

## Chapter 2

# Theory of Mixtures

**Abstract** This chapter lays out the conceptual basis for the study of processes of solid–liquid separation. For the study of flows in rigid and deformable porous media and of suspension sedimentation and transport, we must consider bodies formed of different materials. The appropriate tool to do this is the *Theory of Mixtures*. A rigorous but limited account of the Theory of Mixtures of continuum mechanics is given that postulates that each point in space of a body is simultaneously occupied by a finite number of particles, one for each component of the mixture. In this way, the mixture can be represented as a superposition of continuous media, each following its own movement with the restriction imposed by the interaction between components. An introduction discusses the conditions that a multi-component body must fulfill to be considered a continuum. The concepts of body, component, mixture, deformation and rate of deformation are introduced and discussed. Mass and momentum balance equations are formulated for each component of the mixture and the need to establish constitutive equations to complete a dynamic process is discussed.

To study the flow in rigid and deformable porous media and for the study of sedimentation and transport of suspensions, it is convenient to consider a body formed of different materials. The appropriate tool to do this is the *Theory of Mixtures*. There is not one but several Theories of Mixtures, and here we will follow the developments of Truesdell and Toupin (1960), Truesdell (1965, 1984).

The Theory of Mixtures postulates that each point in space is simultaneously occupied by a finite number of particles, one for each component of the mixture. In this way, the mixture may be represented as a superposition of continuous media, each following its own movement with the restriction imposed by the interaction between components. This means that each component will obey the laws of conservation of mass and momentum, incorporating terms to account for the interchange of mass and momentum between components. To obtain a rational theory, we must require that the properties of the mixture follow the same laws as a body of a single component, that is, that the mixture behaves as a single component body. Concha and Barrientos (1993), Concha (2001).

Treatment similar or alternative to this treatment may be found in many articles and books, such as Bowen (1976), Atkin and Crain (1976), Bedford and Drumheller (1983), Drew (1983), Truesdell (1984), Ungarish (1993), Rajagopal and Tao (1995), Drew and Passman (1998).

## 2.1 Kinematics

### 2.1.1 Body, Configuration and Type of Mixture

The term *mixture* denote a body  $B$  formed by  $n$  components  $B_\alpha \subset B$ ,  $\alpha = 1, 2, \dots, n$ . The elements of  $B_\alpha$  are called *particles* and are denoted by  $p_\alpha$ . Each body occupies a determined region of the Euclidian three-dimensional space  $E_3$  called *configuration* of the body. The elements of the configurations are points  $X_\alpha \in E_3$ , whose positions are given by the position vector  $\mathbf{r}$ . Thus, the position of a particle  $p_\alpha \in B_\alpha$  is given by:

$$\mathbf{r} = \chi_\alpha(p_\alpha), \quad \alpha = 1, 2, \dots, n \quad (2.1)$$

To investigate the properties of  $\chi_\alpha$  see Bowen (1976). The configuration  $\chi(B)$  of the mixture is:

$$\chi(B) = \bigcup_\alpha \chi_\alpha(B_\alpha) \quad (2.2)$$

The volume of  $\chi(B)$  is called the material volume and is denoted by  $V_m := V(\chi(B))$ . To every body  $B_\alpha$  we can assign a positive, continuous and additive function  $m_\alpha$  that measures the amount of matter it contains, such that:

$$m(B) = \sum_{\alpha=1}^n m_\alpha(B_\alpha) \quad (2.3)$$

where  $m_\alpha$  and  $m(B)$  are the *masses* of the  $\alpha$  component and of the mixture respectively. Due to the continuous nature of mass, we can define a *mass density*  $\bar{\rho}_\alpha(\mathbf{r}, t)$  at point  $\mathbf{r}$  and time  $t$  in the form:

$$\bar{\rho}_\alpha(\mathbf{r}, t) = \lim_{k \rightarrow \infty} \frac{m_\alpha(P_k)}{V_m(P_k)}, \quad \alpha = 1, 2, \dots, n \quad (2.4)$$

where  $P_{k+1} \subset P_k$  are part of the mixture having the position  $\mathbf{r}$  in common at time  $t$ . Due to the hypothesis that mass for a continuum is an absolutely continuous function of volume, the function  $\bar{\rho}_\alpha$  exists almost everywhere in  $B$ , see Drew and Passman (1999). This mass density is called the *apparent density* of  $B_\alpha$ . The total mass of  $B_\alpha$  can be written in terms of  $\bar{\rho}_\alpha$  by:

$$m_\alpha = \int_{V_m(t)} \bar{\rho}_\alpha(\mathbf{r}, t) dV \quad (2.5)$$

For each body  $B_\alpha$  we select a reference configuration  $\chi_{\alpha K}$ , such that in that configuration it is the only component of the mixture (pure state). Let  $\rho_{\alpha K}$  be the mass density of the  $\alpha$  component in the reference configuration and call it *material density*. Then we can write:

$$m_\alpha = \int_{V_m(t)} \bar{\rho}_\alpha(\mathbf{r}, t) dV = \int_{V_K} \rho_{\alpha K}(\mathbf{R}) dV \quad (2.6)$$

The material density of  $B_\alpha$  in the actual configuration is denoted by  $\rho_\alpha(\mathbf{r}, t)$  and defines by the function  $\varphi_\alpha(\mathbf{r}, t)$ :

$$\varphi_\alpha(\mathbf{r}, t) = \frac{\bar{\rho}_\alpha(\mathbf{r}, t)}{\rho_\alpha(\mathbf{r}, t)}, \quad \alpha = 1, 2, \dots, n \quad (2.7)$$

Substituting into Eq. (2.5) yields:

$$m_\alpha = \int_{V_m(t)} \bar{\rho}_\alpha dV = \int_{V_m(t)} \rho_\alpha \varphi_\alpha dV \quad (2.8)$$

The new element of volume  $dV_\alpha := \varphi_\alpha dV$  is defined such that:

$$m_\alpha = \int_{V_m(t)} \bar{\rho}_\alpha dV = \int_{V_\alpha} \rho_\alpha dV_\alpha \quad (2.9)$$

The volume  $V_\alpha(t)$  is called the partial volume of  $\alpha$  and the function  $\varphi_\alpha(\mathbf{r}, t)$  the volume fraction of  $B_\alpha$  in the present configuration. Since the sum of the partial volumes give the total volume,  $\varphi_\alpha$  should obey the restriction:

$$\sum_{\alpha=1}^n \varphi_\alpha(\mathbf{r}, t) = 1 \quad (2.10)$$

We can distinguish two types of mixtures: homogeneous and heterogeneous. Homogeneous mixtures fulfil completely the condition of continuity for the material because the mixing between components occurs at the molecular level. Those mixtures are frequently called *solutions*. For homogeneous mixtures,  $\bar{\rho}_\alpha$  is the concentration of the component  $B_\alpha$ . In heterogeneous mixtures, the mixing of the components is at the macroscopic level, and for them to be considered as a continuum, the size of the integration volume  $V_m$  in the previous equations must be greater than that of the mixing level. These mixtures are also called *multiphase mixtures* because each component can be identified as a different phase. In these types of mixtures,  $\varphi_\alpha(\mathbf{r}, t)$  is a measure of the local structure of the mixture, and  $\bar{\rho}_\alpha$  is called the *bulk density*.

It is sometimes convenient to define another reference configuration for  $B_\alpha$ , such as  $\chi_{\alpha c}$ , with material volume  $V_c$ , that may or may not correspond to a certain instant in the motion of the mixture. The mass density of  $B_\alpha$  in this new reference configuration is denoted by  $\bar{\rho}_{\alpha c}$ , which is related to  $\bar{\rho}_{\alpha K}$  in the following way:

$$m_\alpha = \int_{V_c} \bar{\rho}_{\alpha c} dV = \int_{V_\kappa} \rho_{\alpha \kappa} dV_\alpha \quad (2.11)$$

### 2.1.2 Deformation and Motion

The position of the particle in space is denoted by the *material point*  $p_\alpha$  in the reference configuration  $\chi_{\alpha \kappa}$ :

$$\mathbf{R}_\alpha = \chi_{\alpha \kappa}(p_\alpha) \quad (2.12)$$

We assume that (2.12) has an inverse such that

$$p_\alpha = \chi_{\alpha \kappa}^{-1}(\mathbf{R}_\alpha) \quad (2.13)$$

The *motion* of  $p_\alpha \in B_\alpha$  is a continuous sequence of configurations over time:

$$\mathbf{r} = \chi_\alpha(p_\alpha, t), \quad \alpha = 1, 2, \dots, n \quad (2.14)$$

Substituting (2.13) into (2.14) yields:

$$\mathbf{r} = \mathbf{f}_\alpha(\mathbf{R}_\alpha, t) \quad (2.15)$$

where  $\mathbf{f}_\alpha$  is the *deformation function* of the  $\alpha$  component:

$$\mathbf{f}_\alpha = \chi_\alpha \circ \chi_{\alpha \kappa}^{-1} \quad (2.16)$$

We require  $\mathbf{f}_\alpha$  to be twice differentiable and to have an inverse, such that:

$$\mathbf{R}_\alpha = \mathbf{f}_\alpha^{-1}(\mathbf{r}, t) \quad (2.17)$$

For a given particle  $p_\alpha \in B_\alpha$ , that is, for a constant  $\mathbf{R}_\alpha$  and a variable  $t$ , the deformation function, Eq. (2.15), represents the trajectory of the particle in time, and for a constant time, the same equation represents the deformation of the body  $B_\alpha$  from the reference configuration  $\chi_{\alpha \kappa}$  to the current configuration  $\chi_{\alpha t}$ .

