SCHOOL OF BIO AND CHEMICAL ENGINEERING
DEPARTMENT OF CHEMICAL ENGINEERING

UNIT – I – Computational Fluid Dynamics – SCHA1403

I. Overview of CFD and Conservation Laws

Computational fluid dynamics deals with equations that represent a balance process for mass, momentum, energy and chemical species. Many students have seen these differential equations before in advanced courses in fluid dynamics or in convective heat and mass transfer. These notes review the derivation process for the basic balance equations with a view to their eventual conversion to numerical methods in computational fluid dynamics.

One of the useful facts about the various balance equations for various quantities is their similar form. This means that a numerical algorithm developed from one particular balance quantity, say momentum, can be applied to another balance quantity, say energy. With this goal in mind, the derivation of the basic differential equations provided in these notes is aimed at demonstrating the similarity of the various quantities for which we derive a balance equation.

We represent the various quantities such a mass, momentum, energy and mass of an individual chemical species by the general symbol, $\square$. We then derive a "balance equation" for $\square$, which is valid for any quantity. We then have to consider the particular physics of the different quantities in the balance equations.

Continuity Equation

We use simple laws. Mass is conserved. Newton's second law tells us that the rate of change of momentum equals the applied force. The first law of thermodynamics says that the rate of energy change equals the heat added plus the work done on a system. Chemical balances tell us that changes in the mass of individual chemical species are related to sources or sinks provided by chemical reactions. All of these simple laws, applied to a flow system, can be stated in terms of a simple balance equation

$$STORAGE + OUTFLOW - INFLOW = SOURCE \qquad [1\text{-}1]$$

We apply this general balance equation (remembering that the symbol, $\square$ can represent mass, momentum or energy) to a variety of physical quantities such as mass, energy, momentum, and chemical species.

The various quantities that we will be concerned with are shown in Table 1-1.

Table 1-1 – Examples of Quantities that Satisfy a Balance Equation						
S.No	mass	x momentum	y momentum	z momentum	Energy	Species
1	m	Mu	mv	mw	$E + m\mathbf{V}^2/2$	$m^{(K)}$
2	1	U	v	w	$e + \mathbf{V}^2/2$	$W^{(K)}$
In this table, u, v, and w are the x, y and z velocity components, E is the total thermodynamic internal energy, e is the thermodynamic internal energy per unit mass, and $m^{(K)}$ is the mass of a chemical species, K, $W^{(K)}$ is the mass fraction of species K. The other energy term, $m\mathbf{V}^2/2$, is the kinetic energy.						

We will derive the general balance equation for a differential volume in three-dimensional Cartesian coordinate space. The velocity components in the (x, y, z) coordinate directions are denoted as (u, v, w).

The volume of the differential element is $\Delta x\, \Delta y\, \Delta z$. If the density of the fluid is denoted by the symbol ρ, the mass, m, inside this volume is $\rho\, \Delta x\, \Delta y\, \Delta z$ The rate at which the quantity, Φ, is stored (or accumulates) in this volume over time is then given by the following equation.

$$Storage = \frac{\partial \Phi}{\partial t} = \frac{\partial (m\varphi)}{\partial t} = \frac{\partial (\rho \Delta x \Delta y \Delta z \varphi)}{\partial t} = \frac{\partial (\rho \varphi)}{\partial t} \Delta x \Delta y \Delta z \qquad \text{[1-2]}$$

The mass flow across a control volume face is the product of velocity, density and cross sectional area. For example, the x direction flow, with a velocity component u, enters and exits the control volume through an area given by the product the $\Delta y\, \Delta z$. Thus, the mass flow in the x direction is given by the product ($\rho\, u\, \Delta y\, \Delta z$).

If the flowing mass has a particular per-unit-mass property, $\square$, then the flow of the total quantity, Φ, across the boundary is given by the product of the per-unit-mass property, $\square$, times the mass flow rate. This means that the flow of $\square$ across a control volume face is the product of four factors: density, ρ, the per-unit-mass value of the quantity considered, $\square$, the cross sectional area of the face, and the velocity normal to the face. Note that this product has the same dimensions as the storage term, the dimensions of $\square$ divided by dimensions of time.

