CHAPTER 3

COMPUTATIONAL FLUID DYNAMICS AND NUMERICAL MODELING OF PROTON EXCHANGE MEMBRANCE FUEL CELL

3.1 Introduction of Fluid Mechanics

3.1.1 Fluid as a Continuum

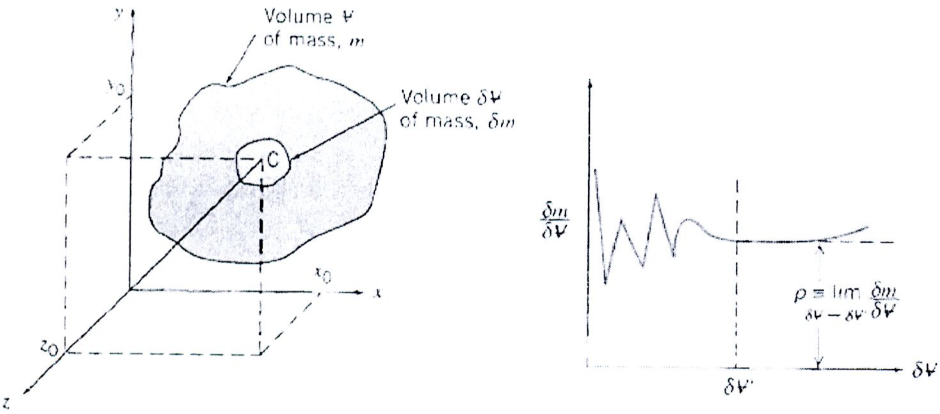
In our definition of a fluid, no mention was made of the molecular structure of matter. All fluids are composed of molecules in constant motion. However, in most engineering applications we are interested in the average or macroscopic effects of many molecules. It is these macroscopic effects that we ordinarily perceive and measure. We thus treat a fluid as an infinitely divisible substance, a continuum, and do not concern ourselves with the behavior of individual molecules.

The concept of a continuum is the basis of classical fluid mechanics. The continuum assumption is valid in treating the behavior of fluids under normal conditions. However, it breaks down whenever the mean free path of the molecules ! becomes the same order of magnitude as the smallest significant characteristic dimension of the problem. In problems such as rarefied gas flow (e.g., as encountered in flights into the upper reaches of the atmosphere), we must abandon the concept of a continuum in favor of the microscopic and statistical points of view.

As a consequence of the continuum assumption, each fluid property is assumed to have a definite value at every point in space. Thus fluid properties such as density, temperature, velocity, and so on, are considered to be continuous functions of position and time.

To illustrate the concept of a property at a point, consider the manner in which we determine the density at a point. A region of fluid is shown in figure 3.1. We are interested in determining the density at the point C, whose coordinates are x_o, y_o, and z_o Density is defined as mass per unit volume. Thus the mean density within volume V would be given by $\rho = m/V$. In general, this will not be equal to the value of the density at point C. To determine the density at point C, we must select a small volume, δV, surrounding point C and determine the ratio $\delta m/\delta V$. The question is, how small can we make the volume δV? Let us answer this question by plotting the ratio $\delta m/\delta V$, and allowing the volume to shrink continuously in size. Assuming that volume δV is initially relatively large (but still small compared with the volume, V) a typical plot of $\delta m/\delta V$ might appear as in figure 3.1b. In other words, δV must be sufficiently large to yield a meaningful, reproducible value for the density at a location and yet small enough to be able to resolve spatial variations in density. The average density tends to approach an asymptotic value as the volume is shrunk to enclose only homogeneous fluid in the immediate neighborhood of point C. When δV becomes so small that it contains only a small number of molecules, it becomes impossible to fix a definite value for $\delta m/\delta V$; the value will vary erratically as molecules cross into and out of the volume. Thus there is a lower limiting value of δV, designated $\delta V'$ in figure 3.1b, allowable for use in defining fluid density at a point.2 The density at a "point" is then defined as

$$\rho = \lim_{\delta v \to \delta V'} \frac{\delta m}{\delta V} \tag{3.1}$$



(a) (b)

Figure 3.1 Definition of density at a point

Since point C was arbitrary, the density at any point in the fluid could be determined in a like manner. If density determinations were made simultaneously at an infinite number of points in the fluid, we would obtain an expression for the density distribution as a function of the space coordinates, $\rho = \rho(x, y, z)$, at the given instant.

Clearly, the density at a point may vary with time as a result of work done on or by the fluid and/or heat transfer to the fluid. Thus the complete representation of density (the field representation) is given by

$$\rho = \rho(x, y, z, t) \tag{3.2}$$

Since density is a scalar quantity, requiring only the specification of a magnitude for a complete description, the field represented by equation 3.2 is a scalar field.

3.1.2 Velocity Field

In dealing with fluids in motion, we shall necessarily be concerned with the description of a velocity field. Refer again to figure 3.1a. Define the fluid velocity at point C as the instantaneous velocity of the center of gravity of the volume, $\delta V'$, instantaneously surrounding point C. If we define a fluid particle as a small mass of fluid of fixed identity of volume $\delta V'$, then the velocity at point C is defined as the instantaneous velocity of the fluid particle which, at a given instant, is passing though point C. The velocity at any point in the flow field is defined similarly. At a given instant the velocity field, $\vec{V}$, is a function of the space coordinates x, y, z. The velocity at any point in the flow field might vary from one instant to another. Thus the complete representation of velocity (the velocity field) is given by

$$\vec{V} = \vec{V}\,(x,\ y,\ z,\ t) \tag{3.3}$$

Velocity is a vector quantity, requiring a magnitude and direction for a complete description, so the velocity field is a vector field.

The velocity vector, ii, also can be written in terms of its three scalar components Denoting the components in the x, y, and z directions by u, v, and w, then

$$\vec{V} = \mathrm{u}\hat{i} + \mathrm{v}\hat{j} + \mathrm{w}\hat{k} \tag{3.4}$$

In general, each component, u, v, and w, will be a function of x, y, z, and t.

If properties at every point in a flow field do not change with time, the flow is termed steady. Stated mathematically, the definition of steady flow is

$$\frac{\partial \eta}{\partial t} = 0$$

where η represents any fluid property. For steady flow,

$$\frac{\partial \rho}{\partial t} = 0 \qquad \text{or} \qquad \rho = \rho\ (x,\ y,\ z,)$$

and

$$\frac{\partial \vec{V}}{\partial t} = 0 \qquad \text{or} \qquad \vec{V} = \vec{V}\ (x,\ y,\ z,)$$

Thus, in steady flow, any property may vary from point to point in the field, but all properties remain constant with time at every point.

3.1.3 One-Two-, and Three-Dimensional Flows

A flow is classified as one-, two-, or three-dimensional depending on the number of space coordinates required to specify the velocity field. Equation 3.3 indicates that the velocity field may be a function of three space coordinates and time. Such a flow field is termed three-dimensional (it is also unsteady) because the velocity at any point in the flow field depends on the three coordinates required to locate the point in space.

Although most flow fields are inherently three-dimensional, analysis based on fewer dimensions is frequently meaningful. Consider, for example, the steady flow through a long straight pipe of constant cross section. Far from the entrance to the pipe the velocity distribution may be described by

$$u = u_{max}\left[1-\left(\frac{r}{R}\right)\right]^2 \qquad (3.5)$$

This profile is shown in figure 3.2, where cylindrical coordinates r, θ, and x are used to locate any point in the flow field. The velocity field is a function of r only; it is independent of coordinates x and θ. Thus this is a one-dimensional flow.

An example of a two-dimensional flow is illustrated in figure 3.3; the velocity distribution is depicted for a flow between diverging straight walls that are imagined to be infinite in extent (in the z direction). Since the channel is considered to be infinite in the z direction, the velocity field will be identical in all planes perpendicular to the z axis. Consequently, the velocity field is a function only of space coordinates x and y; the flow field is classified as two-dimensional.

As you might suspect, the complexity of analysis increases considerably with the number of dimensions of the flow field. For many problems encountered in engineering, a one-dimensional analysis is adequate to provide approximate solutions of engineering accuracy.

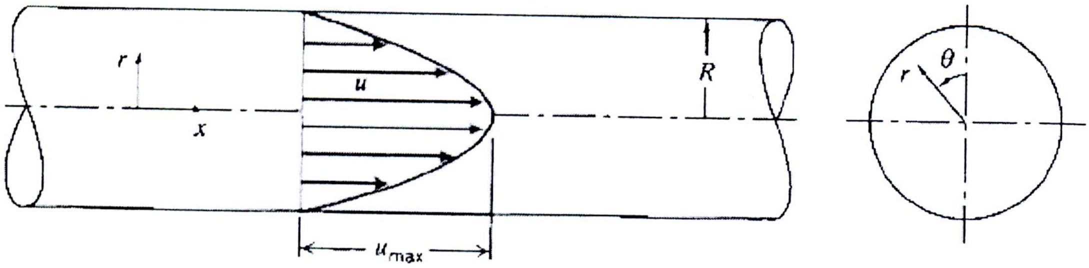


Figure 3.2 Example of one-dimensional flow.