#### Spatial and material coordinates

The Cartesian components  $x_i$  of  $\mathbf{r}$  and  $X_i^\alpha$  of  $\mathbf{R}_\alpha$  are the *spatial* and *material* coordinates of  $p_\alpha$ :

$$\mathbf{r} = x_i \mathbf{e}_i \quad \text{and} \quad \mathbf{R}_\alpha = X_i^\alpha \mathbf{e}_i \quad (2.18)$$

Any property  $G_\alpha$  of the body  $B_\alpha$  can be described in terms of material or spatial coordinates. For  $G_\alpha(p_\alpha, t)$  we can write either:

$$G_\alpha = G_\alpha(\chi_{\alpha \kappa}^{-1}(\mathbf{R}_\alpha, t)) \equiv g_{\alpha 1}(\mathbf{R}_\alpha, t), \quad \text{or} \quad (2.19)$$

$$G_\alpha = G_\alpha(\chi_\alpha^{-1}(\mathbf{r}, t)) \equiv g_{\alpha 2}(\mathbf{r}, t) \quad (2.20)$$

Of course the properties  $g_{\alpha 1}(\mathbf{R}_\alpha, t)$  and  $g_{\alpha 2}(\mathbf{r}, t)$  are equivalent. We refer to the first notation as the *material property* and to the second as the *spatial property*  $G$  of the body  $B_\alpha$ .

Since the property  $G_\alpha$  is the function of two variables  $(\mathbf{R}_\alpha, t)$  or  $(\mathbf{r}, t)$ , it is possible to obtain the *partial derivatives of  $G$  with respect to each of these variables  $\mathbf{R}_\alpha$  or  $\mathbf{r}$* . The *gradient* of  $G_\alpha$  is the partial derivative of  $G_\alpha$  with respect to the space variable. Since there are two such variables, there will be two gradients:

$$\text{Material gradient} \quad \frac{\partial G_\alpha}{\partial \mathbf{R}_\alpha} = \frac{\partial(g_{\alpha 1}(\mathbf{R}_\alpha, t))}{\partial \mathbf{R}_\alpha} = \frac{\partial g_{\alpha 1}}{\partial X_i^\alpha} \mathbf{e}_i \equiv \text{grad} G_\alpha \quad (2.21)$$

$$\text{Spatial gradient} \quad \frac{\partial G_\alpha}{\partial \mathbf{r}} = \frac{\partial(g_{\alpha 2}(\mathbf{r}, t))}{\partial \mathbf{r}} = \frac{\partial g_{\alpha 2}}{\partial x_i} \mathbf{e}_i \equiv \text{grad} G_\alpha \equiv \nabla G_\alpha \quad (2.22)$$

In the same way, we can define material and spatial time derivatives of  $G_\alpha$ :

$$\text{Material derivative} \quad \left. \frac{\partial G_\alpha}{\partial t} \right|_{\mathbf{R}_\alpha} = \frac{\partial(g_{\alpha 1}(\mathbf{R}_\alpha, t))}{\partial t} = \left. \frac{\partial g_{\alpha 2}(\mathbf{r}, t)}{\partial t} \right|_{\mathbf{R}_\alpha} \equiv \frac{DG_\alpha}{Dt} \equiv \dot{G}_\alpha \quad (2.23)$$

$$\text{Spatial derivative} \quad \frac{\partial G_\alpha}{\partial t} = \frac{\partial g_{\alpha 2}(\mathbf{r}, t)}{\partial t} = \left. \frac{\partial g_{\alpha 1}(\mathbf{R}_\alpha, t)}{\partial t} \right|_{\mathbf{r}} \quad (2.24)$$

The material derivative represents the derivative of  $G_\alpha$  with respect to time holding the material point  $\mathbf{R}_\alpha$  fixed, while the spatial derivative is the derivative of  $G_\alpha$  with respect to time holding the place  $\mathbf{r}$  fixed.

The relationship between the material and the spatial derivatives is obtained by applying the chain rule of differentiation to Eq. (2.23):

$$\begin{aligned} \dot{G}_\alpha &= \left. \frac{\partial g_{\alpha 2}(\mathbf{r}, t)}{\partial t} \right|_{\mathbf{R}_\alpha} = \frac{\partial g_{\alpha 2}(\mathbf{r}, t)}{\partial t} + \frac{\partial g_{\alpha 2}(\mathbf{r}, t)}{\partial \mathbf{r}} \cdot \left. \frac{\partial \mathbf{r}}{\partial t} \right|_{\mathbf{R}_\alpha} \\ &= \frac{\partial g_{\alpha 2}}{\partial t} + \nabla g_{\alpha 2} \cdot \dot{\mathbf{r}} \\ &= \frac{\partial g_{\alpha 2}}{\partial t} + \nabla G_\alpha \cdot \dot{\mathbf{r}} \end{aligned} \quad (2.25)$$

where  $\dot{\mathbf{r}}$  (with a point above) is the material derivative of the deformation function  $\mathbf{r} = \mathbf{f}_\alpha(\mathbf{R}_\alpha, t)$ .

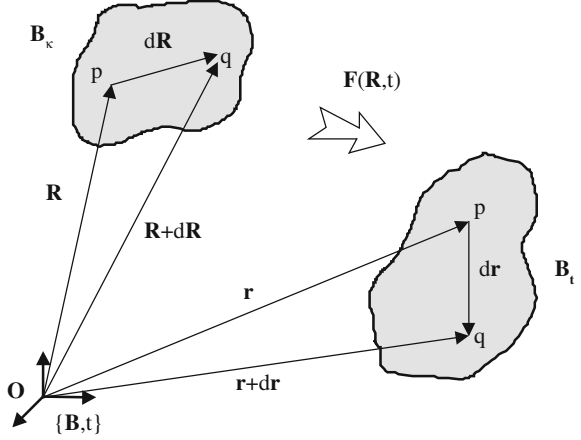
### Gradient of deformation tensor

Consider two particles  $p_\alpha, q_\alpha \in B_\alpha$  having the positions  $\mathbf{R}_\alpha$  and  $\mathbf{R}_\alpha + d\mathbf{R}_\alpha$  in the reference configuration; see Fig. 2.1. At time  $t$ , their positions are:

$$\mathbf{r} = \mathbf{f}_\alpha(\mathbf{R}_\alpha, t) \quad \text{and} \quad \mathbf{r} + d\mathbf{r} = \mathbf{f}_\alpha(\mathbf{R}_\alpha + d\mathbf{R}_\alpha, t) \quad (2.26)$$

The position of  $q_\alpha$  at time  $t$  can be approximated in the vicinity of  $\mathbf{r}$  by a linear function of  $d\mathbf{R}_\alpha$ :

**Fig. 2.1** Deformation of a body from the reference configuration  $B_{\kappa}$  to the present configuration  $B_t$



$$f_{\alpha}(\mathbf{R}_{\alpha} + d\mathbf{R}_{\alpha}, t) \approx f_{\alpha}(\mathbf{R}_{\alpha}, t) + \frac{\partial f_{\alpha}}{\partial \mathbf{R}_{\alpha}} \cdot d\mathbf{R}_{\alpha} \quad (2.27)$$

Then, from (2.26) and (2.27) we see that:

$$d\mathbf{r} = \frac{\partial f_{\alpha}}{\partial \mathbf{R}_{\alpha}} \cdot d\mathbf{R}_{\alpha} \quad (2.28)$$

The tensor  $\partial f_{\alpha} / \partial \mathbf{R}_{\alpha}$ , that approximates the deformation function of  $f_{\alpha}$  in the neighbourhood of  $\mathbf{r}$  is called the gradient of the *deformation tensor* of the  $\alpha$  component, and is denoted by:

$$\mathbf{F}_{\alpha}(\mathbf{R}_{\alpha}, t) = \frac{\partial f_{\alpha}(\mathbf{R}_{\alpha}, t)}{\partial \mathbf{R}_{\alpha}} = \text{grad } \mathbf{r} \quad (2.29)$$

To ensure the existence of an inverse,  $\det \mathbf{F}_{\alpha} \neq 0$ . In Cartesian and matrix notation the deformation tensor can be written in the form:

$$\mathbf{F}_{\alpha}(\mathbf{R}_{\alpha}, t) = \frac{\partial \mathbf{r}}{\partial \mathbf{R}_{\alpha}} = \mathbf{B}^T \begin{bmatrix} \frac{\partial x_1}{\partial X_1} & \frac{\partial x_1}{\partial X_2} & \frac{\partial x_1}{\partial X_3} \\ \frac{\partial x_2}{\partial X_1} & \frac{\partial x_2}{\partial X_2} & \frac{\partial x_2}{\partial X_3} \\ \frac{\partial x_3}{\partial X_1} & \frac{\partial x_3}{\partial X_2} & \frac{\partial x_3}{\partial X_3} \end{bmatrix} \mathbf{B} \quad (2.30)$$

where  $\mathbf{B}$  is the basis of orthogonal unit vectors.

Equation (2.28) represents the transformation of a line element  $d\mathbf{R}_{\alpha}$  from the reference configuration to the present configuration  $d\mathbf{r}$ :

$$d\mathbf{r} = \mathbf{F}_{\alpha}(\mathbf{R}_{\alpha}, t) \cdot d\mathbf{R}_{\alpha} \quad (2.31)$$

A deformation is called homogeneous if  $\mathbf{F}_{\alpha}$  is independent of  $\mathbf{R}_{\alpha}$ .

### Change of reference configuration

The deformation quantified by  $F_\alpha(\mathbf{R}_\alpha, t)$  depends on the reference configuration chosen. Since this reference configuration is arbitrary, it is convenient to know how a change of reference configuration affects  $F_\alpha$ .

