Chapter 4

Mass and energy conservation

The conservation equations are derived using two basic principles — the conservation laws and the constitutive relations. The conservation laws are based on the law of conservation of mass, which states that mass is conserved, and the Newton's law for the conservation of momentum, which states that the rate of change of momentum is equal to the sum of the applied forces. However, there is a complication when these are applied to flow systems, because fluids are transported with the mean flow, and so it is necessary to apply the conservation principles in a reference frame moving with the fluid. Therefore, the time derivatives used in the conservation equations have to be defined a little more carefully. So we will first consider the concept of 'substantial derivatives' before we proceed to deriving the conservation equations. Substantial derivatives will be illustrated using a position dependent concentration field as an example.

4.1 Conservation equations in Cartesian coordinates

4.1.1 Partial derivative

The partial time derivative of the concentration is the rate of change of concentration at a fixed location in space. Fix the location of observation, and determine the change in the concentration with time at this position. If the concentration at the position x at time t is $c(x, t)$ and the concentration at position x at time $t + \Delta t$ is $c(x, t + \Delta t)$, the 'partial derivative' is writtten as

$$\frac{\partial c}{\partial t} = \lim_{\Delta t \to 0} \frac{c(x_1, x_2, x_3, t + \Delta t) - c(x_1, x_2, x_3, t)}{\Delta t} \tag{4.1}$$

4.1.2 Substantial derivative

Though the partial derivative is defined as the change in the value of the concentration at a point in the fluid, this does not reflect the change in the concentration in material volumes, because these material volumes are convected with the flow. Therefore, the volume of fluid which was located at (x_1, x_2, x_3) at time t would have moved to a new position $(x_1 + v_1\Delta t, x_2 + v_2\Delta t, x_3 + v_3\Delta t)$ at time $t + \Delta t$. The substantial derivative determines the change in concentration on material volumes that are moving with the fluid. If the fluid is moving only in one direction, the substantial derivative is defined as

$$\begin{aligned}
\frac{Dc}{Dt} &= \lim_{\Delta t \to 0} \frac{c(x_1 + v_1\Delta t, x_2 + v_2\Delta t, x_3 + v_3\Delta t, t + \Delta t) - c(x, t)}{\Delta t} \\
&= \frac{\partial c}{\partial t} + \frac{dx_1}{dt}\frac{\partial c}{\partial x} + \frac{dx_2}{dt}\frac{\partial c}{\partial x_2} + \frac{dx_3}{dt}\frac{\partial c}{\partial x_3} \\
&= \frac{\partial c}{\partial t} + v_1\frac{\partial c}{\partial x_1} + v_2\frac{\partial c}{\partial x_2} + v_3\frac{\partial c}{\partial x_3}
\end{aligned} \tag{4.2}$$

In a three dimensional flow, there are three components of the velocity field, and the substantial derivative contains terms due to each of these three components.

$$\frac{Dc}{Dt} = \frac{\partial c}{\partial t} + v_1\frac{\partial c}{\partial x_1} + v_2\frac{\partial c}{\partial x_2} + u_3\frac{\partial c}{\partial x_3} \tag{4.3}$$

4.1.3 Conservation of mass

The mass conservation equation simply states that mass cannot be created or destroyed. Therefore, for any volume of fluid,

$$\left(\begin{array}{l}\text{Rate of mass} \\ \text{accumulation}\end{array}\right) = \left(\begin{array}{l}\text{Rate of mass} \\ \text{IN}\end{array}\right) - \left(\begin{array}{l}\text{Rate of mass} \\ \text{OUT}\end{array}\right) \tag{4.4}$$

Consider the volume of fluid shown in figure 4.1. This volume has a total volume $\Delta x_1 \Delta x_2 \Delta x_3$, and it has six faces. The rate of mass in through the face at x is $(\rho v_1)|_{x_1} \Delta x_2 \Delta x_3$, while the rate of mass out at $x_1 + \Delta x_1$

is $(\rho v_1)|_{x_1+\Delta x_1}\Delta x_2\Delta x_3$. Similar expressions can be written for the rates of mass flow through the other four faces. The total increase in mass for this volume is $(\partial\rho/\partial t)\Delta x_1\Delta x_2\Delta x_3$. Therefore, the mass conservation equation states that

$$\begin{aligned}\Delta x_1\Delta x_2\Delta x_3\frac{\partial\rho}{\partial t} &= \Delta x_2\Delta x_3[(\rho v_1)|_{x_1} - (\rho v_1)|_{x_1+\Delta x_1}] \\ &\quad +\Delta x_1\Delta x_3[(\rho v_2)|_{x_2} - (\rho v_2)|_{x_2+\Delta x_2}] \\ &= \Delta x_1\Delta x_2[(\rho v_3)|_{x_3} - (\rho v_3)|_{x_3+\Delta x_3}] \end{aligned} \tag{4.5}$$

Dividing by $\Delta x_1\Delta x_2\Delta x_3$, and taking the limit as these approach zero, we get

$$\frac{\partial\rho}{\partial t} = -\left(\frac{\partial(\rho v_1)}{\partial x_1} + \frac{\partial(\rho v_2)}{\partial x_2} + \frac{\partial(\rho v_3)}{\partial x_3}\right) \tag{4.6}$$

The above equation can often be written using the substantial derivative

$$\frac{\partial\rho}{\partial t} + \left(v_1\frac{\partial\rho}{\partial x_1} + v_2\frac{\partial\rho}{\partial x_2} + v_3\frac{\partial\rho}{\partial x_3}\right) = -\rho\left(\frac{\partial v_1}{\partial x_1} + \frac{\partial v_2}{\partial x_2} + \frac{\partial v_3}{\partial x_3}\right) \tag{4.7}$$

The left side of the above equation is the substantial derivative, while the right side can be written as

$$\frac{D\rho}{Dt} = -\rho(\nabla.\mathbf{v}) \tag{4.8}$$

where the dot product has the usual connotation, and the operator ∇ is defined as

$$\nabla = \mathbf{e}_1\frac{\partial}{\partial x_1} + \mathbf{e}_2\frac{\partial}{\partial x_2} + \mathbf{e}_3\frac{\partial}{\partial x_3} \tag{4.9}$$

The above equation describes the change in density for a material element of fluid which is moving along with the mean flow. A special case is when the density does not change, so that $(D\rho/Dt)$ is identically zero. In this case, the continuity equation reduces to

$$\frac{\partial v_1}{\partial x_1} + \frac{\partial v_2}{\partial x_2} + \frac{\partial v_3}{\partial x_3} = 0 \tag{4.10}$$

This is just the symmetric part of the rate of deformation tensor. As we had seen in the previous lecture, this symmetric part corresponds to volumetric compression or expansion. Therefore, if this is zero, it implies that there is

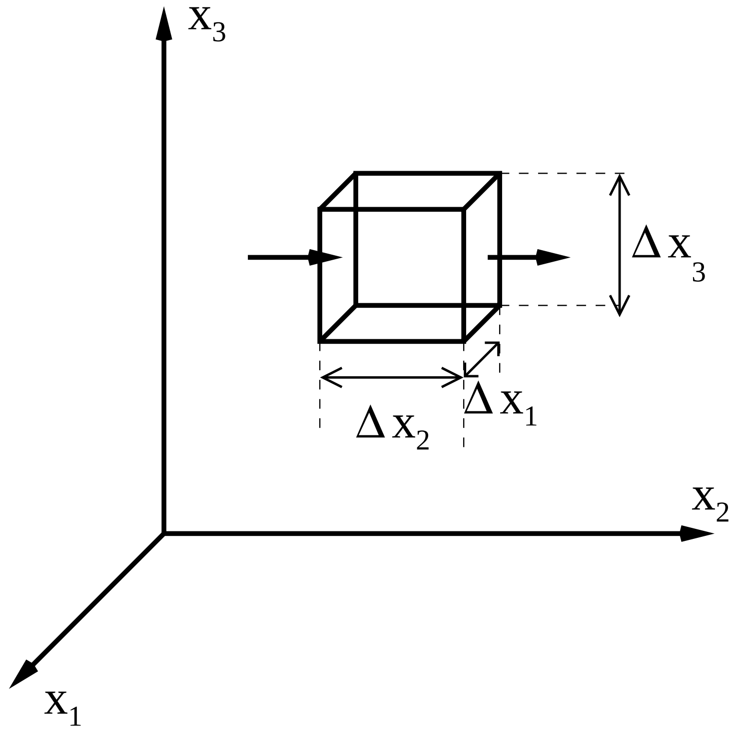

Figure 4.1: Control volume used for calculating mass and momentum balance.

no volumetric expansion or compression, and if mass is conserved then the density has to be a constant. Fluids which obey this condition are called 'incompressible' fluids. Most fluids that we use in practical applications are incompressible fluids; in fact all liquids can be considered incompressible for practical purposes. Compressibility effects only become important in gases when the speed of the gas approaches the speed of sound, 332 m/s.