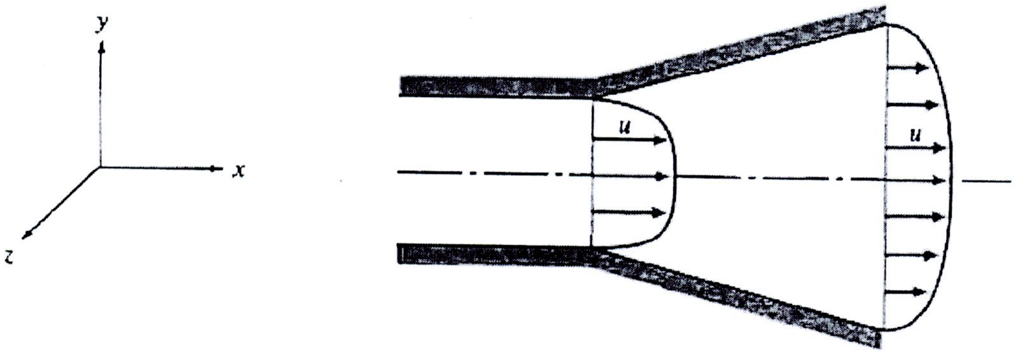


Figure 3.3 Example of two-dimensional flow.

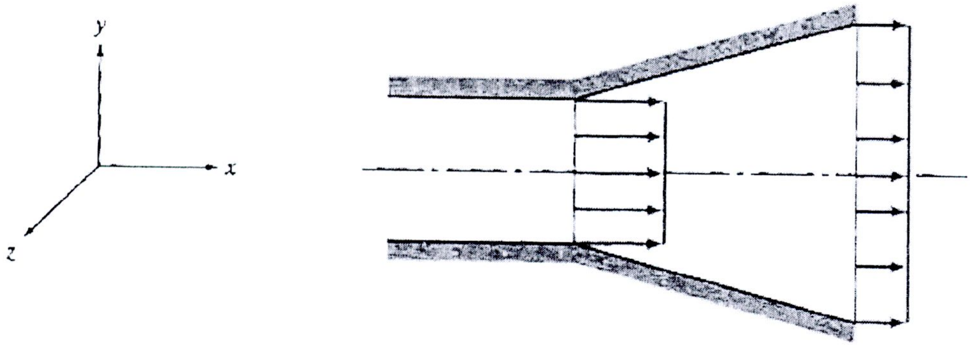


Figure 3.4 Example of uniform flow at a section.

Since all fluids satisfying the continuum assumption must have zero relative velocity at a solid surface (to satisfy the no-slip condition), most flows are inherently two or three-dimensional. For purposes of analysis it often is convenient to introduce the notion of uniform flow at a given cross section. In a flow that is uniform at a given cross section, the velocity is constant across any section normal to the flow. Under this assumption, the two-dimensional flow of figure 3.3 is modeled as the flow shown in figure 3.4. In the flow of figure 3.4, the velocity field is a function of x alone, and thus the flow model is one-dimensional. (Other properties, such as density or pressure, also may be assumed uniform at a section, if appropriate.)

The term uniform flow field (as opposed to uniform flow at a cross section) is used to describe a flow in which the magnitude and direction of the velocity vector are constant, i.e., independent of all space coordinates, throughout the entire flow field.

3.1.4 Laminar and Turbulent Flows

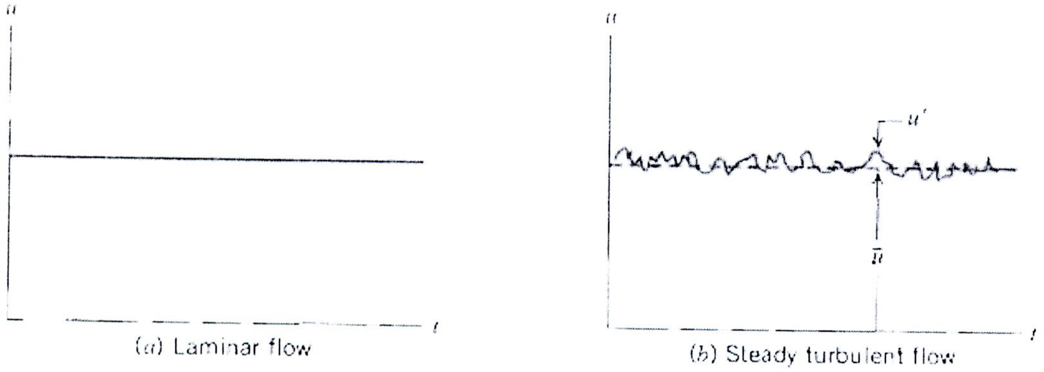
Viscous flow regimes are classified as laminar or turbulent on the basis of flow structure. In the laminar regime, flow structure is characterized by smooth motion in laminar, or layers. Flow structure in the turbulent regime is characterized by random, three-dimensional motions of fluid particles in addition to the mean motion.

In laminar flow there is no macroscopic mixing of adjacent fluid layers. A thin filament of dye injected into a laminar flow appears as a single line; there is no dispersion of dye throughout the flow, except the slow diffusion due to molecular motion. On the other hand, a dye filament injected into a turbulent flow disperses quickly throughout the flow field; the line of dye breaks up into myriad entangled threads of dye. This behavior of turbulent flow is caused by the velocity fluctuations present; the macroscopic mixing of fluid particles from adjacent layers of fluid results in rapid dispersion of the dye. The straight filament of smoke rising from a cigarette in still surroundings gives a clear picture of laminar flow. As the smoke continues to rise, it breaks up into random, haphazard motions; this is an example of turbulent flow.

One can obtain a more quantitative picture of the difference between laminar and turbulent flow by examining the output from a sensitive velocity-measuring device immersed in the flow. If one measures the x component of velocity at a fixed location in a pipe for both laminar and turbulent steady flow, the traces of velocity versus time appear as shown in figure 3.5. For steady laminar flow, the velocity at a point remains constant with time. In turbulent flow the velocity trace indicates random fluctuations of the instantaneous velocity, u, about the time mean velocity, $\bar{u}$. We can consider the instantaneous velocity, u, as the sum of the time mean velocity, $\bar{u}$, and the fluctuating component, u',

$$u = \bar{u} + u' \tag{3.6}$$

Because the flow is steady, the mean velocity, u, does not vary with time



(a) Laminar flow

(b) Steady turbulent flow

Figure 3.5 Variation of axial velocity with time.

Although many turbulent flows of interest are steady in the mean (u is not a function of time), the presence of the random, high-frequency velocity fluctuations makes the analysis of turbulent flows extremely difficult. In a one-dimensional laminar flow, the shear stress is related to the velocity gradient by the simple relation

$$\tau_{yx} = \mu \frac{du}{dy} \tag{3.7}$$

For a turbulent flow in which the mean velocity field is one-dimensional, no such simple relation is valid. Random, three-dimensional velocity fluctuations (u', v', and w') transport momentum across the mean flow streamlines, increasing the effective shear stress. Consequently, in turbulent flow there is no universal relationship between the stress field and the mean velocity field. Thus in turbulent flows we must rely heavily on semi-empirical theories and on experimental data.

3.1.5 Reynolds Number

In fluid mechanics, the Reynolds number Re is a dimensionless number that gives a measure of the ratio of inertial forces to viscous forces and consequently quantifies the relative importance of these two types of forces for given flow conditions. Reynolds numbers frequently arise when performing dimensional analysis of fluid dynamics problems, and as such can be used to determine dynamic similitude between different experimental cases. They are also used to characterize different flow regimes, such as laminar or turbulent flow: laminar flow occurs at low Reynolds numbers, where viscous forces are dominant, and is characterized by smooth, constant fluid motion; turbulent flow occurs at high Reynolds numbers and is dominated by inertial forces, which tend to produce chaotic eddies, vortices and other flow instabilities.

Reynolds number can be defined for a number of different situations where a fluid is in relative motion to a surface (the definition of the Reynolds number is not to be confused with the Reynolds Equation or lubrication equation). These definitions generally include the fluid properties of density and viscosity, plus a velocity and a characteristic length or characteristic dimension. This dimension is a matter of convention – for example a radius or diameters are equally valid for spheres or circles, but one is chosen by convention. For aircraft or ships, the length or width can be used. For flow in a pipe or a sphere moving in a fluid the internal diameter is generally used today. Other shapes (such as rectangular pipes or non-spherical objects) have an equivalent diameter defined. For fluids of variable density (e.g. compressible gases) or variable viscosity (non-Newtonian fluids) special rules apply. The velocity may also be a matter of convention in some circumstances, notably stirred vessels.

$$R_e = \frac{\rho V L}{\mu} = \frac{V L}{\nu} \tag{3.7}$$

where V is the mean velocity of the object relative to the fluid (SI units: m/s)
L is a characteristic linear dimension, (travelled length of the fluid; hydraulic diameter when dealing with river systems) (m)
ρ is the density of the fluid (kg/m³)
μ is the dynamic viscosity of the fluid (Pa•s or N•s/m² or kg/(m•s))
ν is the kinematic viscosity ($\nu = \mu / \rho$) (m²/s)

For flow in a pipe or tube, the Reynolds number is generally defined as:

$$R_e = \frac{\rho V D_H}{\mu} = \frac{V D_H}{\nu} = \frac{Q D_H}{\nu A} \tag{3.8}$$

where D_H is the hydraulic diameter of the pipe (m).
Q is the volumetric flow rate (m^3/s)
A is the pipe cross-sectional area (m²).

For shapes such as squares, rectangular or annular ducts (where the height and width are comparable) the characteristic dimension for internal flow situations is taken to be the hydraulic diameter, DH, defined as 4 times the cross-sectional area (of the fluid), divided by the wetted perimeter. The wetted perimeter for a channel is the total perimeter of all channel walls that are in contact with the flow. This means the length of the water exposed to air is NOT included in the wetted perimeter

$$D_H = \frac{4A}{P} \tag{3.9}$$

For a circular pipe, the hydraulic diameter is exactly equal to the inside pipe diameter, as can be shown mathematically.

