

# Chapter 2

## Preliminaries

### 2.1 Mathematical Foundation

#### 2.1.1 Notation Rules and Algebra with Vectors and Tensors

In the mathematical formulation of quantities and fields there are two types of notation which we shall use through the book: *symbolic (or Gibbs')* notation as well as *index notation*. For the sake of convenience and to provide suitably abstract formulations we mostly prefer the symbolic notation. Let  $\mathbf{a}$  and  $\mathbf{b}$  be vectors in a (real) space of dimension  $D$ , we write with (all used symbols are summarized in the Appendix A)

$$\mathbf{a} = \begin{pmatrix} a_1 \\ a_2 \\ \vdots \\ a_D \end{pmatrix} = a_i, \quad \mathbf{b} = \begin{pmatrix} b_1 \\ b_2 \\ \vdots \\ b_D \end{pmatrix} = b_i \quad (1 \leq i \leq D) \quad (2.1)$$

for the *scalar (or dot) product*

$$\mathbf{a} \cdot \mathbf{b} = a_i b_i \quad (1 \leq i \leq D) \quad (2.2)$$

using *Einstein's summation convention* according to  $a_i b_i = \sum_{i=1}^D a_i b_i$  in which repeated indices are summed,

for the *vector (or cross) product*

$$\mathbf{a} \times \mathbf{b} = \varepsilon_{ijk} a_i b_j \mathbf{e}_k = \det \begin{pmatrix} a_1 & a_2 & \dots & a_D \\ b_1 & b_2 & \dots & b_D \\ \mathbf{e}_1 & \mathbf{e}_2 & \dots & \mathbf{e}_D \end{pmatrix} \quad (1 \leq i, j, k \leq D) \quad (2.3)$$

where  $\varepsilon_{ijk}$  is the *permutation symbol* (also known as the Levi-Civita tensor  $\epsilon$ ) defined as

$$\varepsilon_{ijk} = \begin{cases} 1 & \text{if } (ijk) \text{ is an even (cyclic) permutation, e.g., } \varepsilon_{123} = \varepsilon_{231} = \varepsilon_{312} = 1 \\ -1 & \text{if } (ijk) \text{ is an odd (noncyclic) permutation, e.g., } \varepsilon_{213} = \varepsilon_{321} = \varepsilon_{132} = -1 \\ 0 & \text{if two or more subscripts of } (ijk) \text{ are the same, e.g., } \varepsilon_{111} = \varepsilon_{112} = \varepsilon_{313} = 0 \end{cases} \quad (2.4)$$

and  $\mathbf{e}_i$  ( $1 \leq i \leq D$ ) are *base vectors* given as

$$\mathbf{e}_1 = \begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix} \quad \mathbf{e}_2 = \begin{pmatrix} 0 \\ 1 \\ \vdots \\ 0 \end{pmatrix} \quad \dots \quad \mathbf{e}_D = \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 1 \end{pmatrix} \quad (2.5)$$

where

$$\mathbf{e}_i \cdot \mathbf{e}_j = \delta = \delta_{ij} \quad (2.6)$$

with the *Kronecker symbol* (unit or identity matrix)

$$\delta = \begin{pmatrix} 1 & 0 & \dots & 0 \\ 0 & 1 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & 1 \end{pmatrix} \quad \delta_{ij} = \begin{cases} 1 & \text{when } i = j \\ 0 & \text{when } i \neq j \end{cases} \quad (2.7)$$

and for the *dyadic (or tensor) product*

$$\mathbf{a} \otimes \mathbf{b} = a_i b_j = \begin{pmatrix} a_1 b_1 & a_1 b_2 & \dots & a_1 b_D \\ a_2 b_1 & a_2 b_2 & \dots & a_2 b_D \\ \vdots & \vdots & \ddots & \vdots \\ a_D b_1 & a_D b_2 & \dots & a_D b_D \end{pmatrix} \quad (1 \leq i, j \leq D) \quad (2.8)$$

which results in a second-order tensor  $\mathbf{A} = \mathbf{a} \otimes \mathbf{b}$ . The multiplication symbol  $\otimes$  in the dyadic product is often omitted and the tensor product of (2.8) is then simply denoted by  $\mathbf{A} = \mathbf{a}\mathbf{b}$ . We note that the components  $a_1, a_2, \dots, a_D$  of  $\mathbf{a}$  in (2.1) are themselves *scalars* and the vector  $\mathbf{a}$  can also be formed via summation

$$\mathbf{a} = a_i \mathbf{e}_i \quad (1 \leq i \leq D) \quad (2.9)$$

We further note that (2.9) is a symbolic vector expression. In such a context  $a_i$  are scalars and not seen as a vector symbol used in the index notation. An equivalent

expression for (2.9) reads  $a_i = \delta_{ij}a_j$  in the index notation. In generalization, the following convention for vector multiplication holds in symbolic notation:

$$\begin{aligned} a_i \mathbf{e}_i & \text{ results in a vector, where } a_i \text{ represent vector components (scalars),} \\ (a_i) \cdot \mathbf{e}_i & \text{ results in a scalar, where } (a_i) \text{ represents a vector,} \\ (a_{ij}) \cdot \mathbf{e}_j & \text{ results in a vector, where } (a_{ij}) \text{ represents a second-order tensor.} \end{aligned} \quad (2.10)$$

The *norm (or magnitude)*  $a$  of vector  $\mathbf{a}$  is given by

$$a = \|\mathbf{a}\| = \sqrt{\mathbf{a} \cdot \mathbf{a}} = \sqrt{a_i a_i} \quad (2.11)$$

If  $\|\mathbf{a}\| = 1$  it is called a *unit vector* such as  $\mathbf{e}_i$ .

Furthermore, we can find the *normalized vector* for  $\mathbf{a}$  according to

$$\hat{\mathbf{a}} = \frac{\mathbf{a}}{\|\mathbf{a}\|} = \frac{a_i}{\sqrt{a_j a_j}} \mathbf{e}_i \quad (2.12)$$

It becomes clear that  $\hat{\mathbf{a}}$  is itself a unit vector because  $\|\hat{\mathbf{a}}\| = 1$ . The *transpose* of vector  $\mathbf{a}$  changes a column vector to a row vector and a row vector to a column vector, respectively,

$$\mathbf{a}^T = (a_1 \ a_2 \ \dots \ a_D) \quad (a_1 \ a_2 \ \dots \ a_D)^T = \begin{pmatrix} a_1 \\ a_2 \\ \vdots \\ a_D \end{pmatrix} \quad (2.13)$$

Let  $\mathbf{A} = \sum_i \sum_j A_{ij} \mathbf{e}_i \otimes \mathbf{e}_j$  and  $\mathbf{B} = \sum_i \sum_j B_{ij} \mathbf{e}_i \otimes \mathbf{e}_j$  be two second-order tensors of dimension  $D$  ( $1 \leq i, j \leq D$ )

$$\mathbf{A} = \begin{pmatrix} A_{11} & A_{12} & \dots & A_{1D} \\ A_{21} & A_{22} & \dots & A_{2D} \\ \vdots & \vdots & \ddots & \vdots \\ A_{D1} & A_{D2} & \dots & A_{DD} \end{pmatrix} \quad \mathbf{B} = \begin{pmatrix} B_{11} & B_{12} & \dots & B_{1D} \\ B_{21} & B_{22} & \dots & B_{2D} \\ \vdots & \vdots & \ddots & \vdots \\ B_{D1} & B_{D2} & \dots & B_{DD} \end{pmatrix} \quad (2.14)$$

then, their scalar product is written as a *double dot product* (or colon product) in the form

$$\mathbf{A} : \mathbf{B} = \sum_i^D \sum_j^D A_{ij} B_{ji} \quad (2.15)$$

which results in a scalar. The norm of such a second-order tensor  $\mathbf{A}$  is defined as

$$\|\mathbf{A}\| = \sqrt{\mathbf{A} : \mathbf{A}^T} = \sqrt{\sum_i \sum_j (A_{ij})^2} \quad (2.16)$$

where the transpose  $\mathbf{A}^T$  of the tensor  $\mathbf{A}$  is given by  $(A_{ij})^T = (A_{ji})$ :

$$\mathbf{A}^T = \begin{pmatrix} A_{11} & A_{21} & \cdots & A_{D1} \\ A_{12} & A_{22} & \cdots & A_{D2} \\ \vdots & \vdots & \ddots & \vdots \\ A_{1D} & A_{2D} & \cdots & A_{DD} \end{pmatrix} \quad (2.17)$$

A second-order tensor  $\mathbf{A} = A_{ij}$  is a *symmetric tensor* for which the following is valid

$$\mathbf{A} = \mathbf{A}^T \quad A_{ij} = A_{ji} \quad (2.18)$$

Any tensor  $\mathbf{A}$  can be written as a sum of symmetric and antisymmetric parts

$$\mathbf{A} = \frac{1}{2}(\mathbf{A} + \mathbf{A}^T) + \frac{1}{2}(\mathbf{A} - \mathbf{A}^T) = \frac{1}{2}(\mathbf{B}_s + \mathbf{B}_a) \quad (2.19)$$

The scalar product of a tensor  $\mathbf{A}$  with a vector  $\mathbf{a}$  is:

$$\mathbf{A} \cdot \mathbf{a} = \sum_i^D \mathbf{e}_i \sum_j^D A_{ij} a_j \quad (2.20)$$

In contrast, the scalar product of a vector  $\mathbf{a}$  with a tensor  $\mathbf{A}$  is:

$$\mathbf{a} \cdot \mathbf{A} = \sum_i^D \mathbf{e}_i \sum_j^D a_j A_{ji} \quad (2.21)$$

A tensor  $\mathbf{A}$  is *diagonal* if the components outside the main diagonal are all zero, i.e.,  $A_{ij} = 0$  for  $i \neq j$ . It is written as

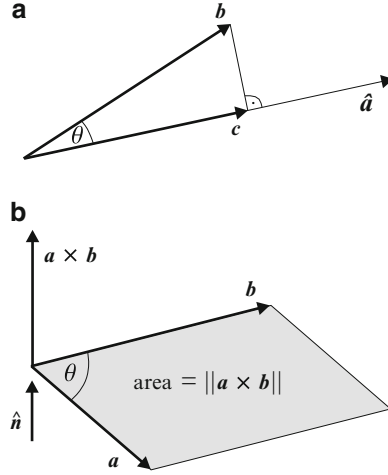
$$\mathbf{A} = [A_{11}, A_{22}, \dots, A_{DD}] = \begin{pmatrix} A_{11} & 0 & \cdots & 0 \\ 0 & A_{22} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & A_{DD} \end{pmatrix} \quad (2.22)$$

Any diagonal tensor is also a symmetric tensor.

