantity

$$\nu_{\varepsilon_1, \varepsilon_2}(\mathbf{x}, t) := \frac{1}{\rho_0 V_{\varepsilon_2}} \int_{S_{\varepsilon_2}(\mathbf{x})} \rho_{\varepsilon_1}(\mathbf{y}, t) dy \tag{2.23}$$

is essentially the mass of liquid within spherical region  $S_{\varepsilon_2}(\mathbf{x})$  divided by the mass of fluid within this sphere if filled with liquid (in the absence of the porous body). Clearly this ratio is a measure of the pore space within  $S_{\varepsilon_2}(\mathbf{x})$  in the locality of  $\mathbf{x}$  at instant  $t$ . That is,  $\nu_{\varepsilon_1, \varepsilon_2}$  is a measure of *porosity*. Notice that porosity is accordingly a quantity that depends upon *two* scales (one to delineate the porous structure and the other the scale at which gross averaging is implemented). Further, porosity is a *field*: that is, it is to be expected to vary with location and time. If the porous body is *rigid*, time-dependence will disappear.

### 2.3. The motion map associated with $w$

Fields  $\rho_w$  and  $\mathbf{v}_w$  are defined at instant  $t$  in region  $\mathcal{R}_w(t)$ : see (2.1), (2.2), (2.9) and (2.18). For a given instant  $t_0$  and any point  $\hat{\mathbf{x}} \in \mathcal{R}_w(t_0)$  consider the initial-value problem for function  $\chi_w^0(\cdot, t)$ :

$$\dot{\chi}_w^0(\hat{\mathbf{x}}, t) = \mathbf{v}_w(\chi_w^0(\hat{\mathbf{x}}, t), t) \tag{2.24}$$

where

$$\chi_w^0(\hat{\mathbf{x}}, t) = \hat{\mathbf{x}}.$$

The function  $\chi_w^0$  is termed the **motion appropriate to  $w$  and the situation at instant  $t_0$** . (To trace out the path of  $\chi_w^0(\hat{\mathbf{x}}, t)$  as  $t$  evolves, we start at instant  $t_0$  at location  $\hat{\mathbf{x}}$ , and move at subsequent times in such a way that our velocity coincides with the instantaneous value of  $\mathbf{v}_w$  wherever we are.)

*Remark 2.6.* In Continuum Mechanics a material system (or ‘body’) is considered to be made up of a set of ‘material points’. At any instant  $t$  each material point  $\mathbf{X}$  is located at a geometrical point and the totality of

such points is the region  $\mathcal{R}_t$  occupied by the body at this instant. If  $\mathbf{X}$  is located at  $\hat{\mathbf{x}}$  at instant  $t_0$  then its location  $\mathbf{x}$  at subsequent time  $t$  is denoted by  $\chi_0(\mathbf{X}, t)$ . The function (here  $I$  denotes any time interval)

$$\chi_0 : \mathcal{R}_{t_0} \times I \rightarrow \mathcal{E} \quad (2.25)$$

is termed the motion of the body over time interval  $I$  with respect to the configuration at instant  $t_0$ . The velocity field  $\mathbf{v}$  is *defined* on the trajectory of  $\chi_0$  by

$$\mathbf{v}(\mathbf{x}, t) := \dot{\chi}_0(\hat{\mathbf{x}}, t) \quad (2.26)$$

where

$$\chi_0(\hat{\mathbf{x}}, t_0) = \hat{\mathbf{x}}.$$

Accordingly the procedure for deriving fields introduced in Section 2.1. via weighting functions can be reconciled with (2.26) by identifying with each  $\hat{\mathbf{x}} \in \mathcal{R}_w(t_0)$  a ‘material point’. However, the more fundamental physical approach is that from the molecular perspective, which has revealed the notion of material point to be scale-dependent. Indeed, such notion is a *mathematical artefact*, associated with visualising gross mass transport at a (any!) given length scale. In particular, the foregoing viewpoint renders clear the following observations:

- (i) The trajectory of a material point should not be confused with that of any individual molecule modelled as a particle. Molecular mass centres exhibit erratic behaviour in all condensed phases, and in fluids rapid molecular diffusion means the near-neighbours of any given molecule are continually changing very rapidly. In a solid, however, near-neighbours remain such, and a region of scale  $\varepsilon$  marked or ‘doped’ in some way will, roughly speaking, move to a good approximation as an  $\varepsilon$ -scale material point associated with a location within this region.
- (ii) Given two molecular species which are mixed at the molecular level, there are three  $\varepsilon$ -scale velocity fields which may be considered. Each species gives rise to such a field, and the system taken as a whole yields a third field. The motions of each of the three systems, at scale  $\varepsilon$ , may be treated in terms of three categories of material point—one for each system in question. Accordingly, at a given *geometrical* point occupied by the whole system, there will be located simultaneously three material points. Interpreting the latter as other than mathematical artefacts can lead to conceptual difficulties.

*Remark 2.7.* Let  $\mathcal{M}^p$  and  $\mathcal{M}^f$  denote the material systems which consist, respectively, of porous body molecules and fluid molecules, and let  $R_\varepsilon^p$  and  $R_\varepsilon^f$  represent the regions occupied by these systems<sup>5)</sup> at scale  $\varepsilon$ . Accordingly the corresponding mass density and velocity fields  $\rho_\varepsilon^p$  and  $\mathbf{v}_\varepsilon^p$  ( $\rho_\varepsilon^f$  and  $\mathbf{v}_\varepsilon^f$ ) are defined in  $R_\varepsilon^p(R_\varepsilon^f)$  and satisfy

$$\frac{\partial \rho_\varepsilon^p}{\partial t} + \operatorname{div}\{\rho_\varepsilon^p \mathbf{v}_\varepsilon^p\} = 0 \quad \text{in } \mathcal{R}_\varepsilon^p \tag{2.27}$$

and

$$\frac{\partial \rho_\varepsilon^f}{\partial t} + \operatorname{div}\{\rho_\varepsilon^f \mathbf{v}_\varepsilon^f\} = 0 \quad \text{in } \mathcal{R}_\varepsilon^f. \tag{2.28}$$

Recall Remark 2.5 in which the two scales  $\varepsilon_1$  (at which pore detail is manifest) and  $\varepsilon_2$  (greater than typical pore size and porous body structural dimension) were introduced. Then

$$\varepsilon_1 \ll \varepsilon_2, \tag{2.29}$$

and we can make the following observations.

O.1. If the porous body is immersed in fluid which also permeates all pores, then

$$\mathcal{R}_{\varepsilon_2}^p \subset \mathcal{R}_{\varepsilon_2}^f, \tag{2.30}$$

since if  $\mathbf{x} \in \mathcal{R}_{\varepsilon_2}^p$  then sphere  $S_{\varepsilon_2}(\mathbf{x})$  will contain fluid molecules and hence  $\rho_{\varepsilon_2}^f(\mathbf{x}) > 0$  and thus  $\mathbf{x} \in \mathcal{R}_{\varepsilon_2}^f$ . In particular, fields  $\rho_{\varepsilon_2}^f$  and  $\mathbf{v}_{\varepsilon_2}^f$  are defined *everywhere* in  $\mathcal{R}_{\varepsilon_2}^p$  (which includes all points within the porous body region  $\mathcal{R}_{\varepsilon_1}^p$  delineated at scale  $\varepsilon_1$ ).

O.2. If

$$\mathcal{I}_{\varepsilon_1}^{pf} := \mathcal{R}_{\varepsilon_1}^p \cap \mathcal{R}_{\varepsilon_1}^f \tag{2.31}$$

and  $\mathbf{x} \in \mathcal{I}_{\varepsilon_1}^{pf}$  then sphere  $S_{\varepsilon_1}(\mathbf{x})$  will contain both porous body *and* fluid molecules. Accordingly if no fluid molecules are to be found within the geometric region  $(\mathcal{R}_{\varepsilon_1}^p)^g$  occupied by ‘p’ molecules at scale  $\varepsilon_1$ , (see (2.22)) then

$$\mathcal{I}_{\varepsilon_1}^{pf} = \{\mathbf{x} : d(\mathbf{x}, \partial(\mathcal{R}_{\varepsilon_1}^p)^g) \leq \varepsilon_1\}. \tag{2.32}$$

Said differently, the *interfacial region*  $\mathcal{I}_{\varepsilon_1}^{pf}$  at scale  $\varepsilon_1$  is the region which consists of all points distant no greater than  $\varepsilon_1$  from the porous body geometric boundary at scale  $\varepsilon_1$ . However, in view of (2.29) the volume of this

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<sup>5)</sup>Of course, these regions are in general time-dependent: such dependence has been suppressed for brevity.

interfacial region will be very small compared with that of the pore space. Thus the fluid and porous body fields are (see (2.31)) defined in essentially distinct regions.

O.3.  $\mathbf{v}_{\varepsilon_1}^f$  values describe the meandering motion of fluid through the pores, while  $\mathbf{v}_{\varepsilon_2}^f$  values correspond to a larger scale average motion associated with an overall drift/creep/seepage of fluid through the porous body. In Chapter 4 these two motions will be related in detail.



### 3. Linear momentum balance

#### 3.1. Linear Momentum Balance for $\mathcal{M}$

The motion of a particle  $P_i$  in any material system  $\mathcal{M}$  is assumed to be governed, in an inertial frame, by

$$\sum_{j \neq i} \mathbf{f}_{ij} + \mathbf{b}_i = \frac{d}{dt} \{m_i \mathbf{v}_i\}. \tag{3.1}$$

Here  $\mathbf{f}_{ij}$  denotes the force exerted on  $P_i$  by  $P_j$  and the sum is taken over all particles except  $P_i$ ;  $\mathbf{b}_i$  represents the resultant force on  $P_i$  from the material universe outwith  $\mathcal{M}$ . Clearly (3.1) yields, on summing over *all* particles and multiplying throughout by  $w(\mathbf{x}_i - \mathbf{x})$ ,

$$\begin{aligned} \sum_i \sum_{j \neq i} \mathbf{f}_{ij} w(\mathbf{x}_i - \mathbf{x}) + \sum_i \mathbf{b}_i w(\mathbf{x}_i - \mathbf{x}) &= \sum_i \frac{d}{dt} \{m_i \mathbf{v}_i\} w(\mathbf{x}_i - \mathbf{x}) \\ &= \frac{\partial}{\partial t} \left\{ \sum_i m_i \mathbf{v}_i w(\mathbf{x}_i - \mathbf{x}) \right\} - \sum_i m_i \mathbf{v}_i (\nabla w \cdot \mathbf{v}_i). \end{aligned} \tag{3.2}$$

Here  $\mathbf{x}$  denotes an arbitrary point and the ‘ $i$ ’ sum is over all particles. Thus<sup>6)</sup>

$$\mathbf{f}_w + \mathbf{b}_w = \frac{\partial}{\partial t} \{ \rho_w \mathbf{v}_w \} + \text{div } \mathbf{D}_w, \tag{3.3}$$

where

$$\mathbf{f}_w(\mathbf{x}, t) := \sum_i \sum_{j \neq i} \mathbf{f}_{ij}(t) w(\mathbf{x}_i(t) - \mathbf{x}), \tag{3.4}$$

$$\mathbf{b}_w(\mathbf{x}, t) := \sum_i \mathbf{b}_i(t) w(\mathbf{x}_i(t) - \mathbf{x}), \tag{3.5}$$

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<sup>6)</sup>In deriving term  $\text{div } \mathbf{D}_w$  it has been noted that  $m_i \mathbf{v}_i (\nabla w \cdot \mathbf{v}_i) = (m_i \mathbf{v}_i \otimes \mathbf{v}_i) \nabla w$  and  $m_i \mathbf{v}_i \otimes \mathbf{v}_i$  is independent of spatial variable  $\mathbf{x}$ . Thus  $\text{div} (m_i (\mathbf{v}_i \otimes \mathbf{v}_i) w) = m_i (\mathbf{v}_i \otimes \mathbf{v}_i) \nabla w$ .

and

$$\mathbf{D}_w(\mathbf{x}, t) := \sum_i m_i \mathbf{v}_i(t) \otimes \mathbf{v}_i(t) w(\mathbf{x}_i(t) - \mathbf{x}). \quad (3.6)$$

Fields  $\mathbf{f}_w$  and  $\mathbf{b}_w$  are termed densities of **interaction force** and **external body force**, respectively.

*Remark 3.1.* The sum in the definition of  $\mathbf{f}_w$  may be written, on suppressing time dependence and noting that, for choice of suitably-small  $h$  in (2.15)  $w$  is essentially given by (2.12), as

$$\sum_i \sum_{j \neq i} \mathbf{f}_{ij} w(\mathbf{x}_i - \mathbf{x}) = \sum_{\substack{P_i \text{ in} \\ S_\varepsilon(\mathbf{x})}} \left\{ \sum_{\substack{P_j \text{ in} \\ S_\varepsilon(\mathbf{x}), j \neq i}} \mathbf{f}_{ij} + \sum_{\substack{P_j \text{ outside} \\ S_\varepsilon(\mathbf{x})}} \mathbf{f}_{ij} \right\} V_\varepsilon^{-1}.$$

Now

$$\sum_{\substack{P_i, P_j \text{ in} \\ S_\varepsilon(\mathbf{x}) \\ j \neq i}} \mathbf{f}_{ij} = \frac{1}{2} \left\{ \sum_{\substack{P_i, P_j \text{ in} \\ S_\varepsilon(\mathbf{x}) \\ j \neq i}} (\mathbf{f}_{ij} + \mathbf{f}_{ji}) \right\} = \mathbf{0}$$

if we make the assumption

$$\mathbf{f}_{ij} + \mathbf{f}_{ji} = \mathbf{0}. \quad (3.7)$$

It follows that *force density*  $\mathbf{f}_w(\mathbf{x})$  is the resultant force exerted by particles outside  $S_\varepsilon(\mathbf{x})$  upon particles inside  $S_\varepsilon(\mathbf{x})$ , divided by the volume of  $S_\varepsilon(\mathbf{x})$ .

