Chapter 3: Equations of Change

In the last chapter, we presented examples of microscopic balances in one or two dimensions for various elementary examples. In this chapter we present the general balance equations in multidimensional case. The balances, also called equations of changes can be written in cartesian, cylindrical or spherical coordinates. We will explicitly derive the balance equations in cartesian coordinates and present the corresponding equations in cylindrical and spherical coordinates. The reader can consult the books in reference for more details. Once the equations are presented we show through various examples how they can be used in a systematic way to model distributed parameter models.

3.1 Total Mass balance

Our control volume is the elementary volume $\Delta x \Delta y \Delta z$ shown in Figure 3.1. The volume is assumed to be fixed in space. To write the mass balance around the volume we need to consider the mass entering in the three directions x, y, and z.
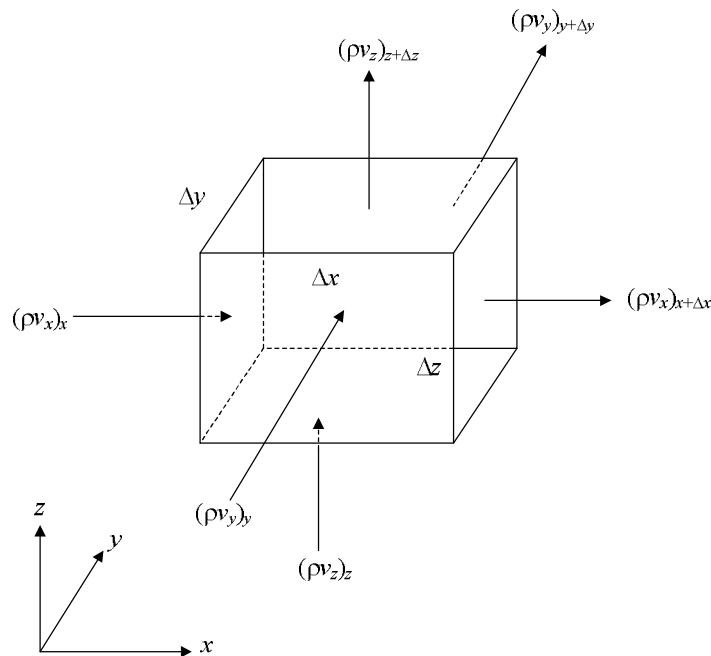

Figure 0-1 Total Mass balance in Cartesian coordinates

Mass in:

The mass entering in the x-direction at the cross sectional area ($\Delta y\Delta z$) is

$$(\rho v_x)|_x \, \Delta y\Delta z\Delta t \tag{3.1}$$

The mass entering in the y-direction at the cross sectional area ($\Delta x\Delta z$) is

$$(\rho v_y)|_y \, \Delta x\Delta z\Delta t \tag{3.2}$$

The mass entering in the z-direction at the cross sectional area ($\Delta x\Delta y$) is

$$(\rho v_z)|_z \, \Delta x \, \Delta y \, \Delta t \tag{3.3}$$

Mass out:

The mass exiting in the x-direction is:

$$(\rho v_x)|_{x+\Delta x} \, \Delta y\Delta z\Delta t \tag{3.4}$$

The mass exiting in the y-direction is:

$$(\rho v_y)|_{y+\Delta y} \, \Delta x\Delta z\Delta t \tag{3.5}$$

The mass exiting in the z-direction is:

$$(\rho v_z)|_{z+\Delta z} \, \Delta x\Delta y \, \Delta t \tag{3.6}$$

Rate of accumulation:

The rate of accumulation of mass in the elementary volume is:

$$(\rho)|_{t+\Delta t} \, \Delta x \, \Delta y \, \Delta z - (\rho)|_t \, \Delta x \, \Delta y \, \Delta z \tag{3.7}$$

Since there is no generation of mass, applying the general balance equation Eq. 1.2 and rearranging gives:

$$(\rho|_{t+\Delta t} - \rho|_t)\, \Delta x\, \Delta y\, \Delta z = (\rho v_x|_x - \rho v_x|_{x+\Delta x})\Delta y \Delta z \Delta t + (\rho v_y|_y - \rho v_y|_{y+\Delta y})\Delta x \Delta z \Delta t$$
$$+ (\rho v_z|_z - \rho v_z|_{z+\Delta z})\, \Delta x\, \Delta y\, \Delta t \tag{3.8}$$

Dividing the equation by $\Delta x\, \Delta y\, \Delta z \Delta t$ results in:

$$\frac{\rho|_{t+\Delta t} - \rho|_t}{\Delta t} = \frac{\rho v_x|_x - \rho v_x|_{x+\Delta x}}{\Delta x} + \frac{\rho v_y|_y - \rho v_y|_{y+\Delta y}}{\Delta y} + \frac{\rho v_z|_z - \rho v_z|_{z+\Delta z}}{\Delta z} \tag{3.9}$$

By taking the limits as $\Delta y, \Delta x, \Delta, z$ and Δt goes to zero, we obtain the following equation of change:

$$\frac{\partial \rho}{\partial t} = -\frac{\partial \rho v_x}{\partial x} - \frac{\partial \rho v_y}{\partial y} - \frac{\partial \rho v_z}{\partial z} \tag{3.10}$$

Expanding the partial derivative of each term yields after some rearrangement:

$$\frac{\partial \rho}{\partial t} + v_x \frac{\partial \rho}{\partial x} + v_y \frac{\partial \rho}{\partial y} + v_z \frac{\partial \rho}{\partial z} = -\rho\left(\frac{\partial v_x}{\partial x} + \frac{\partial v_y}{\partial y} + \frac{\partial v_z}{\partial z}\right) \tag{3.11}$$

This is the general form of the mass balance in cartesian coordinates. The equation is also known as the continuity equation. If the fluid is incompressible then the density is assumed constant, both in time and position. That means the partial derivatives of ρ are all zero. The total continuity equation (Eq. 3.11) is equivalent to:

$$0 = -\rho\left(\frac{\partial v_x}{\partial x} + \frac{\partial v_y}{\partial y} + \frac{\partial v_z}{\partial z}\right) \tag{3.12}$$

or simply:

$$0 = \frac{\partial v_x}{\partial x} + \frac{\partial v_y}{\partial y} + \frac{\partial v_z}{\partial z}$$

<div align="right">(3.13)</div>

3.2 Component Balance Equation

We consider a fluid consisting of species A, B ... , and where a chemical reaction is generating the species A at a rate r_A ($kg/m^3 s$). The fluid is in motion with mass-average velocity $v = n_t/\rho$ (m/s) where $n_t = n_A + n_B + ...$ ($kg/m^2 s$) is the total mass flux and ρ ($kg/m^3 s$) is the density of the mixture. Our objective is to establish the component balance equation of A as it diffuses in all directions x,y,z (Figure 3.2).
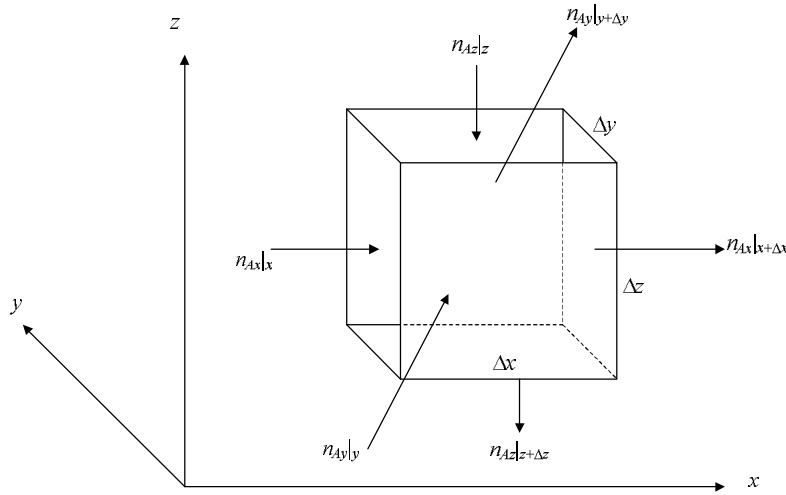