For the coordinate system shown, we define inflows as occurring at a particular face designated as x, y or z. The outflows then occur at the face in the increasing coordinate direction. These faces are denoted as x+ Δx, y + Δy, and z + Δz. The $\square$ inflow in the x direction would be given by the following expression: ρ u $\square$ |$_x$ Δy Δz. Similar terms apply in the y and z directions. Summing the terms for each coordinate direction gives the total inflow.

$$Inflow = \rho\, u\, \varphi\big|_x \Delta y\, \Delta z \;\; + \rho\, v\, \varphi\big|_y \Delta x\, \Delta z \;\; + \rho\, w\, \varphi\big|_z \Delta y\, \Delta x \qquad\qquad [1\text{-}3]$$

The expression for the outflow is similar. The only difference is the subscript indicating that the outflow occurs at a different face of the control volume.

$$Outflow = \rho\, u\, \varphi\big|_{x+\Delta x} \Delta y\, \Delta z \;\; + \rho\, v\, \varphi\big|_{y+\Delta y} \Delta x\, \Delta z \;\; + \rho\, w\, \varphi\big|_{z+\Delta z} \Delta y\, \Delta x \qquad [1\text{-}4]$$

The source term, S_φ, must be defined for each individual physical quantity that satisfies a balance equation. For the mass balance, the source term is zero. In the balance equation for the ith chemical species, the source term is the chemical production of species i. The dimensions of S_φ are (phi dimensions) per unit volume, per unit time. This source term in the balance equation, with dimensions of (phi dimensions) per unit time, is written as follows.

$$Source = \mathsf{S}_\varphi\, \Delta x\, \Delta y\, \Delta z \qquad\qquad [1\text{-}5]$$

All the terms in the equations [1-2] to [1-5] are to be substituted into equation [1-1] where they will be added to each other or subtracted from each other. In this case, each term must have the same dimensions. The storage term in equation [1-2] obviously has

the dimensions of □-dimensions per unit time. In order to have consistent dimensions when equations [1-2] to [1-5] are substituted into equation [1-1], all the terms in equations [1-2] to [1-5] must have these dimensions.

For example, consider the storage term in the energy balance equation. In this equation, □ represents the energy E, so the □ -dimensions would be energy dimensions. In the SI system, the energy would have units of joules (J), and the units for □ would be J/kg. The ρφ product would have units of J/m^3. The derivative of the ρ□□ product with respect to time would have units of J/m^3-s. Multiplying this term by $\Delta x \Delta y \Delta z$ gives the final units for the storage term in the energy equation as J/s.

A similar analysis can be done for both the inflow and outflow terms. The dimensions of ρu□$\Delta y \Delta z$ are (mass/length^3)(length/time)(□□-dimensions/mass)(length^2) which equates to □-dimensions divided by time dimensions. For the energy equation, this would be joules per second, which is consistent with what we found earlier for the storage (or transient) term. Thus all terms in equation [1-1] to [1-5] will have dimensions of □ divided by dimensions of time. If the source term in equation [1-5] must have dimensions of □ divided by dimensions of time, the S_φ term must have dimensions of □ divided by dimensions of time and divided by dimensions of volume. In the energy equation, the S_φ term would then have units of $J/s\text{-}m^3$.

Combining all the quantities in equations [1-2] to [1-5], according to the verbal equation [1-1] and dividing by the volume, $\Delta x \Delta y \Delta z$, gives the following result.

$$\frac{\partial \rho \varphi}{\partial t} + \frac{\rho\, u\, \varphi|_{x+\Delta x} - \rho\, u\, \varphi|_x}{\Delta x} + \frac{\rho\, v\, \varphi|_{y+\Delta y} - \rho\, v\, \varphi|_y}{\Delta y} + \frac{\rho\, w\, \varphi|_{z+\Delta z} - \rho\, w\, \varphi|_z}{\Delta z} = \mathsf{S}_\varphi \quad [1\text{-}6]$$

Taking the limit as the differentials approach zero gives the definitions of the partial derivative. This limit results in the following differential equation.

$$\frac{\partial \rho \varphi}{\partial t} + \frac{\partial \rho\, u \varphi}{\partial x} + \frac{\partial \rho\, v \varphi}{\partial y} + \frac{\partial \rho\, w \varphi}{\partial z} = S_\varphi^* \qquad [1\text{-}7]$$

Where we have defined

$$S_\varphi^* = \lim_{\Delta x \Delta y \Delta z \to 0} S_\varphi \qquad [1\text{-}8]$$

Notation to Simplify Multidimensional Equations

The repetition in the directional terms is simplified by notation known as Cartesian tensor notation (sometimes called the Einstein convention). In this notation, the coordinate directions and velocity components are given numerical subscripts. The repetition of an index implies summation over all three coordinate directions (two directions in a two-dimensional problem.) The usual coordinate system (x, y, z) is written as (x_1, x_2, x_3). The velocity components that we have written as (u, v, w) could also be written as (u_x, u_y, u_z). In Cartesian tensor notation, the velocity components are written as (u_1, u_2, u_3). Using the numerical notation for the spatial coordinates and the velocity components we can rewrite equation [1-7] as follows.