### 2.1.2 Relations for Scalar and Vector Products

If  $\hat{\mathbf{a}}$  and  $\hat{\mathbf{b}}$  are unit vectors in the directions of  $\mathbf{a}$  and  $\mathbf{b}$ , respectively, then

$$\hat{\mathbf{a}} \cdot \hat{\mathbf{b}} = \cos \theta \quad (2.23)$$



**Fig. 2.1** (a) Projection of  $\mathbf{b}$  onto the unit vector  $\hat{\mathbf{a}}$  and (b) vector product  $\mathbf{a} \times \mathbf{b}$

where  $\theta$  represents the angle between the two directions. Since  $\mathbf{a} = \|\mathbf{a}\| \hat{\mathbf{a}}$  and  $\mathbf{b} = \|\mathbf{b}\| \hat{\mathbf{b}}$  we find for the scalar product (2.2) with (2.23)

$$\mathbf{a} \cdot \mathbf{b} = \|\mathbf{a}\| \|\mathbf{b}\| \cos \theta \quad (2.24)$$

This form of the scalar product is useful to formulate the *projection* of a vector onto a given direction. Assuming we have a unit vector  $\hat{\mathbf{a}}$  and another vector  $\mathbf{b}$ , we project  $\mathbf{b}$  perpendicularly onto  $\hat{\mathbf{a}}$ , as shown in Fig. 2.1, and call the resulting projected vector  $\mathbf{c}$ . We find

$$\begin{aligned} \|\mathbf{c}\| &= \|\mathbf{b}\| \cos \theta \\ &= \|\mathbf{b}\| \left( \frac{\hat{\mathbf{a}} \cdot \mathbf{b}}{\|\hat{\mathbf{a}}\| \|\mathbf{b}\|} \right) \\ &= \hat{\mathbf{a}} \cdot \mathbf{b} = \frac{\mathbf{a} \cdot \mathbf{b}}{\|\mathbf{a}\|} \end{aligned} \quad (2.25)$$

The interpretation of (2.25) is that the scalar product of the unit vector in the direction of vector  $\mathbf{a}$  and the vector  $\mathbf{b}$  yields the length of the projection of  $\mathbf{b}$  onto  $\hat{\mathbf{a}}$  (see Fig. 2.1). If the angle  $\theta$  between the two vectors  $\mathbf{a}$  and  $\mathbf{b}$  is a right angle,  $\theta = \pi/2$ , then  $\cos \theta = 0$ . Such vectors are said to be *orthogonal* and the condition for *orthogonality* is

$$\mathbf{a} \cdot \mathbf{b} = 0 \quad (2.26)$$

The *square* of a vector  $\mathbf{a}$  results from the scalar product (2.24) with (2.11)

$$\mathbf{a} \cdot \mathbf{a} = \|\mathbf{a}\| \|\mathbf{a}\| \cos 0 = a^2 \quad (2.27)$$

The cross product  $\mathbf{a} \times \mathbf{b}$  of vectors  $\mathbf{a}$  and  $\mathbf{b}$  forms a vector of magnitude  $\|\mathbf{a}\| \|\mathbf{b}\| \sin \theta$  normal to the plane defined by  $\mathbf{a}$  and  $\mathbf{b}$ :

$$\mathbf{a} \times \mathbf{b} = \|\mathbf{a}\| \|\mathbf{b}\| \sin \theta \hat{\mathbf{n}} \quad (2.28)$$

where the unit vector  $\hat{\mathbf{n}}$  is normal to the plane  $\mathbf{a}$  and  $\mathbf{b}$  and  $\|\mathbf{a} \times \mathbf{b}\|$  is the area of the parallelogram that the vectors  $\mathbf{a}$  and  $\mathbf{b}$  span.

### 2.1.3 Coordinate System and Spatial Vector

To position physical objects in space and to define their spatial motion, the  $D$ -dimensional Euclidean space  $\Re^D$  ( $D = 1, 2, 3$ ) is used as reference system. We employ an orthogonal Cartesian coordinate system as shown in Fig. 2.2 in which a position  $P$  is defined by the Cartesian coordinate vector  $\mathbf{x}$ , viz.,

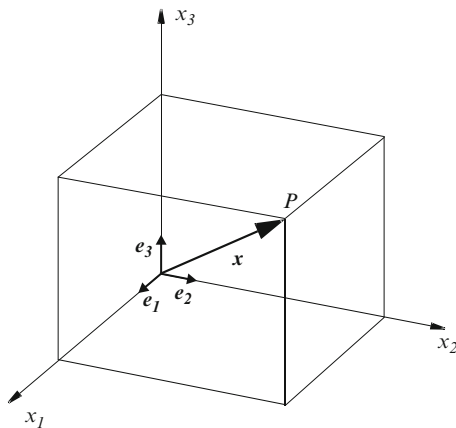
$$\mathbf{x} = \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} x \\ y \\ z \end{pmatrix} \quad \text{in } \Re^3 \text{ (3D)} \quad (2.29)$$

In  $\Re^2$  (2D) and  $\Re^1$  (1D) it is  $\mathbf{x}^T = (x_1 \ x_2) = (x \ y)$  and  $\mathbf{x}^T = (x_1) = (x)$ , respectively. If we want to identify positions of a list of points  $\mathbf{x}_l \in \Re^D$  ( $l = 1, 2, \dots, N_p$ ) labeled by a (nodal) index  $l$ , their coordinates are written as

$$\mathbf{x}_l = \begin{pmatrix} x_{1l} \\ x_{2l} \\ x_{3l} \end{pmatrix} = \begin{pmatrix} x_l \\ y_l \\ z_l \end{pmatrix} \quad \text{in } \Re^3 \text{ (3D), } (l = 1, 2, \dots, N_p) \quad (2.30)$$

where  $N_p$  is the number of the listed points. It follows that the components of the coordinate vector are themselves vectors consisting of an ordered list of (discrete) numbers, i.e.,  $\mathbf{x}_l^T = (x_{1l} \ x_{2l} \ \dots \ x_{lN_p})$ , and so forth. With the coordinate vector  $\mathbf{x} = x_i \mathbf{e}_i$  we find that the corresponding base vectors  $\mathbf{e}_i$  are formed from the tangent vectors  $\bar{\mathbf{e}}_i$  to the coordinate lines of the  $\mathbf{x}$ -coordinates, viz.,

$$\begin{aligned} \mathbf{e}_i &= \widehat{\bar{\mathbf{e}}_i} = \frac{\bar{\mathbf{e}}_i}{\|\bar{\mathbf{e}}_i\|} \\ \bar{\mathbf{e}}_i &= \frac{\partial \mathbf{x}}{\partial x_i} \end{aligned} \quad (2.31)$$



**Fig. 2.2** Cartesian coordinate system in  $\mathbb{R}^3$ . The position  $P$  is represented by the vector  $\mathbf{x} = x_i \mathbf{e}_i$

We note that the Cartesian coordinate system is orthogonal with  $\mathbf{e}_i \cdot \mathbf{e}_j = 0$  ( $i \neq j$ ), cf. (2.26).

### 2.1.4 Eulerian and Lagrangian Coordinates

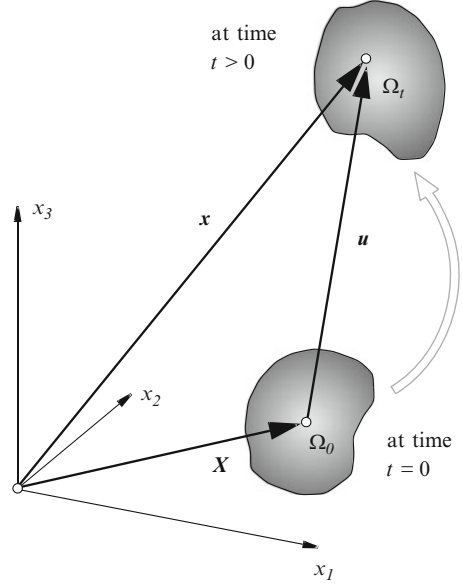
Following the concepts of continuum mechanics we use the term *point* to indicate a location in space  $\mathbb{R}^D$  and the term *particle* to denote a *point in a continuum*. While points are fixed in space and independent of time  $t$ , positions of particles may vary with time  $t$ . This provides a distinction between two kinds of coordinates:

- (a) *Spatial (Eulerian) coordinates*  $\mathbf{x}$ , that define points in space with respect to a fixed frame of reference.
- (b) *Material (Lagrangian) coordinates*  $\mathbf{X}$ , that are assigned to particles of a continuum. Usually,  $\mathbf{X}$  is selected as the initial position vector of a considered particle, i.e.,  $\mathbf{X} \equiv \mathbf{x}|_{t=0}$ .

As a particle moves, its coordinates  $\mathbf{x}$  vary in time  $t$ , whereas its material coordinates  $\mathbf{X}$  remain unchanged. Such a motion is described by

$$\mathbf{x} = \mathbf{x}(\mathbf{X}, t) \quad (2.32)$$

which is known as the *Lagrangian formulation of motion*. Figure 2.3 shows a spatial domain  $\Omega_0$  occupied at  $t = 0$  by a continuum with material coordinates  $\mathbf{X}$ . At a later time  $t > 0$ , the domain occupied by the same continuum is  $\Omega_t$ . The domain  $\Omega_t$  represents the *deformed configuration* of the continuum initially in  $\Omega_0$ .

**Fig. 2.3** Motion of a particle

The *Eulerian formulation of motion* is obtained if (2.32) is inverted to yield the initial position (i.e., material coordinates) of a particle which at time  $t$  is at position  $\mathbf{x}$ :

$$\mathbf{X} = \mathbf{X}(\mathbf{x}, t) \quad (2.33)$$

A necessary and sufficient condition for the existence of (2.33) is given, if the Jacobian

$$\mathbf{J} = \frac{\partial \mathbf{x}}{\partial \mathbf{X}} = \begin{pmatrix} \frac{\partial x_1}{\partial X_1} & \frac{\partial x_2}{\partial X_1} & \frac{\partial x_3}{\partial X_1} \\ \frac{\partial x_1}{\partial X_2} & \frac{\partial x_2}{\partial X_2} & \frac{\partial x_3}{\partial X_2} \\ \frac{\partial x_1}{\partial X_3} & \frac{\partial x_2}{\partial X_3} & \frac{\partial x_3}{\partial X_3} \end{pmatrix} \quad (2.34)$$

differs from zero. The *displacement* vector  $\mathbf{u}$  (Fig. 2.3) is defined as the difference between the position vector  $\mathbf{x}$  of a moving particle at a given time  $t$  and its initial position vector  $\mathbf{X}$ :

$$\mathbf{u} = \mathbf{x} - \mathbf{X} \quad (2.35)$$

The need for a mathematical description based on a fixed domain and spatial reference renders the Eulerian formulation an ideal candidate to describe flow fields.