Defining the **notional**<sup>7)</sup> **thermal velocity** of  $P_i$  at  $\mathbf{x}$  (which depends upon the choice of  $w$ ) by

$$\hat{\mathbf{v}}_i(\mathbf{x}, t) := \mathbf{v}_i(t) - \mathbf{v}_w(\mathbf{x}, t) \quad (3.8)$$

we have, using (2.1), (2.2) and (2.4),

$$\sum_i m_i \hat{\mathbf{v}}_i(\mathbf{x}, t) w(\mathbf{x}_i(t) - \mathbf{x}) = \mathbf{p}_w(\mathbf{x}, t) - \rho_w(\mathbf{x}, t) \mathbf{v}_w(\mathbf{x}, t) = \mathbf{0}. \quad (3.9)$$

Accordingly, from (3.6), (3.8), (3.9) and (2.1),

$$\mathbf{D}_w = \mathcal{D}_w + \mathbf{0} \otimes \mathbf{v}_w + \mathbf{v}_w \otimes \mathbf{0} + \rho_w \mathbf{v}_w \otimes \mathbf{v}_w, \quad (3.10)$$

<sup>7)</sup>The notional thermal velocity  $\hat{\mathbf{v}}_i(\mathbf{x}, t)$  of a molecule at  $\mathbf{x}$  (at time  $t$ ) approximates its actual thermal velocity  $\tilde{\mathbf{v}}_i(t) := \mathbf{v}_i(t) - \mathbf{v}_w(\mathbf{x}_i(t))$ .

where the **notional thermal stress tensor** field  $\mathcal{D}_w$  takes values given by

$$\mathcal{D}_w(\mathbf{x}, t) := \sum_i m_i \hat{\mathbf{v}}_i(\mathbf{x}, t) \otimes \hat{\mathbf{v}}_i(\mathbf{x}, t) w(\mathbf{x}_i(t) - \mathbf{x}). \tag{3.11}$$

Hence (3.3) may be expressed in the form<sup>8)</sup>

$$-\operatorname{div} \mathcal{D}_w + \mathbf{f}_w + \mathbf{b}_w = \frac{\partial}{\partial t} \{ \rho_w \mathbf{v}_w \} + \operatorname{div} \{ \rho_w \mathbf{v}_w \otimes \mathbf{v}_w \} \tag{3.12}$$

$$= \rho_w \left[ \frac{\partial \mathbf{v}_w}{\partial t} + (\nabla \mathbf{v}_w) \mathbf{v}_w \right], \tag{3.13}$$

on invoking (2.10). Thus, defining the ( $w$ -dependent) acceleration field  $\mathbf{a}_w$  by

$$\mathbf{a}_w := \dot{\mathbf{v}}_w := \frac{\partial \mathbf{v}_w}{\partial t} + (\nabla \mathbf{v}_w) \mathbf{v}_w, \tag{3.14}$$

linear momentum balance has been established in the form

$$-\operatorname{div} \mathcal{D}_w + \mathbf{f}_w + \mathbf{b}_w = \rho_w \mathbf{a}_w. \tag{3.15}$$

Modulo a certain property of interactions, delineated below,  $\mathbf{f}_w$  may be expressed as the divergence of a tensor-valued field  $\mathbf{T}_w^-$  as follows. As a consequence of (2.3),

$$\int_{\mathcal{E}} w(\mathbf{y} - \mathbf{x}_0) d\mathbf{y} = 1 \tag{3.16}$$

for any given point  $\mathbf{x}_0$ . Accordingly we may write

$$\mathbf{f}_w(\mathbf{x}, t) = \int_{\mathcal{E}} \mathbf{g}(\mathbf{x}, \mathbf{y}, t) d\mathbf{y}, \tag{3.17}$$

where

$$\mathbf{g}(\mathbf{x}, \mathbf{y}, t) := \sum_i \sum_{j \neq i} \mathbf{f}_{ij}(t) w(\mathbf{x}_i(t) - \mathbf{x}) w(\mathbf{x}_j(t) - \mathbf{y}). \tag{3.18}$$

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<sup>8)</sup>Use is here made of the results

$$\operatorname{div}(\rho \mathbf{v} \otimes \mathbf{v}) \equiv \rho \operatorname{div}(\mathbf{v} \otimes \mathbf{v}) + (\mathbf{v} \otimes \mathbf{v}) \nabla \rho \equiv \rho \{ (\operatorname{div} \mathbf{v}) \mathbf{v} + (\nabla \mathbf{v}) \mathbf{v} \} + (\mathbf{v} \cdot \nabla \rho) \mathbf{v}.$$

On suppressing time-dependence for brevity, and assuming (3.7) holds for all  $i, j$ , we have

$$\begin{aligned} \mathbf{g}(\mathbf{y}, \mathbf{x}) &= \sum_{\substack{i \\ i \neq j}} \sum_j \mathbf{f}_{ij} w(\mathbf{x}_i - \mathbf{y}) w(\mathbf{x}_j - \mathbf{x}) \\ &= \sum_{\substack{i \\ j \neq i}} \sum_j \mathbf{f}_{ji} w(\mathbf{x}_j - \mathbf{y}) w(\mathbf{x}_i - \mathbf{x}) \\ &= - \sum_{\substack{j \\ j \neq i}} \sum_i \mathbf{f}_{ij} w(\mathbf{x}_j - \mathbf{y}) w(\mathbf{x}_i - \mathbf{x}) = -\mathbf{g}(\mathbf{x}, \mathbf{y}). \end{aligned}$$

The second equality is merely a re-labelling of indices and the third inequality follows from (3.7). Thus

$$\mathbf{g}(\mathbf{y}, \mathbf{x}) = -\mathbf{g}(\mathbf{x}, \mathbf{y}). \quad (3.19)$$

Provided that, for some positive number  $\delta$ ,  $\mathbf{g}(\mathbf{x}, \mathbf{y}) |\mathbf{x}|^{3+\delta} |\mathbf{y}|^{3+\delta}$  remains bounded for all  $\mathbf{x}$  and  $\mathbf{y}$ , and the same property holds for first derivatives of  $\mathbf{g}$ , then a theorem due to Walter Noll (see Noll [5]) furnishes the *existence* of a tensor field  $\mathbf{T}_w^-$  (the **interaction stress tensor field**) for which<sup>9)</sup>

$$\mathbf{f}_w = \operatorname{div} \mathbf{T}_w^-. \quad (3.20)$$

Further, this theorem furnishes the explicit form

$$\mathbf{T}_w^-(\mathbf{x}) := -\frac{1}{2} \int_{\mathcal{V}} \int_0^1 \mathbf{g}(\mathbf{x} + \alpha \mathbf{u}, \mathbf{x} - (1 - \alpha) \mathbf{u}) \otimes \mathbf{u} \, d\alpha \, d\mathbf{u}, \quad (3.21)$$

<sup>9)</sup>If  $\mathbf{A}$  denotes a field whose values are linear transformations and  $\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3$  denotes an orthonormal basis, then  $\operatorname{div} \mathbf{A}$  is that vector field for which

$$(\operatorname{div} \mathbf{A}) \cdot \mathbf{e}_i = \sum_{j=1}^3 A_{ij,j} \quad \text{where } A_{ij} := \mathbf{e}_i \cdot \mathbf{A} \mathbf{e}_j.$$

whence

$$\mathbf{T}_w^-(\mathbf{x}) = -\frac{1}{2} \int_V \int_0^1 \sum_{i \neq j} \mathbf{f}_{ij} \otimes \mathbf{u} w(\mathbf{x}_i - \mathbf{x} - \alpha \mathbf{u}) w(\mathbf{x}_j - \mathbf{x} + (1 - \alpha)\mathbf{u}) d\alpha du. \quad (3.22)$$

$$= -\frac{1}{2} \sum_{i \neq j} \mathbf{f}_{ij} \otimes \int_V \int_0^1 \mathbf{u} w(\mathbf{x}_i - \mathbf{x} - \alpha \mathbf{u}) w(\mathbf{x}_j - \mathbf{x} + (1 - \alpha)\mathbf{u}) d\alpha du. \quad (3.23)$$

From (3.15) and (3.20) linear momentum balance is expressible as

$$\operatorname{div} \mathbf{T}_w + \mathbf{b}_w = \rho_w \mathbf{a}_w, \quad (3.24)$$

where the (Cauchy) stress tensor field (cf. (3.11) and (3.23))

$$\mathbf{T}_w := \mathbf{T}_w^- - \mathcal{D}_w. \quad (3.25)$$

*Remark 3.2.* The conditions upon  $\mathbf{g}$  sufficient to obtain (3.20) are not restrictive. Indeed, it suffices that the derivative of  $w$  be bounded (although mollification involves large values of this derivative, such *are* bounded) and that interactions be governed by pairwise potentials which are bounded below (in such case any single interaction will be bounded by a particle-independent bound governed by the total energy of the system).

*Remark 3.3.* Integrating balance (3.24) over a region  $\mathcal{R}$  with outward unit normal  $\mathbf{n}$  on its boundary  $\partial R$  yields, upon invoking the divergence theorem,

$$\int_{\partial R} \mathbf{T}_w \mathbf{n} + \int_R \mathbf{b}_w = \int_R \rho_w \mathbf{a}_w = \frac{d}{dt} \left\{ \int_{R_t} \rho_w \mathbf{v}_w \right\}, \quad (3.26)$$

where  $\mathcal{R}_t$  denotes that deforming region which coincides with  $\mathcal{R}$  at instant  $t$  and whose boundary points move with the motion  $\chi_w^0$  related to  $\mathbf{v}_w$  by (2.24). Equation (3.26) is the form of balance which is *postulated* to hold for arbitrary regions in standard developments of Continuum Mechanics, with integrand  $\mathbf{T}_w \mathbf{n}$  replaced by the so-called **traction** field  $\mathbf{t}$ . Field  $\mathbf{t}$  is interpreted as delivering the force per unit area exerted by material of the body in question which lies *outside*  $\mathcal{R}$  upon material of the body *inside*  $\mathcal{R}$ . If  $\mathbf{t}$  depends continuously upon position and  $\mathbf{n}$  then the arbitrary nature of  $\mathcal{R}$  enables the *existence* of a tensor field  $\mathbf{T}$  to be shown for which

$$\mathbf{T} \mathbf{n} = \mathbf{t}. \quad (3.27)$$

Consequently (3.26) holds and then (3.24) is *deduced*.

The molecular viewpoint together with weighting function methodology led directly to (3.24) with two significant physical insights missing from the purely continuum approach:

- (i) *fields are manifestly scale-dependent, and*
- (ii) *there are two contributions to  $\mathbf{T}_w$ , one associated with molecular interactions ( $\mathbf{T}_w^-$ ) and the other with thermal motions ( $-\mathcal{D}_w$ ).*

In this context it should be noted that in a moderately-rarefied gas molecular interactions occur only intermittently (via binary 'collisions') and  $\mathbf{T}_w^-$  is negligible. In such case

$$\mathbf{T}_w = -\mathcal{D}_w \quad (3.28)$$

and the interpretation of  $\mathbf{T}_w \mathbf{n}$  as a traction is incorrect.

*Exercise 3.1.* Show that  $-\mathcal{D}_w$  is 'pressure-like' in that

$$\mathcal{D}_w \mathbf{n} \cdot \mathbf{n} > 0 \quad (3.29)$$

for all unit vectors  $\mathbf{n}$ . If

$$\mathcal{D}_w = P\mathbf{1} \quad (3.30)$$

and the velocity field vanishes (that is,  $\mathbf{v}_w = \mathbf{0}$ ) show, by taking the trace of relation (3.30), that

$$P(\mathbf{x})V_\epsilon = \frac{2}{3} \times \{\text{kinetic energy of molecules in } S_\epsilon(\mathbf{x})\}. \quad (3.31)$$

### 3.2. Linear momentum balance for fluid in a porous body

#### 3.2.1. The general form of balance

Recall (see Remark 2.7) that  $\mathcal{M}^f$  and  $\mathcal{M}^p$  denote the material systems consisting of fluid molecules and porous body molecules, respectively. Now consider balance (3.24) for system  $\mathcal{M}^f$ . In such case term  $\mathbf{b}_w$  represents the effect upon fluid molecules which derives from non-fluid molecules (see (3.5)). There are accordingly contributions from terrestrial gravitation and from interactions with porous body molecules. Specifically,

$$\mathbf{b}_i(t) = \sum_{P_\alpha \in \mathcal{M}^p} \mathbf{F}_{i\alpha}(t) + m_i \mathbf{g}, \quad (3.32)$$

where the sum is taken over all porous body molecules  $P_\alpha$ ,  $\mathbf{F}_{i\alpha}$  denotes the force on  $P_i \in \mathcal{M}^f$  due to  $P_\alpha \in \mathcal{M}^p$ , and  $\mathbf{g}$  represents the acceleration due to gravity. It follows from (3.5) that<sup>10)</sup>

$$\mathbf{b}_w^f = \mathbf{F}_w^{fp} + \rho_w^f \mathbf{g}, \tag{3.33}$$

where

$$\mathbf{F}_w^{fp}(\mathbf{x}, t) := \sum_{P_\alpha \in \mathcal{M}^p} \sum_{P_i \in \mathcal{M}^f} \mathbf{F}_{i\alpha}(t) w(\mathbf{x}_i(t) - \mathbf{x}). \tag{3.34}$$

Thus  $\mathbf{F}_w^{fp}$  is the body force density associated with the effect upon fluid of the porous body. Specifically,  $\mathbf{F}_w^{fp}(\mathbf{x}, t)$  denotes the resultant force (at instant  $t$ ) exerted by all porous body molecules upon fluid molecules within  $\mathcal{S}_\varepsilon(\mathbf{x})$ , divided by  $V_\varepsilon$ . Of course,  $\rho_w^f$  denotes the fluid mass density.

Balance (3.24) may be re-written, using (3.14) and (3.33), in the form

$$\operatorname{div} \mathbf{T}_w^f + \mathbf{F}_w^{fp} + \rho_w^f \mathbf{g} = \rho_w^f \left\{ \frac{\partial \mathbf{v}_w^f}{\partial t} + (\nabla \mathbf{v}_w^f) \mathbf{v}_w^f \right\}. \tag{3.35}$$

*Remark 3.4.* The physical interpretations of the fields which appear in (3.35) depend crucially upon the spatial scale  $\varepsilon$  associated with the weighting function  $w$ . This is because these fields are only defined, at instant  $t$ , in region  $\mathcal{R}_w^f(t)$ : see (2.18) with  $\rho_w = \rho_w^f$ . With choice  $w = w_\varepsilon$  the appropriate region is  $\mathcal{R}_\varepsilon^f(t)$ : see (2.19) with  $\mathbf{x}_i(t)$  the instantaneous location of a fluid molecule. As discussed in Remark 2.5, choices  $\varepsilon = \varepsilon_1$  and  $\varepsilon = \varepsilon_2$  yield very different regions: the former yields the pore space in which fluid is to be found, while the latter yields that region all points of which lie within  $\varepsilon_2$  of a fluid molecule and hence (since  $\varepsilon_2$  is much greater than typical pore size and structural dimension of the porous body) includes points within the region  $\mathcal{R}_{\varepsilon_1}^p(t)$ : see (2.19) with  $\mathbf{x}_i(t)$  the location of a porous body molecule. In the following two subsections the interpretations of fields at each of the scales  $\varepsilon_1$  and  $\varepsilon_2$  are discussed. Chapter 4 will link these two continuum descriptions in the context of incompressible liquid saturating a rigid porous body.