Figure 0-2 Mass balance of component A

Mass of A in:

The mass of species A entering the x-direction at the cross sectional ($\Delta y \Delta z$) is:

$$(n_{Ax})|_x \, \Delta y \Delta z \Delta t$$

<div align="right">(3.14)</div>

where n_{Ax} kg/m^2 is the flux transferred in the x-direction

Similarly the mass of A entering the y and z direction are respectively:

$$(n_{Ay})|_y \, \Delta x \Delta z \Delta t$$

<div align="right">(3.15)</div>

$$(n_{Az})|_z \, \Delta x \, \Delta y \, \Delta t \qquad\qquad (3.16)$$

Mass of A out:

The mass of species A exiting the x, y and z direction are respectively

$$(n_{Ax})|_{x+\Delta x} \, \Delta y \Delta z \Delta t \qquad\qquad (3.17)$$

$$(n_{Ay})|_{y+\Delta y} \, \Delta x \Delta z \Delta t \qquad\qquad (3.18)$$

$$(n_{Az})|_{z+\Delta z} \, \Delta x \, \Delta y \, \Delta t \qquad\qquad (3.19)$$

The rate of accumulation is:

$$\rho_A|_{t+\Delta t} \, \Delta x \, \Delta y \, \Delta z - \rho_A|_t \, \Delta x \, \Delta y \, \Delta z \qquad\qquad (3.20)$$

The rate of generation is:

$$-r_A \Delta x \, \Delta y \, \Delta z \Delta t \qquad\qquad (3.21)$$

Applying the general balance equation (Eq. 1.3) yields:

$$(\rho_A|_{t+\Delta t} - \rho_A|_t) \, \Delta x \, \Delta y \, \Delta z = (n_{Ax}|_{x+\Delta x} - n_{Ax}|_x)\Delta y \Delta z \Delta t + (n_{Ay}|_{y+\Delta y} - n_{Ay}|_y)\Delta x \Delta z \Delta t$$
$$+ \, (n_{Az}|_{z+\Delta z} - n_{Az}|_z)\Delta x \Delta y \Delta t + r_A \Delta x \, \Delta y \, \Delta z \Delta t \qquad (3.22)$$

Dividing each term by $\Delta x \Delta y \Delta z \Delta t$ and letting each of these terms goes to zero yields:

$$\frac{\partial \rho_A}{\partial t} + \frac{\partial n_{Ax}}{\partial t} + \frac{\partial n_{Ay}}{\partial t} + \frac{\partial n_{Az}}{\partial t} = r_A$$
$$\qquad\qquad (3.23)$$

We know from Section 1.11.1, that the flux n_A is the sum of a term due to convection $(\rho_A v)$ and a term due to diffusion j_A $(kg/m^2 s)$:

$$n_A = \rho_A v + j_A \qquad\qquad (3.24)$$

Substituting the different flux in Eq. 3.23 gives:

$$\frac{\partial \rho_A}{\partial t} + \frac{\partial(\rho_A v_x)}{\partial x} + \frac{\partial(\rho_A v_y)}{\partial y} + \frac{\partial(\rho_A v_z)}{\partial z} + \frac{\partial j_{Ax}}{\partial x} + \frac{\partial j_{Ay}}{\partial y} + \frac{\partial j_{Az}}{\partial z} = r_A \tag{3.25}$$

For a binary mixture (A,B), Fick's law gives the flux in the u-direction as :

$$j_{Au} = -\rho D_{AB} \frac{\partial w_A}{\partial u} \tag{3.26}$$

where $w_A = \rho_A/\rho$. Expanding Eq. 3.25 and substituting for the fluxes yield:

$$\frac{\partial \rho_A}{\partial t} + \rho_A \left(\frac{\partial v_x}{\partial x} + \frac{\partial v_y}{\partial y} + \frac{\partial v_z}{\partial z} \right) + \left(v_x \frac{\partial \rho_A}{\partial x} + v_y \frac{\partial \rho_A}{\partial y} + v_z \frac{\partial \rho_A}{\partial z} \right)$$

$$- \left(\frac{\partial}{\partial x} (\frac{\partial \rho D_{AB} w_A}{\partial x}) + \frac{\partial}{\partial y} (\frac{\partial \rho D_{AB} w_A}{\partial y}) + \frac{\partial}{\partial z} (\frac{\partial \rho D_{AB} w_A}{\partial z}) \right) = r_A \tag{3.27}$$

This is the general component balance or equation of continuity for species A. This equation can be further reduced according to the nature of properties of the fluid involved. If the binary mixture is a dilute liquid and can be considered incompressible, then density ρ and diffusivity D_{AB} are constant. Substituting the continuity equation (Eq. 3.13) in the last equation gives:

$$\frac{\partial \rho_A}{\partial t} + \left(v_x \frac{\partial \rho_A}{\partial x} + v_y \frac{\partial \rho_A}{\partial y} + v_z \frac{\partial \rho_A}{\partial z} \right) - D_{AB} \left(\frac{\partial^2 \rho_A}{\partial x^2} + \frac{\partial^2 \rho_A}{\partial y^2} + \frac{\partial^2 \rho_A}{\partial z^2} \right) = r_A \tag{3.28}$$

This equation can also be written in molar units by dividing it by the molecular weight M_A to yield:

$$\underbrace{\frac{\partial C_A}{\partial t}}_{accumulation} + \underbrace{\left(v_x \frac{\partial C_A}{\partial x} + v_y \frac{\partial C_A}{\partial y} + v_z \frac{\partial C_A}{\partial z} \right)}_{Convection} - D_{AB} \underbrace{\left(\frac{\partial^2 C_A}{\partial x^2} + \frac{\partial^2 C_A}{\partial y^2} + \frac{\partial^2 C_A}{\partial z^2} \right)}_{Diffusion} = \underbrace{R_A}_{reaction} \tag{3.29}$$

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The component balance equation is composed then of a transient term, a convective term, a diffusive term and a reaction term.