$$\frac{\partial \rho \varphi}{\partial t} + \frac{\partial \rho u \varphi}{\partial x} + \frac{\partial \rho v \varphi}{\partial y} + \frac{\partial \rho w \varphi}{\partial z} = \frac{\partial \rho \varphi}{\partial t} + \frac{\partial \rho u_1 \varphi}{\partial x_1} + \frac{\partial \rho u_2 \varphi}{\partial x_2} + \frac{\partial \rho u_3 \varphi}{\partial x_3} = S_\varphi \qquad [1\text{-}9]$$

With a conventional summation notation, we could write the second part of equation [1-9] as follows.

$$\frac{\partial \rho \varphi}{\partial t} + \sum_{i=1}^{3} \frac{\partial \rho u_i \varphi}{\partial x_i} = S_\varphi \qquad [1\text{-}10]$$

In the Cartesian tensor notation the summation symbol is not used. Summation over repeated indices is implied. This we would write equation [1-10] as follows in this notation.

$$\frac{\partial \rho \varphi}{\partial t} + \frac{\partial \rho u_i \varphi}{\partial x_i} = S_\varphi \qquad [1\text{-}11]$$

Equation [1-11] is the same as equations [1-7] and [1-10]; it is just using a more compact notation to show that there are similar terms in each coordinate direction.

Forces on a Fluid Element – The Source Term for Momentum

The source term for the momentum balance equation comes from Newton's second law expressed as the statement that the net force is the rate of change of momentum. Thus, the balance equation for the momentum must have a source term has the dimensions of force. The analysis of forces on a fluid element considers two kinds of forces. Forces such as gravity or electromagnetic forces that act over the entire volume of the body are called body forces. In contrast, forces such as pressure and viscous stresses act on the surfaces of a fluid element.

The main body force that is considered in fluid dynamics problems is gravity. The general body force is written as ρB. When written this way, B must have dimensions of acceleration. This can be seen as follows. The source term for all balance terms, $\square$, must have dimensions of $\square$ per unit time, per unit volume. Since the dimensions of momentum are mass times distance over time, the dimensions of the source term for momentum (momentum per unit volume per unit time) must be (mass times distance over time) per unit volume per unit time. Thus the source term represented by $\rho\mathbf{B}$ has dimensions of mass divided by distance-squared and time-squared. Since the dimensions of ρ are mass over distance-cubed, the resulting dimensions for $\mathbf{B}$ must be distance over time-squared or acceleration. Since the body force has three directional components we will write these components as B_x, B_y, and B_z. Alternatively, using the Cartesian tensor notation, we will write these components, in general, as B_i, i= 1, 2, 3.

Surface forces are represented by the notation σ_{ij}, which denotes the normal or shear stress force on a face of the fluid facing direction i. This force is resolved into a component in each coordinate direction. The j subscript denotes a particular direction. For example, σ_{yx} denotes a force, acting in the x direction, on a control volume surface, facing the y direction.

By convention, the force or stress is considered positive when it is exerted by the fluid above an element on the fluid below an element. The net force on a fluid element due to a single component is the difference between forces on two sides of an element. For example, the force on the y faces acting in the x direction is shown in the diagram on the next page.

Since stress is the force per unit area, the force that results from the stress, $\sigma_{yx,}$, is σ_{yx} times the area $\Delta x\,\Delta z$. The net force in the x direction, due to the stress on the y-facing faces of the element is given by $[\sigma_{yx}|_{y+\Delta y} - -\sigma_{yx}|_{y}]\,\Delta x\,\Delta z$. If we divide this net force (from one face in one direction) by the control element volume, $\Delta x\,\Delta y\,\Delta z$, we get the result shown in equation [1-12] for the net force per unit volume.

$$\frac{Net\ yFace,\ xDirection\ force}{Unit\ Volume} = \frac{\sigma_{yx}\big|_{y+\Delta y} - \sigma_{yx}\big|_{y}}{\Delta x\,\Delta y\,\Delta z}\,\Delta x\,\Delta z = \frac{\sigma_{yx}\big|_{y+\Delta y} - \sigma_{yx}\big|_{y}}{\Delta y} \quad [1\text{-}12]$$

In order to get the correct source term in the differential equation, we have to use the definition in equation [1-8], which requires that we take the limit as the control volume approaches zero. In this limit, the last term in equation [1-12] becomes the partial derivative.