### 3.2.2. Linear momentum balance at scale $\varepsilon = \varepsilon_1$

Molecular interactions are short-range. Indeed, such interactions are considered to be very long range if they extend to  $100 = 10^{-8}$  m. If  $\varepsilon_1 > 100$

<sup>10)</sup>Superscript ‘f’ has been added to label all fluid-related fields.

then the effect of porous body molecules upon fluid molecules will be confined to those between such molecules which lie within the interfacial region  $\mathcal{I}_{\varepsilon_1}^{pf}$  (see (2.31)). Thus the form of (3.35) with  $w = w_{\varepsilon_1}$  appropriate to the region

$$-\mathcal{R}_{\varepsilon_1}^f := \mathcal{R}_{\varepsilon_1}^f - \mathcal{I}_{\varepsilon_1}^{pf} \quad (3.36)$$

has  $\mathbf{F}_w^{fp} = \mathbf{0}$ . Accordingly, *in this region* (3.35) is a balance of linear momentum for fluid *only*. The form of  $\mathbf{T}_w^f$  (which will now be denoted by  $\mathbf{T}_{\varepsilon_1}^f$  to emphasise the associated scale) depends upon whether the fluid is in a gaseous or liquid phase. For a moderately rarefied gaseous phase  $\mathbf{T}_{\varepsilon_1}^f$  will be a density-dependent pressure: see (3.28) and (3.30). That is,

$$\mathbf{T}_{\varepsilon_1}^f = -P(\rho_{\varepsilon_1}^f)\mathbf{1}. \quad (3.37)$$

For incompressible Newtonian liquid phases,  $\rho_{\varepsilon_1}^f$  is constant and

$$\mathbf{T}_{\varepsilon_1}^f = -P\mathbf{1} + \mu(\nabla\mathbf{v}_{\varepsilon_1}^f + (\nabla\mathbf{v}_{\varepsilon_1}^f)^T), \quad (3.38)$$

where  $P$  denotes pressure and  $\mu$  is the viscosity. Relation (3.35) in this case is accordingly the Navier-Stokes equation

$$-\nabla P + \mu\Delta\mathbf{v}_{\varepsilon_1}^f + \rho_{\varepsilon_1}^f\mathbf{g} = \rho_{\varepsilon_1}^f \left\{ \frac{\partial\mathbf{v}_{\varepsilon_1}^f}{\partial t} + (\nabla\mathbf{v}_{\varepsilon_1}^f)\mathbf{v}_{\varepsilon_1}^f \right\}. \quad (3.39)$$

*Remark 3.5.* In many important situations a fluid is to be found in both gaseous and liquid phases within a porous body. Of course, where such phases co-exist there are interfaces in which surface tension is to be found. The situation is further complicated by the possibility of net evaporation or condensation at such interfaces. The modelling of the behaviour of such systems (and of mixtures of different liquids and fluids in pores) at scale  $\varepsilon_2$  will be discussed in Chapter 6.

*Remark 3.6.* The behaviour of fluid in  $\mathcal{I}_{\varepsilon_1}^{pf}$  will not be discussed here. In Chapter 4 the *effect* of the porous body upon fluid flow (which we have seen derives entirely from  $\mathcal{I}_{\varepsilon_1}^{pf}$  interactions) will be modelled via the standard non-slip and non-penetration conditions of fluid dynamics, and behaviour within  $\mathcal{I}_{\varepsilon_1}^{pf}$  will be neglected. More particularly, in Chapter 4 the  $\varepsilon_1$ -scale behaviour of an incompressible Newtonian fluid will be modelled by relation (3.39). This relation will be assumed to hold<sup>11)</sup> in  $\mathcal{R}_{\varepsilon_1}^f - (\mathcal{R}_{\varepsilon_1}^p)^g$  and subject to the non-slip, non-penetration, boundary condition

$$\mathbf{v}_{\varepsilon_1}^f = \mathbf{0} \quad \text{on} \quad \partial(\mathcal{R}_{\varepsilon_1}^p)^g. \quad (3.40)$$

<sup>11)</sup> $(\mathcal{R}_{\varepsilon_1}^p)^g$  denotes the geometric region associated with the porous body at scale  $\varepsilon_1$ .



3.2.3. *Linear momentum balance at scale  $\varepsilon = \varepsilon_2$*

To emphasise scale-dependence we re-write (3.35) as

$$\operatorname{div} \mathbf{T}_{\varepsilon_2}^f + \mathbf{F}_{\varepsilon_2}^{fp} + \rho_{\varepsilon_2}^f \mathbf{g} = \rho_{\varepsilon_2}^f \left\{ \frac{\partial \mathbf{v}_{\varepsilon_2}^f}{\partial t} + (\nabla_{\mathbf{v}_{\varepsilon_2}^f}) \mathbf{v}_{\varepsilon_2}^f \right\}. \tag{3.41}$$

The stress tensor (see 3.25)

$$\mathbf{T}_{\varepsilon_2}^f = (\mathbf{T}_{\varepsilon_2}^f)^- - \mathcal{D}_{\varepsilon_2}^f \tag{3.42}$$

where (see (3.20))

$$\operatorname{div}(\mathbf{T}_{\varepsilon_2}^f)^- = \mathbf{f}_{\varepsilon_2}^f. \tag{3.43}$$

Recalling Remark 3.1,  $\mathbf{f}_{\varepsilon_2}^f(\mathbf{x}, t)$  denotes the force exerted (at instant  $t$ ) upon fluid molecules within  $S_{\varepsilon_2}(\mathbf{x})$  by fluid molecules outside  $S_{\varepsilon_2}(\mathbf{x})$  divided by  $V_{\varepsilon_2}$ . (See Figure 5).

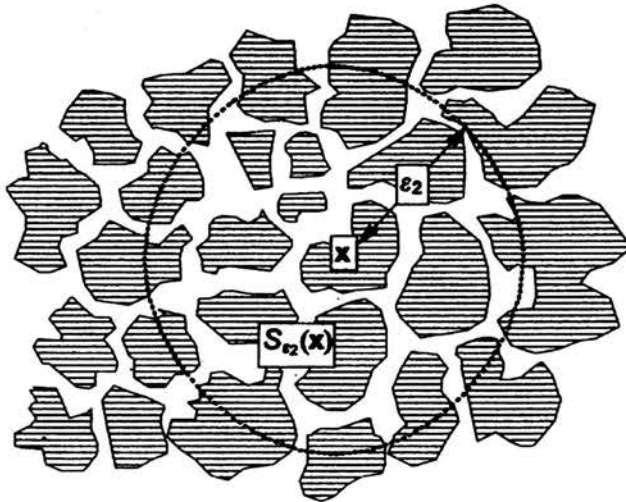


Figure 5: The shaded region represents the region  $\mathcal{R}_{\varepsilon_1}^p$  occupied by the porous body at scale  $\varepsilon_1$  and the dotted curve denotes the boundary of sphere  $S_{\varepsilon_2}(\mathbf{x})$ . Force density  $\mathbf{f}_{\varepsilon_2}(\mathbf{x}, t)$  is the force exerted by fluid in the unshaded region *outside*  $S_{\varepsilon_2}(\mathbf{x})$  upon fluid in the unshaded region *within*  $S_{\varepsilon_2}(\mathbf{x})$ , divided by the volume of  $S_{\varepsilon_2}(\mathbf{x})$ .

The definition of  $\mathcal{D}_{\varepsilon_2}^f(\mathbf{x}, t)$  differs from its  $\varepsilon_1$ -scale counterpart in two respects. Firstly, the weighting of contributions in its definition (see (3.11)) is  $V_{\varepsilon_2}^{-1}$  and fluid molecules are only to be found within pore space within

$\mathcal{S}_{\varepsilon_2}(\mathbf{x})$ . Secondly, the notional thermal velocity (see (3.8)) is computed with respect to  $\mathbf{v}_w^f = \mathbf{v}_{\varepsilon_2}^f$  rather than  $\mathbf{v}_w^f = \mathbf{v}_{\varepsilon_1}^f$ . For creeping flow such distinction is not significant since molecular speeds are of order  $10^3 \text{ ms}^{-1}$  at room temperature and the overwhelmingly dominant contribution to  $\mathcal{D}_w^f$  stems from individual molecular velocities. (Said differently, neglect of  $\mathbf{v}_{\varepsilon_2}^f$  and  $\mathbf{v}_{\varepsilon_1}^f$  in the appropriate forms of (3.11) will affect values of  $\mathcal{D}_{\varepsilon_2}^f$  and  $\mathcal{D}_{\varepsilon_1}^f$  negligibly, in general.)

Term  $\mathbf{F}_{\varepsilon_2}^{fp}(\mathbf{x}, t)$  represents the effect of porous body molecules upon fluid molecules within  $\mathcal{S}_{\varepsilon_2}(\mathbf{x})$ . In view of the short-range nature of molecular interactions this effect is localised at the boundaries of pores occupied by fluid within  $\mathcal{S}_{\varepsilon_2}(\mathbf{x})$ . As can be visualised from Figure 5, such effect will represent the resistance to the passage of fluid through the porous body. This resistance stems from two sources:

- (i) the porous body boundary forms an obstacle which constrains the fluid flow as a consequence of being unable to penetrate this boundary, and
- (ii) the porous body boundary exerts a 'drag' on fluid moving over it.

As will be seen in Chapter 4, source (i) takes the form of a 'back-pressure' exerted by pore boundaries within  $\mathcal{S}_{\varepsilon_2}(\mathbf{x})$  (this is the 'reaction' to the pressure exerted by the fluid on such boundaries) while the effect of (ii) is proportional to viscosity.

#### 4. Flow of an incompressible, linearly-viscous, fluid through a porous body it saturates

At scale  $\varepsilon_1$  pore details are manifest, yet continuum modelling is sensible since  $\varepsilon_1$  is much greater than the scale at which individual molecular behaviour is apparent or significant. Accordingly, the flow through a rigid porous body of an incompressible linearly-viscous fluid is adequately modelled by the Navier-Stokes equations

$$-\nabla P + \mu \Delta \mathbf{v} + \rho_0 \mathbf{g} = \frac{\partial}{\partial t} \{\rho_0 \mathbf{v}\} + \operatorname{div}\{\rho_0 \mathbf{v} \otimes \mathbf{v}\}, \quad (4.1)$$

where

$$\operatorname{div} \mathbf{v} = 0. \quad (4.2)$$

Here  $P$  denotes the pressure,  $\mu$  viscosity,  $\mathbf{v}$  the ( $\varepsilon_1$ -scale) velocity,  $\rho_0$  the (constant) mass density, and  $\mathbf{g}$  the acceleration due to gravity. Of course, (4.2) is the consequence of mass conservation and incompressibility.

Equations (4.1) and (4.2) hold in the (fixed) region  $R$  consisting of all pore space and immediate vicinity of the porous body. These equations are supplemented by the boundary condition

$$\mathbf{v} = \mathbf{0} \quad \text{on} \quad \partial R, \quad (4.3)$$

which expresses the non-slip and non-penetration of fluid at pore 'walls'.

*Question:* How can we average relation (4.1) at a scale large compared with pore size and porous body structural dimension? Here we are trying to average *fields* rather than discrete molecular quantities.

*Answer:* Use weighting functions! To do so we define, for a given field  $f$  and weighting function  $w$ , the  $w$ -average  $\langle f \rangle_w$  of  $f$  by

$$\langle f \rangle_w(\mathbf{x}) := \int_{\varepsilon} f(\mathbf{y}) w(\mathbf{y} - \mathbf{x}) d\mathbf{y}. \quad (4.4)$$

Here  $\mathcal{E}$  denotes Euclidean space and  $\mathbf{y}$  a typical point in  $\mathcal{E}$ . To ensure that  $\langle f \rangle_w$  has the same physical dimensions as  $f$  it is necessary for the values of  $w$  to have dimension  $L^{-3}$ . Further, so that the average of any constant-valued function should yield this same function, it is necessary and sufficient that normalisation condition (2.3) should hold.

*Remark 4.1* To see the link between (4.4) and our previous weighted sums, consider the microscopic density distribution (on suppressing time-dependence)

$$\rho_{\text{mic}}(\mathbf{x}) := \sum_i m_i \delta(\mathbf{x}_i - \mathbf{x}), \quad (4.5)$$

where ‘ $\delta$ ’ denotes the Dirac delta distribution. Formal integration of (4.5) yields (see (2.1))

$$\begin{aligned} \langle \rho_{\text{mic}} \rangle_w(\mathbf{x}) &:= \int_{\mathcal{E}} \rho_{\text{mic}}(\mathbf{y}) w(\mathbf{y} - \mathbf{x}) d\mathbf{y} \\ &= \sum_i^N m_i \int_{\mathcal{E}} \delta(\mathbf{x}_i - \mathbf{y}) w(\mathbf{y} - \mathbf{x}) d\mathbf{y} \\ &= \sum_i^N m_i w(\mathbf{x}_i - \mathbf{x}) = \rho_w(\mathbf{x}). \end{aligned} \quad (4.6)$$

*Remark 4.2.* To obtain the averaged form of (4.1), each term is evaluated at  $\mathbf{y}$ , multiplied by  $w(\mathbf{y} - \mathbf{x})$ , and integrated over  $\mathcal{E}$ . However, the fields in (4.1) are defined only in the pore space and immediate vicinity of the body, denoted by  $R$ . In evaluating integrals over  $\mathcal{E}$ , these fields are considered to vanish outside  $R$ . The averaging of (4.1) requires that  $\langle \nabla P \rangle_w$ ,  $\langle \Delta \mathbf{v} \rangle_w$ ,  $\langle \rho_0 \mathbf{g} \rangle_w$ ,  $\langle \frac{\partial}{\partial t} \{ \rho_0 \mathbf{v} \} \rangle_w$  and  $\langle \text{div} \{ \rho_0 \mathbf{v} \otimes \mathbf{v} \} \rangle_w$  be computed.