4.1.4 Diffusion equation for the concentration field

The diffusion equation for the concentration field, c, can be determined in a manner similar to that for the density from equation 4.1. However, in this case, the transport across the cubic faces takes place due to mean convection as well as due to the diffusion flux across the surfaces.

$$\begin{aligned}\Delta x_1 \Delta x_2 \Delta x_3 \frac{\partial c}{\partial t} &= \Delta x_2 \Delta x_3 [(c v_1 + j_1)|_{x_1} - (c v_1 + j_1)|_{x_1 + \Delta x_1}] \\ &\quad + \Delta x_1 \Delta x_3 [(c v_2 + j_2)|_{x_2} - (c v_2 + j_2)|_{x_2 + \Delta x_2}] \\ &= \Delta x_1 \Delta x_2 [(c v_3 + j_3)|_{x_3} - (c v_3 + j_3)|_{x_3 + \Delta x_3}] \end{aligned} \tag{4.11}$$

Dividing throughout by $\Delta x_1 \Delta x_2 \Delta x_3$, the equation for the concentration field is

$$\frac{\partial c}{\partial t} + \frac{\partial (c v_1)}{\partial x_1} + \frac{\partial (c v_2)}{\partial x_2} + \frac{\partial (c v_3)}{\partial x_3} = - \frac{\partial j_1}{\partial x_1} - \frac{\partial j_2}{\partial x_2} - \frac{\partial j_3}{\partial x_3} \tag{4.12}$$

This equation can also be written as

$$\frac{\partial c}{\partial t} + \nabla . (c \mathbf{u}) = - \nabla . \mathbf{j} \tag{4.13}$$

where the vector flux, $\mathbf{j}$, is

$$\mathbf{j} = j_1 \mathbf{e}_1 + j_2 \mathbf{e}_2 + j_3 \mathbf{e}_3 \tag{4.14}$$

The flux is expressed in terms of the concentration field as

$$\mathbf{j} = D \nabla c = D \left(\mathbf{e}_1 \frac{\partial c}{\partial x_1} + \mathbf{e}_2 \frac{\partial c}{\partial x_2} + \mathbf{e}_3 \frac{\partial c}{\partial x_3} \right) \tag{4.15}$$

Using this, the equation for the concentration field is

$$\frac{\partial c}{\partial t} + \nabla . (c \mathbf{u}) = \nabla . (D \nabla c) \tag{4.16}$$

If the diffusion coefficient is a constant, the equation for the concentration field becomes

$$\frac{\partial c}{\partial t} + \nabla . (c \mathbf{u}) = D \nabla^2 c \tag{4.17}$$

where

$$\nabla^2 = \left(\frac{\partial}{\partial x_1^2} + \frac{\partial}{\partial x_2^2} + \frac{\partial}{\partial x_3^2} \right) \tag{4.18}$$

The concentration equation assumes a slightly different form if it is expressed in terms of the mass fraction instead of the concentration (mass per unit volume) of the component in a solution. The concentration is related to the mass fraction w by $c = \rho w$, so the equation for the mass fraction is

$$\frac{\partial (\rho w)}{\partial t} + \nabla . (\rho w \mathbf{v}) = D \nabla^2 (\rho w) \tag{4.19}$$

From this, if we subtract w times the mass conservation equation, we get

$$\rho\left(\frac{\partial w}{\partial t}+\mathbf{v}.\nabla w\right)=D\nabla^2(\rho w) \tag{4.20}$$

or

$$\rho\frac{Dw}{Dt}=D\nabla^2(\rho w) \tag{4.21}$$

4.1.5 Energy conservation equation

The conservation equation for the energy density e, derived using procedures similar to that for the concentration equation, is

$$\frac{\partial e}{\partial t}+\nabla.(e\mathbf{u})=\nabla.(K\nabla T) \tag{4.22}$$

where K is the thermal conductivity, and $K\nabla T$ is the energy flux due to temperature gradients. The energy density e is given by $(\rho C_p T)$, where T is the absolute temperature. With this, the energy equation becomes

$$\frac{\partial(\rho C_p T)}{\partial t}+\nabla.(\rho C_p T\mathbf{v})=\nabla.(K\nabla T) \tag{4.23}$$

From this, we can subtract $C_pT\times$ the mass conservation equation, to obtain

$$\rho C_p\left(\frac{\partial T}{\partial t}+\mathbf{v}.\nabla T\right)=\nabla.(K\nabla T) \tag{4.24}$$

4.2 Elements of vector calculus

The derivative of a function $f(x)$ of one independent variable, shown in figure 4.2 (a), at a point x is given by the ratio of the difference in the abcissa, Δf, and the variation in the ordinate, Δx.

$$\frac{df(x)}{dx}=\lim_{\Delta x\to 0}\frac{\Delta f}{\Delta x} \tag{4.25}$$

The integral of a function $g(x)$ between two points, x_i and x_f, is the area under the curve, as shown in figure 4.2 (b). The integral of the derivative of

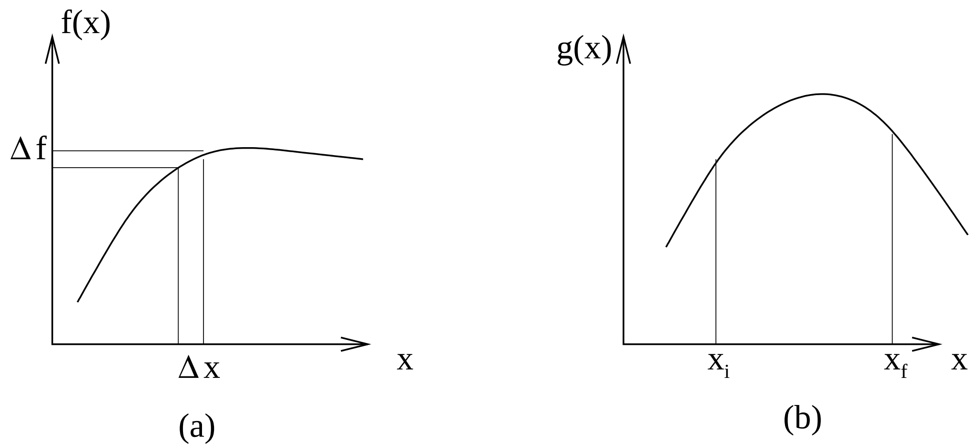

Figure 4.2: Elements of calculus in one dimension.

the function is equal to the difference in the values of the function between the end points.

$$\int_{x_i}^{x_f} dx \frac{df}{dx} = f(x_f) - f(x_i) \tag{4.26}$$

In the three dimensional coordinate system that has been used in this chapter, we have encountered the 'gradient' operator

$$\nabla = \mathbf{e}_1 \frac{\partial}{\partial x_1} + \mathbf{e}_2 \frac{\partial}{\partial x_2} + \mathbf{e}_3 \frac{\partial}{\partial x_3} \tag{4.27}$$

and this operator has been used in two ways, i. e., the gradient acting on a scalar which results in a vector, $\mathbf{j} = -D\nabla c$, as well as the dot product between the gradient operator and a vector, resulting in a tensor, $\nabla.\mathbf{j}$. The latter is called the 'divergence of a vector', div$\mathbf{j}$. A third type of derivative, the 'curl of a vector', curl$\mathbf{A}$, is defined as

$$\begin{aligned} \mathrm{curl}\mathbf{A} &= \begin{vmatrix} \mathbf{e}_1 & \mathbf{e}_2 & \mathbf{e}_3 \\ (\partial/\partial x_1) & (\partial/\partial x_2) & (\partial/\partial x_3) \\ A_1 & A_2 & A_3 \end{vmatrix} \\ &= \mathbf{e}_1 \left(\frac{\partial A_2}{\partial x_3} - \frac{\partial A_3}{\partial x_2} \right) + \mathbf{e}_2 \left(\frac{\partial A_3}{\partial x_1} - \frac{\partial A_1}{\partial x_3} \right) \mathbf{e}_3 \left(\frac{\partial A_1}{\partial x_2} - \frac{\partial A_2}{\partial x_1} \right) \end{aligned} \tag{4.28}$$

These differential operators are usually defined in terms of the underlying coordinate system, in this case a Cartesian coordinate system. However,

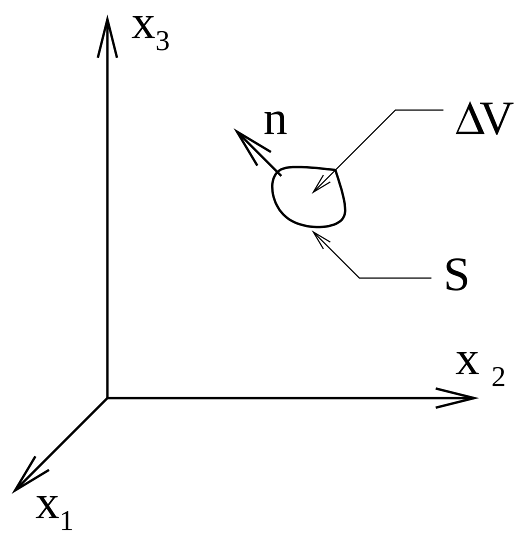

Figure 4.3: Control volume used in definition of gradient, divergence and curl.

these operators can be defined without making reference to the underlying coordinate system, just as a vector can be defined without making reference to the underlying coordinate system, even though the components of a vector do depend on the coordinate system. In a similar manner, integral relations similar to 4.26 can be defined for these operators which are independent of the underlying coordinate system. We shall briefly examine the definition and physical interpration of these operators, as well as the integral relations for each of them.

4.2.1 Gradient

The gradient of a scalar, Φ, at a point $\mathbf{x}$, is determined by considering a small volume ΔV, which is bounded by the surface S, as shown in figure 4.3. The outward unit normal to the surface is $\mathbf{n}$. The gradient is defined as

$$\mathrm{grad}(\Phi) = \lim_{\Delta V \to 0} \frac{\int_S dS \mathbf{n} \Phi}{\Delta V} \tag{4.29}$$

It is evident that the gradient is a vector, since it is proportional to the integral of the unit normal and the scalar function Φ.