$$\begin{array}{c} Limit \\ \Delta y \to 0 \end{array} \frac{Net\ yFace,\ xDirection\ force}{Unit\ Volume} = \frac{\partial \sigma_{yx}}{\partial y} \quad [1\text{-}13]$$

There will be similar terms for the net x-direction force from faces in the x and z directions. Writing out these terms and combining them with the y-face term gives the net force in the x-direction from surface stresses.

$$Net\ x-direction\ surface\ force\ source = \frac{\partial \sigma_{xx}}{\partial x} + \frac{\partial \sigma_{yx}}{\partial y} + \frac{\partial \sigma_{zx}}{\partial z} \quad [1\text{-}14]$$

If we repeated the analysis for the net surface-force source term in the y and z coordinate directions, we would obtain similar terms. These are shown below.

$$Net\ y-direction\ surface\ force\ source = \frac{\partial \sigma_{xy}}{\partial x} + \frac{\partial \sigma_{yy}}{\partial y} + \frac{\partial \sigma_{zy}}{\partial z} \quad [1\text{-}15]$$

$$Net\ z-direction\ surface\ force\ source = \frac{\partial \sigma_{xz}}{\partial x} + \frac{\partial \sigma_{yz}}{\partial y} + \frac{\partial \sigma_{zz}}{\partial z} \quad [1\text{-}16]$$

Using numerical subscripts we can write each of these terms in the same form. Further, using the Cartesian tensor notation we can write the net forces in one direction, say

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direction j, as a single partial derivative with implied summation over repeated indices. In this manner, equations [1-14] to [1-16] can be written with the following notation.

$$Net\ j-direction\ surface\ force\ source = \frac{\partial \sigma_{1j}}{\partial x_1} + \frac{\partial \sigma_{2j}}{\partial x_2} + \frac{\partial \sigma_{3j}}{\partial x_3} = \frac{\partial \sigma_{ij}}{\partial x_i} \qquad [1\text{-}17]$$

In the final term, the repeated index, i, implies summation. The non-repeated index, j, indicated the direction of the force. In subsequent equations for the work done by the surface forces we will use a summation over the j index as well.

The Mass Balance Equation

As noted in Table 1-1, $\square = 1$ in the balance equation for mass. Since mass is neither produced nor destroyed – we are ignoring the effects of relativity here – the source term $S_\varphi = 0$. Thus, equation [1-10] can be written as follows for conservation of mass.

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_i}{\partial x_i} = 0 \qquad [1\text{-}18]$$

This equation is simple enough so that we can write the full equation without Cartesian tensor notation in a fairly simple manner as follows:

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u}{\partial x} + \frac{\partial \rho v}{\partial y} + \frac{\partial \rho w}{\partial z} = 0 \qquad [1\text{-}19]$$

This is simply obtained from equation [1-18] by using the definition of the Cartesian tensor notation and switching to the use of (x,y,z) and (u,v,w) for the spatial and velocity coordinate systems, respectively. It can also be obtained by setting $\square = 1$ and $S_\varphi = 0$ in equation [1-7]. Equation [1-18] (or its equivalent form in equation [1-19]) is known as the continuity equation.

Using the product rule for differentiation, equation [1-18] may be rewritten as follows

$$\frac{\partial \rho}{\partial t} + u_i \frac{\partial \rho}{\partial x_i} + \rho \frac{\partial u_i}{\partial x_i} = 0 \qquad [1\text{-}20]$$

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Note that both the second and third terms in this equation have repeated indices so that summation over all coordinate directions is implied for each term. Thus, equation [1-20] may be written as follows

$$\frac{\partial \rho}{\partial t} + \rho \left[\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} \right] + u \frac{\partial \rho}{\partial x} + v \frac{\partial \rho}{\partial y} + w \frac{\partial \rho}{\partial z} = 0 \qquad [1\text{-}21]$$

The four terms with density derivatives in this equation are sometimes written as $D\rho/Dt$, which is known as the substantive derivative. For any function, Ψ, this derivative is defined as follows:

$$\frac{D\Psi}{Dt} = \frac{\partial \Psi}{\partial t} + u \frac{\partial \Psi}{\partial x} + v \frac{\partial \Psi}{\partial y} + w \frac{\partial \Psi}{\partial z} \qquad or \qquad \frac{D\Psi}{Dt} = \frac{\partial \Psi}{\partial t} + u_i \frac{\partial \Psi}{\partial x_i} \qquad [1\text{-}22]$$

In the second definition above, the Cartesian tensor notation is used and summation is assumed over the repeated index, i. Physically, the substantive derivative represents the change in properties with time, following a fixed element of mass as it moves through the fluid. This is in contrast to the usual partial derivative (with respect to time) that measures the change in time at a fixed point in space through which the fluid flows.