*Remark 4.3.* To see that we should be clear *a priori* about the choice of  $w$ , consider the  $w$ -average of the gradient of a scalar field  $\phi$  defined on  $R$ . We

have

$$\begin{aligned}
 \langle \nabla \phi \rangle_w(\mathbf{x}) &:= \int_{\mathcal{E}} \nabla \phi(\mathbf{y}) w(\mathbf{y} - \mathbf{x}) d\mathbf{y} \\
 &= \int_R \nabla \phi(\mathbf{y}) w(\mathbf{y} - \mathbf{x}) d\mathbf{y} = \int_R \nabla_{\mathbf{y}}(\phi w) - \phi \nabla_{\mathbf{y}} w \, d\mathbf{y} \\
 &= \int_R \operatorname{div}\{\phi w \mathbf{1}\} + \phi \nabla_{\mathbf{x}} w \, d\mathbf{y} \\
 &= \int_{\partial R} \phi w \mathbf{n} \, dA + \nabla_{\mathbf{x}} \int_R \phi(\mathbf{y}) w(\mathbf{y} - \mathbf{x}) d\mathbf{y}.
 \end{aligned}$$

That is,

$$\langle \nabla \phi \rangle_w(\mathbf{x}) = \int_{\partial R} \phi(\mathbf{y}) w(\mathbf{y} - \mathbf{x}) \mathbf{n}(\mathbf{y}) dA_{\mathbf{y}} + \nabla\{\langle \phi \rangle_w\}(\mathbf{x}). \tag{4.7}$$

Hence the difference between the average of a gradient and the gradient of an average is the integral of  $\phi w \mathbf{n}$  over the pore boundary  $\partial R$  with outward unit normal  $\mathbf{n}$  to  $R$ . (Notice  $\mathbf{n}$  is directed *into* the porous body.) Clearly this difference only derives from points  $\mathbf{y}$  on  $\partial R$  for which  $w(\mathbf{y} - \mathbf{x}) \neq 0$ . For example, if  $w$  is given by (2.12) then only points on  $\partial R$  which lie within a distance of  $\varepsilon$  from  $\mathbf{x}$  contribute to the integral term in (4.7).

Averages in the porous media literature are computed over so-called ‘representative elementary volumes’ (abbreviated to ‘REV’s). These are regions whose characteristic dimensions are large compared to pore and structure size. More precisely, an REV  $C(\mathbf{x})$  ‘centred at point  $\mathbf{x}$ ’ is defined by

$$C(\mathbf{x}) := \{\mathbf{x} + \mathbf{u} : \mathbf{u} \in \mathcal{U}\}. \tag{4.8}$$

Here  $\mathcal{U}$  is a fixed set of displacements which form a neighbourhood of  $\mathbf{0} \in \mathcal{V}$  (the space of all displacements between pairs of points in  $\mathcal{E}$ ) which contains all vectors  $\mathbf{u}$  with norm  $\|\mathbf{u}\| \leq \varepsilon_2$ . If  $V$  denotes the volume of  $C(\mathbf{x})$  (this is the same for all  $\mathbf{x}$ , of course... why?) then the choice of weighting function  $w$  is a mollified version of

$$\left. \begin{aligned}
 \hat{w}(\mathbf{u}) &:= V^{-1} \quad \text{if } \mathbf{u} \in \mathcal{U} \\
 \hat{w}(\mathbf{u}) &:= 0 \quad \text{if } \mathbf{u} \notin \mathcal{U}
 \end{aligned} \right\}. \tag{4.9}$$

As in Chapter 2, mollification is effected over a physically-insignificant region, so that the values of  $\int_{\mathcal{E}} f(\mathbf{y}) w(\mathbf{y} - \mathbf{x}) d\mathbf{y}$  and  $\int_{\mathcal{E}} f(\mathbf{y}) \hat{w}(\mathbf{y} - \mathbf{x}) d\mathbf{y}$  are physically-indistinguishable for the fields with which we deal. Mollification is necessary

in order that  $\nabla w$  should exist: notice  $\nabla \hat{w}$  fails to exist on the boundary of set  $\mathcal{U}$ . Returning to (4.7), we now note that

$$\int_{\partial R} \phi(\mathbf{y})w(\mathbf{y} - \mathbf{x})\mathbf{n}(\mathbf{y})dA_{\mathbf{y}} = \int_{S(\mathbf{x})} \phi(\mathbf{y})w(\mathbf{y} - \mathbf{x})\mathbf{n}(\mathbf{y})dA_{\mathbf{y}} \quad (4.10)$$

where

$$S(\mathbf{x}) := \partial R \cap \{\mathbf{y} : \mathbf{y} - \mathbf{x} \in \mathcal{U}\}. \quad (4.11)$$

Accordingly (4.7) becomes

$$\langle \nabla \phi \rangle_w(\mathbf{x}) = \nabla \{ \langle \phi \rangle_w \}(\mathbf{x}) + \int_{S(\mathbf{x})} \phi(\mathbf{y})w(\mathbf{y} - \mathbf{x})\mathbf{n}(\mathbf{y})dA_{\mathbf{y}}. \quad (4.12)$$

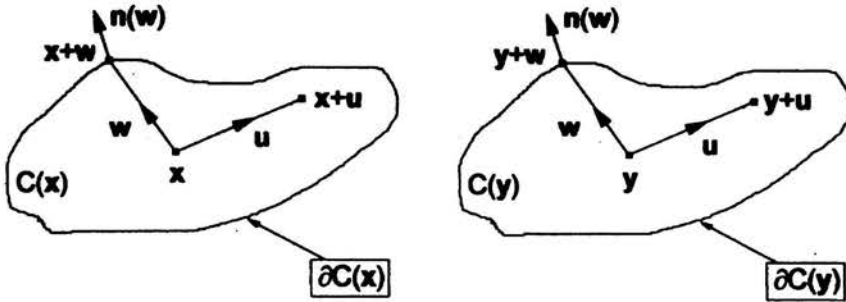


Figure 6: Elementary cells  $C(\mathbf{x})$  and  $C(\mathbf{y})$  centred at points  $\mathbf{x}$  and  $\mathbf{y}$  are depicted,  $\mathbf{u} \in \mathcal{U}$ ,  $\mathbf{w} \in \partial \mathcal{U}$ , and  $\mathbf{n}(\mathbf{w})$  denotes the unit normal at that point on the boundary of the cell which corresponds to  $\mathbf{w}$ .

With reference to the first term in (4.1), choice  $\phi = P$  in (4.12) yields (upon suppressing explicit  $w$ -dependence for simplicity)

$$\langle \nabla P \rangle(\mathbf{x}) = \nabla \{ \langle P \rangle \}(\mathbf{x}) + \int_{S(\mathbf{x})} P(\mathbf{y})\mathbf{n}(\mathbf{y})w(\mathbf{y} - \mathbf{x})dA_{\mathbf{y}}. \quad (4.13)$$

In abbreviated form this may be written as

$$\langle -\nabla P \rangle = -\nabla \{ \langle P \rangle \} - \left( \int_S P \mathbf{n} dA \right) / V \quad (4.14)$$

upon invoking (4.9) *et seq.* Recalling that  $\mathbf{n}$  is that unit normal field on  $\partial R$  which is directed *into* the porous body, the last term in (4.14) represents

an REV-volume averaged ‘back pressure’ exerted *on* the fluid *by* the porous body. This ‘back pressure’ is the reaction to the pressure exerted *on* the pore boundary *by* the fluid.

Further results necessary to effect averages of all terms in (4.1) are contained in

*Proposition 4.1.*

$$\langle \nabla \mathbf{u} \rangle = \nabla \{ \langle \mathbf{u} \rangle \} + \int_S w \mathbf{u} \otimes \mathbf{n} dA, \tag{4.15}$$

$$\langle \operatorname{div} \mathbf{u} \rangle = \{ \operatorname{div} \langle \mathbf{u} \rangle \} + \int_S \mathbf{u} \cdot \mathbf{n} w dA, \tag{4.16}$$

and

$$\langle \operatorname{div} \mathbf{B} \rangle = \operatorname{div} \{ \langle \mathbf{B} \rangle \} + \int_S \mathbf{B} \mathbf{n} w dA. \tag{4.17}$$

Here  $\mathbf{u}$  and  $\mathbf{B}$  are, respectively, vector and tensor-valued functions defined in the region occupied by the fluid which vanish elsewhere. Further,

$$\langle \partial \mathbf{u} / \partial t \rangle = \frac{\partial}{\partial t} \{ \langle \mathbf{u} \rangle \}. \tag{4.18}$$

*Proofs.*

$$\begin{aligned} \langle \nabla \mathbf{u} \rangle (\mathbf{x}) &:= \int_{\mathcal{E}} \nabla \mathbf{u}(\mathbf{y}) w(\mathbf{y} - \mathbf{x}) d\mathbf{y} \\ &= \int_R \nabla \mathbf{u}(\mathbf{y}) w(\mathbf{y} - \mathbf{x}) d\mathbf{y} = \int_R (\nabla_{\mathbf{y}} \{ w \mathbf{u} \} - \mathbf{u} \otimes \nabla_{\mathbf{y}} w) d\mathbf{y}. \end{aligned} \tag{4.19}$$

To simplify the first term in the last integral we note that, for any fixed vector  $\mathbf{k}$ ,

$$\begin{aligned} \left( \int_R \nabla \mathbf{u} \{ w \mathbf{u} \} d\mathbf{y} \right) \mathbf{k} &= \int_R (\nabla_{\mathbf{y}} \{ w \mathbf{u} \}) \mathbf{k} d\mathbf{y} \\ &= \int_R \operatorname{div}_{\mathbf{y}} \{ w \mathbf{u} \otimes \mathbf{k} \} d\mathbf{y} = \int_{\partial R} (w \mathbf{u} \otimes \mathbf{k}) \mathbf{n} dA_{\mathbf{y}} \\ &= \int_{S(\mathbf{x})} (w \mathbf{u} \otimes \mathbf{n}) \mathbf{k} dA_{\mathbf{y}} = \left( \int_{S(\mathbf{x})} w \mathbf{u} \otimes \mathbf{n} dA_{\mathbf{y}} \right) \mathbf{k}. \end{aligned}$$

Hence

$$\int_R \nabla_{\mathbf{y}} \{w\mathbf{u}\} d\mathbf{y} = \int_{S(\mathbf{x})} w\mathbf{u} \otimes \mathbf{n} dA_{\mathbf{y}}. \quad (4.20)$$

The last term in (4.19) is

$$-\int_R \mathbf{u} \otimes \nabla_{\mathbf{y}} w d\mathbf{y} = \int_R \mathbf{u} \otimes \nabla_{\mathbf{x}} w d\mathbf{y} = \int_R \nabla_{\mathbf{x}} \{w\mathbf{u}\} d\mathbf{y} = \nabla_{\mathbf{x}} \left\{ \int_R w\mathbf{u} d\mathbf{y} \right\}. \quad (4.21)$$

Relations (4.19), (4.20) and (4.21) yield (4.15).

Taking the trace of relation (4.15), recalling that  $\operatorname{div} \mathbf{u} := \operatorname{tr}\{\nabla \mathbf{u}\}$ , and noting  $\operatorname{tr}\{\mathbf{u} \otimes \mathbf{n}\} = \mathbf{u} \cdot \mathbf{n}$ , we obtain (4.16).

Similarly,

$$\begin{aligned} \langle \operatorname{div} \mathbf{B} \rangle \{ \mathbf{x} \} &:= \int_{\mathcal{E}} (\operatorname{div} \mathbf{B})(\mathbf{y}) w(\mathbf{y} - \mathbf{x}) d\mathbf{y} = \int_R (\operatorname{div} \mathbf{B})(\mathbf{y}) w(\mathbf{y} - \mathbf{x}) d\mathbf{y} \\ &= \int_R \operatorname{div}_{\mathbf{y}} \{w\mathbf{B}\} - \mathbf{B}(\nabla_{\mathbf{y}} w) d\mathbf{y} \\ &= \int_{\partial R} w\mathbf{B}\mathbf{n} dA_{\mathbf{y}} + \int_R \mathbf{B}\nabla_{\mathbf{x}} w d\mathbf{y} \\ &= \int_{S(\mathbf{x})} w\mathbf{B}\mathbf{n} dA_{\mathbf{y}} + \int_R \operatorname{div}_{\mathbf{x}} \{ \mathbf{B}w \} d\mathbf{y} \\ &= \int_{S(\mathbf{x})} w\mathbf{B}\mathbf{n} dA_{\mathbf{y}} + \operatorname{div}_{\mathbf{x}} \left\{ \int_R \mathbf{B}w d\mathbf{y} \right\}. \end{aligned} \quad (4.22)$$

Thus (4.17) holds.

Finally,

$$\begin{aligned} \langle \partial \mathbf{u} / \partial t \rangle \{ \mathbf{x} \} &:= \int_{\mathcal{E}} \partial \mathbf{u} / \partial t(\mathbf{y}) w(\mathbf{y} - \mathbf{x}) d\mathbf{y} = \int_R \partial \mathbf{u} / \partial t(\mathbf{y}) w(\mathbf{y} - \mathbf{x}) d\mathbf{y} \\ &= \int_R \frac{\partial}{\partial t} \{ \mathbf{u}(\mathbf{y}) w(\mathbf{y} - \mathbf{x}) \} d\mathbf{y} = \frac{\partial}{\partial t} \left\{ \int_R \mathbf{u}(\mathbf{y}) w(\mathbf{y} - \mathbf{x}) d\mathbf{y} \right\} \\ &= \frac{\partial}{\partial t} \left\{ \int_{\mathcal{E}} \mathbf{u}(\mathbf{y}) w(\mathbf{y} - \mathbf{x}) d\mathbf{y} \right\}, \end{aligned} \quad (4.23)$$

which establishes (4.18). Of course, here we have assumed sufficient regularity of field  $\mathbf{u}$  to ensure the interchange of the limiting processes of time-differentiation and spatial integration is justified. (A similar remark is also



in order in respect of relations (4.20) and (4.22) in which spatial integration and spatial differentiation are interchanged.)

*Corollary 4.2.*

Consider the fluid momentum density

$$\mathbf{p} := \rho_0 \mathbf{v}. \tag{4.24}$$

Then

$$\langle \nabla \mathbf{p} \rangle = \nabla \{ \langle \mathbf{p} \rangle \}, \tag{4.25}$$

$$\langle \Delta \mathbf{p} \rangle = \Delta \{ \langle \mathbf{p} \rangle \} + \int_S (\nabla \mathbf{p}) \mathbf{n} w \, dA, \tag{4.26}$$

and

$$\langle \text{div} \{ \mathbf{p} \otimes \mathbf{p} \} \rangle = \text{div} \{ \langle \mathbf{p} \otimes \mathbf{p} \rangle \}. \tag{4.27}$$

*Proofs.*

Setting  $\mathbf{u} = \mathbf{p}$  in (4.15) yields (4.25) on noting that (4.3) implies

$$\mathbf{p} = \mathbf{0} \quad \text{on } \mathcal{S}, \tag{4.28}$$

since  $\mathcal{S}$  is a subset of  $\partial R$ .