3.3 Momentum Balance

We consider a fluid flowing with a velocity $v(t,x,y,z)$ in the cube of Figure 3.3. The flow is assumed laminar. We know from Section 1.11.2 that the momentum is transferred through convection (bulk flow) and by molecular transfer (velocity gradient).
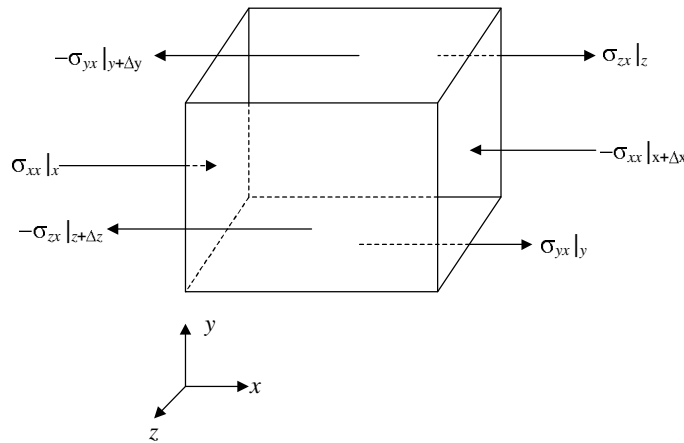

Figure 0-3 Balance of the x-component of the momentum

Since, unlike the mass or the energy, the momentum is a vector that has three components, we will present the derivation of the equation for the conservation of the x-component of the momentum. The balance equations for the y-component and the z-component are obtained in a similar way. To establish the momentum balance for its x-component we need to consider its transfer in the x-direction, y-direction, and z-direction.

Momentum in:

The x-component of momentum entering the boundary at x-direction, by convection is:

$$(\rho v_x v_x)|_x \, \Delta y \Delta z \Delta t \qquad (3.30)$$

The x-component of momentum entering the boundary at y-direction, by convection is:

$$(\rho v_y v_x)|_y \, \Delta x \Delta z \Delta t \qquad (3.31)$$

and it enters the z-direction by convection with a momentum:

$$(\rho v_z v_x)|_z \, \Delta x \Delta y \Delta t \qquad (3.32)$$

The x-component of momentum entering the boundary at x-direction, by molecular diffusion is:

$$(\tau_{xx})|_x \, \Delta y \Delta z \Delta t \qquad (3.33)$$

The x-component of momentum entering the boundary at y-direction, by molecular diffusion is:

$$(\tau_{yx})|_y \, \Delta x \Delta z \Delta t \qquad (3.34)$$

and it enters the z-direction by molecular diffusion with a momentum:

$$(\tau_{zx})|_z \, \Delta x \Delta y \Delta t \qquad (3.35)$$

Momentum out:

The rate of momentum leaving the boundary at $x+\Delta x$, by convection is:

$$(\rho v_x v_x)|_{x+\Delta x} \, \Delta y \Delta z \Delta t \qquad (3.36)$$

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and at boundary $y+\Delta y$,:

$$(\rho v_y v_x)|_{y+\Delta y} \, \Delta x \Delta z \Delta t \tag{3.37}$$

and at boundary $z+\Delta z$:

$$(\rho v_z v_x)|_{z+\Delta z} \, \Delta x \Delta y \Delta t \tag{3.38}$$

The x-component of momentum exiting the boundary $x+\Delta x$, by molecular diffusion is:

$$(\tau_{xx})|_{x+\Delta x} \, \Delta y \Delta z \Delta t \tag{3.39}$$

and at boundary $y+\Delta y$:

$$(\tau_{yx})|_{y+\Delta y} \, \Delta x \Delta z \Delta t \tag{3.40}$$

and at boundary $z+\Delta z$::

$$(\tau_{zx})|_{z+\Delta z} \, \Delta x \Delta y \Delta t \tag{3.41}$$

Forces acting on the volume:

The net fluid pressure force acting on the volume element in the x-direction is:

$$(P|_x - P|_{x+\Delta x}) \, \Delta y \Delta z \Delta t \tag{3.42}$$

The net gravitational force in the x-direction is:

$$\rho g|_x \, \Delta x \, \Delta y \Delta z \, \Delta t \tag{3.43}$$

Accumulation is:

$$(\rho v_x|_{t+\Delta t} - \rho v_x|_t)\, \Delta x\, \Delta y \Delta z \tag{3.44}$$

Substituting all these equations in Eq. 1.5, dividing by $\Delta x\, \Delta y\, \Delta z \Delta t$ and taking the limit of each term goes zero gives:

$$\frac{\partial(\rho v_x)}{\partial t} + \frac{\partial(\rho v_x v_x)}{\partial x} + \frac{\partial(\rho v_x v_y)}{\partial y} + \frac{\partial(\rho v_x v_z)}{\partial z} = -\left(\frac{\partial \tau_{xx}}{\partial x} + \frac{\partial \tau_{yx}}{\partial y} + \frac{\partial \tau_{zx}}{\partial z}\right) - \frac{\partial P}{\partial x} + \rho g_x \tag{3.45}$$

Expanding the partial derivative and rearranging:

$$v_x\left(\frac{\partial \rho}{\partial t} + \frac{\partial \rho v_x}{\partial x} + \frac{\partial \rho v_y}{\partial y} + \frac{\partial \rho v_z}{\partial z}\right) + \rho\left(\frac{\partial v_x}{\partial t} + v_x\frac{\partial v_x}{\partial x} + v_y\frac{\partial v_x}{\partial y} + v_z\frac{\partial v_x}{\partial z}\right) =$$

$$-\left(\frac{\partial \tau_{xx}}{\partial x} + \frac{\partial \tau_{yx}}{\partial y} + \frac{\partial \tau_{zx}}{\partial z}\right) - \frac{\partial P}{\partial x} + \rho g_x \tag{3.46}$$

Using the equation of continuity (Eq. 3.10) for incompressible fluid, Equation (3.46) is reduced to:

$$\rho\left(\frac{\partial v_x}{\partial t} + v_x\frac{\partial v_x}{\partial x} + v_y\frac{\partial v_x}{\partial y} + v_z\frac{\partial v_x}{\partial z}\right) = -\left(\frac{\partial \tau_{xx}}{\partial x} + \frac{\partial \tau_{yx}}{\partial y} + \frac{\partial \tau_{zx}}{\partial z}\right) - \frac{\partial P}{\partial x} + \rho g_x \tag{3.47}$$

Using the assumption of Newtonian fluid, i.e.

$$\tau_{xx} = -\mu\frac{\partial v_x}{\partial x}, \qquad \tau_{yx} = -\mu\frac{\partial v_x}{\partial y}, \qquad \tau_{zx} = -\mu\frac{\partial v_x}{\partial z} \tag{3.48}$$

Equation 3.47 yields:

$$\underbrace{\rho\frac{\partial v_x}{\partial t}}_{\text{accumulation}} + \underbrace{\rho\left(v_x\frac{\partial v_x}{\partial x} + v_y\frac{\partial v_x}{\partial y} + v_z\frac{\partial v_x}{\partial z}\right)}_{\text{transport by bulk flow}} = \underbrace{\mu\left(\frac{\partial^2 v_x}{\partial x^2} + \frac{\partial^2 v_x}{\partial y^2} + \frac{\partial^2 v_x}{\partial z^2}\right)}_{\text{transport by viscous forces}} \underbrace{- \frac{\partial P}{\partial x} + \rho g_x}_{\text{generation}} \tag{3.49}$$