In boundary layer flow over a flat plate, experiments can confirm that, after a certain length of flow, a laminar boundary layer will become unstable and become turbulent. This instability occurs across different scales and with different fluids, usually when, where *x* is the distance from the leading edge of the flat plate, and the flow velocity is the freestream velocity of the fluid outside the boundary layer. For flow in a pipe of diameter D, experimental observations show that for fully developed flow, laminar flow occurs when $R_e < 2300$ and turbulent flow occurs when $R_e > 4000$. In the interval between 2300 and 4000, laminar and turbulent flows are possible 'transition flows, depending on other factors, such as pipe roughness and flow uniformity. This result is generalized to non-circular channels using the hydraulic diameter, allowing a transition Reynolds number to be calculated for other shapes of channel. These transitions Reynolds numbers are also called critical Reynolds numbers. Pressure drops seen for fully developed flow of fluids through pipes can be predicted using the Moody diagram (in figure 3.6) which plots the Darcy–Weisbach friction factor f against Reynolds number R_e and relative roughness $\varepsilon\ /\ D$. The diagram clearly shows the laminar, transition, and turbulent flow regimes as Reynolds number increases. The nature of pipe flow is strongly dependent on whether the flow is laminar or turbulent

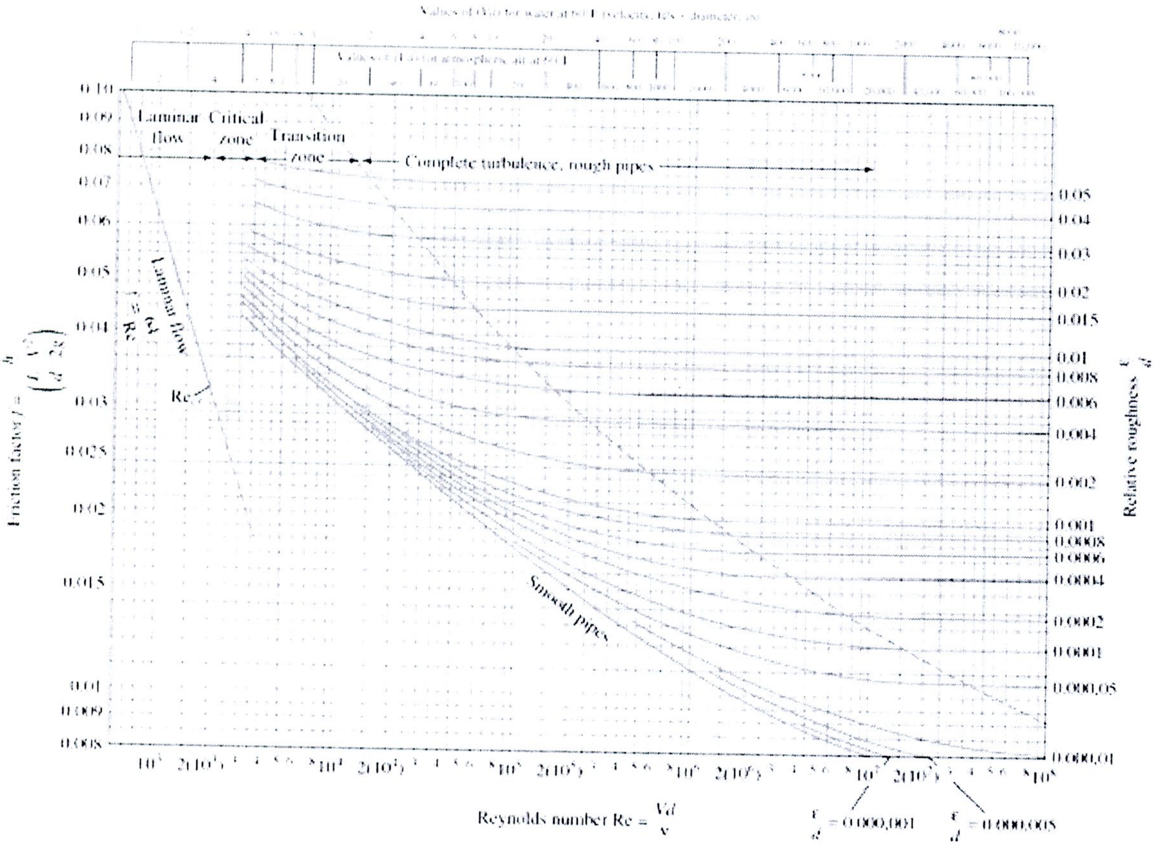


Figure 3.6 moody diagram (Fox & McDonald, 1998)

3.1.6 Bernoulli Equation and Darcy's Equation

Bernoulli's principle can be applied to various types of fluid flow, resulting in what is loosely denoted as Bernoulli's equation. In fact, there are different forms of the Bernoulli equation for different types of flow. The simple form of Bernoulli's principle is valid for incompressible flows (e.g. most liquid flows) and also for compressible flows (e.g. gases) moving at low Mach numbers. More advanced forms may in some cases be applied to compressible flows at higher Mach numbers (see the derivations of the Bernoulli equation). Bernoulli's principle can be derived from the principle of conservation of energy. This states that, in a steady flow, the sum of all forms of mechanical energy in a fluid along a streamline is the same at all points on that streamline. This requires that the sum of kinetic energy and potential energy remain constant. Thus an increase in the speed of the fluid occurs proportionately with an increase in both its dynamic pressure and kinetic energy, and a decrease in its static pressure and potential energy. If the fluid is flowing out of a reservoir the sum of all forms of energy is the same on all streamlines because in a reservoir the energy per unit volume (the sum of pressure and gravitational potential ρ g h) is the same everywhere. Equation of Bernoulli is generally defined as:

$$\frac{P_1}{\rho g} + Z_1 + \frac{V_1^2}{2g} - h_L = \frac{P_2}{\rho g} + Z_2 + \frac{V_2^2}{2g} \tag{3.10}$$

where Z is level at point i (m).
h_L is head loss (m)

Darcy's equation can be applied to flow of liquid through a pipe is resisted by viscous shear stresses within the liquid and the turbulence that occurs along the internal walls of the pipe, created by the roughness of the pipe material. This resistance is usually known as pipe friction and is measured is feet or meters head of the fluid, thus the term head loss is also used to express the resistance to flow. The flow of liquid through a pipe is resisted by viscous shear stresses within the liquid and the turbulence that occurs along the internal walls of the pipe, created by the roughness of the pipe material. This resistance is usually known as pipe friction and is measured is feet or meters head of the fluid, thus the term head loss is also used to express the resistance to flow. Head loss can be divided in major loss and minor loss.

Major loss due to friction and it can be calculated with

$$(h_L)_{major} = f\frac{LV^2}{2gD_H} \tag{3.11}$$

Where $(h_L)_{major}$ is major head loss due to friction (m)
L is the length of the pipe (m)
D_H is the hydraulic diameter of the pipe (m)
V is the average velocity of the fluid flow (m/s)
f is a dimensionless coefficient called the Darcy friction factor

Which friction factor formula may be applicable depends upon the type of flow that exists:

- Laminar flow
- Transition between laminar and turbulent flow
- Fully turbulent flow in smooth conduits
- Fully turbulent flow in rough conduits
- Free surface flow.

Laminar flow

The Darcy friction factor for laminar flow (Reynolds number less than 2000) is given by the following formula:

$$f = \frac{64}{R_e} \qquad (3.12)$$

Where f is the Darcy friction factor
R_e is the Reynolds number.

Transition flow

Transition (neither fully laminar nor fully turbulent) flow occurs in the range of Reynolds numbers between 2300 and 4000. The value of the Darcy friction factor may be subject to large uncertainties in this flow regime.

Turbulent flow in smooth conduits

Empirical correlations exist for this flow regime. Such correlations are included in the ASHRAE Handbook of Fundamentals.

Turbulent flow in rough conduits

The Darcy friction factor for fully turbulent flow (Reynolds number greater than 4000) in rough conduits is given by the Colebrook equation.

Free surface flow

The last formula in the Colebrook equation section of this article is for free surface flow. The approximations elsewhere in this article are not applicable for this type of flow.

Minor loss due to change of velocity in bends, valves and similar and it can be calculated with

$$(h_L)_{\min or} = K\frac{V^2}{2g} \qquad (3.13)$$

Where $(h_L)_{\text{minor}}$ is minor head loss due to friction (m)
K is coefficient in head loss, $K = f_t\frac{L_e}{D_H}$

f_t can be find in Moody diagram and L_e is Equivalent Length.

3.2 Conservation Laws of Fluid Motion and Boundary Conditions

The mathematical basis can be develop for a comprehensive general purpose model of fluid flow and heat transfer from the basic principles of conservation of mass, momentum and energy. This leads to the governing equations of fluid flow and a discussion of the necessary auxiliary conditions -initial and boundary conditions.

The governing equations of fluid flow represent mathematical statements of the conservation laws of physics. The fluid will be regarded as a continuum. For the analysis of fluid flows at macroscopic length scales (say 1 μm and larger) the molecular structure of matter and molecular motions may be ignored. We describe the behavior of the fluid in terms of macroscopic properties, such as velocity, pressure, density and temperature, and their space and time derivatives. These may be thought of as averages over suitably large numbers of molecules. A fluid particle or point in a fluid is then the smallest possible element of fluid whose macroscopic properties are not influenced by individual molecules.

3.2.1 Mass Conservation

The first step in the derivation of the mass conservation equation is to write down a mass balance for the fluid element.