Since

$$\Delta \mathbf{p} := \text{div} \{ \nabla \mathbf{p} \}, \tag{4.29}$$

setting  $\mathbf{B} = \nabla \mathbf{p}$  in (4.17) yields

$$\langle \Delta \mathbf{p} \rangle = \text{div} \{ \langle \nabla \mathbf{p} \rangle \} + \int_S (\nabla \mathbf{p}) \mathbf{n} w \, dA. \tag{4.30}$$

However, from (4.25),

$$\text{div} \{ \langle \nabla \mathbf{p} \rangle \} = \text{div} \{ \nabla \{ \langle \mathbf{p} \rangle \} \} =: \Delta \{ \langle \mathbf{p} \rangle \}. \tag{4.31}$$

Result (4.26) follows from (4.30) and (4.31).

With  $\mathbf{B} = \mathbf{p} \otimes \mathbf{p}$ , relation (4.17) yields

$$\langle \text{div} \{ \mathbf{p} \otimes \mathbf{p} \} \rangle = \text{div} \{ \langle \mathbf{p} \otimes \mathbf{p} \rangle \} + \int_S (\mathbf{p} \otimes \mathbf{p}) \mathbf{n} w \, dA. \tag{4.32}$$

Relation (4.32) yields (4.27) on noting (4.28).

The Navier-Stokes equation (4.1) that we wish to average may be written in the form

$$-\nabla P + (\mu/\rho_0)\Delta \mathbf{p} + \rho_0 \mathbf{g} = \frac{\partial}{\partial t} \{\mathbf{p}\} + \left(\frac{1}{\rho_0}\right) \operatorname{div}\{\mathbf{p} \otimes \mathbf{p}\}, \quad (4.33)$$

since  $\rho_0$  is constant. Using (4.14), (4.26), (4.27) and (4.18) with  $\mathbf{u} = \mathbf{p}$ , we obtain

$$\begin{aligned} & -\nabla\{\langle P \rangle\} - \left(\int_S P \mathbf{n}\right) / V + (\mu/\rho_0)[\Delta\{\langle \mathbf{p} \rangle\} + \int_S (\nabla \mathbf{p}) \mathbf{n} w dA] \\ & + \int_R \rho_0 \mathbf{g} w d\mathbf{y} = \frac{\partial}{\partial t} \{\langle \mathbf{p} \rangle\} + \left(\frac{1}{\rho_0}\right) \operatorname{div}\{\langle \mathbf{p} \otimes \mathbf{p} \rangle\}. \end{aligned} \quad (4.34)$$

*Remark 4.4.* It is tempting to note that  $\rho_0 \mathbf{g}$  is constant and invoke normalisation to write

$$\int_R \rho_0 \mathbf{g} w(\mathbf{y} - \mathbf{x}) d\mathbf{y} = \rho_0 \mathbf{g}.$$

*This is not correct*, however, since the domain of integration is the pore space  $R$  and not all space  $\mathcal{E}$ . Indeed, for a general field point  $\mathbf{x}$  (notice  $\mathbf{x}$  may be located in the pore space or porous body) the integration is effectively over that pore space within the REV  $C(\mathbf{x})$ : see (4.8). Specifically,

$$\int_R w(\mathbf{y} - \mathbf{x}) d\mathbf{y} = \left(\int_{R \cap C(\mathbf{x})} 1 d\mathbf{y}\right) / V. \quad (4.35)$$

The value of the integral over  $R \cap C(\mathbf{x})$  is the volume of the pore space within  $C(\mathbf{x})$ , so that the right-hand side of (4.35) represents the pore space volume within  $C(\mathbf{x})$  divided by the volume of  $C(\mathbf{x})$ . Of course, this is the relevant measure of *porosity*,  $\nu$  say. That is,

$$\nu(\mathbf{x}) := \int_R w(\mathbf{y} - \mathbf{x}) d\mathbf{y} = \langle 1 - \chi_B \rangle, \quad (4.36)$$

where  $\chi_B$  denotes the characteristic function for the porous body which occupies the fixed region  $B$  at scale  $\varepsilon_1$ . [Thus  $\chi_B(\mathbf{y}) = 1$  if  $\mathbf{y} \in B$ ,  $\chi_B(\mathbf{y}) = 0$  if  $\mathbf{y} \notin B$ .] Accordingly,

$$\int_R \rho_0 \mathbf{g} w(\mathbf{y} - \mathbf{x}) d\mathbf{y} = \rho_0 g \nu(\mathbf{x}). \quad (4.37)$$

As noted in the Introduction,  $\nu$  depends upon *two* length scales, namely  $\varepsilon_1$  and  $\varepsilon_2$ . The former is the scale at which the pore boundary is delineated (and hence employed in the definition of  $R$  in (4.37)), while the latter is the REV scale embodied in the choice of  $w$ .

Relation (4.34) may be written as

$$\begin{aligned} -\nabla\{\langle P \rangle\} + (\mu/\rho_0)\Delta\{\langle \mathbf{p} \rangle\} + \rho_0 \nu \mathbf{g} + \mathbf{f}^{fp} \\ = \frac{\partial}{\partial t} \{\langle \mathbf{p} \rangle\} + \operatorname{div}\{\rho_0^{-1}\langle \mathbf{p} \otimes \mathbf{p} \rangle\}, \end{aligned} \tag{4.38}$$

where

$$\mathbf{f}^{fp} := \int_S (-P\mathbf{1} + (\mu/\rho_0)\nabla\mathbf{p})\mathbf{n}w \, dA. \tag{4.39}$$

In order to obtain a relation which resembles (4.33) as closely as possible, we re-write (4.38) as

$$\begin{aligned} -\nabla\{\langle P \rangle\} + (\mu/\rho_0)\Delta\{\langle \mathbf{p} \rangle\} + \rho_0 \nu \mathbf{g} + \mathbf{f}^{fp} - \operatorname{div} \mathcal{D} \\ = \frac{\partial}{\partial t} \{\langle \mathbf{p} \rangle\} + \operatorname{div}\{\langle \rho \rangle^{-1}\langle \mathbf{p} \otimes \mathbf{p} \rangle\}, \end{aligned} \tag{4.40}$$

where

$$\mathcal{D} := \rho_0^{-1}\langle \mathbf{p} \otimes \mathbf{p} \rangle - \langle \rho \rangle^{-1}(\langle \mathbf{p} \rangle \otimes \langle \mathbf{p} \rangle). \tag{4.41}$$

Here, using (4.36),

$$\langle \rho \rangle(\mathbf{x}) := \int_R \rho_0 w(\mathbf{y} - \mathbf{x})d\mathbf{y} = \rho_0 \int_R w(\mathbf{y} - \mathbf{x})d\mathbf{y} = \rho_0 \nu(\mathbf{x}). \tag{4.42}$$

*Remark 4.5.* Relation (4.40) may be written in several equivalent ways upon introducing two candidate velocity fields,  $\mathbf{V}$  and  $\mathbf{Q}$ , via

$$\mathbf{V} := \langle \mathbf{p} \rangle / \langle \rho \rangle \tag{4.43}$$

and

$$\mathbf{Q} := \langle \mathbf{p} \rangle / \rho_0. \tag{4.44}$$

Of course, from (4.42), (4.43) and (4.44) we have

$$\mathbf{Q} = \nu\mathbf{V}. \tag{4.45}$$

Velocity  $\mathbf{V}$  is the natural choice (cf. (2.9)) and leads from (4.40) to

$$\begin{aligned} -\nabla\{\langle P \rangle\} + \mu\Delta\{\nu\mathbf{V}\} + \langle \rho \rangle\mathbf{g} + \mathbf{f}^{fp} - \operatorname{div} \mathcal{D} \\ = \frac{\partial}{\partial t} \{\langle \rho \rangle\mathbf{V}\} + \operatorname{div}\{\langle \rho \rangle\mathbf{V} \otimes \mathbf{V}\}. \end{aligned} \tag{4.46}$$

The equivalent formulation in terms of  $\mathbf{Q}$  is

$$\begin{aligned} -\nabla\{\langle P \rangle\} + \mu\Delta\mathbf{Q} + \rho_0\nu\mathbf{g} + \mathbf{f}^{fp} - \operatorname{div}\mathcal{D} \\ = \frac{\partial}{\partial t}\{\rho_0\mathbf{Q}\} + \operatorname{div}\{(\rho_0/\nu)(\mathbf{Q} \otimes \mathbf{Q})\}. \end{aligned} \quad (4.47)$$

Relations (4.46) and (4.47) may be compared with (4.1). To obtain the analogue of (4.2) we note that, from (4.16) and (4.3),

$$\begin{aligned} 0 = \langle \operatorname{div} \mathbf{v} \rangle &= \operatorname{div}\{\langle \mathbf{v} \rangle\} = \operatorname{div}\{\langle \rho_0 \mathbf{v} \rangle / \rho_0\} \\ &= \operatorname{div}\{\langle \mathbf{p} \rangle / \rho_0\} = \operatorname{div}\{\langle \rho \rangle \mathbf{V} / \rho_0\} \\ &= \operatorname{div}\{\nu \mathbf{V}\}. \end{aligned} \quad (4.48)$$

Thus from (4.45)

$$\operatorname{div} \mathbf{Q} = 0, \quad (4.49)$$

while

$$\nu \operatorname{div} \mathbf{V} + \nabla\nu \cdot \mathbf{V} = 0. \quad (4.50)$$

Clearly (4.50) indicates that

$$\text{in general } \operatorname{div} \mathbf{V} \neq 0. \quad (4.51)$$

*Remark 4.6.* It is of passing interest to note that (4.47) may be written as

$$\operatorname{div} \mathbf{T} + \rho_0\nu\mathbf{g} + \mathbf{f}^{fp} = \frac{\partial}{\partial t}\{\rho_0\mathbf{Q}\} + \operatorname{div}\{(\rho_0/\nu)\mathbf{Q} \otimes \mathbf{Q}\}, \quad (4.52)$$

where

$$\mathbf{T} := -\langle P \rangle \mathbf{1} + \mu[\nabla\mathbf{Q} + (\nabla\mathbf{Q})^T] - \mathcal{D}. \quad (4.53)$$

This is a consequence of the identities

$$\operatorname{div}\{(\nabla\mathbf{Q})^T\} \equiv \nabla\{\operatorname{div} \mathbf{Q}\}, \quad \operatorname{div}\{\langle P \rangle \mathbf{1}\} = \nabla\{\langle P \rangle\}, \quad (4.54)$$

and relation (4.49).

In the case of *creeping flow*, (4.1) becomes

$$-\nabla P + \mu\Delta\mathbf{v} + \rho_0\mathbf{g} = \frac{\partial}{\partial t}\{\rho_0\mathbf{v}\} \quad (4.55)$$

while (4.46) and (4.47) become, respectively,

$$-\nabla\{\langle P \rangle\} + \mu\Delta\{\nu\mathbf{V}\} + \langle \rho \rangle \mathbf{g} + \mathbf{f}^{fp} = \frac{\partial}{\partial t}\{\langle \rho \rangle \mathbf{V}\} \quad (4.56)$$

and

$$-\nabla\{\langle P \rangle\} + \mu\Delta\mathbf{Q} + \rho_0\nu\mathbf{g} + \mathbf{f}^{fp} = \frac{\partial}{\partial t}\{\rho_0\mathbf{Q}\}. \tag{4.57}$$

In view of (4.49) it is thus choice  $\mathbf{Q}$  which results, at least for creeping flow, in the closest match between the original Navier-Stokes equations and their averaged counterparts.

*Remark 4.7.* The velocity field  $\mathbf{Q}$  has a very important physical interpretation in the context of the foregoing, namely flow of an incompressible liquid through a rigid porous solid that it saturates. To see this it is instructive to consider mass conservation of *any* fluid which is contained within a rigid porous solid. This is given by

$$\partial\rho/\partial t + \operatorname{div}\mathbf{p} = 0, \tag{4.58}$$

a relation which holds throughout all pore space. (As we saw in (2.8), such a relation holds irrespective of whether the fluid is in liquid, vapour, or a mixture of the two separated by interfaces.) Averaging (4.58), using (4.16) with  $\mathbf{u} = \mathbf{p}$ , and noting (4.18) also holds for scalar fields (and hence for  $\rho$  in particular), we obtain

$$\partial\{\langle\rho\rangle\}/\partial t + \operatorname{div}\{\langle\mathbf{p}\rangle\} = 0. \tag{4.59}$$

Integrating (4.59) over any fixed region  $\mathcal{P}$  yields

$$\int_{\mathcal{P}} \partial\{\langle\rho\rangle\}/\partial t \, dV = - \int_{\partial\mathcal{P}} \langle\mathbf{p}\rangle \cdot \mathbf{n} \, dA \tag{4.60}$$

on using the divergence theorem. Since the left-hand side of (4.60) is expressible as the rate of *increase* of mass within  $\mathcal{P}$ ,  $\langle\mathbf{p}\rangle \cdot \mathbf{n}$  has the interpretation of mass flux across  $\partial\mathcal{P}$  in the direction of  $\mathbf{n}$ . That is,  $\langle\mathbf{p}\rangle \cdot \mathbf{n} \, \Delta A$  is to be interpreted, for small areas  $\Delta A$ , as delivering the mass flow per unit time, across a planar surface of area  $\Delta A$ , to which  $\mathbf{n}$  is a normal, in the direction of  $\mathbf{n}$ . From (4.44) this flow rate is  $\rho_0\mathbf{Q} \cdot \mathbf{n} \, \Delta A$  in the context of incompressible flow, and so the *volume* of fluid crossing ‘ $\Delta A$ ’ per unit time in the ‘ $\mathbf{n}$ ’ direction is  $\mathbf{Q} \cdot \mathbf{n} \, \Delta A$ . For this reason (and in this context)  $\mathbf{Q}$  is termed the *volumetric flux vector*.