Accordingly, the Eulerian concept is preferred in our analysis. It requires, however, that the flow and transport quantities be *continuous* throughout the domain  $\Omega$ . Let us consider a property  $f = f(\mathbf{x}, t)$  in the Eulerian description, which is linked to the considered particle in  $\Omega$ . Using (2.32) we obtain the relationship between the two respective coordinate systems

$$f(\mathbf{x}, t) = f[\mathbf{x}(\mathbf{X}, t), t] \quad (2.36)$$

and the rate of change of  $f$  in a Lagrangian description

$$\frac{Df}{Dt} = \frac{\partial f}{\partial t} \Big|_{\mathbf{X}=\text{const}} \quad (2.37)$$

defining the derivative with respect to time  $t$  keeping  $\mathbf{X}$  constant. The derivative  $D/Dt$  represents the rate of change as observed when moving with the particle and is called *material derivative*. In the Eulerian description we can derive

$$\begin{aligned} \frac{Df[\mathbf{x}(\mathbf{X}, t), t]}{Dt} &= \frac{\partial f}{\partial t} \Big|_{\mathbf{x}=\text{const}} + \frac{\partial f}{\partial \mathbf{x}} \Big|_{t=\text{const}} \cdot \frac{\partial \mathbf{x}(\mathbf{X}, t)}{\partial t} \Big|_{\mathbf{X}=\text{const}} \\ &= \frac{\partial f}{\partial t} + (\mathbf{v} \cdot \nabla) f \end{aligned} \quad (2.38)$$

where

$$\mathbf{v} = \dot{\mathbf{x}} = \frac{\partial \mathbf{x}}{\partial t} \Big|_{\mathbf{X}=\text{const}} \quad (2.39)$$

is the *velocity* of the particle and

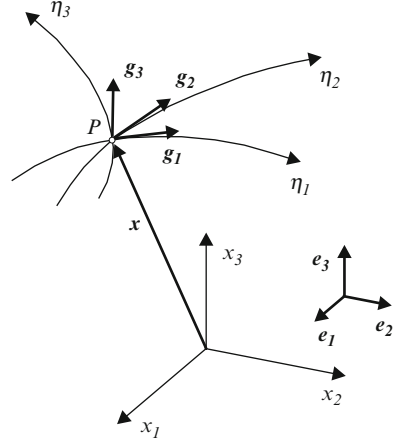
$$\nabla = \frac{\partial}{\partial \mathbf{x}} = \mathbf{e}_i \frac{\partial}{\partial x_i} \quad (2.40)$$

is the *gradient (or Nabla) operator* which represents a  $D$ –dimensional vector.

### 2.1.5 Coordinate Transformations

Physical quantities in form of scalars, vectors and tensors have to be coordinate-invariant properties. In transforming between different coordinate systems the quantities have to remain unchanged. It is important to determine the relations between sets of components relative to different coordinate systems. The introduction of different coordinate systems is often useful to simplify the analysis. In our applications we need to use *orthogonal coordinate systems*, i.e., systems where the coordinate lines are orthogonal, for example cylindrical coordinates or local finite-element coordinates.

**Fig. 2.4** Transformed coordinate system  $\eta$



### 2.1.5.1 Mapping

Introducing the general coordinates

$$\eta = \begin{pmatrix} \eta_1 \\ \eta_2 \\ \eta_3 \end{pmatrix} \quad (2.41)$$

$$\mathbf{x} = \eta_i \mathbf{g}_i$$

where  $\mathbf{g}_i$  are the base vectors of the  $\eta$ -system (Fig. 2.4), a one-to-one mapping between the  $\eta$ -space and the Euclidean  $\mathbf{x}$ -space must exist:

$$\mathbf{x}(\eta) \Leftrightarrow \eta(\mathbf{x}) \quad (2.42)$$

The corresponding tangent vectors  $\bar{\mathbf{g}}_i$  (2.41) of the  $\eta$ -coordinates provide, cf. (2.31)

$$\bar{\mathbf{g}}_i = \frac{\partial \mathbf{x}}{\partial \eta_i} = \frac{\partial \mathbf{x}}{\partial x_k} \cdot \left( \frac{\partial x_k}{\partial \eta_i} \right) = \left( \frac{\partial x_k}{\partial \eta_i} \right) \cdot \bar{\mathbf{e}}_k = (J_{ik}) \cdot \bar{\mathbf{e}}_k \quad (2.43)$$

where the Jacobian matrix  $\mathbf{J}$

$$\mathbf{J} = \frac{\partial \mathbf{x}}{\partial \eta} = J_{ij} = \frac{\partial x_j}{\partial \eta_i} = \begin{pmatrix} \frac{\partial x_1}{\partial \eta_1} & \frac{\partial x_2}{\partial \eta_1} & \frac{\partial x_3}{\partial \eta_1} \\ \frac{\partial x_1}{\partial \eta_2} & \frac{\partial x_2}{\partial \eta_2} & \frac{\partial x_3}{\partial \eta_2} \\ \frac{\partial x_1}{\partial \eta_3} & \frac{\partial x_2}{\partial \eta_3} & \frac{\partial x_3}{\partial \eta_3} \end{pmatrix} = \begin{pmatrix} J_{11} & J_{12} & J_{13} \\ J_{21} & J_{22} & J_{23} \\ J_{31} & J_{32} & J_{33} \end{pmatrix} \quad (2.44)$$

must be non-zero to perform the reverse transformation

$$\bar{\mathbf{e}}_k = \left( \frac{\partial \eta_i}{\partial x_k} \right) \cdot \bar{\mathbf{g}}_i = (J_{ki})^{-1} \cdot \bar{\mathbf{g}}_i \quad (2.45)$$

We note that the base vectors are derived from the tangent vectors, viz.,

$$\mathbf{g}_i = \frac{\bar{\mathbf{g}}_i}{\|\bar{\mathbf{g}}_i\|} \quad \mathbf{e}_i = \frac{\bar{\mathbf{e}}_i}{\|\bar{\mathbf{e}}_i\|} \quad (2.46)$$

With  $\mathbf{a}^x$  denoting an arbitrary vector in the  $x$ -system, the corresponding vector  $\mathbf{a}^\eta$  expressed in the transformed  $\eta$ -system can be obtained via projection, cf. (2.25)

$$\mathbf{a}^\eta = \begin{pmatrix} \mathbf{a}^x \cdot \mathbf{g}_1 \\ \mathbf{a}^x \cdot \mathbf{g}_2 \\ \mathbf{a}^x \cdot \mathbf{g}_3 \end{pmatrix} \quad (2.47)$$

According to (2.45) a Cartesian vector  $\mathbf{a}^x$  can be expressed by the vector components  $a_i^\eta$  written in the  $\eta$ -coordinate system:

$$\mathbf{a}^x = \begin{pmatrix} a_1^x \\ a_2^x \\ a_3^x \end{pmatrix} = \begin{pmatrix} (J_{1i})^{-1} a_i^\eta \\ (J_{2i})^{-1} a_i^\eta \\ (J_{3i})^{-1} a_i^\eta \end{pmatrix} \quad a_i^\eta = \begin{pmatrix} a_1^\eta \\ a_2^\eta \\ a_3^\eta \end{pmatrix} = \mathbf{a}^\eta \quad (2.48)$$

### 2.1.5.2 Cylindrical Coordinate System

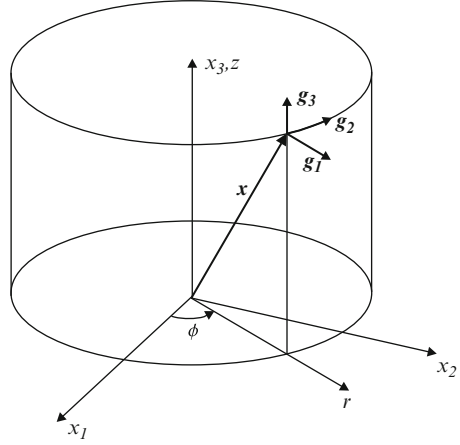
We apply *cylindrical coordinates*  $\boldsymbol{\eta}^T = (r \ \phi \ z)$ , where the mapping  $\mathbf{x}(\boldsymbol{\eta})$  is given by

$$\mathbf{x} = \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} r \cos \phi \\ r \sin \phi \\ z \end{pmatrix} \quad (2.49)$$

in which  $(r, \phi, z)$  correspond to the radial, azimuthal and axial coordinates, respectively (see Fig. 2.5). For cylindrical coordinates the Jacobian  $\mathbf{J}$  yields

$$\mathbf{J} = \begin{pmatrix} \cos \phi & \sin \phi & 0 \\ -r \sin \phi & r \cos \phi & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad \mathbf{J}^{-1} = \frac{1}{|\mathbf{J}|} \begin{pmatrix} r \cos \phi & -\sin \phi & 0 \\ r \sin \phi & \cos \phi & 0 \\ 0 & 0 & r \end{pmatrix} \quad |\mathbf{J}| = r \quad (2.50)$$

**Fig. 2.5** Cylindrical coordinates  $(r, \phi, z)$



where the determinant of matrix  $\mathbf{J}$  is denoted by  $|\mathbf{J}| = \det \mathbf{J}$ . According to (2.43) and (2.50) we obtain the base vectors  $\mathbf{g}_i$  to express cylindrical coordinates via Cartesian coordinates

$$\begin{aligned} \mathbf{g}_1^T &= \frac{(J_{11} \ J_{12} \ J_{13})}{\|(J_{11} \ J_{12} \ J_{13})\|} = (\cos \phi \ \sin \phi \ 0) \\ \mathbf{g}_2^T &= \frac{(J_{21} \ J_{22} \ J_{23})}{\|(J_{21} \ J_{22} \ J_{23})\|} = (-\sin \phi \ \cos \phi \ 0) \\ \mathbf{g}_3^T &= \frac{(J_{31} \ J_{32} \ J_{33})}{\|(J_{31} \ J_{32} \ J_{33})\|} = (0 \ 0 \ 1) \end{aligned} \quad (2.51)$$

It can easily be shown that the spatial derivatives with respect to the cylindrical coordinates such as  $\frac{\partial \mathbf{g}_i}{\partial r}$ ,  $\frac{\partial \mathbf{g}_i}{\partial \phi}$  and  $\frac{\partial \mathbf{g}_i}{\partial z}$  become zero, except for

$$\begin{aligned} \frac{\partial \mathbf{g}_1^T}{\partial \phi} &= (-\sin \phi \ \cos \phi \ 0) = \mathbf{g}_2^T \\ \frac{\partial \mathbf{g}_2^T}{\partial \phi} &= (-\cos \phi \ -\sin \phi \ 0) = -\mathbf{g}_1^T \end{aligned} \quad (2.52)$$

Exemplified for the Nabla operator (2.40) we can find the transformation by using (2.48) and (2.50):

$$\nabla = \begin{pmatrix} \frac{\partial}{\partial x_1} \\ \frac{\partial}{\partial x_2} \\ \frac{\partial}{\partial x_3} \end{pmatrix} = \begin{pmatrix} \cos \phi \frac{\partial}{\partial r} - \frac{1}{r} \sin \phi \frac{\partial}{\partial \phi} \\ \sin \phi \frac{\partial}{\partial r} + \frac{1}{r} \cos \phi \frac{\partial}{\partial \phi} \\ \frac{\partial}{\partial z} \end{pmatrix} \quad (2.53)$$

Taking into account (2.47), the Nabla operator in the  $\boldsymbol{\eta}$ -system is built from  $(\nabla_i) \cdot \mathbf{g}_i$  and finally results with (2.53) and (2.51) in

$$\nabla = \begin{pmatrix} \frac{\partial}{\partial r} \\ \frac{1}{r} \frac{\partial}{\partial \phi} \\ \frac{\partial}{\partial z} \end{pmatrix} \quad (2.54)$$