The value of the gradient in Cartesian coordinates is determined by considering a cubic volume $\Delta x_1 \Delta x_2 \Delta x_3$ about the point $\mathbf{x} = (x_1, x_2, x_3)$, as shown in figure 4.4. This volume has six faces, and the surface integral in 4.29 is the sum of the contributions due to these six faces. The directions of the outward unit normals should be noted; the outward unit normal to the face A at $(x_2 + \Delta x_2/2)$ is $+\mathbf{e}_1$, while the outward unit normal to the face B at $(x_2 - \Delta x_2/2)$ is $-\mathbf{e}_2$. Similarly, the outward unit normals to the faces at $(x_1 + \Delta x_1/2)$ and $(x_3 + \Delta x_3/2)$ are $\mathbf{e}_1$ and $\mathbf{e}_3$ respectively, while the outward unit normals to the faces at $(x_1 - \Delta x_1/2)$ and $(x_3 - \Delta x_3/2)$ are $-\mathbf{e}_1$ and $-\mathbf{e}_3$ respectively. With these, the surface integral in 4.29 becomes

$$\begin{aligned}
&\int_S dS \mathbf{n} \Phi \\
&= \mathbf{e}_1 \Delta x_2 \Delta x_3 (\Phi(x_1 + \Delta x_1/2, x_2, x_3) - \Phi(x_1 - \Delta x_1/2, x_2, x_3)) \\
&\quad + \mathbf{e}_2 \Delta x_1 \Delta x_3 (\Phi(x_1, x_2 + \Delta x_2/2, x_3) - \Phi(x_1, x_2 - \Delta x_2/2, x_3)) \\
&\quad + \mathbf{e}_3 \Delta x_1 \Delta x_3 (\Phi(x_1, x_2, x_3 + \Delta x_3/2) - \Phi(x_1, x_2, x_3 - \Delta x_3/2)) \qquad (4.30)
\end{aligned}$$

When this surface integral is divided by the volume $\Delta x_1 \Delta x_2 \Delta x_3$, and the limit $\Delta x_1, \Delta x_2, \Delta x_3 \to 0$ is taken, we get the definition of the gradient,

$$\begin{aligned}
\mathrm{grad}(\Phi) &= \mathbf{e}_1 \frac{\partial \Phi}{\partial x_1} + \mathbf{e}_2 \frac{\partial \Phi}{\partial x_2} + \mathbf{e}_3 \frac{\partial \Phi}{\partial x_3} \\
&= \nabla \Phi \qquad (4.31)
\end{aligned}$$

The physical significance of the gradient is as follows. The variation in the scalar Φ, due to a small variation in the position vector $\Delta \mathbf{x}$ a point, can be written as the dot product of the gradient of Φ and the vector displacement.

$$\begin{aligned}
&\Phi(\mathbf{x} + \Delta \mathbf{x}) - \Phi(\mathbf{x}) \\
&= \Delta x_1 \frac{\partial \Phi}{\partial x_1} + \Delta x_2 \frac{\partial \Phi}{\partial x_2} + \Delta x_3 \frac{\partial \Phi}{\partial x_3} \\
&= (\mathbf{e}_1 \Delta x_1 + \mathbf{e}_2 \Delta x_2 + \mathbf{e}_3 \Delta x_3) . \left(\mathbf{e}_1 \frac{\partial \Phi}{\partial x_1} + \mathbf{e}_2 \frac{\partial \Phi}{\partial x_2} + \mathbf{e}_3 \frac{\partial \Phi}{\partial x_3} \right) \\
&= \Delta \mathbf{x} . (\nabla \Phi) \qquad (4.32)
\end{aligned}$$

Two important results arise from the above relation.

1. The gradient provides the direction of maximum variation of the scalar Φ. In equation 4.32, if we keep the magnitude of the displacement $|\Delta \mathbf{x}|$

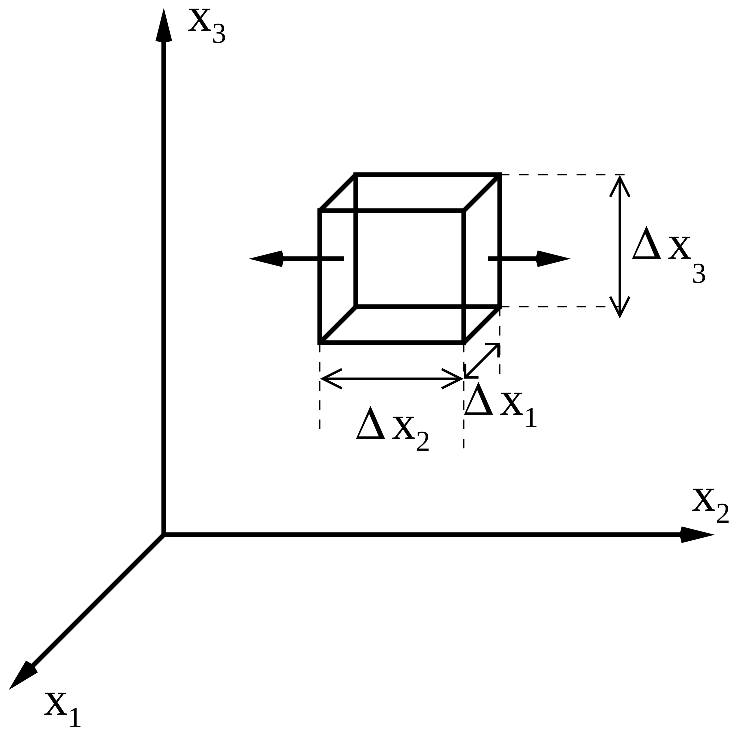

Figure 4.4: Control volume used for calculating the gradient and divergence.

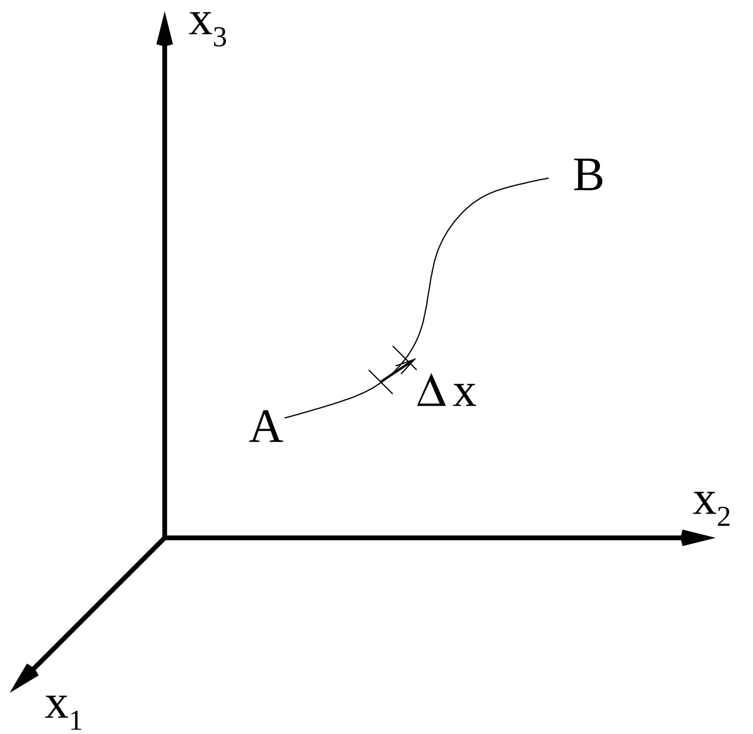

Figure 4.5: The line integral of the gardient of a scalar over a path is equal to the difference in the value of the gradient at the end points.

a constant, and vary the direction, then the dot product $(\Delta\mathbf{x}.\nabla\Phi)$ is a maximum when $\Delta\mathbf{x}$ and $\nabla\Phi$ are in the same direction. Thus, the direction of the gradient is the direction of the maximum variation of the function.

2. If the displacement $\Delta\mathbf{x}$ is perpendicular to $\nabla\Phi$, then there is no variation in the function Φ due to the displacement. Thus, the gradient vector is perpendicular to the surface of constant Φ.

The variation in the scalar Φ in equation 4.32 was defined for a differential displacement Δx. This can be used to obtain the variation in Φ for two points separated by a macroscopic distance, by connecting the two points by a path and summing the variation in Φ over the differential displacements $\mathbf{x}^{(i)}$ along this path, as shown in figure 4.5.

$$\begin{aligned} \Phi(\mathbf{x}_B) - \Phi(\mathbf{x}_A) &= \sum_i \Delta\mathbf{x}^{(i)}.\nabla\Phi \\ &= \int_{\mathbf{x}_A}^{\mathbf{x}_B} d\mathbf{x}.\nabla\Phi \end{aligned} \tag{4.33}$$

This is the equilvalent of the integral relation 4.26 for the gradient. A consequence of this is that since the difference in Φ between $\mathbf{x}_A$ and $\mathbf{x}_B$ is independent of the path used to reach $\mathbf{x}_B$ from $\mathbf{x}_A$, the integral $\int d\mathbf{x}.\nabla\Phi$ is equal for all paths between the two points $\mathbf{x}_A$ and $\mathbf{x}_B$. Another consequence is that the integral of the gradient over a closed path is always equal to zero.

4.2.2 Divergence

The divergence of a vector is also defined by considering a small differential volume ΔV shown in figure 4.3. The divergence is defined as

$$\mathrm{div}(\mathbf{A}) = \lim_{\Delta V \to 0} \frac{\int_S dS\mathbf{n}.\mathbf{A}}{\Delta V} \tag{4.34}$$

It is evident that the divergence of a vector is a scalar, since it in obtained by taking the dot product of the vector and the unit normal to the surface. By a construction similar to that used for deriving equation 4.30 using figure 4.4, it can easily be inferred that the divergence in Cartesian coordinates is

$$\begin{aligned} \mathrm{div}(\mathbf{A}) &= \frac{\partial A_1}{\partial x_1} + \frac{\partial A_2}{\partial x_2} + \frac{\partial A_3}{\partial x_3} \\ &= \nabla.\mathbf{A} \end{aligned} \tag{4.35}$$

The divergence of a vector, literally, provides the divergence of the vector from a point.

The integral theorem for the divergence operator, called the ‘divergence theorem’, states that for a vector field $\mathbf{A}$, the following equality applies for any volume V which has a bounding surface S,

$$\int_V dV\nabla.\mathbf{A} = \int_S dS\mathbf{n}.\mathbf{A} \tag{4.36}$$

where $\mathbf{n}$ is the outward unit normal to the surface. Note that equation 4.36 relates the volume integral of the divergence of the vector field to the integral of $\mathbf{n}.\mathbf{A}$ over the surface. Therefore, in order to evaluate the integral of the divergence of A over a volume, it is not necessary to know the value of A throughout the volume, but it is sufficient to know the value of A on the surface bounding the volume.