Consider two reference configurations  $B_{\alpha K}$  and  $B_{\alpha C}$ , and the actual configuration  $B_{\alpha I}$  of the body  $B_\alpha$ . Call  $F_{\alpha K}$ ,  $F_{\alpha C}$  and  $P_\alpha$  the gradient of deformation tensors to go from  $B_{\alpha K}$  to  $B_{\alpha I}$ , from  $B_{\alpha C}$  to  $B_{\alpha I}$  and  $B_{\alpha K}$  to  $B_{\alpha C}$  respectively; see Fig. 2.2. We can write:

$$d\mathbf{r} = \mathbf{F}_{\alpha K} \cdot d\mathbf{R}_{\alpha K} = \mathbf{F}_{\alpha C} \cdot d\mathbf{R}_{\alpha C} \quad \text{and} \quad d\mathbf{R}_{\alpha C} = \mathbf{P}_\alpha \cdot d\mathbf{R}_{\alpha K}$$

$$\text{Then} \quad d\mathbf{r} = \mathbf{F}_{\alpha K} \cdot d\mathbf{R}_{\alpha K} = \mathbf{F} \circ (\mathbf{P}_\alpha \cdot d\mathbf{R}_{\alpha K}),$$

$$\text{and therefore} \quad \mathbf{F}_{\alpha K} = \mathbf{F}_{\alpha C} \circ \mathbf{P}_\alpha \quad (2.32)$$

### Dilatation

Consider an element of material volume  $dV_{\alpha K}$  in the form of a parallelepiped in the reference configuration; see Fig. 2.3, then:

$$dV_{\alpha K} = d\mathbf{R}_{\alpha 1} \cdot d\mathbf{R}_{\alpha 2} \times d\mathbf{R}_{\alpha 3} \equiv [d\mathbf{R}_{\alpha 1}, d\mathbf{R}_{\alpha 2}, d\mathbf{R}_{\alpha 3}]$$

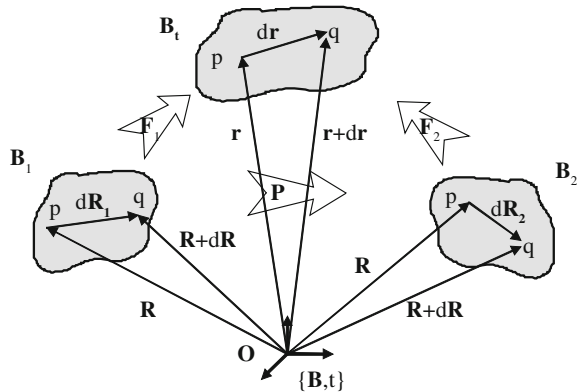
After the deformation, the volume becomes:

$$dV_m = d\mathbf{r}_1 \cdot d\mathbf{r}_2 \times d\mathbf{r}_3 \equiv [d\mathbf{r}_1, d\mathbf{r}_2, d\mathbf{r}_3]$$

Using (2.31):

$$\begin{aligned} dV_m &= [\mathbf{F}_{\alpha 1} \cdot d\mathbf{R}_{\alpha 1}, \mathbf{F}_{\alpha 2} \cdot d\mathbf{R}_{\alpha 2}, \mathbf{F}_{\alpha 3} \cdot d\mathbf{R}_{\alpha 3}] \\ &= \det \mathbf{F}_\alpha [d\mathbf{R}_{\alpha 1}, d\mathbf{R}_{\alpha 2}, d\mathbf{R}_{\alpha 3}] \\ &= \det \mathbf{F}_\alpha dV_{\alpha K} \end{aligned} \quad (2.33)$$

**Fig. 2.2** Change of reference configuration



The quotient between the elements of volume before and after the deformation is called the *dilatation* of the body and is denoted by  $J_\alpha$ , then:

$$J_\alpha = \det \mathbf{F}_\alpha \quad (2.34)$$

The physical meaning of dilatation, expressed by (2.33), shows that  $\det \mathbf{F}_\alpha \geq 0$ .

### Rigid deformation

A special type of deformation is the *rigid deformation* defined as a deformation in which the distances between the particles in a body do not change. Consider two particles  $p_\alpha, q_\alpha \in B_\alpha$  which, during the deformation, maintain their distance. Call  $d\mathbf{R}_\alpha = ds_{\alpha\kappa} \mathbf{e}_\kappa$  and  $d\mathbf{r} = ds \mathbf{e}$ , refer to Fig. 2.1 and write:

$$\begin{aligned} d_{\alpha s}^2 - ds_{\alpha\kappa}^2 &= 0 \\ d\mathbf{r} \cdot d\mathbf{r} - d\mathbf{R}_\alpha \cdot d\mathbf{R}_\alpha &= 0 \\ (\mathbf{F}_\alpha \cdot d\mathbf{R}_\alpha)(\mathbf{F}_\alpha \cdot d\mathbf{R}_\alpha) - d\mathbf{R}_\alpha \cdot \mathbf{I} \cdot d\mathbf{R}_\alpha &= 0 \\ d\mathbf{R}_\alpha \cdot (\mathbf{F}_\alpha^T \cdot \mathbf{F}_\alpha - \mathbf{I}) \cdot d\mathbf{R}_\alpha &= 0 \end{aligned}$$

Therefore, a rigid deformation should obey:

$$\mathbf{F}_\alpha^T \cdot \mathbf{F}_\alpha = \mathbf{I} \quad (2.35)$$

There are two cases for which (2.35) is valid: if  $\mathbf{F}_\alpha = \mathbf{I}$ , which represents a *translation*, and  $\mathbf{F}_\alpha = \mathbf{Q}_\alpha$ , **which is a rotation**.

### Stretching

Since for the deformation function  $\mathbf{f}_\alpha(\mathbf{R}_\alpha, t)$ ,  $\det \mathbf{F}_\alpha \geq 0$ , the polar decomposition (Gurtin 1981) may be applied to  $\mathbf{f}_\alpha$ :

$$\mathbf{F}_\alpha = \mathbf{Q}_\alpha \cdot \mathbf{U}_\alpha = \mathbf{V}$$

Then,

$$\mathbf{U}_\alpha^2 = \mathbf{F}_\alpha^T \cdot \mathbf{F}_\alpha = \mathbf{C}_\alpha \quad \text{and} \quad \mathbf{V}_\alpha^2 = \mathbf{F}_\alpha \cdot \mathbf{F}_\alpha^2 = \mathbf{B}_\alpha \quad (2.37)$$

Since  $\mathbf{U}_\alpha$  and  $\mathbf{V}_\alpha$  are symmetric and positive definite tensors and  $\mathbf{Q}_\alpha$  is an orthogonal tensor, it can be shown that the characteristic values of  $\mathbf{U}_\alpha$  and  $\mathbf{V}_\alpha$  are the same:

$$\mathbf{U}_\alpha = \sum_{k=1}^n \lambda_k \mathbf{u}_k \mathbf{u}_k \quad \text{and} \quad \mathbf{V}_\alpha = \sum_{k=1}^n \lambda_k \mathbf{v}_k \mathbf{v}_k \quad (2.38)$$

and that the characteristic vectors are related by de rotation:

$$\mathbf{v}_k = \mathbf{Q}_\alpha \cdot \mathbf{u}_k \quad (2.39)$$

### Velocity and acceleration

The velocity and acceleration of a particle  $p_\alpha \in B_\alpha$  are the first and second material derivatives of the deformation function  $\mathbf{r} = \mathbf{f}_\alpha(\mathbf{R}_\alpha, t)$ :

$$\mathbf{v}_\alpha = \frac{D\mathbf{f}_\alpha(\mathbf{R}_\alpha, t)}{Dt} = \frac{D_\alpha \mathbf{r}}{Dt} = \dot{\mathbf{r}}(\mathbf{R}_\alpha, t) \quad (2.40)$$

$$\mathbf{a}_\alpha = \dot{\mathbf{v}}_\alpha = \frac{D_\alpha \mathbf{v}_\alpha}{Dt} = \frac{D_\alpha^2 \mathbf{r}}{Dt^2} \quad (2.41)$$

If the flow field is expressed in spatial coordinates, the acceleration is:

$$\mathbf{a}_\alpha = \frac{D_\alpha \mathbf{v}_\alpha}{Dt} = \left. \frac{\partial \mathbf{v}_\alpha(\mathbf{R}_\alpha, t)}{\partial t} \right|_{\mathbf{r}} + \frac{\partial \mathbf{v}_\alpha(\mathbf{R}_\alpha, t)}{\partial \mathbf{r}} \cdot \frac{\partial \mathbf{r}(\mathbf{R}_\alpha, t)}{\partial t} = \frac{\partial \mathbf{v}_\alpha}{\partial t} + \nabla \mathbf{v}_\alpha \cdot \mathbf{v}_\alpha \quad (2.42)$$

### Velocity gradient: rate of dilatation, stretching and spin

Consider two particles  $p_\alpha, q_\alpha \in B_\alpha$ . If  $p_\alpha$  has a velocity of  $\mathbf{v}_\alpha(\mathbf{r}, t)$ , the velocity  $\mathbf{v}_\alpha(\mathbf{r} + d\mathbf{r}, t)$  of  $q_\alpha$ , can be approximated by:

$$\mathbf{v}_\alpha(\mathbf{r} + d\mathbf{r}, t) = \mathbf{v}_\alpha(\mathbf{r}, t) + \frac{\partial \mathbf{v}_\alpha(\mathbf{r}, t)}{\partial \mathbf{r}} \cdot d\mathbf{r} \quad (2.43)$$