Let  $\mathbf{a}$  be a vector in cylindrical coordinates  $\mathbf{a}^T = (a_r \ a_\phi \ a_z)$ , then the scalar product  $\nabla \cdot \mathbf{a}$  results in cylindrical coordinates using (2.54) and (2.52):

$$\begin{aligned} \nabla \cdot \mathbf{a} &= (\mathbf{g}_1 \frac{\partial}{\partial r} + \mathbf{g}_2 \frac{1}{r} \frac{\partial}{\partial \phi} + \mathbf{g}_3 \frac{\partial}{\partial z}) \cdot (\mathbf{g}_1 a_r + \mathbf{g}_2 a_\phi + \mathbf{g}_3 a_z) \\ &= \frac{1}{r} \frac{\partial(r a_r)}{\partial r} + \frac{1}{r} \frac{\partial a_\phi}{\partial \phi} + \frac{\partial a_z}{\partial z} \end{aligned} \quad (2.55)$$

In the same way we find for the vector product  $\nabla \times \mathbf{a}$  in cylindrical coordinates

$$\nabla \times \mathbf{a} = \begin{pmatrix} \frac{1}{r} \frac{\partial a_z}{\partial \phi} - \frac{\partial a_\phi}{\partial z} \\ \frac{\partial a_r}{\partial z} - \frac{\partial a_z}{\partial r} \\ \frac{1}{r} \left[ \frac{\partial}{\partial r} (r a_\phi) - \frac{\partial a_r}{\partial \phi} \right] \end{pmatrix} \quad (2.56)$$

### 2.1.5.3 Rotated Coordinate System

Another orthogonal coordinate transformation of interest is the *rotation* of  $\mathbf{x}$ -coordinates in the form

$$\boldsymbol{\eta} = \mathbf{A} \cdot \mathbf{x} \quad \text{with the rotation matrix} \quad \mathbf{A} = \begin{pmatrix} A_{11} & A_{12} & A_{13} \\ A_{21} & A_{22} & A_{23} \\ A_{31} & A_{32} & A_{33} \end{pmatrix} \quad (2.57)$$

and, accordingly

$$\mathbf{x} = \mathbf{A}^{-1} \cdot \boldsymbol{\eta} \quad \text{with} \quad \mathbf{A}^{-1} = \frac{1}{|\mathbf{A}|} \begin{pmatrix} A_{22}A_{33} - A_{32}A_{23} & A_{32}A_{13} - A_{12}A_{33} & A_{12}A_{23} - A_{22}A_{13} \\ A_{31}A_{23} - A_{21}A_{33} & A_{11}A_{33} - A_{31}A_{13} & A_{21}A_{13} - A_{11}A_{23} \\ A_{21}A_{32} - A_{31}A_{22} & A_{31}A_{12} - A_{11}A_{32} & A_{11}A_{22} - A_{21}A_{12} \end{pmatrix} \quad (2.58)$$

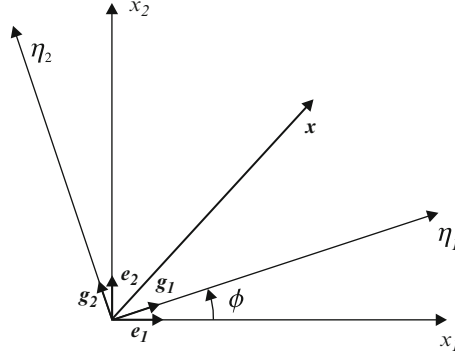
and

$$|\mathbf{A}| = A_{11}(A_{22}A_{33} - A_{32}A_{23}) + A_{21}(A_{32}A_{13} - A_{12}A_{33}) + A_{31}(A_{12}A_{23} - A_{22}A_{13}) \quad (2.59)$$

where  $A_{ij}$  are *directional cosines* which are given by

$$A_{ij} \equiv \cos(\mathbf{g}_i, \mathbf{e}_j) \quad (2.60)$$

For a rotation about the  $x_3$ -axis we get (Fig. 2.6)



**Fig. 2.6** Rotation of coordinates around  $x_3$ -axis as a 2D orthogonal coordinate transformation

$$A = \begin{pmatrix} \cos \phi & \sin \phi & 0 \\ -\sin \phi & \cos \phi & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad (2.61)$$

and a full rotation about all three axes in the 3D space the rotation matrix  $A$  yields [194]

$$A = \begin{pmatrix} \cos \psi \cos \phi - \cos \theta \sin \phi \sin \psi & \cos \psi \sin \phi + \cos \theta \cos \phi \sin \psi & \sin \psi \sin \theta \\ -\sin \psi \cos \phi - \cos \theta \sin \phi \cos \psi & -\sin \psi \sin \phi + \cos \theta \cos \phi \cos \psi & \cos \psi \sin \theta \\ \sin \theta \sin \phi & -\sin \theta \cos \phi & \cos \theta \end{pmatrix} \quad (2.62)$$

where  $(\phi, \theta, \psi)$  are the *Eulerian angles* as defined in Fig. 2.7.

#### 2.1.5.4 Volume, Surface and Line Integral Elements

In Cartesian coordinates the elements of volume  $d\Omega$ , surface  $d\Gamma$  and line  $dS$  are

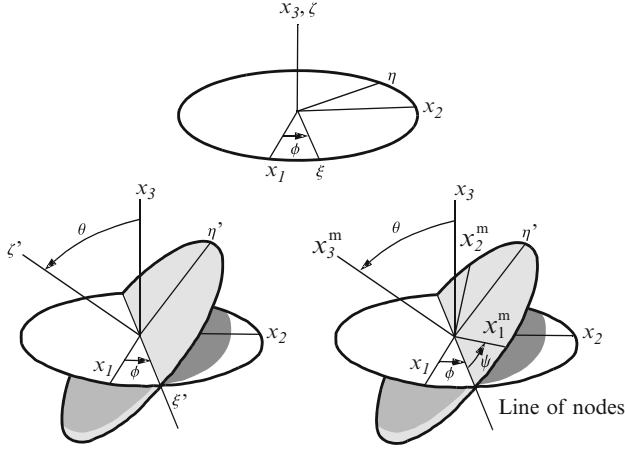
$$\begin{aligned} d\Omega &= dx_1 dx_2 dx_3 \\ d\Gamma &= dx_i dx_j \quad (i \neq j, 1 \leq i, j \leq 3) \\ dS &= dx_i \end{aligned} \quad (2.63)$$

Since

$$\mathbf{x} = \mathbf{x}(\boldsymbol{\eta}) \quad x_i = x_i(\eta_1, \eta_2, \eta_3) \quad (2.64)$$

then by partial differentiation we can derive

$$d\mathbf{x} = \frac{\partial \mathbf{x}}{\partial \boldsymbol{\eta}} \cdot d\boldsymbol{\eta} = \mathbf{J} \cdot d\boldsymbol{\eta} \quad dx_i = \frac{\partial x_i}{\partial \eta_j} d\eta_j = J_{ij} \eta_j \quad (2.65)$$



**Fig. 2.7** The rotations defining the Eulerian angles in 3D. Note that  $(\xi, \eta, \zeta)$  and  $(\xi', \eta', \zeta')$  represent intermediate stages of a sequential rotation of the axes (Modified from [194])

Let  $d\mathbf{x}_i$  be the vectors with components  $(\partial x_i / \partial \eta_j) d\eta_j$  for  $(j = 1, 2, 3)$ , then we obtain for the volume element  $d\Omega$

$$\begin{aligned} d\Omega &= (d\mathbf{x}_1 \times d\mathbf{x}_2) \cdot d\mathbf{x}_3 \\ &= |\mathbf{J}| d\eta_1 d\eta_2 d\eta_3 \end{aligned} \quad (2.66)$$

for the surface element  $d\Gamma$  for instance

$$\begin{aligned} d\Gamma &= \|d\mathbf{x}_1 \times d\mathbf{x}_2\| \\ &= \left\| \begin{pmatrix} J_{12}J_{23} - J_{22}J_{13} \\ J_{21}J_{13} - J_{11}J_{23} \\ J_{11}J_{22} - J_{21}J_{12} \end{pmatrix} \right\|_{\eta_3} d\eta_1 d\eta_2 \end{aligned} \quad (2.67)$$

and for the line element  $dS$  for instance

$$\begin{aligned} dS &= \|d\mathbf{x}_1\| \\ &= \left\| \begin{pmatrix} J_{11} \\ J_{12} \\ J_{13} \end{pmatrix} \right\|_{\eta_2, \eta_3} d\eta_1 = \sqrt{J_{11}^2 + J_{12}^2 + J_{13}^2} \Big|_{\eta_2, \eta_3} d\eta_1 \end{aligned} \quad (2.68)$$

where  $|\mathbf{J}|$  is the determinant of the Jacobian (2.44) and  $\|\cdot\|$  represents the norm of the vector resulting from transformed coordinates. It is to be noted that  $d\Gamma$  and  $dS$  can also be expressed by different transformed coordinates, e.g.,  $d\Gamma = \|(\cdot)_{\eta_1}\| d\eta_2 d\eta_3$  and so on. For example, by using cylindrical

coordinates  $(r, \phi, z)$  the following integral elements result according to the mapping (2.50):

$$\begin{aligned} d\Omega &= r \, dr \, d\phi \, dz && \text{in the } (r, \phi, z) \text{ space} \\ d\Gamma &= \begin{cases} r \, dr \, d\phi & \text{in the } (r, \phi)\text{-space} \\ dr \, dz & \text{in the } (r, z)\text{-space} \\ r \, d\phi \, dz & \text{in the } (\phi, z)\text{-space} \end{cases} \\ dS &= \begin{cases} dr & \text{in the } r\text{-space} \\ r \, d\phi & \text{in the } \phi\text{-space} \\ dz & \text{in the } z\text{-space} \end{cases} \end{aligned} \quad (2.69)$$

### 2.1.6 Spatial Variables and Their Derivative Operations

For both Cartesian  $\Re^D$  ( $D = 1, 2, 3$ ) and cylindrical coordinate systems

$$\mathbf{x}^T = \begin{cases} (x_1 \, x_2 \, x_3) \\ (x_1 \, x_2) \\ (x_1) \\ (r \, \phi \, z) \end{cases} \text{ for } \begin{cases} 3D \\ 2D \\ 1D \end{cases} \begin{cases} \text{Cartesian} \\ \text{cylindrical} \end{cases} \quad (2.70)$$

a scalar variable  $\psi$  and the velocity  $\mathbf{v}$  (2.39)

$$\mathbf{v} = \begin{cases} \begin{pmatrix} v_1 \\ v_2 \\ v_3 \end{pmatrix} & \text{for Cartesian} \\ \begin{pmatrix} v_r \\ v_\phi \\ v_z \end{pmatrix} & \text{for cylindrical} \end{cases} \quad (2.71)$$

have dependencies in space and time:  $\psi = \psi(\mathbf{x}, t)$ ,  $\mathbf{v} = \mathbf{v}(\mathbf{x}, t)$ . The following derivative operations hold, cf. (2.2), (2.3), (2.40), (2.54), (2.55) and (2.56). The gradient  $\nabla\psi$  is

$$\nabla\psi = \begin{cases} \begin{pmatrix} \frac{\partial\psi}{\partial x_1} & \frac{\partial\psi}{\partial x_2} & \frac{\partial\psi}{\partial x_3} \end{pmatrix}^T & 3D \text{ Cartesian} \\ \begin{pmatrix} \frac{\partial\psi}{\partial x_1} & \frac{\partial\psi}{\partial x_2} \end{pmatrix}^T & 2D \text{ Cartesian} \\ \begin{pmatrix} \frac{\partial\psi}{\partial x_1} \end{pmatrix} & 1D \text{ Cartesian} \\ \begin{pmatrix} \frac{\partial\psi}{\partial r} & \frac{1}{r} \frac{\partial\psi}{\partial \phi} & \frac{\partial\psi}{\partial z} \end{pmatrix}^T & \text{cylindrical } (r, \phi, z) \end{cases} \quad (2.72)$$