The divergence theorem can be proved as follows. Consider the volume V shown in figure 4.6. This volume is sub-divided into a large number of differential elements, $\Delta V^{(1)}, \Delta V^{(2)}, \ldots \Delta V^{(n)}$. For each of these differential elements, the divergence theorem states that

$$\Delta V^{(i)} \nabla.\mathbf{A} = \int_{S^{(i)}} dS \mathbf{n}.\mathbf{A} \tag{4.37}$$

where $S^{(i)}$ is the surface bounding volume $V^{(i)}$. The integral over the volume V can expressed as the sum over the differential elements,

$$\int_V dV \nabla.\mathbf{A} = \sum_{i=1}^{N} \Delta V^{(i)} \nabla.\mathbf{A} = \sum_{i=1}^{N} \int_{S^{(i)}} dS \mathbf{n}.\mathbf{A} \tag{4.38}$$

Let us examine, more closely, the surface integral on the right side of equation 4.38 for two adjacent volumes, $\Delta V^{(i)}$ and $\Delta V^{(i+1)}$. These two volumes have a common surface, S_c in figure **??**. When the surface integral on the right side of 4.38 is determined over these two volumes, the value of the vector A is identical on the common surface, but the outward unit normal to the surface $\mathbf{n}$ for the volumes $\Delta V^{(i)}$ and $\Delta V^{(i+1)}$ are opposite to each other on this surface. Thus the surface integrals on the common surface for the two adjacent volumes are equal in magnitude and opposite in sign, and these cancel when the summation is carried out in equation 4.38. In a similar manner, the surface integrals over all surfaces that separate two adjacent volumes cancel, and we are left with the surface integral on the bounding surface S for the volume V,

$$\int_V dV \nabla.\mathbf{A} = \int_S dS \mathbf{n}.\mathbf{A} \tag{4.39}$$

This proves the divergence theorem.

4.2.3 Curl

The curl of a vector at a point $\mathbf{x}$ is defined by considering a small differential volume ΔV about this point, as shown in figure 4.3. The curl of the vector

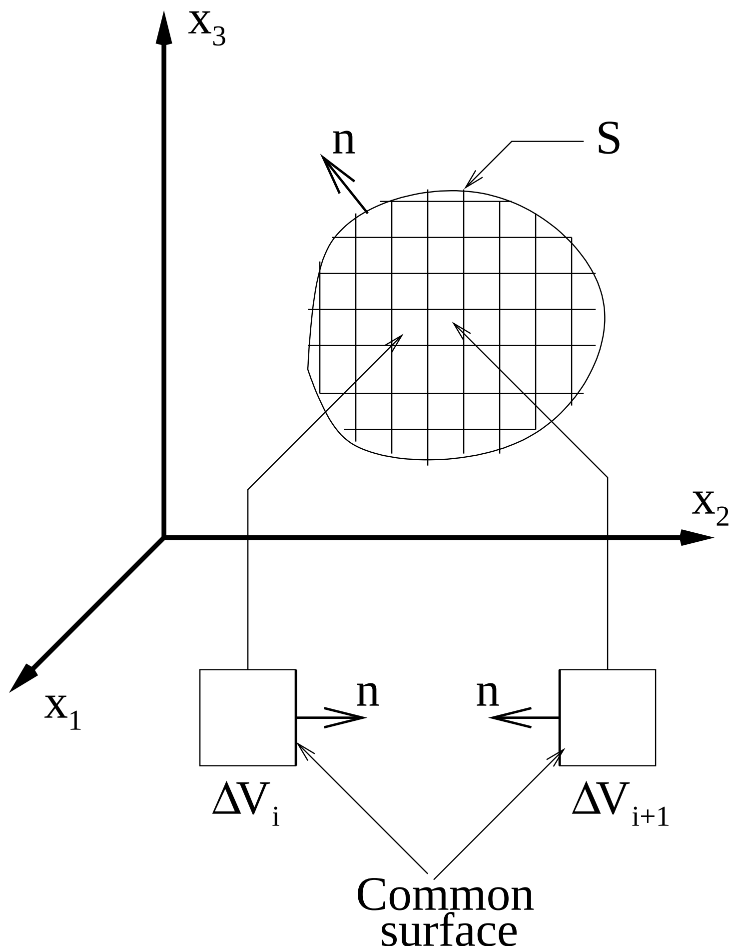

Figure 4.6: Divergence theorem.

is defined as

$$\mathrm{curl}\mathbf{A} = \frac{\int_S \mathbf{n}\times\mathbf{A}}{\Delta V} \tag{4.40}$$

Since the cross product of the unit normal and the vector $\mathbf{A}$ is a vector, the curl operating on a vector results in a vector. The curl of a vector in Cartesian coordinates can be determined using the same construction used for evaluating the gradient (figure 4.4). The surface integral on the left side of equation 4.40 is

$$\begin{aligned}
&\int_S dS\mathbf{n}\times\mathbf{A}\\
&= \Delta x_2\Delta x_3\mathbf{e}_1\times(\mathbf{A}(x_1+\Delta x_1/2,x_2,x_3)-\mathbf{A}(x_1-\Delta x_1/2,x_2,x_3))\\
&\quad +\Delta x_1\Delta x_3\mathbf{e}_2\times(\mathbf{A}(x_1,x_2+\Delta x_2/2,x_3)-\mathbf{A}(x_1,x_2-\Delta x_2/2,x_3))\\
&\quad +\Delta x_1\Delta x_3\mathbf{e}_3\times(\mathbf{A}(x_1,x_2,x_3+\Delta x_3/2)-\mathbf{A}(x_1,x_2,x_3-\Delta x_3/2))
\end{aligned} \tag{4.41}$$

$$\begin{aligned}
&\int_S dS\mathbf{n}\times\mathbf{A}\\
&= \Delta x_2\Delta x_3\mathbf{e}_3\times(A_2(x_1+\Delta x_1/2,x_2,x_3)-A_2(x_1-\Delta x_1/2,x_2,x_3))\\
&\quad -\Delta x_2\Delta x_3\mathbf{e}_2\times(A_3(x_1+\Delta x_1/2,x_2,x_3)-A_3(x_1-\Delta x_1/2,x_2,x_3))\\
&\quad +\Delta x_1\Delta x_3\mathbf{e}_1\times(A_3(x_1,x_2+\Delta x_2/2,x_3)-A_3(x_1,x_2-\Delta x_2/2,x_3))\\
&\quad -\Delta x_1\Delta x_3\mathbf{e}_3\times(A_1(x_1,x_2+\Delta x_2/2,x_3)-A_1(x_1,x_2-\Delta x_2/2,x_3))\\
&\quad +\Delta x_1\Delta x_3\mathbf{e}_2\times(A_1(x_1,x_2,x_3+\Delta x_3/2)-A_1(x_1,x_2,x_3-\Delta x_3/2))\\
&\quad -\Delta x_1\Delta x_3\mathbf{e}_1\times(A_2(x_1,x_2,x_3+\Delta x_3/2)-A_2(x_1,x_2,x_3-\Delta x_3/2))
\end{aligned} \tag{4.42}$$

The above equation is simplified by converting the difference equation to a differential equation in the limit $(\Delta x_1\to 0,\Delta x_2\to 0,\Delta x_3\to 0)$, and then divided by $(\Delta x_1\Delta x_2\Delta x_3)$, to provide

$$\begin{aligned}
\mathrm{curl}(A) &= \mathbf{e}_1\left(\frac{\partial A_3}{\partial x_2}-\frac{\partial A_2}{\partial x_3}\right)+\mathbf{e}_2\left(\frac{\partial A_1}{\partial x_3}-\frac{\partial A_3}{\partial x_1}\right)+\mathbf{e}_3\left(\frac{\partial A_2}{\partial x_1}-\frac{\partial A_1}{\partial x_2}\right)\\
&= \nabla\times\mathbf{A}
\end{aligned} \tag{4.43}$$

The curl of a vector field provides the extent of circulation in the vector field.

The integral theorem for the curl of the vector, called the 'Stokes theorem', relates the integral of $\mathbf{n}.\nabla\times\mathbf{A}$ over a surface S to the integral of $\mathbf{A}$

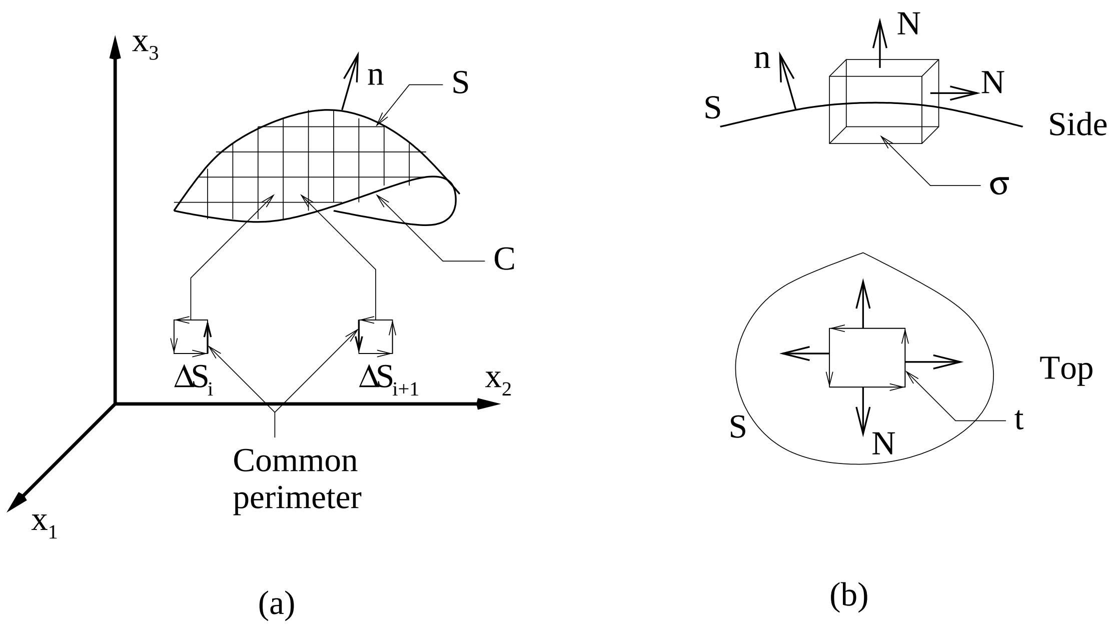

Figure 4.7: Configuration used for the definition of the curl (a), and the construction used for deriving the Stokes theorem (b).

over the closed perimeter of the surface C, as shown in figure 4.7(a).

$$\int_S dS\mathbf{n}.\nabla \times \mathbf{A} = \oint_C d\mathbf{x}.\mathbf{A} \tag{4.44}$$

where C is a closed loop which is the perimeter of S, and $d\mathbf{x}$ is the differential vector displacement on this closed loop.