Since  $\mathbf{v}_\alpha(\mathbf{r} + d\mathbf{r}, t) = \mathbf{v}_\alpha(\mathbf{r}, t) + d\mathbf{v}_\alpha$ , in analogy to [2.26–2.28](#),

$$d\mathbf{v}_\alpha = \frac{\partial \mathbf{v}_\alpha(\mathbf{r}, t)}{\partial \mathbf{r}} \cdot d\mathbf{r} \equiv \mathbf{L}_\alpha(\mathbf{r}, t) \cdot d\mathbf{r} \quad (2.44)$$

The linear function  $\mathbf{L}_\alpha := \partial \mathbf{v}_\alpha / \partial \mathbf{r}$  is called the *velocity gradient tensor*. In Cartesian tensor and matrix notations  $\mathbf{L}_\alpha$  can be written in the form:

$$\mathbf{L}_\alpha = \nabla \mathbf{v}_\alpha = \frac{\partial v_{\alpha i}}{\partial x_j} \mathbf{e}_i \mathbf{e}_j = \mathbf{B}^T \begin{bmatrix} \frac{\partial v_{\alpha 1}}{\partial x_1} & \frac{\partial v_{\alpha 1}}{\partial x_2} & \frac{\partial v_{\alpha 1}}{\partial x_3} \\ \frac{\partial v_{\alpha 2}}{\partial x_1} & \frac{\partial v_{\alpha 2}}{\partial x_2} & \frac{\partial v_{\alpha 2}}{\partial x_3} \\ \frac{\partial v_{\alpha 3}}{\partial x_1} & \frac{\partial v_{\alpha 3}}{\partial x_2} & \frac{\partial v_{\alpha 3}}{\partial x_3} \end{bmatrix} \mathbf{B} \quad (2.45)$$

The relationship between  $\mathbf{L}_\alpha$  and  $\mathbf{F}_\alpha$  can be obtained by calculating  $\dot{\mathbf{v}}_\alpha = d\dot{\mathbf{r}}$  from Eq. (2.31):

$$\begin{aligned} d\dot{\mathbf{v}} &= d\dot{\mathbf{r}} = \frac{D}{Dt}(\mathbf{F}_\alpha \cdot d\mathbf{R}_\alpha) \\ &= \dot{\mathbf{F}}_\alpha \cdot d\mathbf{R}_\alpha = \dot{\mathbf{F}}_\alpha \cdot \mathbf{F}_\alpha^{-1} d\mathbf{r} \\ &= \mathbf{L}_\alpha \cdot d\mathbf{r} \end{aligned}$$

Therefore:

$$\mathbf{L}_\alpha = \dot{\mathbf{F}}_\alpha \mathbf{F}_\alpha^{-1} \quad (2.46)$$

The velocity gradient can be separated into three irreducible parts, which are mutually orthogonal:

$$\mathbf{L}_\alpha = \underbrace{\frac{1}{3}(\text{tr } \mathbf{L}_\alpha) \mathbf{I}}_{\text{Rate of expansion or rate of dilatation tensor.}} + \underbrace{\left\{ \frac{1}{2}(\mathbf{L}_\alpha + \mathbf{L}_\alpha^T) - \frac{1}{3}(\text{tr } \mathbf{L}_\alpha) \mathbf{I} \right\}}_{\text{Rate of shear tensor or stretching tensor.}} + \underbrace{\frac{1}{2}(\mathbf{L}_\alpha - \mathbf{L}_\alpha^T)}_{\text{Rate of rotation tensor or spin tensor.}} \quad (2.47)$$

To show that  $\text{tr } \mathbf{L}_\alpha$  represents the rate of dilatation, calculate the following:

$$\begin{aligned} \text{tr } \mathbf{L}_\alpha &= \text{tr } \nabla \mathbf{v}_\alpha = \frac{\partial v_{\alpha i}}{\partial x_i} \\ &= \nabla \cdot \mathbf{v}_\alpha \end{aligned}$$

On the other hand, take the derivative of the dilatation  $J(\mathbf{r}, t)$ :

$$\begin{aligned} \dot{J}_\alpha &= \frac{D}{Dt}(\det \mathbf{F}_\alpha) \\ &= \det \mathbf{F}_\alpha \text{tr } (\dot{\mathbf{F}}_\alpha \mathbf{F}_\alpha^{-1}) \\ &= \det \mathbf{F}_\alpha \text{tr } \mathbf{L}_\alpha \end{aligned} \quad (2.48)$$

From (2.48) we can write:

$$\text{tr } \mathbf{L}_\alpha = \nabla \cdot \mathbf{v}_\alpha = \frac{\dot{J}}{J} \quad (2.49)$$

Equation (2.49) shows that  $\text{tr } \mathbf{L}_\alpha$  and  $\nabla \cdot \mathbf{v}_\alpha$  have the meaning of *rate of dilatation per unit of dilatation*.

Defining the following terms:

$$\text{Rate of expansion tensor: } \mathbf{L}_{\alpha E} = \frac{1}{3}(\text{tr } \mathbf{L}_\alpha) \mathbf{I} \quad (2.50)$$

$$\text{Rate of shear(stretching:)} \quad \mathbf{D}_\alpha = \left\{ \frac{1}{2}(\mathbf{L}_\alpha + \mathbf{L}_\alpha^T) - \frac{1}{3}(\text{tr } \mathbf{L}_\alpha) \mathbf{I} \right\} \quad (2.51)$$

$$\text{Rate of rotation(spin:)} \quad \mathbf{W}_\alpha = \frac{1}{2}(\mathbf{L}_\alpha - \mathbf{L}_\alpha^T)$$

Equation (2.47) may be written in the form:

$$\begin{array}{ccccccc} \mathbf{L}_\alpha & = & \mathbf{L}_{\alpha E} & + & \mathbf{D}_\alpha & + & \mathbf{W}_\alpha \\ \text{Velocity gradient} & & \text{Rate of expansion} & & \text{Rate of shear tensor} & & \text{Rate of rotation tensor} \\ \text{tensor} & & \text{or rate of dilatation} & & \text{or stretching tensor.} & & \text{or spin tensor.} \\ & & \text{tensor.} & & & & \end{array} \quad (2.52)$$

### 2.1.3 Mass Balance

Let the rate of mass transfer, *per unit volume*, from all other components to  $B_\alpha$  be denoted by  $\bar{g}_\alpha(\mathbf{r}, t)$ . This term  $\bar{g}_\alpha(\mathbf{r}, t)$  receives the name of *mass growth rate* of the  $\alpha$  component. The following balance must be obeyed:

$$\begin{array}{ccc} \frac{d}{dt} \int_{V_m} \bar{\rho}_\alpha dV & = & \int_{V_m} \bar{g}_\alpha dV \\ \text{Mass rate of change of} & & \text{Net rate of generation of} \\ \text{the } \alpha \text{ component in } V_m & & \text{the } \alpha \text{ component in } V_m \end{array} \quad (2.53)$$

where  $dV$  is an element of material volume  $V_m$  of  $B_\alpha$ . Taking the left side of (2.53) to reference configuration yields:

$$\begin{aligned}
\frac{d}{dt} \int_{V_m} \bar{\rho}_\alpha dV &= \int_{V_\kappa} \frac{D}{Dt} (\bar{\rho}_\alpha J_\alpha) dV \\
&= \int_{V_\kappa} (\dot{\bar{\rho}}_\alpha J_\alpha + \bar{\rho}_\alpha \dot{J}_\alpha) dV \\
&= \int_{V_\kappa} (\dot{\bar{\rho}}_\alpha + \bar{\rho}_\alpha \nabla \cdot \mathbf{v}_\alpha) J_\alpha dV \\
&= \int_{V_m} \left( \frac{\partial \bar{\rho}_\alpha}{\partial t} + \nabla \cdot \bar{\rho}_\alpha \mathbf{v}_\alpha \right) dV \\
&= \int_{V_m} \frac{\partial \bar{\rho}_\alpha}{\partial t} dV + \int_{V_m} \nabla \cdot \bar{\rho}_\alpha \mathbf{v}_\alpha dV \\
&= \int_{V_m} \frac{\partial \bar{\rho}_\alpha}{\partial t} dV + \oint_{S_m} \bar{\rho}_\alpha \mathbf{v}_\alpha \cdot \mathbf{n} dV
\end{aligned} \tag{2.54}$$

Substituting in (2.53) gives a new form of the mass balance of  $B_\alpha$ :

$$\int_{V_m} \frac{\partial \bar{\rho}_\alpha}{\partial t} dV + \oint_{S_m} \bar{\rho}_\alpha (\mathbf{v}_\alpha \cdot \mathbf{n}) dV = \int_{V_m} \bar{g}_\alpha dV \tag{2.55}$$

On the other hand, both volume integrals in (2.53) maybe taken to the reference configuration to obtain:

$$\int_{V_\kappa} \left( \frac{D}{Dt} (\bar{\rho}_\alpha J_\alpha) - \bar{g}_\alpha J_\alpha \right) dV = 0 \tag{2.56}$$

Performing the material derivative:

$$\begin{aligned}
\int_{V_\kappa} (\dot{\bar{\rho}}_\alpha J_\alpha + \bar{\rho}_\alpha \dot{J}_\alpha - \bar{g}_\alpha J_\alpha) dV &= 0 \\
\int_{V_\kappa} (\dot{\bar{\rho}}_\alpha J_\alpha + \bar{\rho}_\alpha \nabla \cdot \mathbf{v}_\alpha J_\alpha - \bar{g}_\alpha J_\alpha) dV &= 0 \\
\int_{V_\kappa} (\dot{\bar{\rho}}_\alpha + \bar{\rho}_\alpha \nabla \cdot \mathbf{v}_\alpha - \bar{g}_\alpha) J_\alpha dV &= 0 \\
\int_{V_m} (\dot{\bar{\rho}}_\alpha + \bar{\rho}_\alpha \nabla \cdot \mathbf{v}_\alpha - \bar{g}_\alpha) dV &= 0
\end{aligned}$$

Using the localization theorem (Gurtin 1981) yields:

$$\dot{\bar{\rho}}_\alpha + \bar{\rho}_\alpha \nabla \cdot \mathbf{v}_\alpha = \bar{g}_\alpha \tag{2.57}$$

Writing the material derivative in terms of the spatial derivative and combining the result with the second term of Eq. (2.57) gives:

$$\frac{\partial \bar{\rho}_\alpha}{\partial t} + \nabla \cdot \bar{\rho}_\alpha \mathbf{v}_\alpha = \bar{g}_\alpha \tag{2.58}$$

Equations (2.57) or (2.58) receive the name of *continuity equation*. The last one has a *conservation form*.