The momentum balances in the y-direction and z-direction can be obtained in a similar fashion:

$$\rho \underbrace{\frac{\partial v_y}{\partial t}}_{\text{accumulation}} + \rho \underbrace{\left(v_x \frac{\partial v_y}{\partial x} + v_y \frac{\partial v_y}{\partial y} + v_z \frac{\partial v_y}{\partial z} \right)}_{\text{transport by bulk flow}} = \mu \underbrace{\left(\frac{\partial^2 v_y}{\partial x^2} + \frac{\partial^2 v_y}{\partial y^2} + \frac{\partial^2 v_y}{\partial z^2} \right)}_{\text{transport by viscous forces}} - \underbrace{\frac{\partial P}{\partial y} + \rho g_y}_{\text{generation}} \qquad (3.50)$$

$$\rho \underbrace{\frac{\partial v_z}{\partial t}}_{\text{accumulation}} + \rho \underbrace{\left(v_x \frac{\partial v_z}{\partial x} + v_y \frac{\partial v_z}{\partial y} + v_z \frac{\partial v_z}{\partial z} \right)}_{\text{transport by bulk flow}} = \mu \underbrace{\left(\frac{\partial^2 v_z}{\partial x^2} + \frac{\partial^2 v_z}{\partial y^2} + \frac{\partial^2 v_z}{\partial z^2} \right)}_{\text{transport by viscous forces}} - \underbrace{\frac{\partial P}{\partial z} + \rho g_z}_{\text{generation}} \qquad (3.51)$$

These equations constitute the Navier-Stock's equation.

3.4 Energy balance

In deriving the equation for energy balance we will be guided by the analogy that exists between mass and energy transport mentioned in Section 1.11.3 We will assume constant density, heat capacity and thermal conductivity for the incompressible fluid. The fluid is assumed at constant pressure (Fig 3.4).

The total energy flux is the sum of heat flux and bulk flux:

$$e = q + \rho CpTv \qquad (3.52)$$

Therefore, the energy coming by convection in the x-direction at boundary x is:

$$(q_x + \rho CpTv_x)\Delta y \Delta z \Delta t \qquad (3.53)$$

Similarly the energy entering the y and z directions are

$$(q_y + \rho CpTv_y)\Delta x \Delta z \Delta t \qquad (3.54)$$

$$(q_z + \rho CpTv_z)\, \Delta x\, \Delta y\, \Delta t \qquad (3.55)$$

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The energy leaving the *x, y* and *z* directions are:

$$(q_x + \rho CpTv_x)|_{x+\Delta x}\ \Delta y\Delta z\Delta t \tag{3.56}$$

$$(q_y + \rho CpTv_y)|_{y+\Delta y}\ \Delta x\Delta z\Delta t \tag{3.57}$$

$$(q_z + \rho CpTv_z)|_{z+\Delta z}\ \Delta x\ \Delta y\ \Delta t \tag{3.58}$$

The energy accumulated is approximated by:

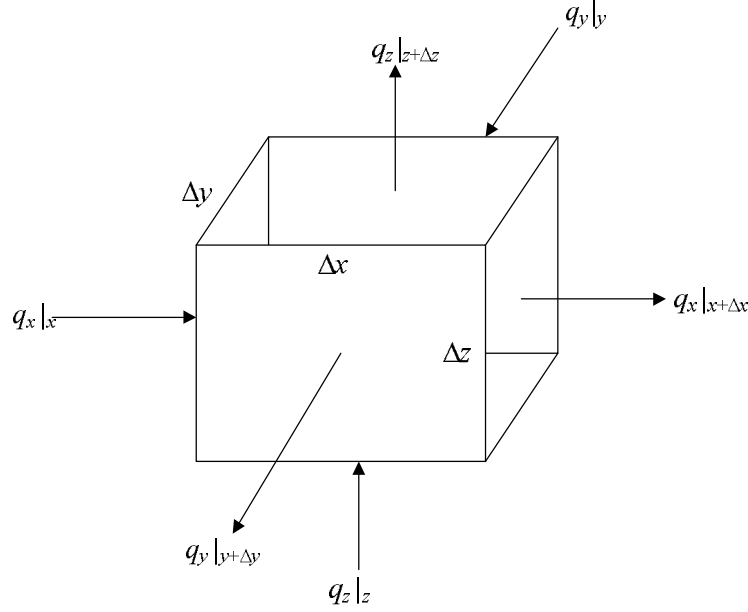$$(\rho CpT|_{t+\Delta t} - \rho CpT|_t)\ \Delta x\ \Delta y\Delta z \tag{3.59}$$

Figure 0-4 Energy Balance in Cartesian coordinates

The rate of generation is Φ_H where Φ_H includes all the sources of heat generation, i.e. reaction, pressure forces, gravity forces, fluid friction, etc. Substituting all these terms in the general energy equation (Eq. 1.7) and dividing the equation by the term $\Delta x\Delta y\Delta z\Delta t$ and letting each of these terms approach zero yield:

$$\frac{\partial(\rho CpT)}{\partial t} + \frac{\partial(\rho CpTv_x)}{\partial x} + \frac{\partial(\rho CpTv_y)}{\partial y} + \frac{\partial(\rho CpTv_z)}{\partial z} + \frac{\partial q_x}{\partial x} + \frac{\partial q_y}{\partial y} + \frac{\partial q_z}{\partial z} = \Phi_H \tag{3.60}$$

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Expanding the partial derivative yields:

$$\rho Cp\left(\frac{\partial T}{\partial t}+v_x\frac{\partial T}{\partial x}+v_y\frac{\partial T}{\partial y}+v_z\frac{\partial T}{\partial z}\right)+\rho CpT\left(\frac{\partial \rho}{\partial t}+\frac{\partial \rho v_x}{\partial x}+\frac{\partial \rho v_y}{\partial y}+\frac{\partial \rho v_z}{\partial z}\right)+\frac{\partial q_x}{\partial x}+\frac{\partial q_y}{\partial y}+\frac{\partial q_z}{\partial z}=\Phi_H$$

(3.61)

Using the equation of continuity (Eq. 3.10) for incompressible fluids the equation is reduced to:

$$\rho Cp\left(\frac{\partial T}{\partial t}+v_x\frac{\partial T}{\partial x}+v_y\frac{\partial T}{\partial y}+v_z\frac{\partial T}{\partial z}\right)+\frac{\partial q_x}{\partial x}+\frac{\partial q_y}{\partial y}+\frac{\partial q_z}{\partial z}=\Phi_H$$

(3.62)

Using Fourier's law:

$$q_u=-k\frac{dT}{du}$$

(3.63)

into the last equation gives:

$$\underbrace{\rho Cp\frac{\partial T}{\partial t}}_{accumulation}+\underbrace{\rho Cp\left(v_x\frac{\partial T}{\partial x}+v_y\frac{\partial T}{\partial y}+v_z\frac{\partial T}{\partial z}\right)}_{\text{Transport by bulk flow}}=\underbrace{k\left(\frac{\partial^2 T}{\partial x^2}+\frac{\partial^2 T}{\partial y^2}+\frac{\partial^2 T}{\partial z^2}\right)}_{\text{Transport by thermal diffusion}}+\underbrace{\Phi_H}_{generation}$$

(3.64)

The energy balance includes as before a transient term, a convection term, a diffusion term, and generation term. For solids, the density is constant and with no velocity, i.e. $v = 0$, the equation is reduced to:

$$\underbrace{\rho Cp\frac{\partial T}{\partial t}}_{accumulation}=\underbrace{k\left(\frac{\partial^2 T}{\partial x^2}+\frac{\partial^2 T}{\partial y^2}+\frac{\partial^2 T}{\partial z^2}\right)}_{\text{Transport by thermal diffusion}}+\underbrace{\Phi_H}_{generation}$$

(3.65)

3.5 Conversion between the coordinates

So far we have shown how to derive the equation of change in Cartesian coordinates. In the same way, the equations of change can be written other coordinate systems such as the cylindrical or spherical coordinates. Alternatively, one can transform the equation of change written in the Cartesian coordinates to the others through the following transformation expressions.