The second-order derivative (Laplacian) operation  $\nabla^2 \psi$  reads to

$$\nabla^2 \psi = \begin{cases} \frac{\partial^2 \psi}{\partial x_1^2} + \frac{\partial^2 \psi}{\partial x_2^2} + \frac{\partial^2 \psi}{\partial x_3^2} & \text{3D Cartesian} \\ \frac{\partial^2 \psi}{\partial x_1^2} + \frac{\partial^2 \psi}{\partial x_2^2} & \text{2D Cartesian} \\ \frac{\partial^2 \psi}{\partial x_1^2} & \text{1D Cartesian} \\ \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial \psi}{\partial r} \right) + \frac{1}{r^2} \frac{\partial^2 \psi}{\partial \phi^2} + \frac{\partial^2 \psi}{\partial z^2} & \text{cylindrical } (r, \phi, z) \end{cases} \quad (2.73)$$

The scalar product  $\nabla \cdot \mathbf{v}$  which is called the *divergence* of the vector  $\mathbf{v}$  is given by

$$\nabla \cdot \mathbf{v} = \begin{cases} \frac{\partial v_1}{\partial x_1} + \frac{\partial v_2}{\partial x_2} + \frac{\partial v_3}{\partial x_3} & \text{3D Cartesian} \\ \frac{\partial v_1}{\partial x_1} + \frac{\partial v_2}{\partial x_2} & \text{2D Cartesian} \\ \frac{\partial v_1}{\partial x_1} & \text{1D Cartesian} \\ \frac{1}{r} \frac{\partial}{\partial r} (r v_r) + \frac{1}{r} \frac{\partial v_\phi}{\partial \phi} + \frac{\partial v_z}{\partial z} & \text{cylindrical } (r, \phi, z) \end{cases} \quad (2.74)$$

The vector product  $\nabla \times \mathbf{v}$  which is called the *curl* of the vector  $\mathbf{v}$ , also known as *vorticity*  $\boldsymbol{\omega}$ , provides

$$\boldsymbol{\omega} = \nabla \times \mathbf{v} = \begin{cases} \begin{pmatrix} \frac{\partial v_3}{\partial x_2} - \frac{\partial v_2}{\partial x_3} \\ \frac{\partial v_1}{\partial x_3} - \frac{\partial v_3}{\partial x_1} \\ \frac{\partial v_2}{\partial x_1} - \frac{\partial v_1}{\partial x_2} \end{pmatrix} & \text{3D Cartesian} \\ \begin{pmatrix} 0 \\ 0 \\ \frac{\partial v_2}{\partial x_1} - \frac{\partial v_1}{\partial x_2} \end{pmatrix} & \text{2D Cartesian} \\ \mathbf{0} & \text{1D Cartesian} \\ \begin{pmatrix} \frac{1}{r} \frac{\partial v_z}{\partial \phi} - \frac{\partial v_\phi}{\partial z} \\ \frac{\partial v_r}{\partial z} - \frac{\partial v_z}{\partial r} \\ \frac{1}{r} \frac{\partial}{\partial r} (r v_\phi) - \frac{1}{r} \frac{\partial v_r}{\partial \phi} \end{pmatrix} & \text{cylindrical } (r, \phi, z) \end{cases} \quad (2.75)$$

which represents the rotation of the vector field  $\mathbf{v}$ . Gradient, divergence and curl, respectively, are sometimes written in other notations, such as

$$\nabla = \mathbf{grad} \quad \nabla \cdot = \text{div} \quad \nabla \times = \mathbf{curl} \quad (2.76)$$

*Axisymmetric problems* written in cylindrical coordinates represent a specific case. Axisymmetry assumes that all flow components along the azimuthal direction  $\phi$  vanish whereby the domain of interest  $\Omega$  is reduced to a 2D meridional domain in  $(r, z)$ . Under such conditions the above relationships (2.71)–(2.75) can be significantly simplified with  $v_\phi = 0$ ,  $\frac{\partial}{\partial \phi} = 0$ .

### 2.1.7 Gauss's Integral Theorem

The Gauss's integral (or divergence) theorem represents the most valuable transformation in tensor analysis. It relates volume integral to surface integral expressions. Let  $\Omega$  be the volume of a domain which is bounded by a piecewise-smooth closed surface  $\Gamma$ , let  $\mathbf{n} (\equiv \hat{\mathbf{n}})$  be the outward-directed unit normal to  $\Gamma$  (Fig. 2.8) and assuming the (scalar) variable  $\psi$  and the vector field  $\mathbf{a}$  have continuous first partial derivatives in  $\Omega$ , then

$$\begin{aligned} \int_{\Omega} \nabla \psi \, d\Omega &= \int_{\Gamma} \psi \, \mathbf{n} \, d\Gamma \\ \int_{\Omega} \nabla \cdot \mathbf{a} \, d\Omega &= \int_{\Gamma} \mathbf{a} \cdot \mathbf{n} \, d\Gamma \\ \int_{\Omega} \nabla \cdot (\mathbf{a}\psi) \, d\Omega &= \int_{\Gamma} \psi (\mathbf{a} \cdot \mathbf{n}) \, d\Gamma \\ \int_{\Omega} \nabla \times \mathbf{a} \, d\Omega &= \int_{\Gamma} \mathbf{a} \times \mathbf{n} \, d\Gamma \\ \int_{\Omega} \nabla \times (\mathbf{a}\psi) \, d\Omega &= \int_{\Gamma} \psi (\mathbf{a} \times \mathbf{n}) \, d\Gamma \end{aligned} \quad (2.77)$$

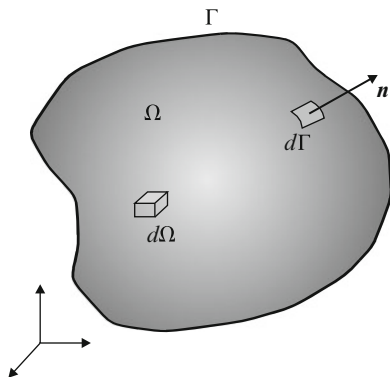
where  $\int_{\Omega} (.) \, d\Omega$  represents a volume integral and  $\int_{\Gamma} (.) \, d\Gamma$  a surface integral. Using partial integration

$$\nabla \cdot (\mathbf{a} \psi) = \mathbf{a} \cdot \nabla \psi + \psi (\nabla \cdot \mathbf{a}) \quad (2.78)$$

we obtain with (2.77)

$$\int_{\Omega} \psi (\nabla \cdot \mathbf{a}) \, d\Omega = - \int_{\Omega} (\nabla \psi \cdot \mathbf{a}) \, d\Omega + \int_{\Gamma} \psi (\mathbf{a} \cdot \mathbf{n}) \, d\Gamma \quad (2.79)$$

**Fig. 2.8** Domain of volume  $\Omega$  with its closed boundary of surface  $\Gamma$  and the outward unit normal  $\mathbf{n}$  to the surface



### 2.1.8 Stokes' Theorem

The Stokes' theorem relates a surface integral  $\Gamma$  over a cap to a line integral  $S$  around a bounding curve. The theorem states that the total circulation  $\mathbf{a} \cdot \mathbf{t}$  of a vector field  $\mathbf{a}$  in form of the line integral is equal to the surface integral of the normal component of  $\nabla \times \mathbf{a}$ :

$$\int_{\Gamma} (\nabla \times \mathbf{a}) \cdot \mathbf{n} d\Gamma = \int_S \mathbf{a} \cdot \mathbf{t} dS \quad (2.80)$$

where  $\mathbf{t}$  is the unit tangent vector.

### 2.1.9 Reynolds' Transport Theorem

The Reynolds' transport theorem (as a generalization of the Leibniz's integral rule) is very useful to compute derivatives of integrated quantities such as

$$\mathcal{F}(t) = \int_{\Omega} f(\mathbf{x}, t) d\Omega \quad (2.81)$$

Let  $\mathbf{v} = \mathbf{v}(\mathbf{x}, t)$  be a fluid vector field and let  $\Omega = \Omega(t)$  be a volume bounded by a closed surface  $\Gamma = \Gamma(t)$  moving with the fluid, then

$$\frac{D}{Dt} \int_{\Omega(t)} f(\mathbf{x}, t) d\Omega = \int_{\Omega(t)} \frac{\partial f}{\partial t} d\Omega + \int_{\Gamma(t)} f(\mathbf{v} \cdot \mathbf{n}) d\Gamma \quad (2.82)$$

or with (2.77)

$$\frac{D}{Dt} \int_{\Omega(t)} f(\mathbf{x}, t) d\Omega = \int_{\Omega(t)} \left[ \frac{\partial f}{\partial t} + \nabla \cdot (\mathbf{v} f) \right] d\Omega \quad (2.83)$$

where  $\frac{D}{Dt}$  is the material derivative (2.38) and  $\mathbf{n}$  is the outward pointing normal vector on the surface  $\Gamma$  (Fig. 2.8).

### 2.1.10 Classification of Vector Fields

A vector field  $\mathbf{v}$  is called *solenoidal*, or divergenceless, if

$$\nabla \cdot \mathbf{v} = 0 \quad (2.84)$$

By Gauss's theorem (2.77) this is equivalent to

$$\int_{\Gamma} \mathbf{v} \cdot \mathbf{n} d\Gamma = 0 \quad (2.85)$$

for any closed surface  $\Gamma$ .

A vector field  $\mathbf{v}$  is called *irrotational*, or curlless, if

$$\boldsymbol{\omega} = \nabla \times \mathbf{v} = \mathbf{0} \quad (2.86)$$

By Stokes' theorem (2.80) this is equivalent to

$$\int_S \mathbf{v} \cdot \mathbf{t} dS = 0 \quad (2.87)$$

for every closed curve  $S$ . A flow satisfying (2.86) is called *potential flow*.

### 2.1.11 Potential Function, Streamfunction, Streamline and Pathline

It is possible to construct scalar functions on which either a solenoidal (2.84) or an irrotational (2.86) vector field can be implicitly satisfied. Assuming the vector field  $\mathbf{v}$  could be the gradient of a (scalar) *potential function*  $\Phi$  in a form such as

$$\mathbf{v} = -\nabla \Phi, \quad (2.88)$$

it is easy to show that (2.88) satisfies irrotationality (2.86), i.e.,  $\boldsymbol{\omega} = \mathbf{0}$ , because  $-\nabla \times \nabla \Phi = \mathbf{0}$ . This is true for all dimensions, cf. (2.75). Introducing (2.88) the potential flow holds with  $\nabla \cdot \mathbf{v}$ :

$$-\nabla^2 \Phi = 0 \quad (2.89)$$

We note that an alternate gradient expression such as  $\mathbf{v} = -K(\mathbf{x})\nabla h$  does not strictly satisfy  $\boldsymbol{\omega} = \mathbf{0}$ , where  $K(\mathbf{x})$  is a spatially dependent coefficient and  $h$  could be a (different) scalar function, which can be seen as a *pseudopotential* function. If (and only if)  $K = \text{const}$ , and hence  $\Phi = K h$ , the flow is irrotational (see [33] for more discussions).