Going back to Eq. (2.56), the localization theorem is used directly on this equation to give:

$$\frac{D}{Dt}(\bar{\rho}_\alpha J_\alpha) = \bar{g}_\alpha J_\alpha \quad (2.59)$$

This expression divided by  $\bar{\rho}_\alpha J_\alpha$  represent the rate *by unit mass* of growth of the mass of the  $\alpha$  component, and is denoted by  $\hat{g}_\alpha = \bar{g}_\alpha / \bar{\rho}_\alpha$ . Integrate with boundary condition  $\bar{\rho}_\alpha(\mathbf{R}_\alpha) = \bar{\rho}_{\alpha\kappa}$  to give:

$$\bar{\rho}_\alpha J_\alpha = \bar{\rho}_{\alpha\kappa} \exp\left(\int_{t_\kappa}^t \hat{g}_\alpha(\tau) d\tau\right) \quad (2.60)$$

In those cases in which there is no mass transfer between components,  $\hat{g}_\alpha = 0$ , Eq. (2.60) reduces to:

$$\bar{\rho}_\alpha J_\alpha = \bar{\rho}_{\alpha\kappa} \quad (2.61)$$

Equation (2.61) is the local mass balance for a body  $B_\alpha$  that deforms from the reference to the actual configuration.

Taking the material derivative of (2.59) we can obtain the continuity equation:

$$\begin{aligned} \dot{\bar{\rho}}_\alpha J_\alpha + \bar{\rho}_\alpha \dot{J}_\alpha &= J_\alpha \bar{g}_\alpha \\ \dot{\bar{\rho}}_\alpha J_\alpha + \bar{\rho}_\alpha \nabla \cdot \mathbf{v}_\alpha J_\alpha &= J_\alpha \bar{g}_\alpha \\ \dot{\bar{\rho}}_\alpha + \bar{\rho}_\alpha \nabla \cdot \mathbf{v}_\alpha &= \bar{g}_\alpha \end{aligned} \quad (2.62)$$

Check this equation with (2.57).

### Mass balance in a discontinuity

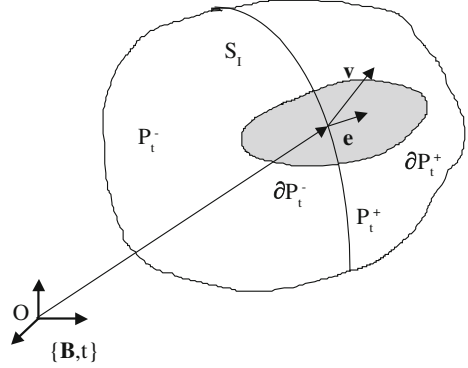
For bodies having discontinuities, the local mass balance equations are not valid. In these cases, it is necessary to analyze the macroscopic mass balance further. Consider a body  $B_\alpha \in B$  having a surface of discontinuity  $S_I$  that separates the body into two parts  $B_\alpha^+$  and  $B_\alpha^-$  in the actual configuration; see Fig. 2.4. The following conditions hold:

$$V_m = V^+ + V^-, \quad S_m = S^+ + S^-, \quad S_I = B_\alpha^+ \cap B_\alpha^- \quad (2.63)$$

Applying the macroscopic balance (2.55) to each side of the body, and noting that the surface of discontinuity is not a material surface, yields:

$$\begin{aligned} \int_{V^+} \frac{\partial \bar{\rho}_\alpha}{\partial t} dV + \int_{V^-} \frac{\partial \bar{\rho}_\alpha}{\partial t} dV + \int_{S^+} \bar{\rho}_\alpha (\mathbf{v}_\alpha \cdot \mathbf{n}) dS + \int_{S_I} \bar{\rho}_\alpha^+ (\mathbf{v}_\alpha^+ - \mathbf{v}_I) \cdot (-\mathbf{e}_I) dS \\ + \int_{S^-} \bar{\rho}_\alpha (\mathbf{v}_\alpha \cdot \mathbf{n}) dS + \int_{S_I} \bar{\rho}_\alpha^- (\mathbf{v}_\alpha^- - \mathbf{v}_I) \cdot \mathbf{e}_I dS = \int_{V^+} \bar{g}_\alpha dV + \int_{V^-} \bar{g}_\alpha dV \end{aligned}$$

**Fig. 2.4** Body  $B_\alpha$  with a surface of discontinuity



Adding the volume and surface integrals and using (2.63), we have:

$$\begin{aligned} \int_{V_m} \frac{\partial \bar{\rho}_\alpha}{\partial t} dV + \int_{S_m} \bar{\rho}_\alpha (\mathbf{v}_\alpha \cdot \mathbf{n}) dS - \int_{S_I} (\bar{\rho}_\alpha^+ (\mathbf{v}_\alpha^+ - \mathbf{v}_I) - \bar{\rho}_\alpha^- (\mathbf{v}_\alpha^- - \mathbf{v}_I)) \cdot \mathbf{e}_I dS \\ = \int_{V^+} \bar{g}_\alpha dV + \int_{V^-} \bar{g}_\alpha dV \end{aligned}$$

Using Eq. (2.55), the previous equation reduces to:

$$\begin{aligned} \int_{S_I} (\bar{\rho}_\alpha^+ (\mathbf{v}_\alpha^+ - \mathbf{v}_I) - \bar{\rho}_\alpha^- (\mathbf{v}_\alpha^- - \mathbf{v}_I)) \cdot \mathbf{e}_I dS = 0 \\ \int_{S_I} [\bar{\rho}_\alpha (\mathbf{v}_\alpha - \mathbf{v}_I) \cdot \mathbf{e}_I] dS = 0 \end{aligned}$$

where the jump of a property  $G$  is defined as  $[G] = G^+ - G^-$ . This equation is called the *macroscopic mass jump balance* at a discontinuity. Using the localization theorem in the previous equation, we obtain the *local mass jump balance* at a discontinuity:

$$[\bar{\rho}_\alpha (\mathbf{v}_\alpha - \mathbf{v}_I) \cdot \mathbf{e}_I] = 0 \quad (2.64)$$

This equation can also be written in the following form called the *Rankin-Hugoniot* jump condition (Bustos et al. 1999):

$$\sigma = \frac{[\bar{\rho}_\alpha \mathbf{v}_\alpha \cdot \mathbf{e}_I]}{[\bar{\rho}_\alpha]} \quad (2.65)$$

where  $\sigma = \mathbf{v}_I \cdot \mathbf{e}_I$  is the displacement velocity of the discontinuity.

### Average properties of the mixture

Adding the continuity Eq. (2.58) and the mass jump balance (2.65) for all components, those properties for the mixture may be obtained:

$$\frac{\partial}{\partial t} \left( \sum_{\alpha=1}^n \bar{\rho}_{\alpha} \right) + \nabla \cdot \sum_{\alpha=1}^n \bar{\rho}_{\alpha} \mathbf{v}_{\alpha} = \sum_{\alpha=1}^n \bar{g}_{\alpha} \quad (2.66)$$

$$\sigma = \frac{\left[ \sum_{\alpha=1}^n \bar{\rho}_{\alpha} \mathbf{v}_{\alpha} \cdot \mathbf{e}_I \right]}{\left[ \sum_{\alpha=1}^n \bar{\rho}_{\alpha} \right]} \quad (2.67)$$

According to the initial postulates, the mixture should follow the laws of a pure material; therefore, the continuity equation and the mass jump condition for the mixture should be:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \rho \mathbf{v} = 0 \quad (2.68)$$

$$\sigma = \frac{[\rho \mathbf{v} \cdot \mathbf{e}_I]}{[\rho]} \quad (2.69)$$

where  $\rho$  and  $\mathbf{v}$  are the *mass density* and *mass average* or *convective velocity* of the mixture. Comparing Eqs. (2.66) and (2.67) with (2.68) and (2.69) respectively, we deduce the following definitions for the mixture properties:

$$\text{Mass density} \quad \rho = \sum_{\alpha=1}^n \bar{\rho}_{\alpha} \quad (2.70)$$

$$\text{Mass average velocity} \quad \mathbf{v} = \frac{\sum_{\alpha=1}^n \bar{\rho}_{\alpha} \mathbf{v}_{\alpha}}{\sum_{\alpha=1}^n \bar{\rho}_{\alpha}} = \frac{\sum_{\alpha=1}^n \bar{\rho}_{\alpha} \mathbf{v}_{\alpha}}{\rho} \quad (2.71)$$

$$\text{Mass growth rate} \quad \sum_{\alpha=1}^n \bar{g}_{\alpha} = 0 \quad (2.72)$$

This last equation indicates that no net production of mass occurs.