Rate of increase of mass in fluid element = Net rate of flow of mass into fluid element

The rate of increase of mass in the fluid element is

$$\frac{\partial}{\partial t}(\rho \delta x \, \delta y \, \delta z) = \frac{\partial \rho}{\partial t} \delta x \, \delta y \, \delta z \qquad (3.14)$$

Next we need to account for the mass flow rate across a face of the element which is given by the product of density, area and the velocity component normal to the face. From Figure 2.2 it can be seen that the net rate of flow of mass into the element across its boundaries is given by

$$\left(\rho u - \frac{\partial(\rho u)}{\partial x}\frac{1}{2}\delta x\right)\delta y \, \delta z - \left(\rho u + \frac{\partial(\rho u)}{\partial x}\frac{1}{2}\delta x\right)\delta y \, \delta z +$$
$$\left(\rho v - \frac{\partial(\rho v)}{\partial y}\frac{1}{2}\delta y\right)\delta x \, \delta z - \left(\rho v + \frac{\partial(\rho v)}{\partial y}\frac{1}{2}\delta y\right)\delta x \, \delta z +$$
$$\left(\rho w - \frac{\partial(\rho w)}{\partial z}\frac{1}{2}\delta z\right)\delta x \, \delta y - \left(\rho w + \frac{\partial(\rho w)}{\partial z}\frac{1}{2}\delta z\right)\delta x \, \delta y$$

Flows which are directed into the element produce an increase of mass in the element and get a positive sign and those flows that are leaving the element are given a negative sign.

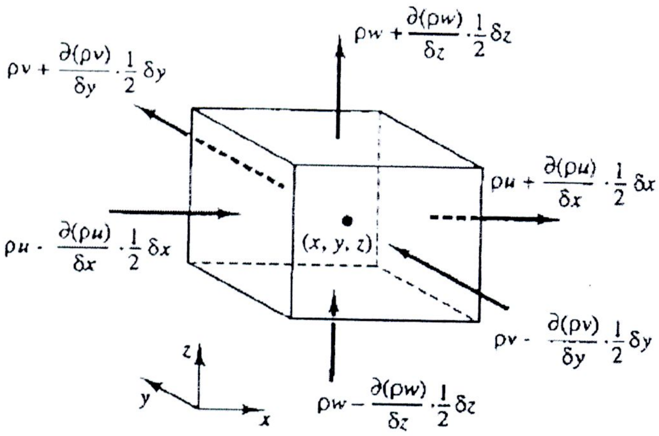


Figure 3.7 Mass flows in and out of fluid element

The rate of increase of mass inside the element is now equated to the net rate of flow of mass into the element across its faces. All terms of the resulting mass balance are arranged on the left hand side of the equals sign and the expression is divided by the element volume $\delta x \delta y \delta z$

This yields

$$\frac{\partial \rho}{\partial t} + \left[\frac{\partial(\rho u)}{\partial x} + \frac{\partial(\rho v)}{\partial y} + \frac{\partial(\rho w)}{\partial z} \right] = 0 \qquad (3.15)$$

or in more compact vector notation

$$\frac{\partial \rho}{\partial t} + \nabla.\left(\rho \vec{V}\right) = 0 \qquad (3.16)$$

When $\vec{V} = u\hat{i} + v\hat{j} + w\hat{k}$

Equation 3.12 is the unsteady, three-dimensional mass conservation or continuity equation at a point in a compressible fluid. The first term on the left hand side is the rate of change in time of the density (mass per unit volume). The second term describes the net flow of mass out of the element across its boundaries and is called the convective term.

$$\nabla\left(\vec{V}\right) = 0 \qquad (3.17)$$

or in longhand notation

$$\left[\frac{\partial u}{\partial x}+\frac{\partial v}{\partial y}+\frac{\partial w}{\partial z}\right]=0 \tag{3.18}$$

3.2.2 Momentum Conservation

Newton's second law states that the rate of change of momentum of a fluid particle equals the sum of the forces on the particle.

Rate of increase of momentum of fluid particle = Sum of forces on fluid particle

The rates of increase of x-, y- and z-momentum per unit volume of a fluid particle are given by $\rho\frac{\partial u}{\partial t}$, $\rho\frac{\partial v}{\partial t}$, $\rho\frac{\partial w}{\partial t}$

We distinguish two types of forces on fluid particles:

• surface forces	- pressure forces
	- viscous forces
• body forces	- gravity force
	- centrifugal force
	- Coriolis force
	- electromagnetic force

It is common practice to highlight the contributions due to the surface forces as separate terms in the momentum equation and to include the effects of body forces as source terms.

The state of stress of a fluid element is defined in terms of the pressure and the nine viscous stress components shown in figure 3.8. The pressure, a normal stress, is denoted by *p*. Viscous stresses are denoted by τ. The usual suffix notation τ_{ij} is applied to indicate the direction of the viscous stresses. The suffices *i* and *j* in τ_{ij} indicate that the stress component acts in the *j*-direction on a surface normal to the *i*-direction.

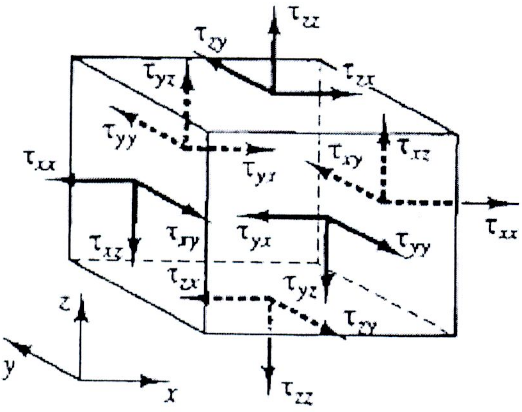


Figure 3.8 Stress components on three faces of fluid element

First we consider the x-components of the forces due to pressure and stress components τ_{xx} τ_{yx} and τ_{zx} shown in figure 3.9. The magnitude of a force resulting from a surface stress is the product of stress and area. Forces aligned with the direction of a co-ordinate axis get a positive sign and those in the opposite direction a negative sign. The net force in the x-direction is the sum of the force components acting in that direction on the fluid element.

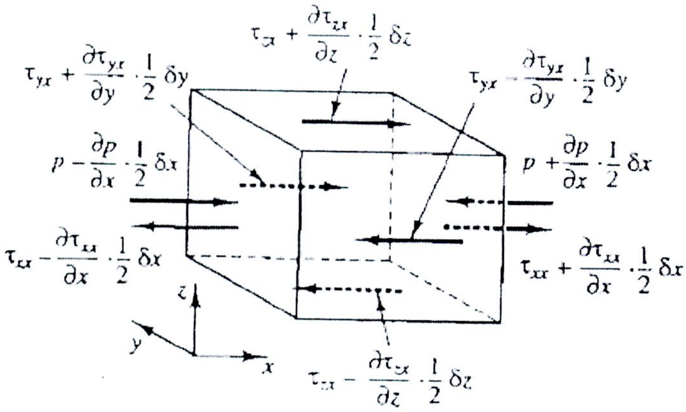


Figure 3.9 Stress components in the x-direction

On the pair of faces (E, W) we have

$$\left[\left(p - \frac{\partial p}{\partial x}\frac{1}{2}\delta x\right) - \left(\tau_{xx} - \frac{\partial \tau_{xx}}{\partial x}\frac{1}{2}\delta x\right)\right]\delta y\,\delta z \;+$$
$$\left[-\left(p + \frac{\partial p}{\partial x}\frac{1}{2}\delta x\right) + \left(\tau_{xx} + \frac{\partial \tau_{xx}}{\partial x}\frac{1}{2}\delta x\right)\right]\delta y\,\delta z = \left(-\frac{\partial p}{\partial x} + \frac{\partial \tau_{xx}}{\partial x}\right)\delta x\,\delta y\,\delta z \tag{3.19}$$

The net force in the x-direction on the pair of faces (N, S) is

$$-\left(\tau_{yx} - \frac{\partial \tau_{yx}}{\partial y}\frac{1}{2}\delta y\right)\delta x\,\delta z + \left(\tau_{yx} + \frac{\partial \tau_{yx}}{\partial y}\frac{1}{2}\delta y\right)\delta x\,\delta z = \frac{\partial \tau_{yx}}{\partial y}\delta x\,\delta y\,\delta z \tag{3.20}$$

Finally the net force in the x-direction on faces T and B is given by

$$-\left(\tau_{zx} - \frac{\partial \tau_{zx}}{\partial z}\frac{1}{2}\delta z\right)\delta x\,\delta y + \left(\tau_{zx} + \frac{\partial \tau_{zx}}{\partial z}\frac{1}{2}\delta z\right)\delta x\,\delta y = \frac{\partial \tau_{zx}}{\partial z}\delta x\,\delta y\,\delta z \tag{3.21}$$

The total force per unit volume on the fluid due to these surface stresses is equal the sum equations 3.19, 3.20, 3.21 divided by the volume

$$\frac{\partial(-p+\tau_{xx})}{\partial x}+\frac{\partial \tau_{yx}}{\partial y}+\frac{\partial \tau_{zx}}{\partial z} \qquad (3.22)$$

Without considering the body forces in further detail their overall effect can be included by defining a source S_{Mx} of x-momentum per unit volume per unit time.

The x-component of the momentum equation is found by setting the rate to change of x-momentum of the fluid particle equal to the total force in the x-direction on the element due to surface stresses plus the rate of increase of x-, y-, z-momentum due to sources

$$\begin{aligned}
&\text{x- axis} \qquad \frac{\partial(\rho u)}{\partial t}=-\frac{\partial p}{\partial x}+\frac{\partial \tau_{xx}}{\partial x}+\frac{\partial \tau_{yx}}{\partial y}+\frac{\partial \tau_{zx}}{\partial z}+S_{Mx}\\
&\text{y- axis} \qquad \frac{\partial(\rho v)}{\partial t}=-\frac{\partial p}{\partial y}+\frac{\partial \tau_{xy}}{\partial x}+\frac{\partial \tau_{yy}}{\partial y}+\frac{\partial \tau_{zy}}{\partial z}+S_{My} \qquad (3.23)\\
&\text{z- axis} \qquad \frac{\partial(\rho w)}{\partial t}=-\frac{\partial p}{\partial z}+\frac{\partial \tau_{xz}}{\partial x}+\frac{\partial \tau_{yz}}{\partial y}+\frac{\partial \tau_{zz}}{\partial z}+S_{Mz}
\end{aligned}$$

The sign associated with the pressure is opposite to that associated with the normal viscous stress, because the usual sign convention takes a tensile stress to be the positive normal stress so that the pressure, which is by definition a compressive normal stress, has a minus sign.