The relations between Cartesian coordinates (x,y,z) and cylindrical coordinates (r,z,θ) (Figures 1.3 and 1.4) are the following:

$$x = rcos(\theta), \quad y = rsin(\theta), \quad z = z \tag{3.66}$$

Therefore;

$$r = \sqrt{x^2 + y^2}, \qquad \theta = \tan^{-1}(\frac{y}{x}) \tag{3.67}$$

The relations between Cartesian coordinates (x,y,z) and spherical coordinates (r,θ,ϕ) (Figures 1.3 and 1.5) are:

$$x = r\sin(\theta)\cos(\phi), \qquad y = r\sin(\theta)\sin(\phi), \qquad z = r\cos(\theta) \tag{3.68}$$

Therefore;

$$r = \sqrt{x^2 + y^2 + z^2}, \qquad \theta = \tan^{-1}(\frac{\sqrt{x^2 + y^2}}{z}), \qquad \phi = \tan^{-1}(\frac{y}{x}) \tag{3.69}$$

Accordingly, we list the following general balance equations in the three coordinates. These equations are written under the assumptions mentioned in previous sections. For the more general case, where density is considered variable the reader can consult the books listed in the references.

3.5.1 Balance Equations in Cartesian Coordinates

Mass Balance

$$\rho(\frac{\partial v_x}{\partial x} + \frac{\partial v_y}{\partial y} + \frac{\partial v_z}{\partial z}) = 0 \tag{3.70}$$

Component balance for component *A* in binary mixture with chemical reaction rate R_A:

$$\frac{\partial C_A}{\partial t} + \left(v_x \frac{\partial C_A}{\partial x} + v_y \frac{\partial C_A}{\partial y} + v_z \frac{\partial C_A}{\partial z} \right) = D_{AB} \left(\frac{\partial^2 C_A}{\partial x^2} + \frac{\partial^2 C_A}{\partial y^2} + \frac{\partial^2 C_A}{\partial z^2} \right) + R_A \tag{3.71}$$

Energy balance

$$\rho Cp \frac{\partial T}{\partial t} + \rho Cp(v_x \frac{\partial T}{\partial x} + v_y \frac{\partial T}{\partial y} + v_z \frac{\partial T}{\partial z}) = k(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} + \frac{\partial^2 T}{\partial z^2}) + \Phi_H \tag{3.72}$$

Momentum balance

- x component

$$\rho \frac{\partial v_x}{\partial t} + \rho(v_x \frac{\partial v_x}{\partial x} + v_y \frac{\partial v_x}{\partial y} + v_z \frac{\partial v_x}{\partial z}) = \mu(\frac{\partial^2 v_x}{\partial x^2} + \frac{\partial^2 v_x}{\partial y^2} + \frac{\partial^2 v_x}{\partial z^2}) - \frac{\partial P}{\partial x} + \rho g_x \tag{3.73}$$

- y component:

$$\rho \frac{\partial v_y}{\partial t} + \rho(v_x \frac{\partial v_y}{\partial x} + v_y \frac{\partial v_y}{\partial y} + v_z \frac{\partial v_y}{\partial z}) = \mu(\frac{\partial^2 v_y}{\partial x^2} + \frac{\partial^2 v_y}{\partial y^2} + \frac{\partial^2 v_y}{\partial z^2}) - \frac{\partial P}{\partial y} + \rho g_y \tag{3.74}$$

- z component

$$\rho\frac{\partial v_z}{\partial t} + \rho(v_x\frac{\partial v_z}{\partial x} + v_y\frac{\partial v_z}{\partial y} + v_z\frac{\partial v_z}{\partial z}) = \mu(\frac{\partial^2 v_z}{\partial x^2} + \frac{\partial^2 v_z}{\partial y^2} + \frac{\partial^2 v_z}{\partial z^2}) - \frac{\partial P}{\partial z} + \rho g_z \tag{3.75}$$

3.5.2 Balance Equations in Cylindrical Coordinates

Mass balance

$$\rho(\frac{1}{r}\frac{\partial rv_r}{\partial r} + \frac{1}{r}\frac{\partial v_\theta}{\partial \theta} + \frac{\partial v_z}{\partial z}) = 0 \tag{3.76}$$

Component balance for component A in binary mixture (A-B) with reaction rate R_A:

$$\frac{\partial C_A}{\partial t} + \left(v_r\frac{\partial C_A}{\partial r} + v_\theta\frac{1}{r}\frac{\partial C_A}{\partial \theta} + v_z\frac{\partial C_A}{\partial z}\right) = D_{AB}\left(\frac{1}{r}\frac{\partial}{\partial r}(r\frac{\partial C_A}{\partial r}) + \frac{1}{r^2}\frac{\partial^2 C_A}{\partial \theta^2} + \frac{\partial^2 C_A}{\partial z^2})\right) + R_A \tag{3.77}$$

Energy balance

$$\rho Cp\frac{\partial T}{\partial t} + \rho Cp(v_r\frac{\partial T}{\partial r} + v_\theta\frac{1}{r}\frac{\partial T}{\partial \theta} + v_z\frac{\partial T}{\partial z}) = k(\frac{1}{r}\frac{\partial}{\partial r}(r\frac{\partial T}{\partial r}) + \frac{1}{r^2}\frac{\partial^2 T}{\partial \theta^2} + \frac{\partial^2 T}{\partial z^2}) + \Phi_H \tag{3.78}$$

Momentum balance

- r component

$$\rho\frac{\partial v_r}{\partial t} + \rho(v_r\frac{\partial v_r}{\partial r} + \frac{v_\theta}{r}\frac{\partial v_r}{\partial \theta} - \frac{v_\theta^2}{r} + v_z\frac{\partial v_r}{\partial z}) = \tag{3.79}$$

$$\mu(\frac{\partial}{\partial r}(\frac{1}{r}\frac{\partial rv_r}{\partial r}) + \frac{1}{r^2}\frac{\partial^2 v_r}{\partial \theta^2} - \frac{2}{r^2}\frac{\partial v_\theta}{\partial \theta} + \frac{\partial^2 v_r}{\partial z^2}) - \frac{\partial P}{\partial r} + \rho g_r$$

- θ component:

$$\rho \frac{\partial v_\theta}{\partial t} + \rho(v_r \frac{\partial v_\theta}{\partial r} + \frac{v_\theta}{r}\frac{\partial v_\theta}{\partial \theta} + \frac{v_r v_\theta}{r} + v_z \frac{\partial v_\theta}{\partial z}) =$$

(3.80)

$$\mu(\frac{\partial}{\partial r}(\frac{1}{r}\frac{\partial r v_\theta}{\partial r}) + \frac{1}{r^2}\frac{\partial^2 v_\theta}{\partial \theta^2} + \frac{2}{r^2}\frac{\partial v_r}{\partial \theta} + \frac{\partial^2 v_\theta}{\partial z^2}) - \frac{\partial P}{\partial \theta} + \rho g_\theta$$