### Convective diffusion equation

Sometimes it is convenient to express the continuity equation of each component in terms of the *convective mass flux density*  $\mathbf{j}_{\alpha C} = \bar{\rho}_{\alpha} \mathbf{v}_{\alpha}$  of that component. Adding and subtracting the convective flux per unit volume  $\nabla \cdot \bar{\rho}_{\alpha} \mathbf{v}$ , yields:

$$\frac{\partial \bar{\rho}_{\alpha}}{\partial t} + \nabla \cdot \bar{\rho}_{\alpha} \mathbf{v} = -\nabla \cdot \bar{\rho}_{\alpha} (\mathbf{v}_{\alpha} - \mathbf{v}) + \bar{g}_{\alpha}$$

Defining the diffusive flux density by  $\mathbf{j}_{\alpha D} := \bar{\rho}_{\alpha} (\mathbf{v}_{\alpha} - \mathbf{v}) = \bar{\rho}_{\alpha} \mathbf{u}_{\alpha}$ , where  $\mathbf{u}_{\alpha} = \mathbf{v}_{\alpha} - \mathbf{v}$  is the diffusion velocity, we can write:

$$\frac{\partial \bar{\rho}_\alpha}{\partial t} + \nabla \cdot \bar{\rho}_\alpha \mathbf{v} = -\nabla \cdot \bar{\rho}_\alpha (\mathbf{v}_\alpha - \mathbf{u}_\alpha) + \bar{g}_\alpha \quad (2.73)$$

Summing this equation over  $\alpha$  yields.

$$\frac{\partial}{\partial t} \left( \sum_{\alpha=1}^n \bar{\rho}_\alpha \right) + \left( \nabla \cdot \sum_{\alpha=1}^n \bar{\rho}_\alpha \mathbf{v} \right) = -\nabla \cdot (\bar{\rho}_\alpha \mathbf{u}_\alpha) + \sum_{\alpha=1}^n \bar{g}_\alpha$$

Using the definitions (2.70)–(2.72), gives:

$$\sum_{\alpha=1}^n j_{\alpha D} = \sum_{\alpha=1}^n \bar{\rho}_\alpha \mathbf{u}_\alpha = 0 \quad (2.74)$$

### Mass balance for incompressible mixtures

Incompressible mixtures are those having incompressible components, realizing that the mixture itself can be compressible, because the volume fraction of the components may be changing.

Using the concept of volume fraction given in (2.7), the continuity equation can be written in the form:

$$\frac{\partial}{\partial t} (\bar{\rho}_\alpha \varphi_\alpha) + \nabla \cdot (\bar{\rho}_\alpha \varphi_\alpha \mathbf{v}_\alpha) = \bar{g}_\alpha \quad (2.75)$$

$$\sigma = \frac{[\bar{\rho}_\alpha \varphi_\alpha \mathbf{v}_\alpha \cdot \mathbf{e}_I]}{[\bar{\rho}_\alpha \varphi_\alpha]} \quad (2.76)$$

Since, for an incompressible component  $\rho_\alpha$  is constant, dividing by  $\rho_\alpha$  the mass balances become volume balances:

$$\frac{\partial \varphi_\alpha}{\partial t} + \nabla \cdot (\varphi_\alpha \mathbf{v}_\alpha) = \hat{g}_\alpha \varphi_\alpha, \quad \sigma = \frac{[\varphi_\alpha \mathbf{v}_\alpha \cdot \mathbf{e}_I]}{[\varphi_\alpha]} \quad (2.77)$$

Summing all components yields:

$$\frac{\partial}{\partial t} \left( \sum_{\alpha=1}^n \varphi_\alpha \right) + \nabla \cdot \left( \sum_{\alpha=1}^n \varphi_\alpha \mathbf{v}_\alpha \right) = \sum_{\alpha=1}^n \hat{g}_\alpha \varphi_\alpha \quad \sigma = \frac{\left[ \sum_{\alpha=1}^n \varphi_\alpha \mathbf{v}_\alpha \cdot \mathbf{e}_I \right]}{\left[ \sum_{\alpha=1}^n \varphi_\alpha \right]} \quad (2.78)$$

Using the restriction  $\sum_{\alpha=1}^n \varphi_\alpha = 1$ , and defining the volume average velocity  $\mathbf{q}$  by :

$$\mathbf{q} = \sum_{\alpha=1}^n \varphi_\alpha \mathbf{v}_\alpha, \quad (2.79)$$

the mass balance equation and the mass jump condition for the mixture become:

$$\nabla \cdot \mathbf{q} = \sum_{\alpha=1}^n \widehat{g}_\alpha \varphi_\alpha \quad [\mathbf{q} \cdot \mathbf{e}_I] = 0 \quad (2.80)$$

The last equation shows that the volume average velocity suffers no jump across a surface of discontinuity.

## 2.2 Dynamical Processes

### 2.2.1 Linear Momentum Balance

Applying the axiom of linear momentum and the Cauchy stress principle to each body  $B_\alpha$ , we arrive to the *macroscopic balance of linear momentum*:

$$\underbrace{\frac{d}{dt} \int_{V_m} \bar{\rho}_\alpha \mathbf{v}_\alpha dV}_{\text{Rate of change of linear momentum of } B_\alpha} = \underbrace{\int_{S_m} \mathbf{T}_\alpha \cdot \mathbf{n} dS}_{\text{Diffusive flux of linear momentum in } B_\alpha} + \underbrace{\int_{V_m} (\mathbf{b}_\alpha + \mathbf{m}_\alpha + \bar{g}_\alpha \mathbf{v}_\alpha) dV}_{\text{Source of linear momentum due to body forces, interaction forces and mass generation.}} \quad (2.81)$$

where  $\mathbf{T}_\alpha$  is the stress tensor field, called *partial stress* and  $\mathbf{b}_\alpha$  is the body force on  $B_\alpha$ ,  $\mathbf{m}_\alpha$  is the interaction force between components, that is, the force by unit volume exerted on  $B_\alpha$  by all other components and  $\bar{g}_\alpha$  is the rate of mass growth, as defined earlier.

Using the Green-Gauss-Ostrogradsky (GGO) theorem on the surface integral yields:

$$\frac{d}{dt} \int_{V_m} \bar{\rho}_\alpha \mathbf{v}_\alpha dV = \int_{V_m} (\nabla \cdot \mathbf{T}_\alpha + \mathbf{b}_\alpha + \mathbf{m}_\alpha + \bar{g}_\alpha \mathbf{v}_\alpha) dV$$

Making a change of reference configuration on the left-hand side and taking the material derivative:

$$\begin{aligned} \int_{V_{\alpha\kappa}} \left( J_\alpha \frac{D}{Dt} (\bar{\rho}_\alpha \mathbf{v}_\alpha) + \bar{\rho}_\alpha \mathbf{v}_\alpha \frac{DJ_\alpha}{Dt} \right) dV &= \int_{V_m} (\nabla \cdot \mathbf{T}_\alpha + \mathbf{b}_\alpha + \mathbf{m}_\alpha + \bar{g}_\alpha \mathbf{v}_\alpha) dV \\ \int_{V_{\alpha\kappa}} \left( \frac{D}{Dt} (\bar{\rho}_\alpha \mathbf{v}_\alpha) + \bar{\rho}_\alpha \mathbf{v}_\alpha \nabla \cdot \mathbf{v}_\alpha \right) J_\alpha dV &= \int_{V_m} (\nabla \cdot \mathbf{T}_\alpha + \mathbf{b}_\alpha + \mathbf{m}_\alpha + \bar{g}_\alpha \mathbf{v}_\alpha) dV \quad (2.82) \\ \int_{V_m} \left( \frac{D}{Dt} (\bar{\rho}_\alpha \mathbf{v}_\alpha) + \bar{\rho}_\alpha \mathbf{v}_\alpha \nabla \cdot \mathbf{v}_\alpha \right) dV &= \int_{V_m} (\nabla \cdot \mathbf{T}_\alpha + \mathbf{b}_\alpha + \mathbf{m}_\alpha + \bar{g}_\alpha \mathbf{v}_\alpha) dV \end{aligned}$$

Changing the material to spatial derivative yields:

$$\begin{aligned}
\int_{V_m} \left( \frac{\partial}{\partial t} (\bar{\rho}_\alpha \mathbf{v}_\alpha) + \bar{\rho}_\alpha \mathbf{v}_\alpha \cdot \nabla \mathbf{v}_\alpha + \bar{\rho}_\alpha \mathbf{v}_\alpha \nabla \cdot \mathbf{v}_\alpha \right) dV &= \int_{V_m} (\nabla \cdot \mathbf{T}_\alpha + \mathbf{b}_\alpha + \mathbf{m}_\alpha + \bar{g}_\alpha \mathbf{v}_\alpha) dV \\
\int_{V_m} \left( \frac{\partial}{\partial t} (\bar{\rho}_\alpha \mathbf{v}_\alpha) + \nabla \cdot (\bar{\rho}_\alpha \mathbf{v}_\alpha \mathbf{v}_\alpha) \right) dV &= \int_{V_m} (\nabla \cdot \mathbf{T}_\alpha + \mathbf{b}_\alpha + \mathbf{m}_\alpha + \bar{g}_\alpha \mathbf{v}_\alpha) dV \\
\int_{V_m} \left( \frac{\partial}{\partial t} (\bar{\rho}_\alpha \mathbf{v}_\alpha) + \nabla \cdot (\bar{\rho}_\alpha \mathbf{v}_\alpha \mathbf{v}_\alpha) - \nabla \cdot \mathbf{T}_\alpha - \mathbf{b}_\alpha - \mathbf{m}_\alpha - \bar{g}_\alpha \mathbf{v}_\alpha \right) dV &= 0
\end{aligned} \tag{2.83}$$