Using the substantive derivative, the continuity equation may be written as follows.

$$\frac{D\rho}{Dt} + \rho \left[\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} \right] = 0 \qquad \frac{D\rho}{Dt} + \rho \frac{\partial u_i}{\partial x_i} = 0 \qquad \frac{D\rho}{Dt} + \rho \Delta = 0 \qquad [1\text{-}23]$$

Here we have introduced a new term, Δ, that is called the dilatation. Its definition is shown in the equation below. For a constant density fluid the continuity equation can be written as follows.

$$\Delta \equiv \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} = 0 \qquad or \qquad \Delta \equiv \frac{\partial u_i}{\partial x_i} = 0 \qquad [1\text{-}24]$$

In a vector definition, the dilatation represents the divergence of velocity. In a physical sense, the dilatation represents the relative change in density with time as we follow a

fixed mass of fluid through the flow. If there is a change in density, there must be a net inflow or outflow of mass to accommodate this change.

Alternative Form for the General Balance Equation and the Conservation Form

The general balance equation may be written in an alternative form as shown below. We start with equation [1-11] and apply the chain rule of differentiation to obtain the following result.

$$\rho \frac{\partial \varphi}{\partial t} + \varphi \left[\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_i}{\partial x_i} \right] + \rho u_i \frac{\partial \varphi}{\partial x_i} = S_\varphi \qquad [1\text{-}25]$$

The term in brackets is just the continuity equation as shown in equation [1-18]. Since the right-hand side of this equation is zero, the bracketed term in equation [1-25] is zero, and we may write the general balance equation as follows.

$$\rho \frac{\partial \varphi}{\partial t} + \rho u_i \frac{\partial \varphi}{\partial x_i} = S_\varphi \qquad [1\text{-}26]$$

Equation [1-26] is the starting point for many analyses in fluid dynamics and convective heat and mass transfer. It is a valid balance equation. However, researchers in computational fluid dynamics have found that the finite-difference schemes derived from this equation have problems in their solution. In particular, the finite-difference equations derived from the form of equation [1-26] will not conserve mass. (For any balance equation with a zero source term, the quantity, □, in the balance equation should be conserved. In this special case, balance equations are sometimes called conservation equations.) However, finite-difference equations based on the original balance equation form in equation [1-11] will conserve mass. Because of this, all derivations of finite-difference equations for computational fluid dynamics start with equation [1-11]. This equation is sometimes called the conservation form because it conserves mass when converted to a finite difference formulation.[*] Using this nomenclature we will call equation [1-26] the "non-conservation" form.

The process of deriving equation [1-26] is a two-way street. If we have an equation in the form given by equation [1-26] we can reverse the derivation to get the form given by equation [1-11].

The Momentum Balance Equation

The total net force in direction j is the sum of the body force and the net surface force in that direction. If we add the body force, ρB_j, in direction j, to the net surface force in that direction, given by equation [1-17] we have the following expression in Cartesian tensor notation.

$$Net\ j-direction\ source\ term = \frac{\partial \sigma_{1j}}{\partial x_1} + \frac{\partial \sigma_{2j}}{\partial x_2} + \frac{\partial \sigma_{3j}}{\partial x_3} + \rho B_j = \frac{\partial \sigma_{ij}}{\partial x_i} + \rho B_j \quad [1\text{-}27]$$

With this force term, the general balance equation [1-11] for the momentum per unit mass in direction j ($\Box = u_j$) can be written as shown below. There are three such equations, one for each coordinate direction.

$$\frac{\partial \rho u_j}{\partial t} + \frac{\partial \rho u_i u_j}{\partial x_i} = \frac{\partial \sigma_{ij}}{\partial x_i} + \rho B_j \qquad j = 1, \text{K}\ 3 \qquad [1\text{-}28]$$

For a Newtonian fluid, the stress, σ_{ij}, is given by the following equation

$$\sigma_{ij} = -P\delta_{ij} + \mu\left[\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right] + (\kappa - \frac{2}{3}\mu)\Delta\delta_{ij} \qquad [1\text{-}29]$$

Here P is the usual thermodynamic pressure; δ_{ij} is called the Kronecker delta. It is 1 if i=j and zero otherwise. The symbols μ and κ are called the dynamic and bulk viscosities; the latter is only important in high frequency sound wave problems and will not be considered further in these notes.If you find this notation confusing, you should write equation [1-29] for σ_{xy}, the net surface force on the x face in the y direction. To do this, you first write equation [1-29] with i = 1 and j = 2 as subscripts. (What is the value of δ_{12} according to the definition of δ?) Next, substitute x for i and y for j in the subscripts for σ. Finally, substitute u and v for u_1 and u_2, respectively, and substitute x and y for x_1 and x_2, respectively. The result will have a notation that is more readable than the notation in

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equation [1-29]. However, this more obvious notation for directions requires you to write nine such equations, all of which will have the same form as equation [1-29], to represent all the surface force terms.