- z component

$$\rho \frac{\partial v_z}{\partial t} + \rho(v_r \frac{\partial v_z}{\partial r} + \frac{v_\theta}{r}\frac{\partial v_z}{\partial \theta} + v_z \frac{\partial v_z}{\partial z}) = \mu(\frac{1}{r}\frac{\partial}{\partial r}(r\frac{\partial v_z}{\partial r}) + \frac{1}{r^2}\frac{\partial^2 v_z}{\partial \theta^2} + \frac{\partial^2 v_z}{\partial z^2}) - \frac{\partial P}{\partial z} + \rho g_z$$

(3.81)

3.5.3 Balance Equations in Spherical Coordinates

Mass Balance

$$\rho\left(\frac{1}{r^2}\frac{\partial(r^2 v_r)}{\partial r} + \frac{1}{r\sin(\theta)}\frac{\partial(v_\theta \sin(\theta))}{\partial \theta} + \frac{1}{r\sin(\theta)}\frac{\partial v_\phi}{\partial \phi}\right) = 0$$

(3.82)

Component balance for component A in binary mixture (A-B) with reaction rate R_A :

$$\frac{\partial C_A}{\partial t} + \left(v_r \frac{\partial C_A}{\partial r} + \frac{v_\theta}{r}\frac{\partial C_A}{\partial \theta} + \frac{v_\phi}{r\sin(\theta)}\frac{\partial C_A}{\partial \phi}\right) =$$

$$D_{AB}\left(\frac{1}{r^2}\frac{\partial}{\partial r}(r^2 \frac{\partial C_A}{\partial r}) + \frac{1}{r^2 \sin(\theta)}\frac{\partial}{\partial \theta}(\sin(\theta)\frac{\partial C_A}{\partial \theta}) + \frac{1}{r^2 \sin^2(\theta)}\frac{\partial^2 C_A}{\partial \phi^2}\right) + R_A$$

(3.83)

Energy balance

$$\rho Cp \frac{\partial T}{\partial t} + \rho Cp\left(v_r \frac{\partial T}{\partial r} + \frac{v_\theta}{r}\frac{\partial T}{\partial \theta} + \frac{v_\phi}{r\sin(\theta)}\frac{\partial T}{\partial \phi}\right) =$$

(3.84)

$$k\left(\frac{1}{r^2}\frac{\partial}{\partial r}(r^2 \frac{\partial T}{\partial r}) + \frac{1}{r^2 \sin(\theta)}\frac{\partial}{\partial \theta}(\sin(\theta)\frac{\partial T}{\partial \theta}) + \frac{1}{r^2 \sin^2(\theta)}\frac{\partial^2 T}{\partial \phi^2}\right) + \Phi_H$$

Momentum balance

- r component

$$\rho \frac{\partial v_r}{\partial t} + \rho \left(v_r \frac{\partial v_r}{\partial r} + \frac{v_\theta}{r} \frac{\partial v_r}{\partial \theta} + \frac{v_\phi}{r\sin(\theta)} \frac{\partial v_r}{\partial \phi} - \frac{v_\theta^2 + v_\phi^2}{r} \right) =$$

$$\mu \left(\frac{1}{r^2} \frac{\partial^2}{\partial r^2}(r^2 v_r) + \frac{1}{r^2 \sin(\theta)} \frac{\partial}{\partial \theta}(\sin(\theta) \frac{\partial v_r}{\partial \theta}) + \frac{1}{r^2 \sin^2(\theta)} \frac{\partial^2 v_r}{\partial \phi^2} \right) - \frac{\partial P}{\partial r} + \rho g_r \qquad (3.85)$$

- θ component:

$$\rho \frac{\partial v_\theta}{\partial t} + \rho \left(v_r \frac{\partial v_\theta}{\partial r} + \frac{v_\theta}{r} \frac{\partial v_\theta}{\partial \theta} + \frac{v_\phi}{r\sin(\theta)} \frac{\partial v_\theta}{\partial \phi} + \frac{v_r v_\theta}{r} - \frac{v_\phi^2 \cot(\theta)}{r} \right) =$$

$$\mu \left(\frac{1}{r^2} \frac{\partial}{\partial r}(r^2 \frac{\partial v_\theta}{\partial r}) + \frac{1}{r^2} \frac{\partial}{\partial \theta}(\sin(\theta) \frac{\partial \sin(\theta) v_\theta}{\partial \theta}) + \frac{1}{r^2 \sin^2(\theta)} \frac{\partial^2 v_\theta}{\partial \phi^2} \right)$$

$$+ \frac{2\mu}{r^2} \left(\frac{\partial v_r}{\partial \theta} - \frac{\cos(\theta)}{\sin^2(\theta)} \frac{\partial v_\phi}{\partial \phi} \right) - \frac{1}{r} \frac{\partial P}{\partial \theta} + \rho g_\theta \qquad (3.86)$$

- Φ component

$$\rho \frac{\partial v_\phi}{\partial t} + \rho \left(v_r \frac{\partial v_\phi}{\partial r} + \frac{v_\theta}{r} \frac{\partial v_\phi}{\partial \theta} + \frac{v_\phi}{r\sin(\theta)} \frac{\partial v_\phi}{\partial \phi} + \frac{v_r v_\phi}{r} + \frac{v_\theta v_\phi \cot(\theta)}{r} \right) =$$

$$\mu \left(\frac{1}{r^2} \frac{\partial}{\partial r}(r^2 \frac{\partial v_\phi}{\partial r}) + \frac{1}{r^2} \frac{\partial}{\partial \theta}(\frac{1}{\sin(\theta)} \frac{\partial \sin(\theta) v_\phi}{\partial \theta}) + \frac{1}{r^2 \sin^2(\theta)} \frac{\partial^2 v_\phi}{\partial \phi^2} \right)$$

$$+ \mu \left(\frac{2}{r^2 \sin(\theta)} \frac{\partial v_r}{\partial \phi} + \frac{2\cos(\theta)}{r^2 \sin^2(\theta)} \frac{\partial v_\theta}{\partial \phi} \right) - \frac{1}{r\sin(\theta)} \frac{\partial P}{\partial \phi} + \rho g_\phi \qquad (3.87)$$

3.6 Examples of Application of Equations of change

Practically all the microscopic balance examples treated in the previous chapter can be treated using the equations of change presented in this chapter. In this section we review some of the previous examples and present additional applications.