Using the localization theorem (Gurtin 1981) leads to the *linear momentum balance* in the *conservation form*:

$$\frac{\partial}{\partial t} (\bar{\rho}_\alpha \mathbf{v}_\alpha) + \nabla \cdot (\bar{\rho}_\alpha \mathbf{v}_\alpha \mathbf{v}_\alpha) = \nabla \cdot \mathbf{T}_\alpha + \mathbf{b}_\alpha + \mathbf{m}_\alpha + \bar{g}_\alpha \mathbf{v}_\alpha \tag{2.84}$$

If instead we take the derivative of (2.82) in the following form:

$$\begin{aligned}
\int_{V_m} \left( \frac{D}{Dt} (\bar{\rho}_\alpha \mathbf{v}_\alpha) + \bar{\rho}_\alpha \mathbf{v}_\alpha \nabla \cdot \mathbf{v}_\alpha \right) dV &= \int_{V_m} (\nabla \cdot \mathbf{T}_\alpha + \mathbf{b}_\alpha + \mathbf{m}_\alpha + \bar{g}_\alpha \mathbf{v}_\alpha) dV \\
\int_{V_m} (\dot{\bar{\rho}}_\alpha \mathbf{v}_\alpha + \bar{\rho}_\alpha \dot{\mathbf{v}}_\alpha + \bar{\rho}_\alpha \mathbf{v}_\alpha \nabla \cdot \mathbf{v}_\alpha - \nabla \cdot \mathbf{T}_\alpha - \mathbf{b}_\alpha - \mathbf{m}_\alpha - \bar{g}_\alpha \mathbf{v}_\alpha) dV &= 0 \\
\int_{V_m} \left( \underbrace{(\dot{\bar{\rho}}_\alpha + \bar{\rho}_\alpha \nabla \cdot \mathbf{v}_\alpha - \bar{g}_\alpha)}_{\text{by continuity equation} = 0} \mathbf{v}_\alpha + \bar{\rho}_\alpha \dot{\mathbf{v}}_\alpha - \nabla \cdot \mathbf{T}_\alpha - \mathbf{b}_\alpha - \mathbf{m}_\alpha \right) dV &= 0 \\
\int_{V_m} (\bar{\rho}_\alpha \dot{\mathbf{v}}_\alpha - \nabla \cdot \mathbf{T}_\alpha - \mathbf{b}_\alpha - \mathbf{m}_\alpha) dV &= 0,
\end{aligned}$$

and using the localization theorem:

$$\bar{\rho}_\alpha \dot{\mathbf{v}}_\alpha = \nabla \cdot \mathbf{T}_\alpha + \mathbf{b}_\alpha + \mathbf{m}_\alpha \tag{2.85}$$

### Linear momentum jump balance

In regions having discontinuities, Eqs. (2.84) and (2.85) are still valid on each side of the discontinuity, but they are not valid at the discontinuity. Following a procedure similar to that used previously for the mass jump balance, we write the last equation of (2.83) in the form:

$$\begin{aligned} \int_{V_m} \left( \frac{\partial}{\partial t} (\bar{\rho}_\alpha \mathbf{v}_\alpha) - \mathbf{b}_\alpha - \mathbf{m}_\alpha - \bar{g}_\alpha \mathbf{v}_\alpha \right) dV &= - \int_{V_m} (\nabla \cdot (\bar{\rho}_\alpha \mathbf{v}_\alpha \mathbf{v}_\alpha) - \nabla \cdot \mathbf{T}_\alpha) dV \\ \int_{V_m} \left( \frac{\partial}{\partial t} (\bar{\rho}_\alpha \mathbf{v}_\alpha) - \mathbf{b}_\alpha - \mathbf{m}_\alpha - \bar{g}_\alpha \mathbf{v}_\alpha \right) dV &= - \oint_{S_m} \bar{\rho}_\alpha \mathbf{v}_\alpha (\mathbf{v}_\alpha \cdot \mathbf{n}) dS - \oint_{S_m} \mathbf{T}_\alpha \cdot \mathbf{n} dS \end{aligned}$$

Applying this equation to each side of the discontinuity yields:

$$\begin{aligned} \int_{V^+} \left( \frac{\partial}{\partial t} (\bar{\rho}_\alpha \mathbf{v}_\alpha) - \mathbf{b}_\alpha - \mathbf{m}_\alpha - \bar{g}_\alpha \mathbf{v}_\alpha \right) dV + \int_{V^-} \left( \frac{\partial}{\partial t} (\bar{\rho}_\alpha \mathbf{v}_\alpha) - \mathbf{b}_\alpha - \mathbf{m}_\alpha - \bar{g}_\alpha \mathbf{v}_\alpha \right) dV \\ -x = - \oint_{S^+} \bar{\rho}_\alpha \mathbf{v}_\alpha (\mathbf{v}_\alpha \cdot \mathbf{n}) dS - \oint_{S_I} \bar{\rho}_\alpha^+ \mathbf{v}_\alpha^+ (\mathbf{v}_\alpha^+ - \mathbf{v}_I) \cdot (-\mathbf{e}_I) dS - \oint_{S^-} \bar{\rho}_\alpha \mathbf{v}_\alpha (\mathbf{v}_\alpha \cdot \mathbf{n}) dS \\ - \oint_{S_I} \bar{\rho}_\alpha^- \mathbf{v}_\alpha^- (\mathbf{v}_\alpha^- - \mathbf{v}_I) \cdot \mathbf{e}_I dS - \oint_{S^+} \mathbf{T}_\alpha \cdot \mathbf{n} dS - \int_{S_I} \mathbf{T}_\alpha^+ \cdot (-\mathbf{e}_I) dS - \oint_{S^-} \mathbf{T}_\alpha \cdot \mathbf{n} dS \\ - \int_{S_I} \mathbf{T}_\alpha^- \cdot \mathbf{e}_I dS \end{aligned}$$

Adding integrals with (+) and (-) and defining the jump of a property  $G$  by  $[G] = G^+ - G^-$ , yields:

$$\begin{aligned} \int_{V_m} \left( \frac{\partial}{\partial t} (\bar{\rho}_\alpha \mathbf{v}_\alpha) - \mathbf{b}_\alpha - \mathbf{m}_\alpha - \bar{g}_\alpha \mathbf{v}_\alpha \right) dV - \oint_{S_m} \bar{\rho}_\alpha \mathbf{v}_\alpha (\mathbf{v}_\alpha \cdot \mathbf{n}) dS - \oint_{S_m} \mathbf{T}_\alpha \cdot \mathbf{n} dS \\ = - \int_{S_I} [\bar{\rho}_\alpha \mathbf{v}_\alpha (\mathbf{v}_\alpha - \mathbf{v}_I) \cdot \mathbf{e}_I] dS - \int_{S_I} [\mathbf{T}_\alpha \cdot \mathbf{e}_I] dS \end{aligned} \quad (2.86)$$

The left hand-side of (2.86) is zero by the macroscopic linear momentum balance, so that:

$$\begin{aligned} \int_{S_I} [\bar{\rho}_\alpha \mathbf{v}_\alpha (\mathbf{v}_\alpha - \mathbf{v}_I) \cdot \mathbf{e}_I] dS + \int_{S_I} [\mathbf{T}_\alpha \cdot \mathbf{e}_I] dS &= \int_{S_I} ([\bar{\rho}_\alpha \mathbf{v}_\alpha (\mathbf{v}_\alpha - \mathbf{v}_I) \cdot \mathbf{e}_I] + [\mathbf{T}_\alpha \cdot \mathbf{e}_I]) dS \\ &= 0 \end{aligned}$$

Applying the localization theorem (Gurtin 1981) yields the *linear momentum jump balance* for the  $\alpha$  component:

$$[\bar{\rho}_\alpha \mathbf{v}_\alpha (\mathbf{v}_\alpha - \mathbf{v}_I) \cdot \mathbf{e}_I] - [\mathbf{T}_\alpha \cdot \mathbf{e}_I] = 0, \text{ or } \sigma[\bar{\rho}_\alpha \mathbf{v}_\alpha] = [\bar{\rho}_\alpha \mathbf{v}_\alpha (\mathbf{v}_I \cdot \mathbf{e}_I)] - [\mathbf{T}_\alpha \cdot \mathbf{e}_I] \quad (2.87)$$

where  $\sigma = [\mathbf{v}_I \cdot \mathbf{e}_I]$  is the displacement velocity of the discontinuity.