The effects of surface stresses are accounted for explicitly; the source terms S_{Mx}, S_{My} and S_{Mz} in equation 3.23 include contributions due to body forces only. For example, the body force due to gravity would be modeled by $S_{Mx} = 0$, $S_{My} = 0$ and $S_{Mz} = -\rho g$.

3.2.3 Energy Conservation

The energy equation is derived from the first law of thermodynamics which states that the rate of change of energy of a fluid particle is equal to the rate of heat addition to the fluid particle plus the rate of work done on the particle.

Rate of increase of energy of fluid particle = [Net rate of heat added to fluid particle +
Net rate of work done on fluid particle]

As before we will be deriving an equation for the rate of increase of energy of a fluid particle per unit volume which is given by $\rho\frac{DE}{Dt}$

The rate of work done on the fluid particle in the element by a surface force is equal to the product of the force and velocity component in the direction of the force. For example, the forces given by equation 3.19-3.21 all act in the x-direction. The work done by these forces is given by

$$\left[\left(pu-\frac{\partial(pu)}{\partial x}\frac{1}{2}\delta x\right)-\left(\tau_{xx}u-\frac{\partial(\tau_{xx}u)}{\partial x}\frac{1}{2}\delta x\right)-\left(pu+\frac{\partial(pu)}{\partial x}\frac{1}{2}\delta x\right)+\left(\tau_{xx}u+\frac{\partial(\tau_{xx}u)}{\partial x}\frac{1}{2}\delta x\right)\right]\delta y\delta z+$$

$$\left[-\left(\tau_{yx}u-\frac{\partial(\tau_{yx}u)}{\partial y}\frac{1}{2}\delta y\right)+\left(\tau_{yx}u+\frac{\partial(\tau_{yx}u)}{\partial y}\frac{1}{2}\delta y\right)\right]\delta x\delta z+$$

$$\left[-\left(\tau_{zx}u-\frac{\partial(\tau_{zx}u)}{\partial z}\frac{1}{2}\delta z\right)+\left(\tau_{zx}u+\frac{\partial(\tau_{zx}u)}{\partial z}\frac{1}{2}\delta z\right)\right]\delta x\delta y$$

The net rate of work done by these surface forces acting in the *x*-, *y*-, *z*-direction is given by

$$\text{x-axis}\quad\left[\frac{\partial[u(-p+\tau_{xx})]}{\partial x}+\frac{\partial(u\tau_{yx})}{\partial y}+\frac{\partial(u\tau_{zx})}{\partial z}\right]\delta x\,\delta y\,\delta z$$

$$\text{y-axis}\quad\left[\frac{\partial(v\tau_{xy})}{\partial x}+\frac{\partial[v(-p+\tau_{yy})]}{\partial y}+\frac{\partial(v\tau_{zy})}{\partial z}\right]\delta x\,\delta y\,\delta z \qquad (3.24)$$

$$\text{z-axis}\quad\left[\frac{\partial(w\tau_{xz})}{\partial x}+\frac{\partial(w\tau_{yz})}{\partial y}+\frac{\partial[w(-p+\tau_{zz})]}{\partial z}\right]\delta x\,\delta y\,\delta z$$

The total rate of work done per unit volume on the fluid particle by all the surface forces is given by the sum of equation 3.24 divided by the volume $\delta x\delta y\delta z$. The term containing pressure can be collected together and written more compactly in vector form

$$-\frac{\partial(up)}{\partial x}-\frac{\partial(vp)}{\partial y}-\frac{\partial(wp)}{\partial z}=-\nabla\cdot\left(p\vec{V}\right) \qquad (3.25)$$

This yields the following total rate of work done on the fluid particle by surface stresses:

$$\left[-\nabla\cdot\left(p\vec{V}\right)\right]+\left[\begin{array}{l}\frac{\partial(u\tau_{xx})}{\partial x}+\frac{\partial(u\tau_{yx})}{\partial y}+\frac{\partial(u\tau_{zx})}{\partial z}+\frac{\partial(v\tau_{xy})}{\partial x}+\frac{\partial(v\tau_{yy})}{\partial y}+\frac{\partial(v\tau_{zy})}{\partial z}\\ +\frac{\partial(w\tau_{xz})}{\partial x}+\frac{\partial(w\tau_{yz})}{\partial y}+\frac{\partial(w\tau_{zz})}{\partial z}\end{array}\right] \qquad (3.26)$$

Energy flux due to heat conduction vector *q* has three component q_x, q_y, q_z. Fourier's law of heat conduction relates the heat flux to the local temperature gradient. So

$$
\begin{aligned}
&\text{x-axis} \qquad && q_x = -k\frac{\partial T}{\partial x} \\
&\text{y-axis} && q_y = -k\frac{\partial T}{\partial y} \qquad\qquad (3.27)\\
&\text{z-axis} && q_z = -k\frac{\partial T}{\partial z}
\end{aligned}
$$

Thus far we have not defined the specific energy E of a fluid. Often the energy of a fluid is defined as the sum of internal (thermal) energy e, kinetic energy $\frac{1}{2}(u^2 + y^2 + w^2)$ and gravitational potential energy. This definition takes the view that the fluid element is storing gravitational potential energy. It is also possible to regard the gravitational force as a body force which does work on the fluid element as it moves through the gravity field.

Here we shall take the latter view and include the effects of potential energy changes as a source term. As before we define a source of energy S_E per unit volume per unit time. Conservation of energy of the fluid particle is ensured by equating the rate of change of energy of the fluid particle to the sum of the net rate of work done on the fluid particle and the net rate of heat addition to the fluid and the rate of increase of energy due to sources. The energy equation is

$$
\begin{aligned}
\rho\frac{DE}{Dt} = -\nabla\cdot\left(p\vec{V}\right) - \left[\frac{\partial}{\partial x}\left(k\frac{\partial T}{\partial x}\right) + \frac{\partial}{\partial y}\left(k\frac{\partial T}{\partial y}\right) + \frac{\partial}{\partial z}\left(k\frac{\partial T}{\partial z}\right)\right] + \\
\left[\begin{array}{l}
+\dfrac{\partial(u\tau_{xx})}{\partial x} + \dfrac{\partial(u\tau_{yx})}{\partial y} + \dfrac{\partial(u\tau_{zx})}{\partial z} + \dfrac{\partial(v\tau_{xy})}{\partial x} + \dfrac{\partial(v\tau_{yy})}{\partial y} + \dfrac{\partial(v\tau_{zy})}{\partial z} + \\
\dfrac{\partial(w\tau_{xz})}{\partial x} + \dfrac{\partial(w\tau_{yz})}{\partial y} + \dfrac{\partial(w\tau_{zz})}{\partial z} + S_E
\end{array}\right] \qquad (3.28)
\end{aligned}
$$

In equation 3.24 we have $E = e + \frac{1}{2}(u^2 + v^2 + w^2)$

Although equation 3.28 is a perfectly adequate energy equation it is common practice to extract the changes of the (mechanical) kinetic energy to obtain an equation for internal energy or temperature. The part of the energy equation attributable to the kinetic energy can be found by multiplying the x-momentum by velocity component u, the y-momentum by v and the z-momentum by w from equation 3.19 and adding the results together. It can be shown that this yields the following conservation equation for the kinetic energy

$$\rho \frac{D\left(e+\frac{\vec{V}^2}{2}\right)}{Dt} = -\nabla\cdot\left(p\vec{V}\right) - \left[\frac{\partial}{\partial x}\left(k\frac{\partial T}{\partial x}\right) + \frac{\partial}{\partial y}\left(k\frac{\partial T}{\partial y}\right) + \frac{\partial}{\partial z}\left(k\frac{\partial T}{\partial z}\right)\right] + \left[+\frac{\partial(u\tau_{xx})}{\partial x} + \frac{\partial(u\tau_{yx})}{\partial y} + \frac{\partial(u\tau_{zx})}{\partial z} + \frac{\partial(v\tau_{xy})}{\partial x} + \frac{\partial(v\tau_{yy})}{\partial y} + \frac{\partial(v\tau_{zy})}{\partial z} + \frac{\partial(w\tau_{xz})}{\partial x} + \frac{\partial(w\tau_{yz})}{\partial y} + \frac{\partial(w\tau_{zz})}{\partial z}\right] + \left(\nabla\cdot\vec{V}\right)S_M \tag{3.29}$$

3.2.4 Navier-Stokes Equation

The governing equations contain as further unknowns the viscous stress components. The most useful forms of the conservation equations for fluid flows are obtained by introducing a suitable model for the viscous stresses. In many fluid flows the viscous stresses can be expressed as functions of the local deformation rate (or strain rate). In three-dimensional flows the local rate of deformation is composed of the linear deformation rate and the volumetric deformation rate.

All gases and many liquids are isotropic. Liquids which contain significant quantities of polymer molecules may exhibit anisotropic or directional viscous stress properties as a result of the alignment of the chain-like polymer molecules with the flow. Such fluids are beyond the scope of this introductory course and we shall continue the development by assuming that the fluids are isotropic.