3.6.1 Liquid flow in a Pipe

To model the one dimensional flow through the pipe of an incompressible fluid (Example 2.2.1) we may use the continuity balance. For constant density we have the continuity equation in cylindrical coordinates (Eq. 3.76).

$$\frac{1}{r}\frac{\partial rv_r}{\partial r} + \frac{\partial v_\theta}{r\partial\theta} + \frac{\partial v_z}{\partial z} = 0 \tag{3.88}$$

The plug flow assumptions imply that $v_r = v_\theta = 0$, and the continuity balance is reduced to:

$$\frac{\partial v_z}{\partial z} = 0 \tag{3.89}$$

3.6.2 Diffusion with Chemical Reaction in a Slab Catalyst

To model the steady state diffusion with chemical reaction of species A in a slab catalyst, (Example 2.2.3) we use the equation of change (Eq. 3.71). The fluid properties are assumed constant,

$$\frac{\partial C_A}{\partial t} + v_x\frac{\partial C_A}{\partial x} + v_y\frac{\partial C_A}{\partial y} + v_z\frac{\partial C_A}{\partial z} - D_A(\frac{\partial^2 C_A}{\partial x^2} + \frac{\partial^2 C_A}{\partial y^2} + \frac{\partial^2 C_A}{\partial z^2}) = R_A \tag{3.90}$$

Since the system is at steady state we have $\frac{\partial C_A}{\partial t} = 0$. If we assume that there is no bulk flow then $v_x = v_y = v_z = 0$. For diffusion in the z-direction only, the following holds: $\frac{\partial}{\partial x} = \frac{\partial}{\partial y} = 0$. The equation is then reduces to:

$$-D_A\frac{d^2 C_A}{dz^2} = R_A \tag{3.91}$$

3.6.3 Plug Flow Reactor

The isothermal plug flow reactor (Example 2.2.5) can be modeled using the component balance equation (3.77). The plug flow conditions imply that $v_r = v_\theta = 0$ and $\frac{\partial}{\partial r} = \frac{\partial}{\partial \theta} = 0$. Equation (3.77) is reduced to:

$$\frac{\partial C_A}{\partial t} = -v_z \frac{\partial C_A}{\partial z} + D_{AB} \frac{\partial^2 C_A}{\partial z^2} - R_A$$

(3.92)

For the non-isothermal plug flow reactor (Example 2.2.6), the energy balance is obtained by using Eq. 3.78. For fluid with constant properties and at constant pressure, we have:

$$\rho Cp \frac{\partial T}{\partial t} + \rho Cp (v_r \frac{\partial T}{\partial r} + \frac{v_\theta}{r} \frac{\partial T}{\partial \theta} + v_z \frac{\partial T}{\partial z}) = k(\frac{\partial^2 T}{\partial r^2} + \frac{1}{r} \frac{\partial T}{\partial r} + \frac{1}{r^2} \frac{\partial^2 T}{\partial \theta^2} + \frac{\partial^2 T}{\partial z^2}) + \Phi_H$$

(3.93)

Using the plug-flow assumptions, $v_r = v_\theta = 0$ and $\frac{\partial}{\partial r} = \frac{\partial}{\partial \theta} = 0$, and neglecting the viscous forces, the term Φ_H includes the heat generation by reaction rate R_A and heat exchanged with the cooling jacket, $h_t A(T - T_w)$. Equation (3.93) is reduced to:

$$\rho Cp \frac{\partial T}{\partial t} = -\rho Cp v \frac{\partial T}{\partial z} + k \frac{\partial^2 T}{\partial z^2} - \Delta H_r k_o e^{-E/RT} C_A - h_t \frac{\pi D}{A}(T - T_w)$$

(3.94)

3.6.4 Energy Transport with Heat Generation

Consider the example of a solid cylinder of radius R in which heat is being generated due to some reaction at a uniform rate of Φ_H ($J/m^2 s$). A cooling system is used to remove heat from the system and maintain its surface temperature at the constant value T_w (Figure 3.5). Our objective is to derive the temperature variations in the cylinder. We assume that the solid is of constant density, thermal conductivity and heat capacity. Clearly this is a distributed parameter system since the temperature can vary with time and with all positions in the cylinder. We will use then the equation of change (Eq. 3.78) in cylindrical coordinates for a solid:

$$\frac{\partial T}{\partial t} = \frac{k}{\rho C p}(\frac{\partial^2 T}{\partial r^2} + \frac{1}{r}\frac{\partial T}{\partial r} + \frac{1}{r^2}\frac{\partial^2 T}{\partial \theta^2} + \frac{\partial^2 T}{\partial z^2}) + \frac{\Phi_H}{\rho C p} \tag{3.95}$$
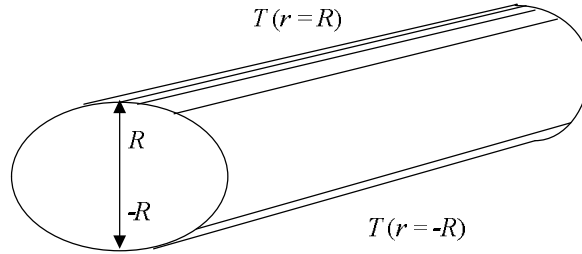

Figure 0-5 Cylindrical solid rod

A number of assumptions can be made:

- The system is at steady state i.e. $\frac{\partial T}{\partial t} = 0$

- The variation of temperature is only allowed in radial directions. Therefore, the terms $\frac{\partial^2 T}{\partial z^2}$ and $\frac{\partial^2 T}{\partial \theta^2}$ are zero.

The energy balance is reduced to:

$$0 = \frac{k}{\rho C p}(\frac{d^2 T}{dr^2} + \frac{1}{r}\frac{dT}{dr}) + \frac{\Phi_H}{\rho C p} \tag{3.96}$$

Or equivalently:

$$(\frac{d^2 T}{dr^2} + \frac{1}{r}\frac{dT}{dr}) = -\frac{\Phi_H}{k} \tag{3.97}$$

with the following boundary conditions:

- The temperature at the wall is constant:

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$$T(r = R) = T_w \tag{3.98}$$

- The maximum temperature will be reached at the center ($r = 0$), therefore:

$$\frac{dT}{dr} = 0 \qquad at \ r = 0 \tag{3.99}$$

Note that Equation (3.97) can also be written as follows:

$$\frac{1}{r}\frac{d}{dr}(r\frac{dT}{dr}) = -\frac{\Phi_H}{k} \tag{3.100}$$

since $q_r = -k \ dT/dr$, this equation is equivalent to:

$$\frac{1}{r}\frac{d}{dr}(rq_r) = -\Phi_H \tag{3.101}$$

The left hand side is the rate of diffusion of heat per unit volume while the right hand side is the rate of heat production per unit volume.

3.6.5 Momentum Transport in a Circular Tube

We revisit example 2.2.2 where we derived the steady state equations for the laminar flow inside a horizontal circular tube. We will see how the model can be obtained using the momentum equation of change. We assume as previously that the fluid is incompressible and Newtonian. The momentum equations of change in cylindrical coordinates are given by Eqs. (3.79-3.81). A number of simplifications are used:

- The flow has only the direction z, i.e. $v_r = v_\theta = 0$.
- The flow is at steady state, $\frac{\partial v_z}{\partial t} = 0$

The momentum equation in cylindrical coordinates Eq. 3.81 is reduced to:

$$\rho v_z \frac{\partial v_z}{\partial z} = \mu \left(\frac{\partial^2 v_z}{\partial r^2} + \frac{1}{r}\frac{\partial v_z}{\partial r} + \frac{1}{r^2}\frac{\partial^2 v_z}{\partial \theta^2} + \frac{\partial^2 v_z}{\partial z^2} \right) - \frac{\partial P}{\partial z} + \rho g_z \tag{3.102}$$

Using the continuity equation (Eq. 3.76), and since $v_r = v_\theta = 0$ gives:

$$\frac{dv_z}{dz} = 0 \tag{3.103}$$

We also note that because the flow is symmetrical around the z-axis we have necessarily no variation of the velocity with θ, i.e.

$$\left(\frac{\partial^2 v_z}{\partial \theta^2} \right) = 0 \tag{3.104}$$

Equation 3.102 is then reduced to

$$\mu \left(\frac{d^2 v_z}{dr^2} + \frac{1}{r}\frac{dv_z}{dr} \right) = \frac{dP}{dz} \tag{3.105}$$

Since the left hand side depends only on r, this equation suggests that $\dfrac{dP}{dz}$ is constant.