### Linear momentum balance for a mixture

Summing Eq. (2.84) for all component results in:

$$\frac{\partial}{\partial t} \sum_{\alpha=1}^n (\bar{\rho}_\alpha \mathbf{v}_\alpha) + \nabla \cdot \sum_{\alpha=1}^n (\bar{\rho}_\alpha \mathbf{v}_\alpha \mathbf{v}_\alpha) = \nabla \cdot \sum_{\alpha=1}^n \mathbf{T}_\alpha + \sum_{\alpha=1}^n (\mathbf{b}_\alpha + \mathbf{m}_\alpha + \bar{g}_\alpha \mathbf{v}_\alpha)$$

Substituting the component velocity by the diffusion velocity by means of equation  $\mathbf{u}_\alpha = \mathbf{v}_\alpha - \mathbf{v}$  in the second term of the left-hands side yields:

$$\begin{aligned} & \frac{\partial}{\partial t} \sum_{\alpha=1}^n (\bar{\rho}_\alpha \mathbf{v}_\alpha) + \nabla \cdot \sum_{\alpha=1}^n (\bar{\rho}_\alpha (\mathbf{u}_\alpha + \mathbf{v})(\mathbf{u}_\alpha + \mathbf{v})) = \nabla \cdot \sum_{\alpha=1}^n \mathbf{T}_\alpha + \sum_{\alpha=1}^n (\mathbf{b}_\alpha + \mathbf{m}_\alpha + \bar{g}_\alpha \mathbf{v}_\alpha) \\ & \frac{\partial}{\partial t} \sum_{\alpha=1}^n (\bar{\rho}_\alpha \mathbf{v}_\alpha) + \nabla \cdot \sum_{\alpha=1}^n (\bar{\rho}_\alpha \mathbf{u}_\alpha \mathbf{v}) + \nabla \cdot \sum_{\alpha=1}^n (\bar{\rho}_\alpha \mathbf{v} \mathbf{u}_\alpha) + \nabla \cdot \sum_{\alpha=1}^n (\bar{\rho}_\alpha \mathbf{v} \mathbf{v}) \\ & = \nabla \cdot \sum_{\alpha=1}^n \mathbf{T}_\alpha - \nabla \cdot \sum_{\alpha=1}^n (\bar{\rho}_\alpha \mathbf{u}_\alpha \mathbf{u}_\alpha) + \sum_{\alpha=1}^n (\mathbf{b}_\alpha + \mathbf{m}_\alpha + \bar{g}_\alpha \mathbf{v}_\alpha) \end{aligned}$$

Using the definitions (2.70)–(2.72) we get:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v} \mathbf{v}) = \nabla \cdot \left( \sum_{\alpha=1}^n \mathbf{T}_\alpha - \sum_{\alpha=1}^n (\bar{\rho}_\alpha \mathbf{u}_\alpha \mathbf{u}_\alpha) \right) + \sum_{\alpha=1}^n (\mathbf{b}_\alpha + \mathbf{m}_\alpha + \bar{g}_\alpha \mathbf{v}_\alpha)$$

For the mixture the linear momentum of a single component should be valid, then:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \rho \mathbf{v} \mathbf{v} = \nabla \cdot \mathbf{T} + \mathbf{b}$$

Comparing the last two equations we conclude that it is necessary that:

$$\mathbf{T} = \mathbf{T}_I - \sum_{\alpha=1}^n \bar{\rho}_\alpha \mathbf{u}_\alpha \mathbf{u}_\alpha, \quad \mathbf{b} = \sum_{\alpha=1}^n \mathbf{b}_\alpha, \quad \sum_{\alpha=1}^n (\mathbf{m}_\alpha + \bar{g}_\alpha \mathbf{v}) = 0 \quad (2.88)$$

$$\text{with} \quad \mathbf{T}_I = \sum_{\alpha=1}^n \mathbf{T}_\alpha \quad (2.89)$$

The term  $\mathbf{T}_I$  receives the name of the internal part of the stress tensor (Truesdell 1984). The last term in (2.88) indicates that no net production of linear momentum exists, and that the growth in one component is done at the expense of the linear momentum of the other components.

### 2.2.2 Angular Momentum Balance

The application of Euler's second law for the angular momentum and Cauchy's stress principle to the  $\alpha$  component of the body gives the *macroscopic angular momentum balance*:

$$\begin{aligned}
\frac{d}{dt} \int_{V_m} ((\mathbf{r} - \mathbf{r}_q) \times \bar{\rho}_\alpha \mathbf{v}_\alpha) dV &= \int_{S_m} ((\mathbf{r} - \mathbf{r}_q) \times \mathbf{T}_\alpha \cdot \mathbf{n}) dS \\
&+ \int_{V_m} ((\mathbf{r} - \mathbf{r}_q) \times (\mathbf{b}_\alpha + \mathbf{m}_\alpha + \bar{g}_\alpha \mathbf{v}_\alpha)) dS + \int_{V_m} \mathbf{a}_{\alpha q} dV
\end{aligned} \tag{2.90}$$

where  $\mathbf{r}_q$  is the position of a fixed point  $Q$  with respect to which the torques and angular momentum are calculated.

When the field variables are smooth and continuous, a procedure similar to that used in the previous section leads to the *local angular momentum balance*:

$$\mathbf{T}_\alpha - \mathbf{T}_\alpha^T = \mathbf{A}_{\alpha q} \tag{2.91}$$

where  $\mathbf{A}_{\alpha q}$  is the skew tensor corresponding to the axial vector  $\bar{\mathbf{a}}_{\alpha q}$ . If we assume that there is no interchange of angular momentum between components,  $\bar{\mathbf{a}}_{\alpha q} = 0$  and the stress tensors for the components are symmetric:

$$\mathbf{T}_\alpha = \mathbf{T}_\alpha^T. \tag{2.92}$$

### 2.2.3 Dynamic Process

Consider a mixture  $B$  formed by component  $B_\alpha \subset B$ , with  $\alpha = 1, 2, \dots, n$ . We say that the following field variables  $\mathbf{r} = \mathbf{f}_\alpha(\mathbf{R}_\alpha, t)$ ,  $\bar{\rho}_\alpha = \bar{\rho}_\alpha(\mathbf{r}, t)$ ,  $\mathbf{T}_\alpha = \mathbf{T}_\alpha(\mathbf{r}, t)$ ,  $\mathbf{b}_\alpha = \mathbf{b}_\alpha(\mathbf{r}, t)$ ,  $\bar{g}_\alpha = \bar{g}_\alpha(\mathbf{r}, t)$  and  $\mathbf{m}_\alpha = \mathbf{m}_\alpha(\mathbf{r}, t)$ , constitute a dynamic process if they obey the following field equations in regions where they are smooth and continuous:

$$\frac{\partial \bar{\rho}_\alpha}{\partial t} + \nabla \cdot (\bar{\rho}_\alpha \mathbf{v}_\alpha) = \bar{g}_\alpha \tag{2.93}$$

$$\frac{\partial}{\partial t} (\bar{\rho}_\alpha \mathbf{v}_\alpha) + \nabla \cdot (\bar{\rho}_\alpha \mathbf{v}_\alpha \mathbf{v}_\alpha) = \nabla \cdot \mathbf{T}_\alpha + \mathbf{m}_\alpha + \bar{\rho}_\alpha \mathbf{v}_\alpha \tag{2.94}$$

and the following jump balance at discontinuities:

$$\sigma[\bar{\rho}_\alpha] = [\bar{\rho}_\alpha \mathbf{v}_\alpha \cdot \mathbf{e}_I], \quad \sigma[\bar{\rho}_\alpha \mathbf{v}_\alpha \cdot \mathbf{e}_I] = [\bar{\rho}_\alpha \mathbf{v}_\alpha \mathbf{v}_\alpha \cdot \mathbf{e}_I] - [\mathbf{T}_\alpha \cdot \mathbf{e}_I] \tag{2.95}$$

For this dynamic process to be complete, *constitutive equations* relating the kinematical with the dynamical variables must be postulated:  $(\mathbf{T}_\alpha, \mathbf{r})$ ,  $(\mathbf{b}_\alpha, \mathbf{r})$ ,  $(\mathbf{m}_\alpha, \mathbf{r})$  and  $(\bar{g}_\alpha, \mathbf{r})$ . A dynamic process for these six field variables  $\mathbf{r}$ ,  $\bar{\rho}_\alpha$ ,  $\mathbf{T}_\alpha$ ,  $\mathbf{b}_\alpha$  and  $\bar{g}_\alpha$  is admissible when the six equations are satisfied.

## References

- Atkin, R. J., & Crain, R. E. (1976). Continuum theories of mixtures: Basic theory and historical development. *The Quarterly Journal of Mechanics and Applied Mathematics*, 29, 209–244.
- Bedford, A., & Drumheller, D. S. (1983). Theories of immiscible and structured mixtures. *International Journal of Engineering Science*, 21(8), 863–960.
- Bowen, R. M. (1976). Theory of mixtures. In A. C. Eringen (Ed.), *Continuum physics* (Vol. III). Waltham: Academic Press.
- Bustos, M. C., Concha, F., Bürger, R., & Tory, E. M. (1999). *Sedimentation and thickening, phenomenological foundation and mathematical theory*. Dordrecht: Kluwer Academic Publications.
- Concha, F., & Barrientos, A. (1993). *Mecánica Racional Moderna, Termomecánica del Medio Continuo* (Vol. 2, pp. 248–266). Dirección de Docencia, Universidad de Concepción.
- Concha, F., (2001). Manual de Filtración y Separación, CIC-Red Cetttec, CETTEM Ltda., Edmundo Larenas 270 Concepción, Chile.
- Drew, D. A. (1983). Mathematical modeling of two-phase flow. *Annual Review of Fluid Mechanics*, 15, 261–291.
- Drew, A. D., & Passman, S.L. (1998). *Theory of multicomponent fluids*. Berlin: Springer.
- Gurtin, M. E. (1981). An Introduction. Academic Press, New York to Continuum Mechanic.
- Rajagopal, K. R., & Tao, L. (1995). Mechanics of mixtures, Worlds Scientific, Singapore.
- Truesdell, C., & Toupin, R. A. (1960). The classical field theories of mechanics. In S. Flügge (Ed.), *Handbook of physics* (Vol. III–1). New York: Springer.
- Truesdell, C. (1965). Sulle basi de la termomecánica, Rend. Acad. Lincei, 22, 33–88, 1957. Traducción al inglés en: Rational Mechanics of Materials, Int. Sci. Rev. Ser. 292–305, Gordon & Breach, New York.
- Truesdell, C. (1984). *Rational thermodynamics* (2nd ed.). New York: Springer.
- Ungsrish, M. (1993). Hydrodynamics of suspensions. Berlin: Springer.

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