The rate of linear deformation of a fluid element has nine components in three dimensions, six of which are independent in isotropic fluids. They are denoted by the symbol e_{ij}. The suffix system is identical to that for stress component. There are three linear elongating deformation components: $e_{xx} = \frac{\partial u}{\partial x}$, $e_{yy} = \frac{\partial v}{\partial y}$, $e_{zz} = \frac{\partial w}{\partial z}$

There are also six shearing linear deformation components:

$$\begin{aligned} &\text{x-axis} \qquad e_{xy} = e_{yx} = \frac{1}{2}\left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x}\right) \\ &\text{y-axis} \qquad e_{xz} = e_{zx} = \frac{1}{2}\left(\frac{\partial u}{\partial z} + \frac{\partial w}{\partial x}\right) \\ &\text{z-axis} \qquad e_{yz} = e_{zy} = \frac{1}{2}\left(\frac{\partial v}{\partial z} + \frac{\partial w}{\partial y}\right) \end{aligned} \tag{3.30}$$

The volumetric deformation is given by

$$\left[\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z}\right] = \nabla\cdot\vec{V} \tag{3.31}$$

In a Newtonian fluid the viscous stresses are proportional to the rates of deformation. The three-dimensional form of Newton's law of viscosity for compressible flows involves two constants of proportionality: the (first) dynamic viscosity, to relate stresses to linear deformations, and the second viscosity, to relate stresses to the volumetric deformation. The nine viscous stress components, 9f which six are independent, are

$$\begin{aligned}
&\text{x-axis} && \tau_{xx} = 2\mu\frac{\partial u}{\partial x} + \lambda\left(\nabla\cdot\vec{V}\right) \\
&\text{y-axis} && \tau_{yy} = 2\mu\frac{\partial v}{\partial y} + \lambda\left(\nabla\cdot\vec{V}\right) \\
&\text{z-axis} && \tau_{zz} = 2\mu\frac{\partial w}{\partial z} + \lambda\left(\nabla\cdot\vec{V}\right) \\
& && \tau_{xy} = \tau_{yx} = \mu\left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x}\right) \\
& && \tau_{xz} = \tau_{zx} = \mu\left(\frac{\partial u}{\partial z} + \frac{\partial w}{\partial x}\right) \\
& && \tau_{yz} = \tau_{zy} = \mu\left(\frac{\partial v}{\partial z} + \frac{\partial w}{\partial y}\right)
\end{aligned} \tag{3.32}$$

Not much is known about the second viscosity, because its effect is small in practice. For gases a good working approximation can be obtained by taking the value $\lambda = -\frac{2}{3}\mu$. Liquids are incompressible so the mass conservation equation is $\nabla\left(\vec{V}\right) = 0$ and the viscous stresses are just twice the local rate of linear deformation times the dynamic viscosity.

Substitution of the above shear stresses in equation 3.32 into equation 3.23 yields the so-called Navier-Stokes equations derived them independently

$$\begin{aligned}
&\text{x-axis} && \rho\frac{Du}{Dt} = -\frac{\partial p}{\partial x} + \frac{\partial}{\partial x}\left[2\mu\frac{\partial u}{\partial x} + \lambda\left(\nabla\cdot\vec{V}\right)\right] + \frac{\partial}{\partial y}\left[\mu\left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x}\right)\right] \\
& && + \frac{\partial}{\partial z}\left[\mu\left(\frac{\partial u}{\partial z} + \frac{\partial w}{\partial x}\right)\right] + S_{Mx} \\
&\text{y-axis} && \rho\frac{Dv}{Dt} = -\frac{\partial p}{\partial y} + \frac{\partial}{\partial x}\left[\mu\left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x}\right)\right] + \frac{\partial}{\partial y}\left[2\mu\frac{\partial v}{\partial y} + \lambda\left(\nabla\cdot\vec{V}\right)\right] \\
& && + \frac{\partial}{\partial z}\left[\mu\left(\frac{\partial v}{\partial z} + \frac{\partial w}{\partial y}\right)\right] + S_{My} \\
&\text{z-axis} && \rho\frac{Dw}{Dt} = -\frac{\partial p}{\partial w} + \frac{\partial}{\partial x}\left[\mu\left(\frac{\partial u}{\partial z} + \frac{\partial w}{\partial x}\right)\right] + \frac{\partial}{\partial y}\left[\mu\left(\frac{\partial v}{\partial z} + \frac{\partial w}{\partial y}\right)\right] \\
& && + \frac{\partial}{\partial z}\left[2\mu\frac{\partial w}{\partial z} + \lambda\left(\nabla\cdot\vec{V}\right)\right] + S_{Mz}
\end{aligned} \tag{3.33}$$

Often it is useful to re-arrange the viscous stress terms as follows

$$\frac{\partial}{\partial x}\left[2\mu\frac{\partial u}{\partial x}+\lambda\left(\nabla\cdot\vec{V}\right)\right]+\frac{\partial}{\partial y}\left[\mu\left(\frac{\partial u}{\partial y}+\frac{\partial v}{\partial x}\right)\right]+\frac{\partial}{\partial z}\left[\mu\left(\frac{\partial u}{\partial z}+\frac{\partial w}{\partial x}\right)\right]=\frac{\partial}{\partial x}\left(\mu\frac{\partial u}{\partial x}\right)+$$
$$\frac{\partial}{\partial y}\left(\mu\frac{\partial v}{\partial y}\right)+\frac{\partial}{\partial z}\left(\mu\frac{\partial w}{\partial z}\right)+\left[\frac{\partial}{\partial x}\left(\mu\frac{\partial u}{\partial x}\right)+\frac{\partial}{\partial y}\left(\mu\frac{\partial v}{\partial x}\right)+\frac{\partial}{\partial z}\left(\mu\frac{\partial w}{\partial x}\right)\right]+ \tag{3.34}$$
$$\frac{\partial\lambda\left(\nabla\cdot\vec{V}\right)}{\partial x}=\nabla\cdot\left(\mu\cdot u\right)+s_{Mx}$$

The viscous stresses in the *y*-and *z*-component equations can be re-cast in a similar manner. We clearly intend to simplify the momentum equations by 'hiding' the two smaller contributions to the viscous stress terms in the momentum source. Defining a new source by

$$S_M = S_M + s_M \tag{3.35}$$

the Navier-Stokes equations can be written in the most useful fonn for the development of the finite volume method:

$$\begin{aligned}
&\text{x-axis} && \rho\frac{Du}{Dt}=-\frac{\partial p}{\partial x}+\nabla\cdot\left(\mu\cdot u\right)+S_{Mx}\\
&\text{y-axis} && \rho\frac{Dv}{Dt}=-\frac{\partial p}{\partial y}+\nabla\cdot\left(\mu\cdot v\right)+S_{My}\\
&\text{z-axis} && \rho\frac{Dw}{Dt}=-\frac{\partial p}{\partial z}+\nabla\cdot\left(\mu\cdot w\right)+S_{Mz}
\end{aligned} \tag{3.36}$$

3.2.5 Heat Transfer and Fourier Law

The law of heat transfer, also known as Fourier's law, states that the time rate of heat transfer through a material is proportional to the negative gradient in the temperature and to the area, at right angles to that gradient, through which the heat is flowing. We can state this law in two equivalent forms: the integral form, in which we look at the amount of energy flowing into or out of a body as a whole, and the differential form, in which we look at the flow rates or fluxes of energy locally, through which the heat is flowing

$$\frac{q_z}{A}=-\alpha\frac{d\left(\rho C_p T\right)}{dZ} \tag{3.37}$$

3.2.6 Fick's Laws of Diffusion

Fick's laws of diffusion describe diffusion and can be used to solve for the diffusion coefficient, which relates the diffusive flux to the concentration, by postulating that the flux goes from regions of high concentration to regions of low concentration, with a magnitude that is proportional to the concentration gradient (spatial derivative). In one (spatial) dimension, this is

$$J_{AZ} = -D_{AB}\frac{dc_A}{dZ} \tag{3.38}$$

where J_{AZ} is flux of component A in z-direction (kgmolA/s.m^2)

D_{AB} is diffusion coefficient of component molecule A in component B (m^2/s)

c_A is concentrate of A (kgmolA/m^3)

3.2.7 The Stefan-Maxwell Equation

The Stefan-Maxwell equation is the only diffusion equation that separates diffusion from convection in a simple way. The flux equation is replaced by the difference in species velocities. The Stefan-Maxwell model is more rigorous, is commonly used in multi component species systems, and is employed quite extensively in the literature. The main disadvantage is that it is difficult to solve mathematically. It may be used to define the gradient in the mole fraction of components

$$\nabla y_i = RT\sum\frac{y_i N_j - y_j N_i}{pD_{ij}^{eff}} \tag{3.39}$$

where y_i is the gas phase mol fraction of species i, and N_i is the superficial gas phase flux of species i averaged over a differential volume element which is small with respect to the overall dimensions of the system, but large with respect to the pore size. D_{ij}^{eff} is the binary diffusion coefficient, and can be defined by

$$D_{ij}^{eff} = \frac{a}{p}\left(\frac{T}{\sqrt{T_{c,i}T_{c,j}}}\right)^{b}\left(p_{c,i}p_{c,j}\right)^{1/3}\left(T_{c,i}T_{c,j}\right)^{5/12}\left(\frac{1}{M}+\frac{1}{Mj}\right)^{1/2}\varepsilon^{1.5} \tag{3.40}$$

where T_c and p_c are the critical temperature and pressure of species i and j, M is the molecular weight of species.