On the other hand, we can find a function  $\Psi$ , called as *streamfunction*, written in 2D and axisymmetric flow as

$$\begin{aligned} v_1 &= \frac{\partial \Psi}{\partial x_2}, \quad v_2 = -\frac{\partial \Psi}{\partial x_1} && \text{2D Cartesian} \\ v_r &= \frac{1}{r} \frac{\partial \Psi}{\partial z}, \quad v_z = -\frac{1}{r} \frac{\partial \Psi}{\partial r} && \text{axisymmetric} \end{aligned} \quad (2.90)$$

which implicitly satisfies the condition of a solenoidal vector field  $\nabla \cdot \mathbf{v} = 0$  (2.84) applied to 2D and axisymmetric problems. Inserting (2.90) into the vorticity equation (2.75) the Laplacian equation holds

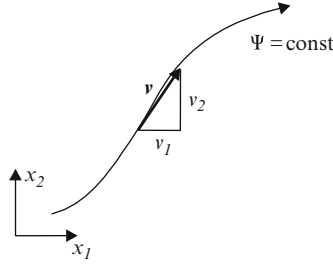
$$-\nabla^2 \Psi = 0 \quad \text{2D and axisymmetric} \quad (2.91)$$

to determine the streamfunction  $\Psi$  for 2D and axisymmetric flows. For 3D problems it is not possible to find a scalar function capable of satisfying a divergenceless velocity,  $\nabla \cdot \mathbf{v} = 0$  similar to 2D. We emphasize that *a streamfunction analog doesn't exist for 3D problems*.

By definition, a *streamline* in a flow is defined as a line, which, at any instant, is tangent to the velocity vector  $\mathbf{v}$ . If  $d\mathbf{x}$  is a differential along a streamline, the tangency condition is expressed by the cross product  $\mathbf{v} \times d\mathbf{x} = \mathbf{0}$ . In 3D Eulerian coordinates it reads to:

$$\frac{dx_1}{v_1(\mathbf{x}, t_a)} = \frac{dx_2}{v_2(\mathbf{x}, t_a)} = \frac{dx_3}{v_3(\mathbf{x}, t_a)} \quad (2.92)$$

where  $t_a$  indicates a certain (fixed) time. The cross product of the two nonzero vectors  $\mathbf{v}$  and  $d\mathbf{x}$  is zero only if they are parallel. Accordingly, a unique direction for the streamline exists at all points in space  $\mathbf{x}$ , provided  $\mathbf{v}$  is not zero. However, an exception is given at so-called stagnation points, where the velocity  $\mathbf{v}$  is zero. At those points streamlines can be split into two or more streamlines. Once the velocity field  $\mathbf{v}$  is known the solution of (2.92) yields a family of streamlines, referred to as the motion pattern. Only in 2D (or axisymmetry) a streamline can be identified as a graph of constant values of streamfunction  $\Psi = \Psi(\mathbf{x})$  (Fig. 2.9).



**Fig. 2.9** The streamfunction  $\Psi$  as a streamline in 2D flow

The streamfunction in 2D must obey the general differential relation:

$$d\Psi = \frac{\partial\Psi}{\partial x_1} dx_1 + \frac{\partial\Psi}{\partial x_2} dx_2 \quad (2.93)$$

Substituting (2.90) into (2.93) gives

$$d\Psi = -v_2 dx_1 + v_1 dx_2 \quad (2.94)$$

Accordingly, for a streamline with constant  $\Psi$ , i.e.  $d\Psi = 0$ , (2.94) becomes

$$\frac{v_2}{v_1} = \frac{dx_2}{dx_1} \Big|_{\Psi=\text{const}} \quad (2.95)$$

showing that the velocity vector is tangent (2.92) to the curve  $\Psi = \text{const}$ .

A *pathline* is a curve (or line) along which a fixed massless particle moves during a sequence of times  $t$ . It is thus the *trajectory* of a particle of fixed identity. In the Eulerian formulation the differential equation for a pathline directly results from (2.39):

$$\frac{d\mathbf{x}}{dt} = \mathbf{v}(\mathbf{x}, t) \quad (2.96)$$

or written in 3D Eulerian coordinates

$$\frac{dx_1}{v_1(\mathbf{x}, t)} = \frac{dx_2}{v_2(\mathbf{x}, t)} = \frac{dx_3}{v_3(\mathbf{x}, t)} = dt \quad (2.97)$$

The solution of (2.96), or (2.97), for a particle location at any time  $t$  can be expressed by

$$\mathbf{x}(t) = \mathbf{x}(t_0) + \int_{t_0}^t \mathbf{v}(\mathbf{x}(t), t) dt \quad (2.98)$$

where  $\mathbf{x}(t_0)$  is the position at initial time  $t_0$ .

Finally, we note that under transient flow conditions, i.e., where the flow field is time-dependent, streamlines and pathlines are commonly distinct. Here we can see an instantaneous picture of the streamlines, as the picture varies continuously. However, for steady-state flow conditions, i.e., where flow characteristics remain invariant with time, streamlines and pathlines coincide.

## 2.2 Classifications and Definitions

Flow and transport processes in the context of subsurface modeling are usually related to terms and descriptions which will be summarized in the following. The most important definitions are presented which we will need to relate to in the subsequent chapters. For a more comprehensive discussion of basic definitions for porous-media and groundwater problems the reader is referred to Bear [34] or Bear and Cheng [38].

### 2.2.1 Water and Aquifer

**Subsurface water** denotes *all* water below the ground surface (Fig. 2.10). This water is contained in the void space of geologic formations of different types. The void space can be fully or partially saturated by water. Subsurface water can be regarded as part of the hydrologic cycle [356].

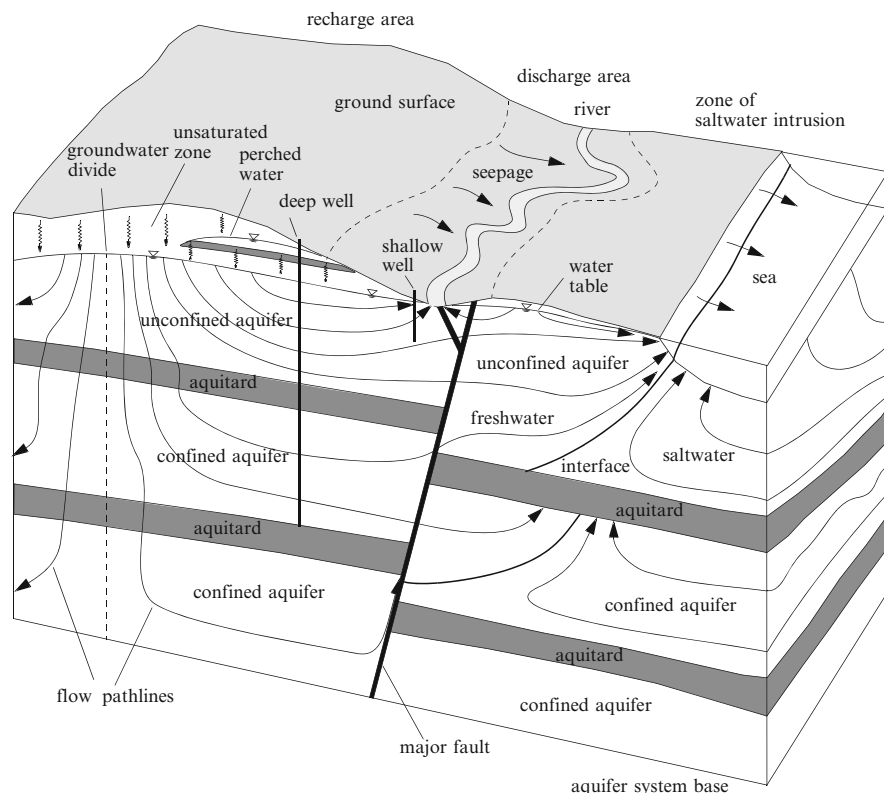
**Groundwater** denotes only this part of the subsurface water that occurs in geologic formations in which the void space is *fully saturated*. Groundwater flows in aquifers and rocks.

**Surface water** denotes all water collecting on the ground or in streams, rivers, lakes, wetlands or oceans. Surface water is usually interrelated to subsurface water where water can be exchanged via infiltration, drainage and seepage.

**Freshwater** represents surface or subsurface water having only low concentrations of salts or other dissolved solids. Commonly, a groundwater resource (without additional specifications) is related to freshwater which is available for drinking and other purposes. Freshwater specifically excludes saltwater. Measuring water salinity by concentrations in parts per million (ppm) – equivalent to g/l – freshwater is usually classified with a concentration smaller than 0.5 ppm.

**Saltwater** is water which contains dissolved salts (mostly NaCl) of different concentrations larger than 0.5 ppm. It can be further categorized into *brackish water* having a salinity in the range of 0.5–30 ppm, *saline water* with a salinity between 30 and 50 ppm and *brine* with a salinity of more than 50 ppm.

**Saltwater intrusion** (or saltwater encroachment) denotes the movement of saltwater into freshwater. In the subsurface it virtually occurs in all coastal aquifers, where the denser saltwater from the sea intrudes into the freshwater aquifer due to



**Fig. 2.10** Illustration of typical flow regimes in a multilayered aquifer system (Modified from [101, 306])

its higher density. It can also be caused by groundwater pumping above or nearby saltwater zones.

**Aquifer** denotes a geologic formation, or a group of formations, of water-bearing permeable rock or sediment layers from which water can be usefully extracted (Fig. 2.10). Aquifers can be confined or unconfined (see further below).

**Aquitard** is a geologic formation which is of a semipervious nature. It transmits water at a very low rate compared to an aquifer. An aquitard separates an aquifer layer from an adjacent aquifer (as exemplified in Fig. 2.10). An aquitard, if completely impermeable, is denoted as *aquiclude* or *aquifuge*.

**Aquifer system** groups a certain number of aquifers separated by aquitards in a multilayered structure (Fig. 2.10).

**Confined aquifer**, also known as *pressure aquifer*, is an aquifer (a) bounded from above and below by impervious formations and an aquifer (b) in which the water pressure reaches such values that the water level measured in a piezometer will rise above the base of the upper confining formation. Water enters a confined aquifer



in a recharge area, which is commonly linked to an unconfined aquifer. A confined aquifer is called a *leaky confined aquifer* if one or both confining formations are semipervious, through which leakage may take place.

**Unconfined aquifer**, also called a *phreatic aquifer*, is bounded from above by the water table or phreatic surface. Usually, a phreatic aquifer is directly recharged from the ground surface above it, except where impervious layers (of limited areal extent) exist between the phreatic surface and the ground surface. Above the phreatic surface a capillary fringe establishes. The base of an unconfined aquifer is considered impervious. An unconfined aquifer is called a *leaky unconfined aquifer* if the lower bounded formation is semipervious.

**Perched groundwater**, or *perched aquifer*, is a special case of a phreatic aquifer. It represents a limited areal extent of water, formed on an impervious, or semipervious, layer (see Fig. 2.10). Perched water may exist only for a limited period of time.