We obtain the momentum balance equation for a Newtonian fluid by substituting the definition of σ_{ij} in equation [1-29] into equation [1-28].

$$\frac{\partial \rho u_j}{\partial t} + \frac{\partial \rho u_i u_j}{\partial x_i} = \frac{\partial}{\partial x_i}\left[-P\delta_{ij} + \mu\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right) + (\kappa - \frac{2}{3}\mu)\Delta\delta_{ij}\right] + \rho B_j \quad j=1, \text{K } 3 \, [1\text{-}30]$$

The right-hand side of this equation has in implied summation in the repeated index i. Since $\delta_{ij}=0$, unless $i = j$, the terms multiplied by δ_{ij} can be written only once. When this is done equation [1-30] can be written as follows:

$$\frac{\partial \rho u_j}{\partial t} + \frac{\partial \rho u_i u_j}{\partial x_i} = -\frac{\partial P}{\partial x_j} + \frac{\partial}{\partial x_i}\left[\mu\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)\right] + \frac{\partial}{\partial x_j}\left[(\kappa - \frac{2}{3}\mu)\Delta\right] + \rho B_j \quad j=1, \text{K } 3 \, [1\text{-}31]$$

The reader who is still unsure of the i and j subscripts can write equation [1-31], three times, once for each coordinate direction. The equation for x-momentum is shown below. The momentum equations for the other two coordinate directions are left as an exercise for the reader.

$$\frac{\partial \rho u}{\partial t} + \frac{\partial \rho uu}{\partial x} + \frac{\partial \rho vu}{\partial y} + \frac{\partial wu}{\partial z} = \rho B_x$$
$$-\frac{\partial P}{\partial x} + 2\frac{\partial}{\partial x}\mu\left(\frac{\partial u}{\partial x}\right) + \frac{\partial}{\partial y}\left[\mu\left(\frac{\partial v}{\partial x} + \frac{\partial u}{\partial y}\right)\right] + \frac{\partial}{\partial z}\left[\mu\left(\frac{\partial w}{\partial x} + \frac{\partial u}{\partial z}\right)\right] + \frac{\partial}{\partial x}\left[(\kappa - \frac{2}{3}\mu)\Delta\right] \quad [1\text{-}32]$$

The original momentum balance in equation [1-28], with σ_{ij} on the right-hand side, is valid for any relation between σ_{ij} and velocity gradients. This equation is starting point for analysis of non-Newtonian fluids. Before such an analysis can proceed, it is necessary to determine the relationship between σ_{ij} and other flow properties. For the remainder of these notes we will use equation [1-28] and consider only Newtonian fluids.

The Energy Balance Equation

The source terms in the balance equation for total energy (thermodynamic plus kinetic plus potential) are the net rate of heat addition plus the net rate at which work is done on the fulid. The heat flow term is written in terms of the heat flux (heat flow per unit area) in a particular direction, i. This directional heat flux is given the symbol q_i. In the simplest flows, this equation is given the Fourier Law for heat conduction.

$$q_i = -k \frac{\partial T}{\partial x_i} \qquad [1\text{-}33]$$

The net contribution to the source term from the heat flow is found from an analysis that is similar to that done for the surface stresses in equations [1-12] and [1-13]. The net heat inflow in the x direction is $q_x|_x - q_x|_{x+\Delta x}$. The heat flow at the $x+\Delta x$ face has a negative sign because the heat flows out of the element at this face if q_x is positive. The x-direction source term is the net heat flow per unit volume.

$$\frac{Net\ x Direction\, heat}{Unit\, Volume} = -\frac{q_x|_{x+\Delta x} - q_x|_x}{\Delta x \Delta y \Delta z} \Delta y \Delta z = -\frac{q_x|_{x+\Delta x} - q_x|_x}{\Delta x} \qquad [1\text{-}34]$$

In order to get the correct source term in the differential equation, we have to use the definition in equation [1-8], which requires that we take the limit as the control volume approaches zero. In this limit, the last term in equation [1-34] becomes the partial derivative.