3.2.8 Darcy's Equation

Darcy's Equation for fluid flow through porous media, which has Continuity equations and transport, and can be defined by

Continuity Equation
$$\varepsilon\frac{\partial\rho}{\partial t} = -(\nabla\cdot\rho v_0) \tag{3.41}$$

Darcy's Equation
$$v_0 = -\frac{\kappa}{\mu}(\nabla p - \rho g) \tag{3.42}$$

where ε is porous of material and κ is permeability

Darcy's equation was come from experimental for explain to slow permeable of particles when combine equation 3.41 and 3.42 can be defined by

$$\left(\frac{\varepsilon\mu}{\kappa}\right)\frac{\partial\rho}{\partial t}=\left(\nabla\cdot\rho(\nabla p-\rho g)\right) \tag{3.43}$$

3.3. Computational Fluid Dynamics of PEMFC

Modeling plays a significant and important role in fuel cell design and development process. Because of its importance, modeling is initiated early into a fuel cell development cycle, as shown in figure 3.10. The flowchart illustrates a typical procedure in fuel cell development, where the process begins with a set of requirements. Requirements include power and energy requirements, environmental operating conditions, size and volume limitations, safety specifications, and others. Along with the requirements, knowledge of materials, processes, and material interactions is necessary to properly construct a fuel cell stack. Once several designs are down selected, modeling of the designs is performed to determine how well the candidate systems satisfy requirements. The modeling helps the designer further down-select designs to fabricate and test. The tests performed on the final designs can either result in a final prototype or result in an iteration of existing designs for improvement. Reliable diagnostics are needed not only to find out what is wrong with the existing design so that it can be improved, but also to calibrate and verify the models and assumptions used in developing them.

This design iteration loop can be quite lengthy and frequent, especially when stringent requirements or poor modeling capabilities exist. On the contrary, improvements in modeling capability can help the designer find and improve on existing designs that satisfy stringent requirements. Hence, modeling has a critical role in the fuel cell design and development process. A designer can use an accurate and robust model to design and develop fuel cell stacks more efficiently and often with better performance and lower manufacturing cost.

Using fuel cell modeling as a successful design tool requires the model to be robust, accurate, and able to provide usable answers quickly. In terms of robustness, the model should be able to predict fuel cell performance under a large range of operating conditions. For example, a PEM fuel cell can be operating at different temperature, humidity level, and fuel mixture. A robust model should be able to predict fuel cell performance under varying conditions. The model must also predict fuel cell performance accurately. It should be mentioned here that accuracy does not necessarily mean that a model should accurately predict the absolute value of all the physical phenomena being modeled at any point in space and time. Instead, a model should accurately predict the relative values or the trends (e.g., an increase in value of one parameter should result in either no, low, moderate, or significant increase or decrease of another parameter). Accuracy can be contributed to using the correct assumptions, using the correct properties and other numerical input parameters, predicting the correct physical phenomena by using the correct governing equations, and being able to match the modeling results with experimental data. However, enhancing model robustness and accuracy often trades off with computational efficiency. To provide answers quickly, the designer must select a model that balances robustness, accuracy, and computational effort.

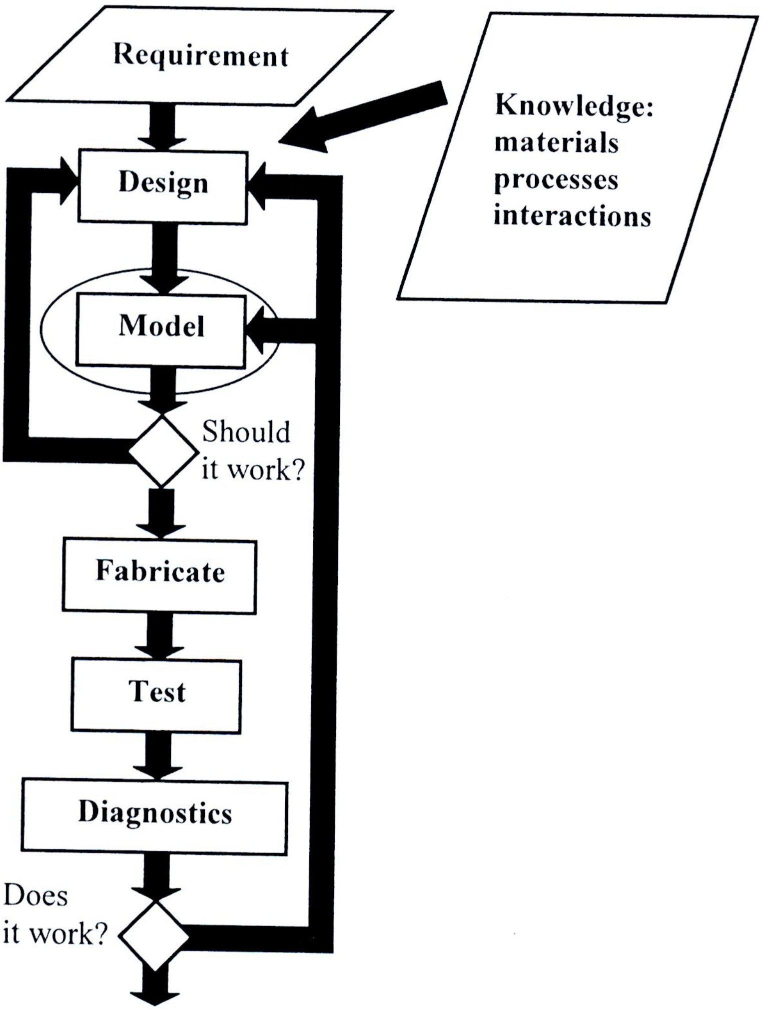


Figure 3.10 Role of modeling and diagnostics in the fuel cell development process.

3.3.1 Modeling Equation

The PEMFC modeling includes the flow field plate, gas diffusion, catalyst layer, membranes and bipolar plate. The numerical calculations are based on solution of the conservation equations of mass, momentum, energy, current and species transport on a computational grid using CFD. The key elements to modeling fuel cells are the transport phenomena in flow channel on polar plate, through porous media, heterogeneous reactions within porous electrodes and the coupling between mass transports, electrochemical reactions and current–potential fields. The result of model can be used to a new flow filed in PEMFC. The model has major assumptions of the modeling are (Fang-Bor Weng et al., 2005):

1. steady state because it was collected data of operating in steady of temperature, voltage and current density,
2. laminar flow which this research used max velocities in 500 cm^3/min and Reynolds number has not over 2300,
3. all gases are treated as ideal gas. At normal conditions such as standard temperature and pressure, most real gases behave qualitatively like an ideal gas. Generally, a gas behaves more like an ideal gas at higher temperature and lower density (i.e. lower pressure) as the work performed by intermolecular forces becomes less significant compared with the particles' kinetic energy, and the size of the molecules becomes less significant compared to the empty space between them.
4. gas phase flow in catalyst layer, gas diffusion layer and channel flow field, without the effects of vaporization and condensation,
5. the Stefan–Maxwell equations for multi-species diffusion,
6. Butler–Volmer equation is used to describe electrochemical reactions within the catalyst layers,
7. Nerst–Planck equation is used for the transport of protons through the membrane,
8. Ohm's law is applied across whole region of the polarization curve,
9. gravity effect is neglected because modeling is small size cause mass is neglected.

Also, empirical equations, particularly those describing water behavior in the polymer membrane and related phenomena, are often used in modeling, in absence of equations that describe the actual physical phenomena. Any model is as good as the assumptions that it is built upon. Assumptions are needed to simplify the model. It is important to understand the assumptions in order to understand the model's limitations and to accurately interpret its results. Common assumptions used in fuel cell modeling are:

- ideal gas properties,
- ideal gas mixtures,
- incompressible flow,
- laminar flow,
- isotropic and homogeneous membrane and electrode structures,
- negligible ohmic potential drop in solid components,
- the mass and energy transport through porous structures of porosity is modeled from macroperspective using the volume-averaged conservation equations.

- **Channel flow field**

According to assumptions, the conservation equations of mass, momentum and species in flow channel can be written as:

Mass conservation:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \left(\rho \vec{U}\right) = 0 \qquad (3.44)$$

Momentum conservation:

$$\begin{aligned} &\text{x – axis} && \frac{\partial \rho u}{\partial t} + \nabla \cdot \left(\rho \vec{U} u\right) = -\frac{\partial p}{\partial x} + \nabla \cdot \left(\mu \nabla u\right) \\ &\text{y – axis} && \frac{\partial \rho v}{\partial t} + \nabla \cdot \left(\rho \vec{U} v\right) = -\frac{\partial p}{\partial y} + \nabla \cdot \left(\mu \nabla v\right) \\ &\text{z – axis} && \frac{\partial \rho w}{\partial t} + \nabla \cdot \left(\rho \vec{U} w\right) = -\frac{\partial p}{\partial z} + \nabla \cdot \left(\mu \nabla w\right) \end{aligned} \tag{3.45}$$

where

ρ = the fluid density, p the pressure and is the μ dynamic viscosity.

Species conservation:

$$\frac{\partial}{\partial t}\left(\varepsilon \rho Y_i\right) + \nabla \cdot \left(\varepsilon \rho U Y_i\right) = \nabla J_i \tag{3.46}$$

where

Y_i = the mass-fraction of i_{th} species and J_i is the diffusive flux.

The species diffusion flux may be written as:

$$\begin{aligned} J_i = {} & \rho D_i \nabla Y_i + \frac{\rho Y_i}{M} D_i \nabla M - \rho Y_i \sum_j D_j \nabla Y_j \\ & - \rho Y_i \frac{\Delta M}{M} \sum_j D_j \nabla Y_j \end{aligned} \tag{3.47}$$

where

M = the mixture molecular weight and D_i is the effective mass diffusion coefficient of species i.

$$D_i = D_{i,FS}\,\varepsilon^{\tau} \tag{3.48}$$

where

$D_{i,FS}$ = the free stream diffusion coefficient of the ith species,
ε = porosity of the medium,
τ = the tortuosity of the medium.