Since equation 4.44 for the definition of a curl involves the integral over a closed surface, whereas the Stokes theorem 4.40 relates the integral over an open surface to the integral over a line, the proof of 4.44 is a little more circuitous than the divergence theorem. Consider the open surface shown in figure 4.7(a), and construct a closed cube which straddles this surface, as shown in figure 4.7(b). The differential area element on the open surface S is denoted by dS, while the differential area element on the closed cube is denoted by $d\sigma$. The normal to the surface S is denoted by $\mathbf{n}$, while the normal to the surface of the cube is denoted by $\mathbf{N}$. From the definition of the curl of a vector $\mathbf{A}$, applied to this cube,

$$\Delta V\mathbf{n}.(\nabla \times \mathbf{A}) = \int_\sigma d\sigma\mathbf{n}.\mathbf{N} \times \mathbf{A} \tag{4.45}$$

The right side of the above equation 4.45 contains the triple product, $\mathbf{n}.\mathbf{N}\times\mathbf{A}$, which can also be written as $\mathbf{A}.\mathbf{n} \times \mathbf{N}$,

$$\Delta V\mathbf{n}.(\nabla \times \mathbf{A}) = \int_\sigma d\sigma\mathbf{A}.\mathbf{n} \times \mathbf{N} \tag{4.46}$$

On the top an bottom surfaces of the cube, the unit vectors $\mathbf{n}$ and $\mathbf{N}$ are in the same or opposite directions, and so the cross product of these two is equal to zero. Therefore, the right side of 4.46 only involves the integral over the sides of the cube.

$$\begin{aligned}\Delta V\mathbf{n}.(\nabla \times \mathbf{A}) &= \int_{\text{sides}} d\sigma\mathbf{A}.\mathbf{n} \times \mathbf{N} \\ &= \int_{\text{sides}} d\sigma\mathbf{A}.\mathbf{t} \end{aligned} \tag{4.47}$$

where $\mathbf{t}$ is the unit vector in the along the curve which is the intersection of the cube and the surface S. The volume $\Delta V = h\Delta S$, where ΔS is the differential area which is the projection of the cube onto the surface S, and h is the height of the cube. Similarly, $d\sigma = hdx$, where dx is the differential displacement along the curve made by the intersection of the cube and the surface S. With these substitutions, equation 4.47 reduces to

$$h \Delta S \mathbf{n}.(\nabla \times \mathbf{A}) = h \oint_{\text{sides}} dx \, \mathbf{A}.\mathbf{t} \tag{4.48}$$

or

$$\begin{aligned} \Delta S \mathbf{n}.(\nabla \times \mathbf{A}) &= \oint dx \, \mathbf{A}.\mathbf{t} \\ &= \oint d\mathbf{x} \, .\mathbf{A} \end{aligned} \tag{4.49}$$

where $d\mathbf{x}$ is the vector displacement along the curve made by the intersection of the cube and the surface S.

Equation 4.49 applies for a differential area element on the surface S. The Stokes theorem for the entire surface can be obtained by dividing the surface into differential area elements ΔS_i, adding the contributions to $\mathbf{n}.(\nabla \times \mathbf{A})$ over all these area elements, as shown in figure 4.7(a).

$$\begin{aligned} \int dS \mathbf{n}.\nabla \times \mathbf{A} &= \sum_i \Delta S_i \mathbf{n}.(\nabla \times \mathbf{A}) \\ &= \oint_{C_i} d\mathbf{x} \, .\mathbf{A} \end{aligned} \tag{4.50}$$

where the curve C_i is the perimeter of the surface element ΔS_i. The right side of equation 4.50 can be simplified as follows. Consider two adjacent area elements ΔS_i and ΔS_{i+1}, as shown in figure 4.7(a). While calculating the integral over the perimenters of these two differential area elements, it is observed that the tangent to the surface along their common periment is opposite in direction for the two area elements, if the tangent is directed in the anticlockwise direction. Therefore, the contribution to the line integral for these two adjacent area elements cancel, and result in zero contribution. A similar result is obtained for all line elements that are in between two adjacent area elements, and the right side of equation 4.50 only contains contributions from the perimeter of the entire surface S,

$$\int dS \mathbf{n}.\nabla \times \mathbf{A} = \oint_C d\mathbf{x} \, . \, \mathbf{A} \tag{4.51}$$

4.3 Conservation equation in spherical coordinates

In the spherical coordinate system, a point is represented by three coordinates, the distance from the origin r, the azimuthal angle θ that the position vetor makes with the x_3 coordinate, and the meridional angle ϕ that the projection of the position vector in the $x_1 - x_2$ plane makes with the x_1 axis, as shown in figure 4.8. The coordinate r is always positive, since it is defined as the distance from the center, and surfaces of constant r are spherical surfaces. The angle θ varies from $0 \leq \theta \leq \pi$, where $\theta = 0$ corresponds to a point on the $+x_3$ axis, while $\theta = \pi$ corresponds to a point on the $-x_3$ axis. Surfaces of constant θ are conical surfaces with subtended angle 2θ. The meridional angle ϕ varies from 0 to 2π, since the projection made by the position vector on the $x_1 - x_2$ plane can rotate over an angle of 2π. The surfaces of constant ϕ are planes perpendicular to the $x_1 - x_2$ plane bounded by the x_3 axis. The coordinates x_1, x_2 and x_3 can be expressed in terms of (r, θ, ϕ) as

$$\begin{aligned} x_1 &= r \sin(\theta) \cos(\phi) \\ x_2 &= r \sin(\theta) \sin(\phi) \\ x_3 &= r \cos(\theta) \end{aligned} \tag{4.52}$$

Conversely, (r, θ, ϕ) are expressed in terms of (x_1, x_2, x_3) as

$$\begin{aligned} r &= (x_1^2 + x_2^2 + x_3^2)^{1/2} \\ \tan(\theta) &= \frac{(x_1^2 + x_2^2)}{x_3} \\ \tan(\phi) &= \frac{x_2}{x_1} \end{aligned} \tag{4.53}$$

In order to obtain conservation equations in a spherical coordinate system, it is first necessary to consider a the appropriate differential volume in the spherical coordinate system. This differential volume, shown in figure 4.9, is bounded by surfaces of constant radius at r and $r + \Delta r$, surfaces at θ and $\theta + \Delta\theta$ along the azimuthal coordinate, and surfaces at ϕ and $\phi + \Delta\phi$ along the meridional coordinate. The width of the control volume along the radial direction is Δr, the width along the azimuthal direction is $r\Delta\theta$ because the radius is r and the subtended angle is $\Delta\theta$, and the width along the meridional direction is $r \sin(\theta)\Delta\phi$, because the radius (distance from the

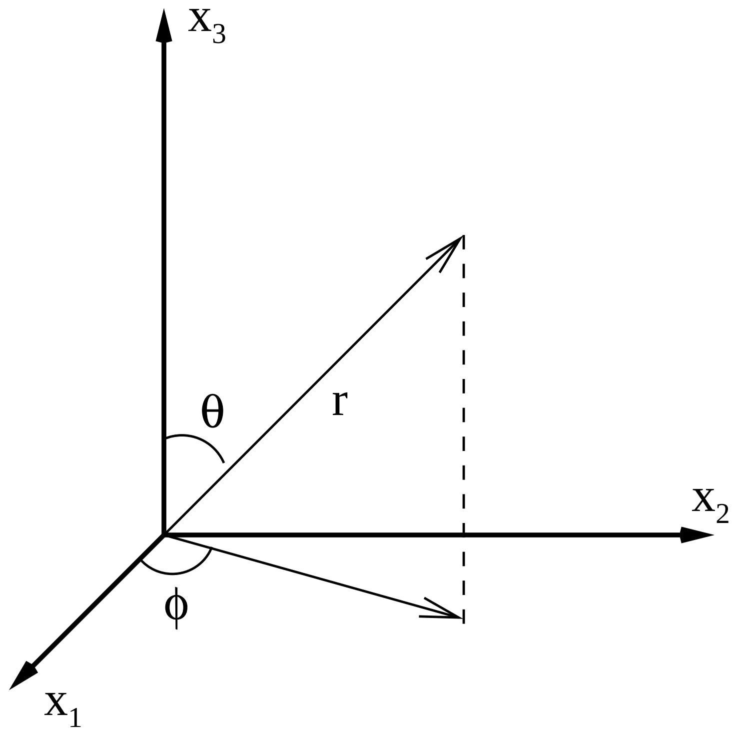

Figure 4.8: Spherical coordinate system.

x_3 axis) is $r\sin(\theta)$ and the subtended angle is $\Delta\phi$. In order to obtain the concentration equation, we consider the change in the total mass of the solute over a time Δt, which is given by

$$(c(r,\theta,\phi,t+\Delta t) - c(r\theta,\phi,t))\,(\Delta r)(r\Delta\theta)(r\sin(\theta)\Delta\phi) \tag{4.54}$$

The total input of solute into the volume through the surface at r is given by

$$((cv_r + j_r)(r\Delta\theta)(r\sin(\theta)\Delta\phi))|_r \tag{4.55}$$

while the output of solute through the surface at $(r+\Delta r)$ is

$$((cv_r + j_r)(r\Delta\theta)(r\sin(\theta)\Delta\phi))|_{r+\Delta r} \tag{4.56}$$