$$\begin{matrix} Limit \\ \Delta x \to 0 \end{matrix} \frac{Net\ x Direction\, heat\, source}{Unit\, Volume} = -\frac{\partial q_x}{\partial x} \qquad [1\text{-}35]$$

This analysis can be repeated in the other two coordinate directions. This gives the total heat source term as the sum of three partial derivatives that can be represented as one using the Cartesian tensor notation.

$$Heat\ Rate = -\frac{\partial q_x}{\partial x} - \frac{\partial q_y}{\partial y} - \frac{\partial q_x}{\partial x} = -\frac{\partial q_i}{\partial x_i} \qquad [1\text{-}36]$$

The derivation of the work term requires an analysis of the body and surface forces. The rate at which work is done at any point in the fluid is the product of the force in a given direction times the velocity component in that direction. For the body-force terms, the

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work rate is simply the product of ρB_j with the velocity component u_j summed over all three coordinate directions.

$$Body\text{-}force\ work\ rate = \rho(uB_x + vB_y + wB_z) = \rho u_i B_i \qquad [1\text{-}37]$$

The analysis of the work done by surface forces is more complex. On each face there are forces acting in all three coordinate directions. These forces must be multiplied by the appropriate velocity component. In addition, the work at the $x_i + \Delta x_i$ face is done on the fluid and is thus positive; at the x_i face, the element does work on the adjacent fluid, so the work term is negative. The difference between there two is the net work. As a specific example, consider the work done on the faces in the y direction.

The work term on each face is given by the following equation:

$$y\text{-}face\ surface\ force\ work = (u\sigma_{yx} + v\sigma_{yy} + w\sigma_{yz})\Delta x\ \Delta z = u_i\sigma_{iy}\ \Delta x\ \Delta z \qquad [1\text{-}38]$$

If we follow the same analysis used for the net heat source term above or the net stress force source term in equations [1-12] and [1-13], we will obtain the following result.

$$Net\ yFace\ Surface\ Force\ Work = \frac{\partial(u\sigma_{yx} + v\sigma_{yy} + w\sigma_{yz})}{\partial y} = \frac{\partial u_i\sigma_{yi}}{\partial y} \qquad [1\text{-}39]$$

A similar analysis in the other coordinate directions provides analogous terms. The total work term is given by adding the terms in all coordinate directions.

$$Net\ Surface\ Force\ Work = \frac{\partial u_i\sigma_{xi}}{\partial x} + \frac{\partial u_i\sigma_{yi}}{\partial y} + \frac{\partial u_i\sigma_{zi}}{\partial z} = \frac{\partial u_i\sigma_{ji}}{\partial x_j} \qquad [1\text{-}40]$$

The final term in equation [1-39] has two repeated indices with an implied summation. Thus, this single term represents the sum of nine different partial derivatives. The reader should ensure that she or he can write out all nine terms using the coordinates x, y, and z, and the corresponding velocity components u, v, and w.

The energy balance equation is another form of the general balance formula given by equation [1-11]. Here the per-unit-mass quantity, φ, in the energy equation is the sum of the (per-unit-mass) thermodynamic internal energy, e, and the kinetic energy, $V^2/2$. The source term is the sum of the heat source from equation [1-36], the body force work from equation [1-37], and the surface force work from equation [1-40]. This gives the following result for the energy balance equation.

$$\frac{\partial \rho(e+V^2/2)}{\partial t}+\frac{\partial \rho u_i(e+V^2/2)}{\partial x_i}=-\frac{\partial q_i}{\partial x_i}+\frac{\partial u_i \sigma_{ji}}{\partial x_j}+\rho u_i B_i \qquad [1\text{-}41]$$

We could stop here, since we now have an energy balance equation. However, many different forms of the energy equation are used in practice. These equations include a separate consideration of the thermodynamic internal energy and kinetic energy balances and the substitution of other thermodynamic properties – enthalpy and temperature – in place of the internal energy. The derivation of these equations is presented below.