We now examine the term  $\mathbf{f}^{fp}$  which represents the force density associated with the resistance to fluid flow from the porous body. From (4.39)

$$\mathbf{f}^{fp} = \hat{\mathbf{f}}^{fp} + \mu\tilde{\mathbf{f}}^{fp}, \tag{4.61}$$

where

$$\hat{\mathbf{f}}^{fp} := - \int_S P \mathbf{n} w dA \quad (4.62)$$

and

$$\tilde{\mathbf{f}}^{fp} := \int_S (\nabla \mathbf{v}) \mathbf{n} w dA. \quad (4.63)$$

The REV *intrinsic* average pressure  $\bar{P}$  (that is, the REV-scale average pressure computed only over the pore space within an REV) is given by

$$\bar{P}(\mathbf{x}) := \int_R P(\mathbf{y}) w(\mathbf{y} - \mathbf{x}) d\mathbf{y} / \int_R w(\mathbf{y} - \mathbf{x}) d\mathbf{y}. \quad (4.64)$$

Thus, from (4.36)

$$\bar{P} = \langle P \rangle / \nu. \quad (4.65)$$

Writing

$$\hat{\mathbf{f}}^{fp}(\mathbf{x}) = - \int_{S(\mathbf{x})} (\bar{P}(\mathbf{x}) + [P(\mathbf{y}) - \bar{P}(\mathbf{x})]) \mathbf{n}(\mathbf{y}) w(\mathbf{y} - \mathbf{x}) dA_{\mathbf{y}} \quad (4.66)$$

yields

$$\hat{\mathbf{f}}^{fp}(\mathbf{x}) = -\bar{P}(\mathbf{x}) \int_{S(\mathbf{x})} \mathbf{n}(\mathbf{y}) w(\mathbf{y} - \mathbf{x}) dA_{\mathbf{y}} + \mathbf{F}^{fp}(\mathbf{x}), \quad (4.67)$$

where

$$\mathbf{F}^{fp}(\mathbf{x}) := - \int_{S(\mathbf{x})} (P(\mathbf{y}) - \bar{P}(\mathbf{x})) \mathbf{n}(\mathbf{y}) w(\mathbf{y} - \mathbf{x}) dA_{\mathbf{y}}. \quad (4.68)$$

Now

$$\begin{aligned} \int_{S(\mathbf{x})} w(\mathbf{y} - \mathbf{x}) \mathbf{n}(\mathbf{y}) dA_{\mathbf{y}} &= \int_R (\operatorname{div}(w\mathbf{1}))(\mathbf{y}) d\mathbf{y} = \int_R \nabla_{\mathbf{y}} w(\mathbf{y} - \mathbf{x}) d\mathbf{y} \\ &= \int_R -\nabla_{\mathbf{x}} w(\mathbf{y} - \mathbf{x}) d\mathbf{y} = -\nabla_{\mathbf{x}} \int_R w(\mathbf{y} - \mathbf{x}) d\mathbf{y} = -(\nabla \nu)(\mathbf{x}). \end{aligned} \quad (4.69)$$

That is,

$$\int_{S(\mathbf{x})} w(\mathbf{y} - \mathbf{x}) \mathbf{n}(\mathbf{y}) dA_{\mathbf{y}} = -(\nabla \nu)(\mathbf{x}). \quad (4.70)$$

Thus (4.67) and (4.70) yield

$$\hat{\mathbf{f}}^{fp} = \bar{P} \nabla \nu + \mathbf{F}^{fp}, \quad (4.71)$$

and, using (4.65),

$$\begin{aligned} -\nabla\{\langle P \rangle\} + \hat{\mathbf{f}}^{fp} &= -\nabla\{\nu \bar{P}\} + \bar{P}\nabla\nu + \mathbf{F}^{fp} \\ &= -\nu\nabla\bar{P} + \mathbf{F}^{fp}. \end{aligned} \tag{4.72}$$

At this point (4.57) is expressible as

$$-\nu\nabla\bar{P} + \mathbf{F}^{fp} + \mu\Delta\mathbf{Q} + \rho_0\nu\mathbf{g} + \mu\tilde{\mathbf{f}}^{fp} = \partial/\partial t\{\rho_0\mathbf{Q}\}. \tag{4.73}$$

For spatially *steady* flow, the right-hand side of (4.73) vanishes. If, additionally,  $\mathbf{F}^{fp}$  is negligible (see Murdoch & Hassanizadeh [6], (4.36) *et seq*), (4.73) becomes

$$-\nu\nabla\bar{P} + \mu\Delta\mathbf{Q} + \rho_0\nu\mathbf{g} + \mu\tilde{\mathbf{f}}^{fp} = \mathbf{0}. \tag{4.74}$$

*Modelling Assumption:* There exists an invertible tensor  $\mathbf{K}$  (the *permeability* tensor) such that

$$\tilde{\mathbf{f}}^{fp} = -\mathbf{K}^{-1}\nu^2(\mathbf{V} - \mathbf{v}_B), \tag{4.75}$$

where  $\mathbf{v}_B$  denotes the REV-scale velocity of the porous body. If the body is at rest then (4.74) becomes

$$-\nabla\bar{P} + (\mu/\nu)\Delta\mathbf{Q} + \rho_0\mathbf{g} - \mu\mathbf{K}^{-1}\mathbf{Q} = \mathbf{0}. \tag{4.76}$$

This is the so-called *Brinkman* equation, with gravity.

In the event that  $\Delta\mathbf{Q}$  and  $\rho_0\mathbf{g}$  are negligible, (4.76) reduces to

$$\nabla\bar{P} = -\mu\mathbf{K}^{-1}\mathbf{Q}. \tag{4.77}$$

If the porous body is isotropic at the REV scale then, for some real-valued function  $k$ ,

$$\mathbf{K} = k\mathbf{1} \tag{4.78}$$

and (4.77) becomes Darcy's 'Law':

$$\nabla\bar{P} = -(\mu/k)\mathbf{Q}. \tag{4.79}$$

*Remark 4.8.* Relation (4.76), and its simplifications (4.77) and (4.79), appear in the literature in alternate forms as a consequence of differing definitions of the permeability tensor. In understanding such relations it is essential that the interpretations of pressure average and velocity field be precise. Here we

emphasise that  $\bar{P}$  is the REV-scale intrinsic pressure average (see text before (4.64)) and  $\mathbf{Q}$  is the volumetric flux vector (see (4.44) and Remark 4.5.).

*Remark 4.9.* The foregoing methodology has been used (see Murdoch & Soliman [7]) to investigate the widely-applied Beavers & Joseph boundary condition for liquid flow over a planar (at REV scale) boundary of a porous body. This study casts doubt on the validity of the accepted condition.

*Remark 4.10.* In cases when a rigid porous body is not saturated by an incompressible liquid, matters are much more complex. The Navier-Stokes equations will hold only where there is such liquid to be found. In general there will be gaseous, interfacial, and liquid phases in pore space. Nevertheless, at scale  $\varepsilon_1$  linear momentum balance for the set of *all* molecules within the region occupied by the porous body at REV scale, but not those of the porous body itself, takes the form (see (3.12), (3.20) and (3.25))

$$\operatorname{div} \mathbf{T} + \rho \mathbf{g} = \frac{\partial}{\partial t} \{\rho \mathbf{v}\} + \operatorname{div} \{\rho \mathbf{v} \otimes \mathbf{v}\}, \quad (4.80)$$

in the event that the only external force is due to gravitation. Averaging (4.80) yields

$$\operatorname{div} \{\langle \mathbf{T} \rangle - \mathcal{D}\} + \int_S (\mathbf{T} \mathbf{n}) w dA + \langle \rho \rangle \mathbf{g} = \frac{\partial}{\partial t} \{\langle \rho \rangle \mathbf{V}\} + \operatorname{div} \{\langle \rho \rangle \mathbf{V} \otimes \mathbf{V}\}, \quad (4.81)$$

where (compare (4.41))

$$\mathcal{D} := \langle \rho \mathbf{v} \otimes \mathbf{v} \rangle - \langle \rho \rangle \mathbf{V} \otimes \mathbf{V}. \quad (4.82)$$

At this point it is necessary to postulate constitutive relations for  $\langle \mathbf{T} \rangle - \mathcal{D}$ , the integral term, and  $\langle \rho \rangle$ . Clearly this matter is highly context-dependent and complex.



## 5. Energy balance

### 5.1. Energy balance for $\mathcal{M}$

The local form of energy balance is obtained from (3.1) by multiplying each term scalarly by  $\mathbf{v}_i w(\mathbf{x}_i - \mathbf{x})$  and then summing over all particles. The balance obtained includes *thermal* quantities: these are quantities whose definitions involve molecular thermal velocities. The *thermal velocity* of  $P_i$  at instant  $t$  (at the scale prescribed by  $w$ ) is<sup>12)</sup>

$$\tilde{\mathbf{v}}_i(t) := \mathbf{v}_i(t) - \mathbf{v}_w(\mathbf{x}_i(t), t). \tag{5.1}$$

So far we have only encountered one thermally-related field,<sup>13)</sup> namely

$$\mathcal{D}_w(\mathbf{x}, t) := \sum_i m_i \hat{\mathbf{v}}_i(\mathbf{x}, t) \otimes \hat{\mathbf{v}}_i(\mathbf{x}, t) w(\mathbf{x}_i(t) - \mathbf{x}). \tag{3.11}$$

Recall

$$\hat{\mathbf{v}}_i(\mathbf{x}, t) := \mathbf{v}_i(t) - \mathbf{v}_w(\mathbf{x}, t), \tag{3.8}$$

so that

$$\begin{aligned} \hat{\mathbf{v}}_i(\mathbf{x}, t) - \tilde{\mathbf{v}}_i(t) &= \mathbf{v}_w(\mathbf{x}_i(t), t) - \mathbf{v}_w(\mathbf{x}, t) \\ &\simeq \nabla \mathbf{v}_w(\mathbf{x}, t)(\mathbf{x}_i(t) - \mathbf{x}). \end{aligned} \tag{5.2}$$

Since contributions to  $\mathcal{D}_w(\mathbf{x}, t)$  come only from particles  $P_i$  near  $\mathbf{x}$  at instant  $t$  (if  $w = w_\epsilon$  then  $\|\mathbf{x}_i(t) - \mathbf{x}\| \leq \epsilon$ ), (5.2) indicates that  $\hat{\mathbf{v}}_i$  approximates  $\tilde{\mathbf{v}}_i$ .

Notice that from (2.2), (2.1) and (2.9)

$$\begin{aligned} \sum_i m_i \hat{\mathbf{v}}_i(\mathbf{x}, t) w(\mathbf{x}_i(t) - \mathbf{x}) &= \mathbf{p}_w(\mathbf{x}, t) - \rho_w(\mathbf{x}, t) \mathbf{v}_w(\mathbf{x}, t) \\ &= \mathbf{0}. \end{aligned} \tag{5.3}$$

<sup>12)</sup>Of course, scale-dependence enters here through the  $w$ -dependent definition (2.9) of  $\mathbf{v}_w$ .

<sup>13)</sup>The characteristic feature of molecular thermal velocities is their erratic nature and large average magnitudes ( $\sim 10^3 \text{ ms}^{-1}$ ) at room temperature. Since  $\tilde{\mathbf{v}}_i(t)$  and  $\hat{\mathbf{v}}_i(\mathbf{x}, t)$  differ only by the difference in the macroscopic velocity at points  $\mathbf{x}_i(t)$  and  $\mathbf{x}$ ,  $\tilde{\mathbf{v}}_i(\mathbf{x}, t)$  will also be erratic, and have large average magnitudes at room temperature.

Multiplying each term in (3.1) scalarly by  $\mathbf{v}_i w(\mathbf{x}_i - \mathbf{x})$  and summing over all particles yields

$$\sum_{i \neq j} \mathbf{f}_{ij} \cdot \mathbf{v}_i w(\mathbf{x}_i - \mathbf{x}) + \sum_i \mathbf{b}_i \cdot \mathbf{v}_i w(\mathbf{x}_i - \mathbf{x}) = \sum_i \frac{d}{dt} \{m_i \mathbf{v}_i\} \cdot \mathbf{v}_i w(\mathbf{x}_i - \mathbf{x}). \quad (5.4)$$

The first term is, using (3.8) and suppressing time dependence,

$$\sum_{i \neq j} \mathbf{f}_{ij} \cdot (\hat{\mathbf{v}}_i(\mathbf{x}) + \mathbf{v}_w(\mathbf{x})) w(\mathbf{x}_i - \mathbf{x}) = q_w(\mathbf{x}) + \mathbf{f}_w(\mathbf{x}) \cdot \mathbf{v}_w(\mathbf{x}), \quad (5.5)$$

where we have recalled (3.4) and

$$q_w(\mathbf{x}, t) := \sum_{i \neq j} \mathbf{f}_{ij}(t) \cdot \hat{\mathbf{v}}_i(\mathbf{x}, t) w(\mathbf{x}_i(t) - \mathbf{x}). \quad (5.6)$$

Similarly the second term in (5.4) is expressible as

$$\sum_i \mathbf{b}_i \cdot (\hat{\mathbf{v}}_i(\mathbf{x}) + \mathbf{v}_w(\mathbf{x})) w(\mathbf{x}_i - \mathbf{x}) = r_w(\mathbf{x}) + \mathbf{b}_w(\mathbf{x}) \cdot \mathbf{v}_w(\mathbf{x}), \quad (5.7)$$

where we have noted (3.5) and

$$r_w(\mathbf{x}, t) := \sum_i \mathbf{b}_i(t) \cdot \hat{\mathbf{v}}_i(\mathbf{x}, t) w(\mathbf{x}_i(t) - \mathbf{x}). \quad (5.8)$$

The right-hand side of (5.4) is

$$\begin{aligned} & \sum_i \frac{d}{dt} \{m_i \mathbf{v}_i\} \cdot \mathbf{v}_i w(\mathbf{x}_i - \mathbf{x}) = \sum_i \frac{d}{dt} \left\{ \frac{1}{2} m_i \mathbf{v}_i^2 \right\} w(\mathbf{x}_i - \mathbf{x}) \\ &= \frac{\partial}{\partial t} \left\{ \sum_i \frac{1}{2} m_i \mathbf{v}_i^2 w(\mathbf{x}_i - \mathbf{x}) \right\} + \operatorname{div} \left\{ \left( \sum_i \frac{1}{2} m_i \mathbf{v}_i^2 \right) \mathbf{v}_i w(\mathbf{x}_i - \mathbf{x}) \right\}. \end{aligned} \quad (5.9)$$