The net accumulation of solute due to the flow through these two surfaces is given by

$$\begin{aligned}((cv_r + j_r)(r\Delta\theta)(r\sin(\theta)\Delta\phi))|_r - ((cv_r + j_r)(r\Delta\theta)(r\sin(\theta)\Delta\phi))|_{r+\Delta r} &= \\ (\Delta\theta)(\sin(\theta)\Delta\phi)\Delta r\left(-\frac{\partial}{\partial r}(r^2(cv_r + j_r))\right)\end{aligned} \tag{4.57}$$

Similar expressions can be obtained for the net accumulation of solute through the surfaces at θ and $\theta+\Delta\theta$,

$$\begin{aligned}((cv_\theta + j_\theta)(\Delta r)(r\sin(\theta)\Delta\phi))|_\theta - ((cv_\theta + j_\theta)(\Delta r)(r\sin(\theta)\Delta\phi))|_{\theta+\Delta\theta} &= \\ (\Delta r)(r\Delta\phi)(\Delta\theta)\left(-\frac{\partial}{\partial\theta}(\sin(\theta)(cv_\theta + j_\theta))\right)\end{aligned} \tag{4.58}$$

and through the surfaces at ϕ and $\phi+\Delta\phi$,

$$\begin{aligned}((cv_\phi + j_\phi)(\Delta r)(r\Delta\theta))|_\phi - ((cv_\phi + j_\phi)(\Delta r)(r\Delta\theta))|_{\phi+\Delta\phi} &= \\ (\Delta r)(r\Delta\theta)(\Delta\phi)\left(-\frac{\partial}{\partial\phi}(cv_\phi + j_\phi)\right)\end{aligned} \tag{4.59}$$

Equating the rate of accumulation of mass to the sum of the Input − Output, and dividing by the volume $(\Delta r)(r\Delta\theta)(r\sin(\theta)\Delta\phi)$, the equation for the concentration field is

$$\frac{\partial c}{\partial t} = -\frac{1}{r^2}\frac{\partial}{\partial r}(r^2(cv_r+j_r)) - \frac{1}{r\sin(\theta)}\frac{\partial}{\partial\theta}(\sin(\theta)(cv_\theta+j_\theta)) - \frac{1}{r\sin(\theta)}\frac{\partial}{\partial\phi}(cv_\phi+j_\phi) \tag{4.60}$$

This equation can be expressed in the form of the diffusion equation 4.13 using the definition of the divergence operator ∇ in spherical coordinates,

$$\nabla.\mathbf{A} = \frac{1}{r^2}\frac{\partial}{\partial r}(r^2 A_r) + \frac{1}{r\sin(\theta)}\frac{\partial}{\partial\theta}(\sin(\theta)A_\theta) + \frac{1}{r\sin(\theta)}\frac{\partial A_\phi}{\partial\phi} \tag{4.61}$$

The components of the fluxes in the three directions are related to the variation of the concentration with position, which in the spherical coordinate system is given by

$$\begin{aligned} j_r &= -D\frac{\partial c}{\partial r} \\ j_\theta &= -D\frac{1}{r}\frac{\partial c}{\partial\theta} \\ j_\phi &= -D\frac{1}{r\sin(\theta)}\frac{\partial c}{\partial\phi} \end{aligned} \tag{4.62}$$

When this is inserted into the conservation equation 4.13, we obtain

$$\frac{\partial c}{\partial t} + \mathbf{nabla}.(c\mathbf{v}) = D\nabla^2 c \tag{4.63}$$

where the Laplacian is defined as

$$\nabla^2 = \left(\frac{1}{r^2}\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r} + \frac{1}{r^2\sin(\theta)}\frac{\partial}{\partial\theta}\sin(\theta)\frac{\partial}{\partial\theta} + \frac{1}{r^2\sin(\theta)^2}\frac{\partial}{\partial\phi^2}\right) \tag{4.64}$$

4.4 Vector calculus in spherical coordinates

In the previous section, we have obtained the gradient and divergence operators in spherical coordinates by carrying out a shell balance for the concentration field. A systemmatic procedure for deriving these operators is derived in the present section, and this procedure can be used for deriving these operators in other orthogonal coordinate systems as well.

4.4.1 Unit vectors

First, it is necessary to derive expressions for the unit vectors in the coordinate system under consideration, and relate these to the unit vectors in

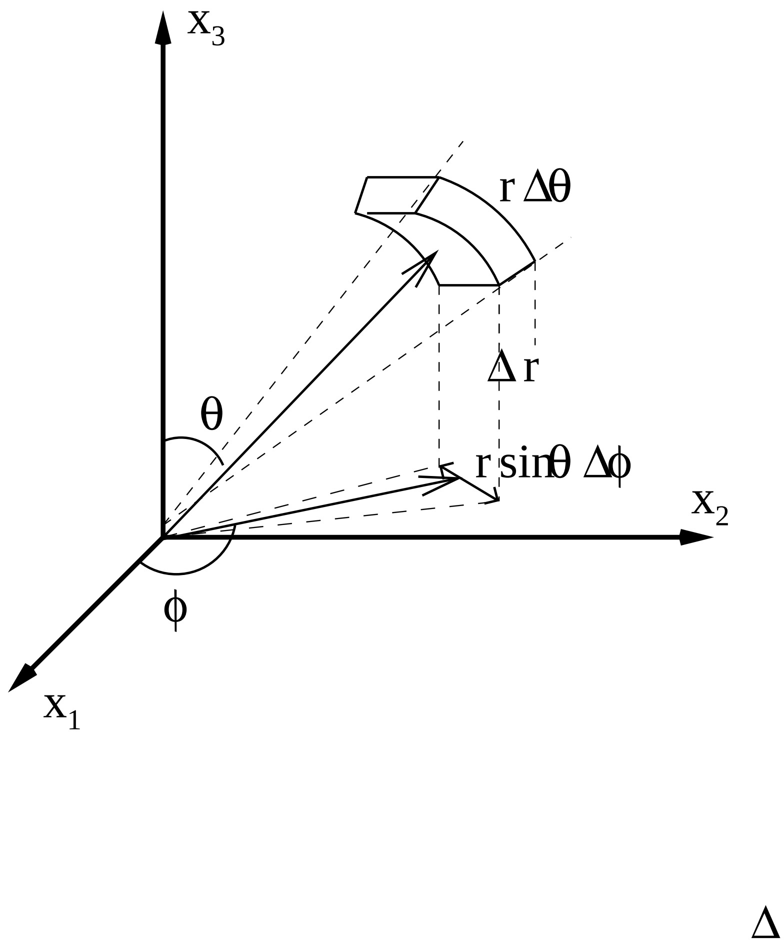

Figure 4.9: Differential volume for deriving conservation equation in spherical coordinate system.

the Cartesian coordinate system. The unit vector $\mathbf{e}_r$ provides the direction of variation of r, and is perpendicular to surfaces of constant r. From the physical significance of the gradient operator, it can be inferred that the unit vector $\mathbf{e}_r$ is along the direction ∇r. However, since it is a unit vector with magnitude 1,

$$\mathbf{e}_r = \frac{\nabla r}{|\nabla r|} \tag{4.65}$$

Using $r = (x_1^2 + x_2^2 + x_3^2)^{1/2}$ (equation 4.53), the gradient of r is

$$\begin{aligned} \nabla r &= \mathbf{e}_1 \frac{\partial r}{\partial x_1} + \mathbf{e}_2 \frac{\partial r}{\partial x_2} + \mathbf{e}_3 \frac{\partial r}{\partial x_3} \\ &= \frac{\mathbf{e}_1 x_1}{(x_1^2 + x_2^2 + x_3^2)^{1/2}} + \frac{\mathbf{e}_2 x_2}{(x_1^2 + x_2^2 + x_3^2)^{1/2}} \frac{\mathbf{e}_2 x_2}{(x_1^2 + x_2^2 + x_3^2)^{1/2}} \end{aligned} \tag{4.66}$$

From the above equation, the magnitude of the gradient is given by $|\nabla r| = 1$, and therefore the unit vector $\mathbf{e}_r$ is

$$\begin{aligned} \mathbf{e}_r &= \frac{\mathbf{e}_1 x_1}{(x_1^2 + x_2^2 + x_3^2)^{1/2}} + \frac{\mathbf{e}_2 x_2}{(x_1^2 + x_2^2 + x_3^2)^{1/2}} \frac{\mathbf{e}_2 x_2}{(x_1^2 + x_2^2 + x_3^2)^{1/2}} \\ &= \sin(\theta)\cos(\phi)\mathbf{e}_1 + \sin(\theta)\sin(\phi)\mathbf{e}_2 + \cos(\theta)\mathbf{e}_3 \end{aligned} \tag{4.67}$$

The θ coordinate is given by $\tan(\theta) = ((x_1^2 + x_2^2)^{1/2}/x_3)$. The unit vector in the θ direction is in the direction or $\nabla\theta$, since it is perpendicular to surfaces of constant θ. However, it is most convenient to calculate the unit vector in the θ direction from $\nabla(\tan(\theta))$, since surfaces of constant θ are also surfaces of constant $\tan(\theta)$. The gradient of $\tan(\theta)$ is given by

$$\nabla \tan(\theta) = \frac{\mathbf{e}_1 x_1}{x_3(x_1^2 + x_2^2)^{1/2}} + \frac{\mathbf{e}_2 x_2}{x_3(x_1^2 + x_2^2)^{1/2}} - \mathbf{e}_3 (x_1^2 + x_2^2)^{1/2} x_3^2 \tag{4.68}$$

and $|\nabla \tan(\theta)$ is

$$\begin{aligned} |\nabla \tan(\theta)| &= \left(\frac{x_1^2}{(x_1^2 + x_2^2)x_3^2} + \frac{x_2^2}{(x_1^2 + x_2^2)x_3^2} + \frac{x_1^2 + x_2^2}{x_3^4} \right)^{1/2} \\ &= \frac{(x_1^2 + x_2^2 + x_3^2)^{1/2}}{x_3^2} \end{aligned} \tag{4.69}$$