**Saturated zone** forms above impervious or semipervious formations. In this zone the entire void space is filled with water. The saturated zone can be bounded from above by a water table, or phreatic surface.

**Unsaturated zone**, or *vadose zone*, describes the zone between ground surface and the underlying phreatic surface, where only part of the void space is occupied by water, the remainder being occupied by a gaseous phase, usually air.

**Infiltration** is the unsaturated downward water flow from the ground surface, percolating through the unsaturated zone and reaching an underlying water table. It is usually driven by natural replenishment from precipitation and snow melt. Its quantity in relation to the total precipitation is influenced, among others, by evaporation, surface runoff, soil characteristics and transpiration through the vegetation. Infiltration can also include seepage from ponds, lakes, ditches, channels and other leakages.

**Groundwater recharge** denotes that amount of infiltrating water which finally reaches the water table of an underlying aquifer. It determines the replenishment of aquifers and represents an important parameter in the use and exploitation of groundwater resources.

**Groundwater divide** is a surface in 3D or a curve in 2D that separates the flow domain into subdomains, on either side of which groundwater moves in opposite directions (see Fig. 2.10).

**Water table**, or *phreatic surface*, is actually the boundary between the unsaturated and saturated zone. It represents the upper surface of the groundwater body. Phreatic surface is a specific representation of a *free surface*.

**Fracture** is part of the void space of a porous-medium domain that has a special spatial configuration: one of its dimensions – the *aperture* – is much smaller than the other two spatial dimensions. Fractures provide pathways for fluid flow and transport through otherwise impermeable or semipervious formations and produce planes, surfaces or even lined interconnections where fluid movement increases and focuses, such as in cracks of rocks, interstices, vugs or tectonic faults.

**Fractured porous rock** defines a pervious rock formation which is composed of an interconnected network of fractures. Thus, the total void space results from fractures

and porous blocks of rock. The flow movement usually dominates in the fracture network. If the surrounded rock contains no void space the term *fractured rock* is used.

### 2.2.2 Terms and Quantities

**Domain** and **boundary** are defined in the  $D$ -dimensional Euclidean space  $\mathbb{R}^D$  ( $D = 1, 2, 3$ ) (see Sect. 2.1.2) and are usually denoted by  $\Omega \subset \mathbb{R}^D$  and  $\Gamma \subset \mathbb{R}^D$ , respectively. The domain  $\Omega$  is completely closed by the boundary  $\Gamma$  (see Fig. 2.8). The boundary  $\Gamma$  can be arbitrarily shaped. It can be composed of different nonoverlapping segments, e.g.,  $\Gamma_D, \Gamma_N, \dots$ , bounding the domain  $\Omega$  both outside and inside. By definition, the boundary  $\Gamma$  is separated from the domain  $\Omega$ . On the other hand, by  $\bar{\Omega}$  we denote the (closure) domain, which completely joins the boundary

$$\bar{\Omega} = \Omega \cup \Gamma \quad \text{with} \quad \Gamma = \Gamma_D \cup \Gamma_N \cup \dots \quad (2.99)$$

On  $\bar{\Omega}$  and  $\Gamma$  initial conditions and boundary conditions have to be specified, respectively.

**Initial conditions** (IC's) specify the values of a time-dependent variable  $\psi = \psi(\mathbf{x}, t)$  in  $\bar{\Omega}$  at initial time  $t_0$ :

$$\psi(\mathbf{x}, t_0) = \psi_0(\mathbf{x}) \quad \text{in} \quad \bar{\Omega} = \Omega \cup \Gamma \quad (2.100)$$

We note that for steady-state problems no IC's are needed, unless the steady-state problem is nonlinear, where IC's are required to initialize an iterative procedure.

**Boundary conditions** (BC's) specify values on the total boundary  $\Gamma$  closing the domain  $\Omega$ . Related to a time-dependent solution variable  $\psi = \psi(\mathbf{x}, t)$  the following types are common:

1. *Dirichlet-type* (1st kind) BC, also termed as *essential boundary condition*, prescribes the value of  $\psi$  on a boundary section  $\Gamma_D$ :

$$\psi(\mathbf{x}, t) = \psi_D(t) \quad \text{on} \quad \Gamma_D \subset \Gamma \quad (2.101)$$

A typical application of a Dirichlet BC is the prescription of a potential value, mass concentration or temperature in dependence on the underlying problem.

2. *Neumann-type* (2nd kind) BC prescribes the normal derivative of  $\psi$  on a boundary section  $\Gamma_N$ :

$$-(\boldsymbol{\alpha} \cdot \nabla \psi) \cdot \mathbf{n} = q_n(t) \quad \text{on} \quad \Gamma_N \subset \Gamma \quad (2.102)$$

where  $\alpha$  is an arbitrary coefficient matrix, which must be  $\|\alpha\| \neq 0$ . The prescribed value  $q_n(t)$  represents a normal flux (positive outward) across the boundary portion  $\Gamma_N$ . If  $q_n = 0$  the Neumann-type BC reduces to a *natural* (no-flux) boundary condition associated with  $\nabla\psi = \mathbf{0}$ . A typical application of a Neumann BC is the description of a diffusive (dispersive/conductive) flux rate of mass or energy in dependence on the underlying problem.

3. *Cauchy-type* and *Robin-type* (3rd kind) BC's combine Dirichlet-type and Neumann-type BC's in different ways. The Cauchy BC represents a weighted arithmetic mean of Dirichlet and Neumann BC according to

$$-(\alpha \cdot \nabla\psi) \cdot \mathbf{n} = -\beta(\psi_C - \psi) \quad \text{on } \Gamma_C \subset \Gamma \quad (2.103)$$

where  $\psi_C = \psi_C(t)$  is a prescribed value of  $\psi$  and  $\beta = \beta(t)$  denotes an additional transfer coefficient. We have chosen the signs in (2.103) in such a way that the flux is directed positive outward if  $\psi > \psi_C$ . If  $\beta$  becomes large the boundary condition tends to a Dirichlet type with  $\psi \rightarrow \psi_C$  on  $\Gamma_C$ . On the other hand, if  $\beta$  becomes small it tends to a natural boundary condition enforcing  $\nabla\psi \rightarrow \mathbf{0}$  on  $\Gamma_C$ . A typical application for Cauchy BC is the leakage of mass through a given boundary section. In contrast, the Robin-type (also called *mixed*) BC is a mixture of Dirichlet and Neumann BC in such a form

$$-(\alpha \cdot \nabla\psi) \cdot \mathbf{n} = q_n - \beta(\psi_C - \psi) \quad \text{on } \Gamma_R \subset \Gamma \quad (2.104)$$

The Robin-type BC is the most general boundary condition and implies all other types of boundary conditions above. A typical application of Robin BC refers to the prescription of a total (diffusive plus advective) mass or energy rate through a given boundary section. If the total (diffusive plus advective) mass or energy rate  $q_n$  is specified in such a form

$$-(\alpha \cdot \nabla\psi - \mathbf{v}\psi) \cdot \mathbf{n} = q_n \quad (2.105)$$

where  $\mathbf{v} \cdot \mathbf{n}$  is the advective velocity normal (outward positive) on  $\Gamma_C$ , (2.105) can be expressed by a Cauchy-type BC (2.103) if we substitute

$$\beta = -\mathbf{v} \cdot \mathbf{n} \quad \text{and} \quad \psi_C = \frac{q_n}{\mathbf{v} \cdot \mathbf{n}} \quad (2.106)$$

We note that the union of  $\Gamma_D$ ,  $\Gamma_N$ ,  $\Gamma_C$  and  $\Gamma_R$  forms the complete boundary  $\Gamma = \Gamma_D \cup \Gamma_N \cup \Gamma_C \cup \Gamma_R$ , where the segments do not overlap each other,  $\Gamma_D \cap \Gamma_N \cap \Gamma_C \cap \Gamma_R = \emptyset$ . Boundary conditions are always required for both transient and steady-state problems. Usually,  $\Gamma_D \neq \emptyset$  at steady-state. Besides these boundary conditions of Dirichlet (2.101), Neumann (2.102), Cauchy (2.103) or Robin (2.104) type, there are more specific boundary conditions, for example *free surface*, *seepage face*, *surface ponding*, *pumping well*, *borehole heat exchanger* or *gradient-type* BC, which represent modifications and in parts nonlinear combinations of the above

conditions and will be described in the context of the problem solutions to be discussed in Chap. 6.

**Transfer** or **leakage** conditions describe the exchange of mass, momentum or energy on specific boundaries. Transfer is a more general term typically used in mass and heat transport, while leakage is commonly used in subsurface hydrology to describe the exchange of flow through external and internal boundaries. Generally expressed, their mathematical formulation reads to

$$q_n = -\beta(\psi_{\text{ex}} - \psi) \quad (2.107)$$

written for the variable  $\psi$ , where  $\beta$  represents a transfer coefficient. Accordingly, the normal exchange rate  $q_n$  is controlled by the difference between an external (known) value  $\psi_{\text{ex}}$  and the internal value of the variable  $\psi$  and can be recognized as a Cauchy-type BC, cf. (2.103), with  $q_n = -(\boldsymbol{\alpha} \cdot \nabla \psi) \cdot \mathbf{n}$ . Applied to the heat transfer, Equation (2.107) is known as *Newton's law of cooling*, where heat transfer occurs at a boundary of a solid with the ambient convecting fluid temperature. Equation (2.107) also represents a leakage condition, where the transfer coefficient is usually replaced by

$$\beta = \frac{K}{b} \quad (2.108)$$

introducing the conductivity  $K$  and the thickness  $b$ . In practice, the transfer coefficient  $\beta$  may be chosen to distinguish between inflowing conditions ( $q_n < 0$ ) and outflowing conditions ( $q_n > 0$ ) introducing the following *dual* functions for the transfer coefficient  $\beta$ :

$$\beta = \begin{cases} \beta_{\text{in}} & \text{for } \psi_{\text{ex}} > \psi \\ \beta_{\text{out}} & \text{for } \psi_{\text{ex}} \leq \psi \end{cases} \quad (2.109)$$

where  $\beta_{\text{in}}$  and  $\beta_{\text{out}}$  denote the in-transfer and the out-transfer coefficients, respectively.

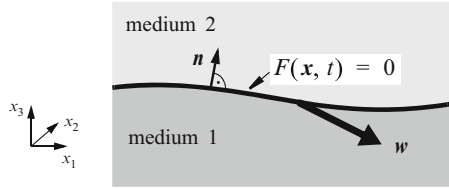
**Resistance** of mass, momentum or heat exchange at a surface is related to the inverse of the transfer coefficient (2.108)

$$\bar{R} = \frac{1}{A\beta} \quad (2.110)$$

where  $A$  corresponds to an exchange area.

**Specific resistance** defines the resistance of mass, momentum or heat exchange per unit length such that

$$R = \bar{R} L = \frac{L}{A\beta} = \frac{1}{S\beta} \quad (2.111)$$



**Fig. 2.11** Interface representation

where  $L$  is a length and  $S = \frac{A}{L}$  is a specific exchange surface. The specific resistance represents a material property.