Therefore:

$$\frac{dp}{dz} = \frac{\Delta P}{L} \tag{3.106}$$

where ΔP is the pressure drop across the tube. Equation 3.105 is equivalent to:

$$\mu \left(\frac{d^2 v_z}{dr^2} + \frac{1}{r}\frac{dv_z}{dr} \right) = \frac{\Delta P}{L} \tag{3.107}$$

with the following conditions identical to those in Example 2.2.2. Note also that Eq. 3.107 can also be written as:

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$$\mu \frac{d}{dr}(\frac{rv_z}{dr}) = \frac{\Delta P}{L}$$

<div align="right">(3.108)</div>

which is also equivalent to:

$$\frac{d(r\tau_{rz})}{rdr} = \frac{\Delta P}{L}$$

<div align="right">(3.109)</div>

where τ_{rz} is the shear stress. The left term is the rate of momentum diffusion per unit volume and the right hand side is in fact the rate of production of momentum (due to pressure drop). Note then the similarity between Eq. 3.109 for momentum transfer with Eq. 3.101 for heat transfer.

3.6.6 Unsteady state Heat Generation

We reconsider Example 3.6.4 but we are interested in the variations of the temperature of the reactor with time as well. This may be needed to compute the heat transferred during start-up or shut-down operations. Keeping the same assumptions as Example 3.3.4 (except the steady state assumption), the energy balance in cylindrical coordinates yields:

$$\rho Cp \frac{\partial T}{\partial t} = k \frac{1}{r} \frac{d}{dr}(r \frac{dT}{dr}) + \frac{\Phi_H}{k}$$

<div align="right">(3.110)</div>

with the initial and boundary conditions:

$$T(R,t) = T_w$$

<div align="right">(3.111)</div>

$$\frac{dT}{dr}\Big|_{r=0} = 0$$

<div align="right">(3.112)</div>

$$T(r,0) = T_w$$

<div align="right">(3.113)</div>

3.6.7 Laminar Flow Heat Transfer with Constant Wall Temperature

We consider a fluid flowing at constant velocity v_z into a horizontal cylindrical tube. The fluid enters with uniform temperature T_i. The wall is assumed at constant temperature T_w. We would like to model the variations of the fluid temperature inside the tube. To apply the energy equation of change (Eq. 3.78) we will assume that the fluid is incompressible, Newtonian and of constant thermal conductivity. Since the system is at steady state $d/dt = 0$ and the flow is one-dimensional $v_r = v_\theta = 0$, the energy equation in cylindrical coordinates Eq. 3.78 is reduced to:

$$\rho C p v_z \frac{\partial T}{\partial t} = k(\frac{\partial^2 T}{\partial r^2} + \frac{1}{r}\frac{\partial T}{\partial r} + \frac{1}{r^2}\frac{\partial^2 T}{\partial \theta^2} + \frac{\partial^2 T}{\partial z^2}) \qquad (3.114)$$
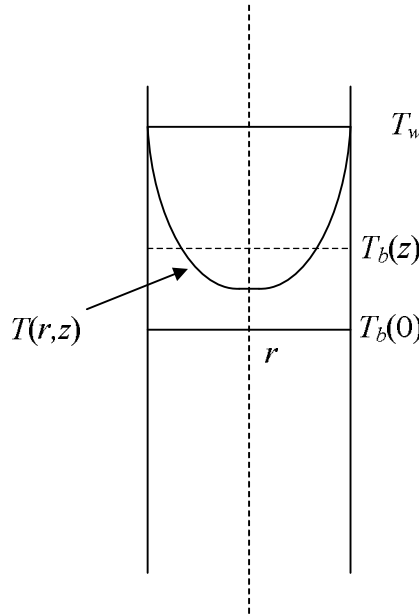

Figure 0-6 heat transfer with constant wall temperature

Since the temperature is symmetrical then $\frac{\partial T}{\partial \theta} = \frac{\partial^2 T}{\partial \theta^2} = 0$. In some cases we can neglect

the conduction term $\frac{\partial^2 T}{\partial z^2}$ compared to the convective term $v_z \frac{\partial T}{\partial z}$. The system is then

described by the following energy and momentum equations:

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$$\rho C p v_z \frac{\partial T}{\partial t} = k(\frac{\partial^2 T}{\partial r^2} + \frac{1}{r}\frac{\partial T}{\partial r})$$

(3.115)

$$\mu \frac{d}{dr}(\frac{rv_z}{dr}) = \frac{\Delta P}{L}$$

(3.116)

These two equations are therefore coupled by v_z, with the previous boundary conditions for v_z,

At $r = R$,	$v_z = 0$	(3.117)
At $r = 0$,	$dv_z/dr = 0$	(3.118)
At $z = 0$,	$T = T_i$	(3.119)
At $r = 0$,	$dT/dr = 0$	(3.120)
At $r = R$,	$T = T_w$	(3.121)

3.6.8 Laminar Flow and Mass Transfer

We consider the example of a fluid flowing through a horizontal pipe with constant velocity v_z. The pipe wall is made of a solute of constant concentration C_{Aw} that dissolved in the fluid. The concentration of the fluid at the entrance z = 0 is C_{Ao}. The regime is assumed laminar and at steady state. The fluid properties are assumed constant. We would like to model the variation of the concentration of A along the axis in the pipe. The component balance for A (Eq. 3.77) is:

$$v_r \frac{\partial C_A}{\partial r} + v_\theta \frac{\partial C_A}{\partial \theta} + v_z \frac{\partial C_A}{\partial z} = D_{AB}(\frac{\partial(r\frac{\partial C_A}{\partial r})}{r\partial r} + \frac{\partial^2 C_A}{r^3 \partial \theta^2} + \frac{\partial^2 C_A}{\partial z^2})$$

(3.122)

Since $v_r = v_\theta = 0$, the balance equation becomes:

$$v_z \frac{\partial C_A}{\partial z} = D_{AB}(\frac{\partial(r\frac{\partial C_A}{\partial r})}{r\partial r} + \frac{\partial^2 C_A}{\partial z^2})$$

(3.123)

If the diffusion term $\dfrac{\partial^2 C_A}{\partial z^2}$ in the z-direction is negligible compared to convection term

$v_z \dfrac{\partial C_A}{\partial z}$ then the last equation reduces to:

$$v_z \frac{\partial C_A}{\partial z} = D_{AB} \left[\frac{\partial (r \frac{\partial C_A}{\partial r})}{r \partial r} \right]$$

(3.124)

The equation (Eq. 3.116) is unchanged.

The two equations are coupled through v_z. The boundary conditions are analogous to the previous example:

At $r = R$,	$v_z = 0$	(3.125)
At $r = 0$,	$dv_z/dr = 0$	(3.126)
At $z = 0$,	$C_A = C_{Ao}$	(3.127)
At $r = 0$,	$dC_A/dr = 0$	(3.128)
At $r = R$,	$C_A = C_{Aw}$	(3.129)

Note the similarity between this example and the heat transfer case of the previous example.