Therefore, the unit vector in the θ direction is

$$\begin{aligned} \mathbf{e}_\theta &= \frac{\mathbf{e}_1 x_1 x_3}{(x_1^2 + x_2^2)^{1/2}(x_1^2 + x_2^2 + x_3^2)^{1/2}} + \frac{\mathbf{e}_2 x_2 x_3}{(x_1^2 + x_2^2)^{1/2}(x_1^2 + x_2^2 + x_3^2)^{1/2}} - \frac{\mathbf{e}_3 (x_1^2 + x_2^2)^{1/2}}{(x_1^2 + x_2^2 + x_3^2)^{1/2}} \\ &= \cos(\theta)\cos(\phi)\mathbf{e}_1 + \cos(\theta)\sin(\phi)\mathbf{e}_2 - \sin(\theta)\mathbf{e}_3 \end{aligned} \tag{4.70}$$

The ϕ coordinate can be expressed in terms of the coordinates in the Cartesian coordinate system using $\tan(\phi) = (x_2/x_1)$. The unit vector in the ϕ direction is perpendicular to surfaces of constant $\tan(\phi)$, and are along the direction of $\nabla \tan(\phi)$, which is given by

$$\nabla \tan(\phi) = -\frac{\mathbf{e}_1 x_2}{x_1^2} + \frac{\mathbf{e}_2}{x_1} \tag{4.71}$$

The magnitude of this gradient is

$$\begin{aligned} |\nabla \tan(\phi) &= \left(\frac{x_2^2}{x_1^4} + \frac{1}{x_1^2}\right)^{1/2} \\ &= \frac{(x_1^2 + x_2^2)^{1/2}}{x_1^2} \end{aligned} \tag{4.72}$$

Therefore, the unit vector in the ϕ direction is given by

$$\begin{aligned} \mathbf{e}_\phi &= -\frac{\mathbf{e}_1 x_2}{(x_1^2 + x_2^2)^{1/2}} + \frac{\mathbf{e}_2 x_1}{(x_1^2 + x_2^2)^{1/2}} \\ &= -\sin(\phi)\mathbf{e}_1 + \cos(\phi)\mathbf{e}_2 \end{aligned} \tag{4.73}$$

It is easily verified that the three unit vectors, $(\mathbf{e}_r, \mathbf{e}_\theta, \mathbf{e}_\phi)$ are orthogonal to each other.

The unit vectors in the Cartesian coordinate system can be expressed in terms of those in the spherical coordinate system using the relation

$$\begin{aligned} \mathbf{e}_1 &= (\mathbf{e}_1.\mathbf{e}_r)\mathbf{e}_r + (\mathbf{e}_1.\mathbf{e}_\theta)\mathbf{e}_\theta + (\mathbf{e}_1.\mathbf{e}_\phi)\mathbf{e}_\phi \\ &= \sin(\theta)\cos(\phi)\mathbf{e}_r + \cos(\theta)\cos(\phi)\mathbf{e}_\theta - \sin(\phi)\mathbf{e}_\phi \\ \mathbf{e}_2 &= (\mathbf{e}_2.\mathbf{e}_r)\mathbf{e}_r + (\mathbf{e}_2.\mathbf{e}_\theta)\mathbf{e}_\theta + (\mathbf{e}_2.\mathbf{e}_\phi)\mathbf{e}_\phi \\ &= \sin(\theta)\sin(\phi)\mathbf{e}_r + \cos(\theta)\sin(\phi)\mathbf{e}_\theta + \cos(\phi)\mathbf{e}_\phi \\ \mathbf{e}_3 &= (\mathbf{e}_3.\mathbf{e}_r)\mathbf{e}_r + (\mathbf{e}_3.\mathbf{e}_\theta)\mathbf{e}_\theta + (\mathbf{e}_3.\mathbf{e}_\phi)\mathbf{e}_\phi \\ &= \cos(\theta)\mathbf{e}_r - \sin(\theta)\mathbf{e}_\theta \end{aligned} \tag{4.74}$$

4.4.2 Derivatives of unit vectors

The unit vectors in a spherical coordinate system depend on position, unlike the Cartesian coordinate system where the unit vectors are independent of position. The variation in the unit vectors with position can be calculated as follows. A differential displacement in the spherical coordinate system can be expressed as

$$\begin{aligned} d\mathbf{x} &= dr\mathbf{e}_r + rd\theta\mathbf{e}_\theta + r\sin(\theta)d\phi\mathbf{e}_\phi \\ &= h_r dr\mathbf{e}_r + h_\theta d\theta\mathbf{e}_\theta + h_\phi d\phi\mathbf{e}_\phi \end{aligned} \tag{4.75}$$

where $h_r = 1, h_\theta = r$ and $h_\phi = r\sin(\theta)$ are called the 'scale factors' for the spherical coordinate system. Scale factors are necessary in the case of spherial coordinates, because the coordinates θ and ϕ do not have units of length. This is in contrast to the Cartesian coordinate system, where all three coordinates have units of length. The derivative of the displacement with respect to r and θ are, respectively,

$$\frac{\partial\mathbf{x}}{\partial r} = h_r\mathbf{e}_r \tag{4.76}$$

$$\frac{\partial\mathbf{x}}{\partial\theta} = h_\theta\mathbf{e}_\theta \tag{4.77}$$

If we take the second derivative of $\mathbf{x}$ with respect to r and ϕ, we get two expressions, the first by taking the derivative of equation 4.76 with θ, and the second by taking the derivative of 4.77 with respect to r.

$$\frac{\partial}{\partial\theta}\frac{\partial\mathbf{x}}{\partial r} = \frac{\partial h_r}{\partial\theta}\mathbf{e}_r + h_r\frac{\partial\mathbf{e}_r}{\partial\theta} \tag{4.78}$$

$$\frac{\partial}{\partial r}\frac{\partial\mathbf{x}}{\partial\theta} = \frac{\partial h_\theta}{\partial r}\mathbf{e}_\theta + h_\theta\frac{\partial\mathbf{e}_\theta}{\partial r} \tag{4.79}$$

Since the value of the second derivative does not depend on the order of differentiation, the right sides of equation 4.78 and equation 4.79 are equal. However, on the right sides of 4.78 and 4.79, $\mathbf{e}_r$ and $\mathbf{e}_\theta$ are perpendicular to each other. Therefore, the equality is satisfied only if

$$\frac{\partial\mathbf{e}_\theta}{\partial r} = \frac{\mathbf{e}_r}{h_\theta}\frac{\partial h_r}{\partial\theta} = 0 \tag{4.80}$$

$$\frac{\partial\mathbf{e}_r}{\partial\theta} = \frac{\mathbf{e}_\theta}{h_r}\frac{\partial h_\theta}{\partial r} = \mathbf{e}_\theta \tag{4.81}$$

The remaining derivatives of the unit vectors with the coordinates can be evaluated in a similar manner.

$$\frac{\partial\mathbf{e}_\phi}{\partial r} = \frac{\mathbf{e}_r}{h_\phi}\frac{\partial h_r}{\partial\phi} = 0 \tag{4.82}$$

$$\frac{\partial \mathbf{e}_r}{\partial \phi} = \frac{\mathbf{e}_\phi}{h_r}\frac{\partial h_\phi}{\partial r} = \sin(\theta)\mathbf{e}_\phi \tag{4.83}$$
$$\frac{\partial \mathbf{e}_\phi}{\partial \theta} = \frac{\mathbf{e}_\theta}{h_\phi}\frac{\partial h_\theta}{\partial \phi} = 0 \tag{4.84}$$
$$\frac{\partial \mathbf{e}_\theta}{\partial \phi} = \frac{\mathbf{e}_\phi}{h_\theta}\frac{\partial h_\phi}{\partial \theta} = \cos(\theta)\mathbf{e}_\phi \tag{4.85}$$

The 'diagonal' derivatives, of the type $(d\mathbf{e}_r/dr)$, can be evaluated using the substitution $\mathbf{e}_r = \mathbf{e}_\theta \times \mathbf{e}_\phi$,

$$\begin{aligned}
\frac{d\mathbf{e}_r}{dr} &= \frac{\partial \mathbf{e}_\theta}{\partial r} \times \mathbf{e}_\phi + \mathbf{e}_\theta \times \frac{\partial \mathbf{e}_\phi}{\partial r} = 0 \\
\frac{d\mathbf{e}_\theta}{d\theta} &= \frac{\partial \mathbf{e}_\phi}{\partial \theta} \times \mathbf{e}_r + \mathbf{e}_\phi \times \frac{\partial \mathbf{e}_r}{\partial \theta} = -\mathbf{e}_r \\
\frac{d\mathbf{e}_\phi}{d\phi} &= \frac{\partial \mathbf{e}_r}{\partial \phi} \times \mathbf{e}_\theta + \mathbf{e}_r \times \frac{\partial \mathbf{e}_\theta}{\partial \phi} = -\sin(\theta)\mathbf{e}_r - \cos(\theta)\mathbf{e}_\theta
\end{aligned} \tag{4.86}$$

4.4.3 Divergence, curl and Laplacian

The gradient operator in spherical coordinates is given by

$$\begin{aligned}
\nabla &= \frac{\mathbf{e}_r}{h_r}\frac{\partial}{\partial r} + \frac{\mathbf{e}_\theta}{h_\theta}\frac{\partial}{\partial \theta} + \frac{\mathbf{e}_\phi}{h_\phi}\frac{\partial}{\partial \phi} \\
&= \mathbf{e}_r\frac{\partial}{\partial r} + \frac{\mathbf{e}_\theta}{r}\frac{\partial}{\partial \theta} + \frac{\mathbf{e}_\phi}{r\sin(\theta)}\frac{\partial}{\partial \phi}
\end{aligned} \tag{4.87}$$

The divergence of a vector $\mathbf{A}$, in spherical coordinates, contains contributions not only due to the variation of the components of A, but also due to the variation of the unit vectors with position.