It is a common practice to use tortuosity value of 1.5 in Equation 3.48, resulting in the so-called Bruggeman model.

- **Gas diffusion layer**

The main assumption is isotropic porous media, their mass and momentum equations are effected by porosity ε and permeability κ. These equations are showed as:

Mass conservation:

$$\frac{\partial}{\partial t}\left(\varepsilon\rho\right)+\nabla\left(\varepsilon\rho U\right)=0 \tag{3.49}$$

Momentum conservation:

$$\frac{\partial}{\partial t}\left(\varepsilon\rho\right)+\nabla\cdot\left(\varepsilon\rho U\cdot U\right)=-\varepsilon\nabla\rho+\nabla\cdot\left(\varepsilon\tau\right)$$
$$+\varepsilon B+\frac{\varepsilon^{2}\mu U}{k} \tag{3.50}$$

where

τ = shear force tensor,
$\vec{U}$ = the flow velocity vector,
ε = porosity of the medium,
B = the body force vector,
κ = a quantity representing the square of the effective volume to surface area ratio of the porous matrix.

The last term in equation 3.51 represents Darcy's drag force imposed by pore walls on the fluid within the pores, and usually results in a significant pressure drop across the porous medium. Species conservation equation in the gas diffusion layer is the same as in flow field. The continuity of current within any material under electro neutral conditions leads to:

$$\nabla\cdot i=0 \tag{3.51}$$

where

i = the current density vector.

- **Catalyst layer**

The mass and momentum equation in the catalyst layer is the same in the gas diffusion layer. The mass conservation equations for individual gas phase species (i.e., for i=1, . . .) may be written as:

$$\frac{\partial}{\partial t}\left(\varepsilon\rho Y_{i}\right)+\nabla\cdot\left(\varepsilon\rho U Y_{i}\right)=\nabla J_{i}+\omega_{i} \tag{3.52}$$

where

Y_i = the mass fractions of the i_{th} species,

$\dot{\omega}_i$ = the production rates of the i_{th} species in the gas phase.

The species diffusion flux may be written same equation 3.52. In the case of electrochemical reaction, the volumetric production rate of a given species is expressed by the ratio of the transfer current, j_T, and the Faraday constant, F:

$$\omega_i = \left(a_i^{''} - a_i^{'}\right)\frac{j_T}{F} \tag{3.53}$$

where

a''_i and a'_i = the stoichiometric coefficients of the products and reactants, respectively,

j_T = obtained from the Butler–Volmer condition.

The continuity of current within any material under electroneutral conditions leads to:

$$\nabla \cdot i = 0 \tag{3.54}$$

where

i =the current density vector.

- **Proton exchange membrane**

In the proton exchange membrane, governing equations are the same as in the catalyst layer, but without any chemical reaction. The membrane proton conductivity is correlated by the experimental data, which are dependent on temperature and water content.

The numerical model describe a detailed three-dimensional of transport phenomena and performance within the PEMFC including gas channel, gas diffusion layer, catalyst layer and membrane.

3.3.2 Potential Drop Across the Cell

The goal in this section is to model the potential losses in the gas diffusion layers and membrane, so that the activation overpotential can be accurately predicted.

- **Ohmic Loss in Gas Diffusion Layers**

The potential loss due to current conduction through the gas diffusion layer can be modeled by an equation similar to the Laplace equation. The potential boundaries are setup to drive the current through these regions,

$$\nabla .(\lambda_e \nabla V) = S_e \tag{3.55}$$

Where S_e is the electron source term equals to the anode and cathode currents for each side respectively. The ohmic loss is then calculated as,

$$\eta_{ohmic}=V_{CL}-V_{ref} \qquad (3.56)$$

Where V_{CL} is the potential at the catalyst layer and V_{ref} is the reference potential set at the interface between the gas diffusion layer and the bipolar plate.

- **Ohmic Loss in Membrane**

Potential loss in the membrane is due to resistance to proton transport across the membrane. This potential loss distribution is also modeled by the Laplace equation similar to the potential loss in the gas diffusion layer regions,

$$\nabla.(\lambda_m \nabla V) = S_m \qquad (3.57)$$

Where S_m is source and sink of protons in the anode catalyst layer and cathode catalyst layer respectively. The protonic loss is then calculated as,

$$\eta_{protonic}=V_{CL,c}-V_{CL,a} \qquad (3.58)$$

Where $V_{CL,c}$ is the potential at the cathode catalyst layer and V_{CL},a is the potential at the anode catalyst layer.

- **Activation Over-potential**

After the ohmic losses in the membrane and gas diffusion electrodes are calculated, activation over-potential can be calculated from the reversible potential and cell potential,

$$\eta_{act,c}=E_{rev}-E_{cell}-\eta_{ohmic,gdl}-\eta_{protonic,mem} \qquad (3.59)$$

The cell reversible potential, E_{rev}, is a thermodynamic property and can be calculated based on Nernst equation. The cell potential, E_{cell}, is the input parameter based on the desired loading condition. Therefore the cathode activation over-potential can be determined. The anode activation over-potential is small and considered negligible in this model.

3.3.3 Electrochemical Kinetics

The local current density is calculated based on the well known Butler-Volmer equation which couples the reactant concentration with the activation over-potential:
Cathode current,

$$i_c = i_{o,c}^{ref}\left(\frac{C_{o_2}}{C_{o,c}^{ref}}\right)^{\gamma_{O_2}}\left[\exp\left(\frac{\alpha_a F}{RT}\eta_{act,c}\right)-\exp\left(-\frac{\alpha_c F}{RT}\eta_{act,c}\right)\right] \qquad (3.60)$$

where , $i_{o,c}^{ref}$ is the cathode reference exchange current density, α_a and α_c are the cathode anodic and cathodic charge transfer coefficients respectively.

Anode current,

$$i_a = i_{o,a}^{ref}\left(\frac{C_{H_2}}{C_{H,c}^{ref}}\right)^{\gamma_{H_2}}\left[\exp\left(\frac{\alpha_a F}{RT}\eta_{act,a}\right)-\exp\left(-\frac{\alpha_c F}{RT}\eta_{act,a}\right)\right] \tag{3.61}$$

However, the anode current is simplified in this model. Since the anode activation overpotential is very small and the hydrogen concentration distribution at the catalyst layer is quite uniform, the local anode current density is set equal to the average cathode current density with the condition that charge must be conserved,

$$I_{total} = \sum_{j=1}^{N_c} i_{c,j} \times V_j = \sum_{j=1}^{N_a} i_{a,j} \times V_j \tag{3.62}$$

Where N_c and N_a are the total number of cells in the cathode and anode catalyst layers respectively; V_j is the cell volume.

3.3.4 Boundary Conditions

Boundary conditions are specified at all external boundaries of the computational domain as well as boundaries for various mass transport and scalar equations inside the computational domain.

- **Inlets**

At the anode and cathode several Dirichlet boundary conditions of velocity, inlet gas stream temperature, mass fraction of each gas component are applied as follows: the inlet velocity is a function of the cell current and stoichiometric flow ratio, MEA area, and channel cross-section area. In other words, the inlet mass flow must be sufficient to supply the amount of reacting species required for a specific current density and stoichiometric flow ratio. In this model, the cell current is predicted from a specified cell voltage, therefore cell current is changing at every iteration, and hence the inlet velocity must be updated at every iteration to keep up with the changing cell current.

- **Outlets**

Pressure boundary conditions are specified at the anode and cathode outlets. The desired cell operating pressures are specified at the anode and cathode outlets. Neumann boundary conditions are applied for other variables, i.e. zero normal gradients are imposed on velocity, temperature, species mass fractions, and the additional scalar equations of the potential fields.

- **External Surfaces**

Symmetry boundary conditions are applied at the surfaces of the computational domain in the *z*-direction. All variables are mathematically symmetric, with no flux across the boundary. At the external surfaces in the *y*-direction, (top and bottom surfaces of the cell), temperature is specified and zero heat flux.

- **Boundary Conditions at the Interfaces inside the Computational Domain**

At the boundary between the gas channel and the bipolar plate, conducting boundary condition is applied to account for heat transfer between these two materials. Perhaps the most difficult boundary conditions to apply are the boundary conditions required for the mass fraction equations and the potential equations at the interfaces between different regions of the cell.

For the oxygen mass fraction equation, a boundary condition must be specified at the interface between the cathode catalyst layer and the membrane to keep the oxygen from entering the membrane.

Similarly, a Neumann type boundary condition was applied at the interface between the anode catalyst layer and the membrane to stop hydrogen from entering the membrane

The potential equations also required a combination of Dirichlet and Neumann boundary conditions at the interfaces in the *y*-direction. Dirichlet boundary conditions are applied at the interface between the bipolar plates and the gas diffusion layers. More specifically, a zero potential boundary is specified at this interface. Neumann boundary conditions are applied at the interface between the gas channels and the gas diffusion layers to give zero potential flux into the gas channels. Mathematically at these interfaces the potential gradient is zero.

Similarly, the protonic potential field requires a set of potential boundary condition and zero flux boundary condition at the anode catalyst layer interface and cathode catalyst layer interface respectively.

3.4 Summary

This chapter ahs presented the theory of computation fluid dynamics (CFD), which used to as a tool in this studied. These included governing equations of fluid flow, heat transfer modeling, chemical reaction and electric modeling. CFD was used for describe to affect parameters of gas flow and chemical reaction in cell. There were gave data used to design flow field for a better performance and building prototypes flow field for experiment. The results was validated with others research and experimental.