Now from (3.8) and (2.1),

$$\begin{aligned} & \sum_i \frac{1}{2} m_i \mathbf{v}_i^2 w(\mathbf{x}_i - \mathbf{x}) = \sum_i \frac{1}{2} m_i (\hat{\mathbf{v}}_i(\mathbf{x}) + \mathbf{v}_w(\mathbf{x}))^2 w(\mathbf{x}_i - \mathbf{x}) \\ &= \rho_w(\mathbf{x}) h_w(\mathbf{x}) + \left( \sum_i m_i \hat{\mathbf{v}}_i(\mathbf{x}) w(\mathbf{x}_i - \mathbf{x}) \right) \cdot \mathbf{v}_w(\mathbf{x}) + \frac{1}{2} \rho_w(\mathbf{x}) \mathbf{v}_w^2(\mathbf{x}), \end{aligned} \quad (5.10)$$

where

$$\rho_w(\mathbf{x}, t)h_w(\mathbf{x}, t) := \sum_i \frac{1}{2} m_i \hat{\mathbf{v}}_i^2(\mathbf{x}, t)w(\mathbf{x}_i(t) - \mathbf{x}). \tag{5.11}$$

From (5.3) the middle term on the right-hand side of (5.10) vanishes. Also, omitting the arguments of  $\hat{\mathbf{v}}_i, \mathbf{v}_w$  and  $w$ ,

$$\begin{aligned} \sum_i \left( \frac{1}{2} m_i \mathbf{v}_i^2 \right) \mathbf{v}_i w &= \sum_i \frac{1}{2} m_i (\hat{\mathbf{v}}_i + \mathbf{v}_w)^2 (\hat{\mathbf{v}}_i + \mathbf{v}_w) w \\ &= \sum_i \frac{1}{2} (m_i \hat{\mathbf{v}}_i^2) \hat{\mathbf{v}}_i w + \left( \sum_i \frac{1}{2} m_i \hat{\mathbf{v}}_i^2 w \right) \mathbf{v}_w + \sum_i m_i (\hat{\mathbf{v}}_i \cdot \mathbf{v}_w) \hat{\mathbf{v}}_i w \\ &\quad + \sum_i m_i (\hat{\mathbf{v}}_i \cdot \mathbf{v}_w) \mathbf{v}_w w + \mathbf{v}_w^2 \sum_i \frac{1}{2} m_i \hat{\mathbf{v}}_i w + \frac{1}{2} (\rho_w \mathbf{v}_w^2) \mathbf{v}_w \end{aligned} \tag{5.12}$$

$$= \mathbf{k}_w + \rho_w h_w \mathbf{v}_w + \mathcal{D}_w \mathbf{v}_w + \mathbf{0} + \mathbf{0} + \frac{1}{2} (\rho_w \mathbf{v}_w^2) \mathbf{v}_w. \tag{5.13}$$

Here

$$\mathbf{k}_w(\mathbf{x}, t) := \sum_i \frac{1}{2} (m_i \hat{\mathbf{v}}_i^2(\mathbf{x}, t)) \hat{\mathbf{v}}_i(\mathbf{x}, t)w(\mathbf{x}_i(t) - \mathbf{x}), \tag{5.14}$$

and we have recalled definitions (5.11), (3.11), (2.1) and the vanishing of two terms as a consequence of (5.3). From (5.4), (5.5), (5.7), (5.9), (5.10) and (5.13),

$$\begin{aligned} q_w + \mathbf{f}_w \cdot \mathbf{v}_w + r_w + \mathbf{b}_w \cdot \mathbf{v}_w \\ = \frac{\partial}{\partial t} \left\{ \rho_w \left( h_w + \frac{1}{2} \mathbf{v}_w^2 \right) \right\} + \text{div} \left\{ \mathbf{k}_w + \rho_w \left( h_w + \frac{1}{2} \mathbf{v}_w^2 \right) \mathbf{v}_w + \mathcal{D}_w \mathbf{v}_w \right\} \end{aligned} \tag{5.15}$$

$$= \rho_w \left\{ \dot{h}_w + \frac{1}{2} \dot{\rho}_w \mathbf{v}_w^2 \right\} + \text{div} \mathbf{k}_w + \text{div}(\mathcal{D}_w \mathbf{v}_w). \tag{5.16}$$

In (5.16) the superposed ‘ $\dot{\cdot}$ ’ indicates a material time derivative,<sup>14)</sup> and in obtaining (5.16) from (5.15) we have invoked the continuity equation (2.10).

<sup>14)</sup>For any scalar field  $\phi$ , using (2.10),

$$\frac{\partial}{\partial t} \{ \rho \phi \} + \text{div} \{ \rho \phi \mathbf{v}_w \} = \rho \dot{\phi},$$

where

$$\dot{\phi} := \partial \phi / \partial t + \nabla \phi \cdot \mathbf{v}_w$$

denotes the material time derivative.

Accordingly, using (3.20), (5.16) becomes

$$q_w + r_w - \operatorname{div} \mathbf{k}_w + (\operatorname{div} \mathbf{T}_w^- + \mathbf{b}_w) \cdot \mathbf{v}_w - \operatorname{div}(\mathcal{D}_w \mathbf{v}_w) = \rho_w \left\{ h_w + \frac{1}{2} \rho_w \mathbf{v}_w^2 \right\}'. \quad (5.17)$$

From (5.6) and the normalisation condition (2.3),

$$q_w(\mathbf{x}) = \int_{\mathcal{E}} \sum_{i \neq j} \mathbf{f}_{ij} \cdot \hat{\mathbf{v}}_i(\mathbf{x}) w(\mathbf{x}_i - \mathbf{x}) w(\mathbf{x}_j - \mathbf{y}) d\mathbf{y}. \quad (5.18)$$

Thus

$$q_w(\mathbf{x}) = \int_{\mathcal{E}} g_w^+(\mathbf{x}, \mathbf{y}) + g_w^-(\mathbf{x}, \mathbf{y}) d\mathbf{y}, \quad (5.19)$$

where

$$g_w^{\pm}(\mathbf{x}, \mathbf{y}) := \frac{1}{2} \sum_{i \neq j} \{ \mathbf{f}_{ij} \cdot \hat{\mathbf{v}}_i(\mathbf{x}) \pm \mathbf{f}_{ji} \cdot \hat{\mathbf{v}}_j(\mathbf{y}) \} w(\mathbf{x}_i - \mathbf{x}) w(\mathbf{x}_j - \mathbf{y}). \quad (5.20)$$

As a consequence of balanced interactions (3.7),

$$g_w^-(\mathbf{y}, \mathbf{x}) = -g_w^-(\mathbf{x}, \mathbf{y}) \quad (5.21)$$

and Noll's Theorem can be invoked to show the existence of a vector field  $\mathbf{q}_w^-$  such that

$$(\operatorname{div} \mathbf{q}_w^-)(\mathbf{x}) = \int_{\mathcal{E}} g_w^-(\mathbf{x}, \mathbf{y}) d\mathbf{y} =: q_w^-(\mathbf{x}). \quad (5.22)$$

Accordingly,

$$q_w = \operatorname{div} \mathbf{q}_w^- + q_w^+, \quad (5.23)$$

where

$$q_w^+(\mathbf{x}) := q_w(\mathbf{x}) - q_w^-(\mathbf{x}) = \int_{\mathcal{E}} g_w^+(\mathbf{x}, \mathbf{y}) d\mathbf{y}. \quad (5.24)$$

Noting

$$(\operatorname{div} \mathbf{T}_w^-) \cdot \mathbf{v}_w = \operatorname{div} \{ (\mathbf{T}_w^-)^T \mathbf{v}_w \} - \mathbf{T}_w^- \cdot \nabla \mathbf{v}_w, \quad (5.25)$$

and defining the *heat flux vector*

$$\mathbf{q}_w := -\mathbf{q}_w^- + \mathbf{k}_w, \quad (5.26)$$

(5.17) may be written in the form (recalling (3.25))

$$\begin{aligned} r_w - \operatorname{div} \mathbf{q}_w + \operatorname{div}(\mathbf{T}_w^T \mathbf{v}_w) + \mathbf{b}_w \cdot \mathbf{v}_w &= -q_w^+ + \mathbf{T}_w^- \cdot \nabla \mathbf{v}_w + \rho_w \left\{ h_w + \frac{1}{2} \mathbf{v}_w^2 \right\}' \end{aligned} \quad (5.27)$$

$$= \rho_w \left\{ e_w + \frac{1}{2} \mathbf{v}_w^2 \right\}' \quad (5.28)$$

Here

$$e_w := \beta_w + h_w, \quad (5.29)$$

where<sup>15)</sup>

$$\dot{\beta}_w := \mathbf{T}_w^- \cdot \nabla \mathbf{v}_w - q_w^-. \quad (5.30)$$

*Remark 5.1.* Integration of (5.28) over a region  $\mathcal{R}$  together with use of the divergence theorem yield (see Remark 3.3)

$$\int_{\partial \mathcal{R}} (-\mathbf{q}_w \cdot \mathbf{n} + \mathbf{T}_w \mathbf{n} \cdot \mathbf{v}_w) + \int_{\mathcal{R}} (r_w + \mathbf{b}_w \cdot \mathbf{v}_w) = \frac{d}{dt} \left\{ \int_{\mathcal{R}_t} \rho_w \left( e_w + \frac{1}{2} \mathbf{v}_w^2 \right) \right\}. \quad (5.31)$$

In Continuum Mechanics balance (5.31) is *postulated* to hold for all regions  $\mathcal{R}$ . The arbitrary nature of  $\mathcal{R}$  then allows local form (5.28) to be *deduced*. As with linear momentum balance, the molecular approach has yielded the local form directly, and furnished explicit, scale-dependent, definitions of all field values in terms of molecular variables.

*Remark 5.2.* The local form of energy balance, namely

$$r_w - \operatorname{div} \mathbf{q}_w + \operatorname{div}(\mathbf{T}_w^T \mathbf{v}_w) + \mathbf{b}_w \cdot \mathbf{v}_w = \rho_w \left\{ e_w + \frac{1}{2} \mathbf{v}_w^2 \right\}' \quad (5.28)$$

is expressible as

$$r_w - \operatorname{div} \mathbf{q}_w + \mathbf{T}_w \cdot \nabla \mathbf{v}_w + \{ \operatorname{div} \mathbf{T}_w + \mathbf{b}_w \} \cdot \mathbf{v}_w = \rho_w \dot{e}_w + \rho_w \dot{\mathbf{v}}_w \cdot \mathbf{v}_w. \quad (5.32)$$

<sup>15)</sup>Relation (5.30) is a consequence of defining

$$\beta_w(\mathbf{x}, t) := \beta_w(\hat{\mathbf{x}}(t), t)$$

in terms of the solution  $\hat{\mathbf{x}}(t)$  to  $\dot{\hat{\mathbf{x}}}(\tau) = \mathbf{v}_w(\hat{\mathbf{x}}(\tau), \tau)$  with  $\hat{\mathbf{x}}(t) = \mathbf{x}$ . Then

$$\beta_w(\mathbf{x}, t) := \int_{t_0}^t \rho_w^{-1} \{ \mathbf{T}_w^- \cdot \nabla \mathbf{v}_w - q_w^+ \} d\tau.$$

Since

$$\dot{\mathbf{v}}_w = \mathbf{a}_w, \quad (5.33)$$

linear momentum balance (3.24) enables (5.32) to be reduced to the form

$$r_w - \operatorname{div} \mathbf{q}_w + \mathbf{T}_w \cdot \nabla \mathbf{v}_w = \rho \dot{e}_w. \quad (5.34)$$

*Remark 5.3.* Noll's theorem delivers the explicit form (see (3.22))

$$\begin{aligned} \mathbf{q}_w^-(\mathbf{x}) := & -\frac{1}{4} \int_{\mathcal{V}} \int_0^1 \sum_{i \neq j} \{ \mathbf{f}_{ij} \cdot \hat{\mathbf{v}}_i(\mathbf{x} + \alpha \mathbf{u}) - \mathbf{f}_{ji} \cdot \hat{\mathbf{v}}_j(\mathbf{x} - (1 - \alpha) \mathbf{u}) \} \\ & \times w(\mathbf{x} + \alpha \mathbf{u} - \mathbf{x}_i) w(\mathbf{x} - (1 - \alpha) \mathbf{u} - \mathbf{x}_j) \mathbf{u} \, d\alpha \, du. \end{aligned} \quad (5.35)$$

*Remark 5.4.* Quantities  $r_w$ ,  $\mathbf{q}_w^-$ ,  $\mathbf{k}_w$  and  $\rho_w h_w$  are of a thermal nature since they involve molecular thermal velocities in their definitions. Term  $r_w$  represents the power expended by external agencies in thermal motions of molecules, while  $\mathbf{k}_w$  represents a diffusion of thermal kinetic energy. It is such thermal kinetic energy which is regarded as *heat*: this is precisely the kinetic theory of heat<sup>16)</sup>. Term  $\rho_w h_w$  is accordingly to be interpreted as the *heat content density* (at the scale represented by  $w$ ).

## 5.2. Energy balance for fluid in a porous body

### 5.2.1. The general form of balance

Recalling (3.32) and (5.8) gives

$$\begin{aligned} r_w(\mathbf{x}, t) &= \sum_i \left\{ \sum_{P_\alpha \in \mathcal{M}^p} \mathbf{F}_{i\alpha}(t) + m_i \mathbf{g} \right\} \cdot \hat{\mathbf{v}}_i(\mathbf{x}, t) w(\mathbf{x}_i(t) - \mathbf{x}) \\ &= r_w^{fp}(\mathbf{x}, t), \end{aligned} \quad (5.36)$$

where (noting (5.3))

$$r_w^{fp}(\mathbf{x}, t) := \sum_i \sum_{P_\alpha \in \mathcal{M}^p} \mathbf{F}_{i\alpha}(t) \cdot \hat{\mathbf{v}}_i(\mathbf{x}, t) w(\mathbf{x}_i(t) - \mathbf{x}). \quad (5.37)$$

Accordingly the reduced form (5.34) of energy balance is

$$r_w^f - \operatorname{div} \mathbf{q}_w^f + \mathbf{T}_w^f \cdot \nabla \mathbf{v}_w^f = \rho_w^f \dot{e}_w^f, \quad (5.38)$$

where superscript  $f$  has been introduced to indicate  $\mathcal{M}^f$  molecules are involved.

<sup>16)</sup>See Brush [8].