$$\nabla.\mathbf{A} = \left(\frac{\mathbf{e}_r}{h_r}\frac{\partial}{\partial r} + \frac{\mathbf{e}_\theta}{h_\theta}\frac{\partial}{\partial \theta} + \frac{\mathbf{e}_\phi}{h_\phi}\frac{\partial}{\partial \phi}\right).(A_r\mathbf{e}_r + A_\theta\mathbf{e}_\theta + A_\phi\mathbf{e}_\phi) \tag{4.88}$$

The contribution to the divergence which is proportional to $(\partial/\partial r)$ can be evaluated as follows,

$$\begin{aligned}
&\frac{\mathbf{e}_r}{h_r}.\frac{\partial(A_r\mathbf{e}_r + A_\theta\mathbf{e}_\theta + A_\phi\mathbf{e}_\phi)}{\partial r} \\
&= \frac{\mathbf{e}_r}{h_r}.\left(\mathbf{e}_r\frac{\partial A_r}{\partial r} + A_r\frac{\partial \mathbf{e}_r}{\partial r} + \mathbf{e}_\theta\frac{\partial A_\theta}{\partial r} + A_\theta\frac{\partial \mathbf{e}_\theta}{\partial r} + \mathbf{e}_\phi\frac{\partial A_\phi}{\partial r} + A_\phi\frac{\partial \mathbf{e}_\phi}{\partial r}\right)
\end{aligned} \tag{4.89}$$

The last two terms on the right side of 4.89 are simplified using the consideration that the unit vectors $\mathbf{e}_r, \mathbf{e}_\theta$ and $\mathbf{e}_\phi$ are orthogonal to each other, and the derivatives of the unit vectors are orthogonal to the unit vectors themselves. Therefore, the only non-zero contributions to the right side of equation 4.89 are

$$\begin{aligned}
& \frac{\mathbf{e}_r}{h_r}.\frac{\partial(A_r\mathbf{e}_r + A_\theta\mathbf{e}_\theta + A_\phi\mathbf{e}_\phi)}{\partial r} \\
&= \frac{\mathbf{e}_r}{h_r}.\left(\mathbf{e}_r\frac{\partial A_r}{\partial r} + A_\theta\frac{\partial \mathbf{e}_\theta}{\partial r} + A_\phi\frac{\partial \mathbf{e}_\phi}{\partial r}\right) \\
&= \frac{\mathbf{e}_r}{h_r}.\left(\mathbf{e}_r\frac{\partial A_r}{\partial r} + A_\theta\frac{\mathbf{e}_r}{h_\theta}\frac{\partial h_r}{\partial \theta} + A_\phi\frac{\mathbf{e}_r}{h_\phi}\frac{\partial h_r}{\partial \phi}\right) \\
\frac{1}{h_r}\frac{\partial A_r}{\partial r} + \frac{A_\theta}{h_\theta}\frac{\partial h_r}{\partial \theta} + \frac{A_\phi}{h_\phi}\frac{\partial h_r}{\partial \phi}
\end{aligned} \tag{4.90}$$

Similar relations can be derived for the derivatives with respect to θ and ϕ, and the final result for the divergence is

$$\begin{aligned}
\nabla.\mathbf{A} &= \frac{1}{h_r}\frac{\partial A_r}{\partial r} + \frac{1}{h_\theta}\frac{\partial A_\theta}{h_\theta} + \frac{1}{h_\phi}\frac{\partial A_\phi}{\partial \phi} \\
&\quad + + \frac{A_\theta}{h_\theta}\frac{\partial h_r}{\partial \theta} + \frac{A_\phi}{h_\phi}\frac{\partial h_r}{\partial \phi} + \frac{A_r}{h_r}\frac{\partial h_\theta}{\partial r} + \frac{A_\phi}{h_\phi}\frac{\partial h_\theta}{\partial \phi} \\
&\quad + \frac{A_r}{h_r}\frac{\partial h_\phi}{\partial r} + \frac{A_\theta}{h_\theta}\frac{\partial h_\phi}{\partial \theta} \\
&= \frac{1}{h_r h_\theta h_\phi}\left(\frac{\partial(A_r h_\theta h_\phi)}{\partial r} + \frac{\partial(A_\theta h_\phi h_r)}{\partial \theta} + \frac{\partial(A_\phi h_r h_\theta)}{\partial \phi}\right) \\
&= \frac{1}{r^2}\frac{\partial(r^2 A_r)}{\partial r} + \frac{1}{r\sin(\theta)}\frac{\partial(\sin(\theta)A_\theta)}{\partial \theta} + \frac{1}{r\sin(\theta)}\frac{\partial A_\phi}{\partial \phi}
\end{aligned} \tag{4.91}$$

The Laplacian is the dot product of two gradient operators, which is obtained by substituting $A_r = (1/h_r)(\partial/\partial r)$, $A_\theta = (1/h_\theta)(\partial/\partial\theta)$ and $A_\phi = (1/h_\phi)(\partial/\partial\phi)$ in equation 4.91,

$$\begin{aligned}
\nabla^2 &= \nabla.\nabla \\
&= \frac{1}{h_r h_\theta h_\phi}\left(\frac{\partial}{\partial r}\frac{h_\theta h_\phi}{h_r}\frac{\partial}{\partial r} + + \frac{\partial}{\partial \theta}\frac{h_\phi h_r}{h_\theta}\frac{\partial}{\partial \theta} + \frac{\partial}{\partial \phi}\frac{h_r h_\theta}{h_\phi}\frac{\partial}{\partial \phi}\right) \\
& \frac{1}{r^2}\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r} + \frac{1}{r^2\sin(\theta)}\frac{\partial}{\partial \theta}\sin(\theta)\frac{\partial}{\partial \theta} + \frac{1}{r^2\sin(\theta)^2}\frac{\partial^2}{\partial \phi^2}
\end{aligned} \tag{4.92}$$

The curl of a vector in spherical coordinates can be evaluated in a similar fashion. We do not provide the details here, since the calculation is algebraically tedious, but just provide the final result.

$$\begin{aligned}
\nabla \times \mathbf{A} &= \frac{1}{h_r h_\theta h_\phi} \begin{vmatrix} h_r \mathbf{e}_r & h_\theta \mathbf{e}_\theta & h_\phi \mathbf{e}_\phi \\ (\partial/\partial r) & (\partial/\partial \theta) & (\partial/\partial \phi) \\ h_r A_r & h_\theta A_\theta & h_\phi A_\phi \end{vmatrix} \\
&= \frac{\mathbf{e}_r}{r \sin(\theta)} \left(\frac{\partial (A_\phi \sin(\theta))}{\partial \theta} - \frac{\partial A_\theta}{\partial \phi} \right) + \frac{\mathbf{e}_\theta}{r} \left(\frac{1}{\sin(\theta)} \frac{\partial A_r}{\partial \phi} - \frac{\partial (r A_\phi)}{\partial r} \right) \\
&\quad + \frac{\mathbf{e}_\phi}{r} \left(\frac{\partial (r A_\theta)}{\partial r} - \frac{\partial A_r}{\partial \theta} \right) \qquad (4.93)
\end{aligned}$$

Problems:

1. Derive an expression for $\nabla^2 \phi$ and $\nabla \times \mathbf{A}$ in terms of the coordinates x_a, x_b and x_c and the scale factors h_a, h_b and h_c for a curvilinear coordinate system.

2. The cylindrical coordinate system consists of the coordinates (r, ϕ, z), where r is the distance from the z axis, and ϕ is the angle made by the position projection of the position vector on the $x - y$ plane with the x axis, as shown in figure 2. For this coordinate system,

   (a) Determine the coordinates (x, y, z) in terms of (r, ϕ, z), and the coordinates (r, ϕ, z) in terms of (x, y, z). How are the unit vectors $(\mathbf{e}_r, \mathbf{e}_\phi, \mathbf{e}_z)$ related to $(\mathbf{e}_x, \mathbf{e}_y, \mathbf{e}_z)$.

   (b) Write down the conservation equation for the concentration field for the appropriate differential volume in cylindrical coordinates. What is the divergence operator $\nabla.$ in this coordinate system?

   (c) Express the flux in terms of the gradient of concentration in the cylindrical coordinate system. What is the Laplacian operator ∇^2 in this coordinate system?

   (d) Solve the differential equation for the concentration in cylindrical coordinates using the separation of variables, in a manner similar to that for spherical coordinate system in class.

3. Consider a two - dimensional coordinate system given by:

$$x = \cosh(\xi) \cos(\eta) \quad y = \sinh(\xi) \sin(\eta) \qquad (4.94)$$

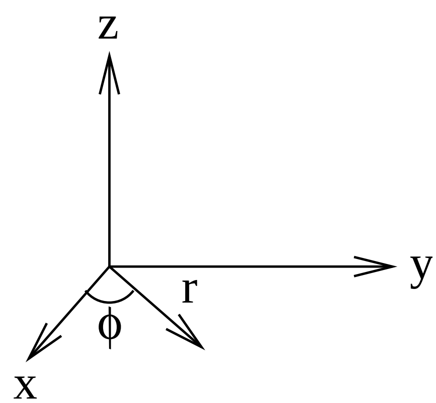

Figure 4.10: Cylindrical coordinate system.

where

$$\cosh(\xi) = \frac{\exp(\xi) + \exp(-\xi)}{2} \quad \sinh(\xi) = \frac{\exp(\xi) - \exp(-\xi)}{2} \tag{4.95}$$

and

$$\frac{\partial \cosh(\xi)}{\partial \xi} = \sinh(\xi) \quad \frac{\partial \sinh(\xi)}{\partial \xi} = \cosh(\xi) \tag{4.96}$$

(a) Derive an expression for $\mathbf{e}_\xi$ and $\mathbf{e}_\eta$ in terms of $\mathbf{e}_x$, $\mathbf{e}_y$, ξ and η. **Note:** In order to determine the unit vectors, it is not necessary to invert the expressions in equation 4.94 to determine $\xi = \xi(x, y)$ and $\eta = \eta(x, y)$.

(b) Is the coordinate system an orthogonal one?

(c) Determine the scale factors h_ξ and h_η.