**Interface**, or *interface boundary* or *surface*, represents a boundary between two media (materials) where the conditions abruptly change (Fig. 2.11). This can be a boundary between different fluids or a boundary between a fluid and a solid. If liquids are immiscible, a distinct sharp interface is maintained between them, even if small quantities of certain components can cross the interphase boundary driven by diffusion. Mathematically, an interface  $F$  can be described by the function:

$$F(\mathbf{x}, t) = 0 \quad (2.112)$$

As the interface moves with a velocity  $\mathbf{w}$ , its shape changes, however, all material points associated with the interface must be conserved, i.e., the material derivative of  $F$  is valid

$$\frac{\partial F}{\partial t} + \mathbf{w} \cdot \nabla F = 0 \quad (2.113)$$

The outward unit vector  $\mathbf{n}$  normal to  $F$  is defined as

$$\mathbf{n} = \frac{\nabla F}{\|\nabla F\|} \quad (2.114)$$

and accordingly it is

$$\mathbf{w} \cdot \mathbf{n} = -\frac{\partial F / \partial t}{\|\nabla F\|} \quad (2.115)$$

**Free surface** is a specific surface of a connected flow domain that is subjected to a constant pressure and a given mass flux crossing the surface. Having a zero mass flux it represents the classic hydrodynamic free-surface condition for an isobaric and impervious boundary. In subsurface flow a phreatic surface represents a free surface.

**Phase**, identified by the index  $\alpha$  (or other Greek indices), is defined as a portion  $\Omega^\alpha$  of space  $\Omega$ , whether connected or non-interconnected, that is separated from other such portions by a well defined surface  $\Gamma^\alpha$ , which represents an interface. A phase

$\alpha$  may be composed of a number of different *chemical species*  $k$ . The phase index  $\alpha$  takes on values of  $s$  and  $f = (l, g)$  corresponding to the solid phase and the two fluid phases of liquid and gas, respectively. Throughout this book,  $\alpha$  (or other Greek indices) ranges as  $\alpha = s, f \in (l, g)$  and the repetition of Greek indices does not imply a summation.

**Energy** in physics represents a quantity that is assigned to a particle, an object and a system of objects. Energy is a scalar physical quantity, which is usually measured in joules (J). There are different forms of energy, e.g., internal or thermal energy and kinetic energy, which are named after the related forces. All forms of energy are equivalent. Energy is subject to a conservation law, the *first law of thermodynamics*. Any form of energy can be transformed into another form, however, in the energy transformation process the total energy remains the same. Energy may neither be created nor destroyed.

**Entropy** is a measure of how disorganized a system is. It is taken as a measure of ‘disorder’: the higher the entropy, the higher the disorder. Disorder means the tendency of a system to get states which are homogeneous and fully mixed throughout space. The highest degree of disorder is the chaos, the most unorganized state. Entropy of a physical system is proportional to the quantity of energy no longer available to do physical work. It is measured in physical units of energy per temperature: joules per kelvin (J/K). Entropy is central to the *second law of thermodynamics*, which states that in an isolated system any activity increases the entropy. The second law of thermodynamics introduces irreversibility: an isolated system cannot pass from a state of higher entropy to a state of lower entropy, e.g., transmission of heat from a cooler medium to a warmer one is impossible. Increases in entropy correspond to irreversible changes in a system. Entropy reaches its maximum at equilibrium state of a physical system.

**Chemical species**, or a *component*, identified by subscript  $k$ , is a part of a phase that consists in an identifiable, chemical constituent, or an assembly of constituents, e.g., ions or molecules. It represents a mixture of a number of independent chemical species ( $k = 1, \dots, N$ ) dissolved in a fluid phase or adsorbed at/absorbed in a solid phase. Chemical species are miscible continuous quantities, which cannot be separated by interface (discontinuity) conditions. Note that Einstein’s summation convention is not applied to the species index  $k$ .

**Extensive quantity**,  $\mathcal{F}_k(t)$ , specified for chemical species  $k$ , such as for mass  $\mathcal{M}_k$ , momentum  $\mathcal{V}_k$ , internal (thermal) energy  $\mathcal{E}_k$ , kinetic energy  $\mathcal{K}_k$  and entropy  $\mathcal{S}_k$ , is given for the domain  $\Omega$  and reads

$$\mathcal{F}_k(t) = \int_{\Omega} f_k(\mathbf{x}, t) d\Omega \quad (2.116)$$

where  $f_k(\mathbf{x}, t)$  is the *intensive quantity* of species  $k$ . Extensive quantities are dependent on the volume  $\Omega$  and listed in Table 2.1.

**Intensive quantity**,  $f_k(\mathbf{x}, t)$  as listed in Table 2.1, is related to the particles occupied in the domain  $\Omega$ . It represents the intensity of an extensive quantity as

**Table 2.1** Extensive  $\mathcal{F}_k$  and intensive  $f_k$  quantities related to species  $k$  (no summation over  $k$ )

Quantity	$\mathcal{F}_k(t)$	$f_k(\mathbf{x}, t)$
Mass	$\mathcal{M}_k$	$\rho_k$
Momentum	$\mathcal{V}_k$	$\rho_k \mathbf{v}_k$
Internal energy	$\mathcal{E}_k$	$\rho_k E_k$
Kinetic energy	$\mathcal{K}_k$	$\rho_k \frac{1}{2} v_k^2$
Entropy	$\mathcal{S}_k$	$\rho_k S_k$

defined by (2.116) and is accordingly independent of the volume  $\Omega$ . In general an intensive quantity that is given per unit volume, is characterized as a *density*. On the other hand, an intensive quantity as given per unit mass, will be denoted as a *specific density*. In Table 2.1 it can be recognized that the velocity  $\mathbf{v}_k$  represents a specific momentum density,  $E_k$  is a specific internal energy density and  $S_k$  is a specific entropy density.

**Density and specific density** represent intensive quantities per unit volume and unit mass, respectively. *Mass density*,  $\rho_k$ , is defined as mass per unit volume, *specific momentum density*,  $\mathbf{v}_k$ , is momentum per unit mass, *specific internal energy density*,  $E_k$ , denotes internal energy per unit mass and *specific entropy density*,  $S_k$ , is entropy per unit mass. Commonly, for short descriptions it is customary to use the word *density* also when we actually mean mass density  $\rho_k$ .

**Concentration** measures the quantity of chemical species  $k$  in a unit volume  $\Omega$  of fluid. It can be expressed in different ways as follows.

**Mass concentration**, denoted by  $C_k$ , expresses the mass of species  $k$  per unit volume of a fluid and is identical to the mass density  $\rho_k$ :

$$C_k \equiv \rho_k = \frac{\mathcal{M}_k}{dV} \quad (2.117)$$

where  $dV$  corresponds to an averaging volume. This measure is preferably used. Usual physical units are g/l (= grams of  $k$  per liter of fluid), or mg/l (= milligrams of  $k$  per liter of fluid).

**Molar concentration**, or *molarity*, denoted by  $[C_k]$ , expresses the number of  $k$ -moles per unit volume of fluid and reads

$$[C_k] = \frac{C_k}{m_k} \quad (2.118)$$

where  $m_k$  is the molecular mass of the  $k$ -species. This measure is common for thermodynamics. Common units are moles of  $k$  per liter of fluid, mol/l or mol/m<sup>3</sup>(= mmol/l).

**Activity** of a species  $k$ , denoted by  $\{C_k\}$ , is related to its molar concentration  $[C_k]$  by

$$\{C_k\} = \gamma_k [C_k] \quad (2.119)$$

where  $\gamma_k$  is the *activity coefficient* of species  $k$ , which is given for an ionic aqueous species for instance by the empirical *Davies relationship* [500] in the form

$$\log_{10} \gamma_k = -\frac{1}{2} z_k^2 \left( \frac{\sqrt{I}}{1 + \sqrt{I}} - 0.3 I \right) \quad (2.120)$$

where  $z_k$  is the charge on the  $k$ th species and  $I$  denotes the *ionic strength* defined by

$$I = \frac{1}{2} \sum_{k=1}^N z_k^2 [C_k] \quad (2.121)$$

For *dilute solutions*,  $\gamma_k \approx 1$  and

$$\{C_k\} \approx [C_k] \quad (2.122)$$

**Mass fraction**, denoted by  $\omega_k$ , is the mass of  $k$ -species per unit mass of fluid. It can be seen as a *specific density* of mass and is expressed as

$$\omega_k = \frac{C_k}{\rho} \equiv \frac{\rho_k}{\rho} \quad \rho = \sum_k \rho_k \quad \sum_k \omega_k = 1 \quad (2.123)$$

where  $\rho$  is the bulk mass density of fluid. This dimensionless measure is often expressed with the physical unit ppm, ‘parts per million’, defining the number of grams of solute per million grams of solution.

**Advection** describes the transport mechanism of a conserved quantity (e.g., mass or heat) due to fluid motion. Advection requires currents in the fluid (or fluid phase). It does not occur in impervious media or stagnant fluids.

**Convection** is sometimes synonymously used with advection. However, it usually refers to more general flow phenomena, in which the fluid motion is additionally influenced or even caused by changes in the fluid (mass) density. One can differentiate between *forced convection* in which the fluid motion is generated by external forces (e.g., pressure/potential gradient, flow source), *free (or natural) convection* in which the flow motion exclusively results from inner buoyant forces due to fluid density changes and *mixed convection* where forced and free convection occur in combination. Throughout the book we will use the term ‘convection’ to indicate transport of quantities within a moving fluid, where variable-density effects are present, while the term ‘advection’ is used to indicate transport of quantities in fluid flow without variable-density effects. With this definition we understand that forced convection is equivalent to advection.

**Diffusion** usually describes the spread of chemical species from regions of higher concentration to regions of lower concentration. It occurs both in fluids and solids. Diffusion in a flowing fluid is independent of the flow direction, i.e., it also acts in the opposite flow direction. More general, diffusion can be understood as a



spreading mechanism driven by gradients of one (or even more) quantity(ies). For instance, thermal diffusion is driven by a temperature gradient, mass diffusion is driven by a concentration gradient, momentum diffusion is driven by a gradient of velocity.

**Conduction** describes a spreading mechanism due to a gradient of a quantity. It is equivalent to diffusion. A hydraulic conduction is controlled by the gradient of a hydraulic potential. A thermal conduction is driven by a temperature gradient.

**Sorption** is a general term which covers both *adsorption* and *absorption*. Adsorption refers to the adherence of chemical species primarily on a solid surface due to adhesion, while absorption refers to a more or less uniform penetration of chemical species into a coexisting phase. Additionally, there is *desorption* which is the reverse of adsorption, i.e., chemical species are detached from the solid surface and reenter a dissolved phase.

**Steady state** describes systems, properties or dependent variables which are unchanging in time  $t$ . A dependent variable  $\psi(\mathbf{x}, t)$  becomes *steady* if the time  $t$  does not appear as an independent variable anymore, i.e.,  $\psi = \psi(\mathbf{x})$ . It implies that its derivative with respect to time is zero:

$$\frac{\partial \psi}{\partial t} = 0 \quad (2.124)$$

FEFLOW

Finite Element Modeling of Flow, Mass and Heat  
Transport in Porous and Fractured Media

Diersch, H.-J.

2014, XXXV, 996 p. 384 illus., 81 illus. in color.,

Hardcover

ISBN: 978-3-642-38738-8