**5.2.2. Energy balance at scale  $\varepsilon = \varepsilon_1$**

As with linear momentum balance at scale  $\varepsilon_1$ , as a consequence of the short-range nature of molecular interactions  $r_w^{fp}$  vanishes in region  $-\mathcal{R}_{\varepsilon_1}^{fp}$  (see (3.36)), and so balance (5.38) reduces to a relation which only involves *fluid* in the region  $-\mathcal{R}_{\varepsilon_1}^f$ . The effect of the porous body is only ‘sensed’ in the  $\varepsilon_1$ -scale interfacial region  $\mathcal{I}_{\varepsilon_1}^{pf}$ . Said differently, except in  $\mathcal{I}_{\varepsilon_1}^{pf}$  standard energy balance for fluids holds in the pore space.

**5.2.3. Energy balance at scale  $\varepsilon = \varepsilon_2$**

Replacing subscript  $w$  by  $\varepsilon_2$  to emphasise the scale involved here, (5.38) becomes

$$r_{\varepsilon_2}^{fp} - \operatorname{div} \mathbf{q}_{\varepsilon_2}^f + \mathbf{T}_{\varepsilon_2}^f \cdot \nabla \mathbf{v}_{\varepsilon_2}^f = \rho_{\varepsilon_2}^f \dot{e}_{\varepsilon_2}^f. \tag{5.39}$$

Term  $r_{\varepsilon_2}^{fp}(\mathbf{x}, t)$  represents the rate at which heat is supplied to fluid in pore space within  $S_{\varepsilon_2}(\mathbf{x})$  at instant  $t$  from the porous body, divided by  $V_{\varepsilon}$ . Of course, this is to be regarded as heat conducted *from* the porous body *to* the fluid if  $r_{\varepsilon_2}^{fp} > 0$  and *vice-versa* if  $r_{\varepsilon_2}^{fp} < 0$ .

Term  $(-\operatorname{div} \mathbf{q}_{\varepsilon_2}^f)(\mathbf{x}, t)$  represents a similar conductive heat supply rate density (at instant  $t$ ) from fluid outside  $S_{\varepsilon_2}(\mathbf{x})$  into fluid inside  $S_{\varepsilon_2}(\mathbf{x})$ . Such conduction is, of course, only effected via pores which are intersected by  $\partial S_{\varepsilon_2}(\mathbf{x})$ . Fields  $\mathbf{T}_{\varepsilon_2}^f$  and  $\mathbf{v}_{\varepsilon_2}^f$  were discussed in §3.2.2. Term  $(\rho_{\varepsilon_2}^f e_{\varepsilon_2}^f)(\mathbf{x}, t)$  represents the binding energy plus thermal kinetic energy associated with fluid within  $S_{\varepsilon_2}(\mathbf{x})$  at instant  $t$  divided by  $V_{\varepsilon}$ . The material time derivative  $\dot{e}_{\varepsilon_2}^f$  is (see footnote 14) that associated with  $\mathbf{v}_{\varepsilon_2}^f$ : that is,

$$\dot{e}_{\varepsilon_2}^f := \frac{\partial e_{\varepsilon_2}^f}{\partial t} + (\nabla e_{\varepsilon_2}^f) \cdot \mathbf{v}_{\varepsilon_2}^f. \tag{5.40}$$

*Exercise 5.1.* Notice the difference between fluid ‘material points’ at scales  $\varepsilon_1$  and  $\varepsilon_2$ . Where are each category of points to be found, and how do they move?

**5.3. Remarks on obtaining  $\varepsilon_2$  scale governing equations from  $\varepsilon_1$ - scale governing equations**

Recalling the discussion of Chapter 4 in which  $\varepsilon_2$ -scale flow equations were derived from the flow of an incompressible Newtonian fluid in pores,

it is natural to attempt the same procedure in an energetic context. To this end we note some difficulties.

- D.1. Once temperature variation is allowed, the notions of 'rigid' porous body and 'incompressible' fluid must be re-appraised. Unless temperature is almost uniform throughout the whole system, thermal expansion must enter into the reckoning.
- D.2. Additional to the non-slip condition at pore boundaries (see (4.3)) heat conduction from  $\mathcal{M}^p$  into  $\mathcal{M}^f$  must be modelled. Said differently an  $\varepsilon_1$ -scale field representing such conduction must be introduced. Here we note that such a condition depends upon how  $\mathcal{M}^p$  and  $\mathcal{M}^f$  behaviour is modelled at scale  $\varepsilon_1$ . Specifically this will involve how heat conduction is modelled for these systems at scale  $\varepsilon_1$ .



## 6. Time- dependent material systems

### 6.1. Preamble

The simplest situation concerning fluid flow in porous bodies is that in which the porous body is rigid, saturated with incompressible liquid, and the temperature is everywhere constant. From a practical viewpoint, modelling of the foregoing must be generalised. One such generalisation is to have pore space occupied by *two* incompressible liquids which do not mix. A motivation here would be oil recovery from shale by displacing oil with water. Another important situation is that of fluid existing in both liquid and gaseous phases within a porous body. In both contexts there will be interfaces (water/oil and liquid/vapour, respectively) and consequent effects of capillarity<sup>17)</sup>. There is also evidence to suggest that ‘common lines’<sup>18)</sup> may play a rôle in these systems. Of course, fluid/fluid interfaces change their molecular populations with time. Thus, in order to employ the molecular viewpoint and averaging methodology used in the foregoing chapters, it is necessary to consider *time-dependent* material systems.

### 6.2. The basic approach

The key idea is to regard the time-dependent system of interest as a subset of a time-*independent* material system  $\mathcal{M}$ . If  $\mathcal{M}$  consists of particles  $P_i$  ( $i = 1, 2, \dots, N$ ) as in previous chapters, then at any instant  $t$ ,

$$\mathcal{M} = \mathcal{M}^+(t) \cup \mathcal{M}^-(t), \quad (6.1)$$

where  $\mathcal{M}^+(t)$  denotes the system of interest at instant  $t$  and

$$\mathcal{M}^-(t) := \mathcal{M} - \mathcal{M}^+(t). \quad (6.2)$$

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<sup>17)</sup>That is, effects associated with surface tension.

<sup>18)</sup>A ‘common line’ is a one-dimensional continuum which models the effect of matter at the common boundary of three phases (for example, oil/water/porous body).

The particle population of  $\mathcal{M}^+(t)$  at instant  $t$  is handled in terms of a 'membership function'  $e_i(t)$ :

$$\begin{cases} e_i(t) = 1 & \text{if } P_i \in \mathcal{M}^+(t) \text{ at instant } t \\ e_i(t) = 0 & \text{if } P_i \notin \mathcal{M}^+(t) \text{ at instant } t. \end{cases} \quad (6.3)$$

The procedure for obtaining continuum equations of balance is to proceed as for time-independent systems, but incorporate factors  $e_i(t)$  and implement an additional averaging in time.

*Remark 6.1.* If continuum field values are to be related to experimental measurements (this is, of course, essential in order to interpret behaviour monitored at a macroscopic scale) then time averaging automatically enters into the reckoning, since no measurement is instantaneous. Accordingly, if measurements are undertaken at scales  $\varepsilon$  and  $\Delta$  of length and time, respectively, then continuum averaging should be undertaken jointly in space and time at these scales. Time averaging has, until this point, been omitted in the interests of simplicity and brevity. Details are to be found in Murdoch & Bedeaux, [9], Murdoch [10] and Murdoch & Hassanizadeh [6].

The  $\Delta$ -time average of a continuous function  $f$  of time is<sup>19)</sup>

$$f_{\Delta}(t) := \frac{1}{\Delta} \int_{t-\Delta}^t f(\tau) d\tau. \quad (6.4)$$

Defining

$$\rho_w(\mathbf{x}, t) := \sum_i m_i e_i(t) w(\mathbf{x}_i(t) - \mathbf{x}) \quad (6.5)$$

and

$$\mathbf{p}_w(\mathbf{x}, t) := \sum_i m_i \mathbf{v}_i(t) e_i(t) w(\mathbf{x}_i(t) - \mathbf{x}) \quad (6.6)$$

it can be shown that the corresponding time-averaged fields  $\rho_{w,\Delta}$  and  $\mathbf{p}_{w,\Delta}$  satisfy

$$\frac{\partial \rho_{w,\Delta}}{\partial t} + \operatorname{div} \mathbf{p}_{w,\Delta} = \mathcal{G}_{w,\Delta}. \quad (6.7)$$

Here  $\mathcal{G}_{w,\Delta}$  represents the net rate of increase of mass for  $\mathcal{M}^+$  (due to mass exchange with  $\mathcal{M}^-$ ) associated with the spatial scale embodied in  $w$  and the time scale  $\Delta$ . Of course (see (2.9)) the corresponding velocity field is

$$\mathbf{v}_{w,\Delta} := \mathbf{P}_{w,\Delta} / \rho_{w,\Delta}. \quad (6.8)$$

<sup>19)</sup>  $f_{\Delta}(t)$  is the mean value of  $f$  over that time interval of duration  $\Delta$  ending at instant  $t$ .

*Exercise 6.1.* Show that if  $f$  is a continuously-differentiable function of time then<sup>20)</sup>

$$\left(\frac{df}{dt}\right)_\Delta = \frac{d}{dt}(f_\Delta). \tag{6.9}$$

Result (6.9) is needed to derive the time derivative term in (6.7). This throws up a problem, since  $\rho_w$  is discontinuous whenever a particle enters or leaves  $\mathcal{M}^+$ . The source of discontinuity is the ‘step function’ nature of  $e_i(t)$  for each  $i$ . Such discontinuities can be ‘mollified’ over time intervals of physically-negligible duration (say  $10^{-20}$  s: such an interval is much smaller than the time scale associated with molecular motion at the molecular level, which is of order  $10^{-13}$  s) in essentially the same way as for weighting function  $w_\epsilon$  (see (2.12) and (2.15)).

The corresponding form of linear momentum balance is obtained by multiplying relation (3.1) by  $w(\mathbf{x}_i(\tau) - \mathbf{x})e_i(\tau)$ , summing over all  $P_i \in \mathcal{M}$ , and taking the  $\Delta$ -time average of the result. The appropriate balance for  $\mathcal{M}^+$  takes the form

$$\text{div } \mathbf{T}_{w,\Delta} + \mathbf{f}_{w,\Delta}^{\text{ext}} + \mathbf{P}_{w,\Delta}^{\text{in}} - \mathbf{P}_{w,\Delta}^{\text{out}} + \mathbf{b}_{w,\Delta} = \rho_{w,\Delta} \dot{\mathbf{v}}_{w,\Delta} + \mathcal{G}_{w,\Delta} \mathbf{v}_{w,\Delta}. \tag{6.10}$$

Here  $\mathbf{T}_{w,\Delta}$ , and  $\mathbf{b}_{w,\Delta}$  represent the stress tensor, and body force density associated with the effect of material other than  $\mathcal{M}$ , respectively. Term  $\mathbf{f}_{w,\Delta}^{\text{ext}}$  denotes the force density associated with the effect on  $\mathcal{M}^+$  particles due to  $\mathcal{M}^-$  particles, and  $\mathbf{P}_{w,\Delta}^{\text{in}}$  ( $\mathbf{P}_{w,\Delta}^{\text{out}}$ ) represents the local rate of supply (depletion) of momentum to  $\mathcal{M}^+$  due to  $\mathcal{M}^- \rightarrow \mathcal{M}^+$  ( $\mathcal{M}^+ \rightarrow \mathcal{M}^-$ ) transitions.

Relations (6.7) and (6.10), together with a corresponding balance of energy, were derived in Murdoch & Hassanizadeh [6] and applied to the situation of two immiscible liquids within a porous body at the REV ( $\epsilon_2$ ) scale. The choices for  $\mathcal{M}^+$  discussed were bulk liquid phases, liquid/liquid interfacial phases, liquid/porous body interfaces, and the common line (liquid/liquid/porous body) phase.

*Remark 6.2.* The balance relations presented in [6] are precise, and all fields are clearly defined in terms of local space-time averages of molecular

<sup>20)</sup>To handle the right-hand side of (6.9) it is essential to notice that if  $a$  and  $b$  are differentiable functions of  $t$  then

$$\frac{d}{dt} \left\{ \int_{a(t)}^{b(t)} f(\tau) d\tau \right\} = f(b(t))db/dt - f(a(t))da/dt.$$

Relevant here are choices  $b(t) = t$  and  $a(t) = t - \Delta$ .

quantities. However, these relations do not deliver a self-contained theory: it is necessary to make *constitutive assumptions* about the nature of certain fields. In (6.10) constitutive relations are needed not only for  $\mathbf{T}_{w,\Delta}$  but also for  $\mathbf{f}_{w,\Delta}^{\text{ext}}$ ,  $\mathbf{P}_{w,\Delta}^{\text{in}} - \mathbf{P}_{w,\Delta}^{\text{out}}$ , and  $\mathcal{G}_{w,\Delta}$ .

## 7. Concluding remarks

*Remark 7.1.* Modelling the behaviour of fluids in porous media is intrinsically difficult because of the lack of detailed knowledge of both pore geometry and just where (and in what phase) fluid is to be found. All that can be hoped for from a continuum description is a rather limited understanding of gross (REV-scale) behaviour.

*Remark 7.2.* More than in any other application of continuum modelling, the scale-dependent nature of the system and its behaviour is *a priori* evident.

*Remark 7.3.* The adoption of an REV-scale continuum approach involves concepts from mixture theory. Such concepts are not always clearly understood: for example, the interpretation of partial stresses in mixture theory, given by early prominent workers in the field (Truesdell & Toupin, [11], Bowen [12]) were incorrect, and led to a paradox (see Gurtin, Oliver & Williams [13]).

*Remark 7.4.* The corpuscular viewpoint adopted here leads to precise understanding of field values, and underpins (and justifies) assumptions made in continuum mechanics. In particular, one is led inevitably to the correct interpretation of partial stress in mixture theory (see Morro & Murdoch, [14]), and to appreciate the distinct contributions to any stress tensor from molecular interactions and from diffusion.

*Remark 7.5.* The molecular perspective and  $\varepsilon$ -scale spatial averaging highlights the existence of a 'layer' of thickness  $2\varepsilon$  located at the boundary of a body. This layer constitutes an interface between the body and its exterior in which field values are to be expected to have a different character to those 'within' the body. (For example, the mass density function goes from a typical bulk value to zero as the interfacial region is traversed.) This suggests modelling the interfacial region in its own right, possibly as a two-dimensional continuum. Such an approach is helpful in analysing boundary conditions. In this context Murdoch & Soliman, [7] studied the Beavers & Joseph boundary condition for liquid flow over a planar boundary of a rigid porous body saturated with the liquid.

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