Alternative Energy Balance Equations

The kinetic energy can be eliminated from the total energy equation as follows. First, we can use the result of equation [1-26] to cast the energy equation in [1-41] into a non-conservation form.

$$\rho\frac{\partial (e+V^2/2)}{\partial t}+\rho u_i\frac{\partial (e+V^2/2)}{\partial x_i}=-\frac{\partial q_i}{\partial x_i}+\frac{\partial u_i \sigma_{ji}}{\partial x_j}+\rho u_i B_i \qquad [1\text{-}42]$$

Similarly, we can use the result of equation [1-26] to write the momentum balance from equation [1-28] in a non-conservation form.

$$\rho\frac{\partial u_j}{\partial t}+\rho u_i\frac{\partial u_j}{\partial x_i}=\frac{\partial \sigma_{ij}}{\partial x_i}+\rho B_j \qquad j=1,\text{K }3 \qquad [1\text{-}43]$$

Equation [1-43] represents three different equations for the conservation of momentum, one in each coordinate direction. The next step in the current derivation is simplified by the use of the Cartesian tensor notation. If we had three equations for x, y, and z momentum, we would multiply the x-momentum equation by u, the y-momentum

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equation by v, the z-momentum equation by w and add the three results. We can obtain the same result by multiplying equation [1-43] by u_j, and applying the summation convention.

$$u_j \left[\rho \frac{\partial u_j}{\partial t} + \rho u_i \frac{\partial u_j}{\partial x_i} = \frac{\partial \sigma_{ij}}{\partial x_i} + \rho B_j \right] \qquad [1\text{-}44]$$

Since each term in equation [1-44] now has a repeated j subscript, we have an implied sum over this subscript. Thus, equation [1-44] represents the task we outlined above of multiplying each momentum balance equation by the corresponding velocity component and adding the results. We can make one further simplification to equation [1-44]. In the two derivatives on the left-hand side we have terms of the form $u_j du_j$. From the summation convention, we know that this term, with its implied summation, is equal to $udu + vdv + wdw = d(u^2/2) + d(v^2/2) + d(w^2/2) = d(u^2 + v^2 + w^2)/2 = d(\mathbf{V}^2/2)$. With this relationship, equation [1-44] may be written as follows.

$$\rho \frac{\partial (\mathbf{V}^2 / 2)}{\partial t} + \rho u_i \frac{\partial (\mathbf{V}^2 / 2)}{\partial x_i} = u_j \frac{\partial \sigma_{ij}}{\partial x_i} + u_j \rho B_j \qquad [1\text{-}45]$$

This equation can be subtracted from the total energy balance in non-conservation form given by equation [1-42] to get a balance equation for the thermodynamic internal energy, e.

$$\rho \frac{\partial e}{\partial t} + \rho u_i \frac{\partial e}{\partial x_i} = -\frac{\partial q_i}{\partial x_i} + \frac{\partial u_i \sigma_{ji}}{\partial x_j} - u_j \frac{\partial \sigma_{ij}}{\partial x_i} = -\frac{\partial q_i}{\partial x_i} + \sigma_{ji} \frac{\partial u_i}{\partial x_j} \qquad [1\text{-}46]$$

Of course we can use the result that the left-hand side of this equation can be written in either the non-conservation form, shown above, or the conservation form. We use the result that the general non-conservation form in equation [1-26] is equivalent to the general conservation form in equation [1-11]. Applying this general result to equation [1-46] gives the equivalent conservation form below.

$$\frac{\partial \rho e}{\partial t} + \frac{\partial \rho u_i e}{\partial x_i} = -\frac{\partial q_i}{\partial x_i} + \sigma_{ji} \frac{\partial u_i}{\partial x_j} \qquad [1\text{-}47]$$

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Further versions of the thermodynamic energy equation can be derived. Equation [1-46] is the usual starting point for these derivations. The first step is to introduce the enthalpy, defined as h = e + P/ρ. Differentiating this enthalpy definition gives the result that dh = de + dP/ρ - Pdρ/ρ². We can use this result to substitute the enthalpy for the internal energy in equation [1-46]. To simplify the derivation, we use the substantive derivative De/Dt.

$$\rho \frac{\partial e}{\partial t} + \rho u_i \frac{\partial e}{\partial x_i} = \rho \frac{De}{Dt} = \rho \left[\frac{Dh}{Dt} - \frac{1}{\rho} \frac{DP}{Dt} + \frac{P}{\rho^2} \frac{D\rho}{Dt} \right] = -\frac{\partial q_i}{\partial x_i} + \sigma_{ji} \frac{\partial u_i}{\partial x_j} \qquad [1\text{-}48]$$

From the continuity equation forms shown in equations [1-23] and [1-24], we can write Dρ/Dt as -ρΔ.

$$\frac{D\rho}{Dt} = -\rho \frac{\partial u_i}{\partial x_i} = -\rho \Delta \qquad [1\text{-}49]$$

Substituting this result into equation [1-48] gives:

$$\rho \frac{Dh}{Dt} = -\frac{\partial q_i}{\partial x_i} + \sigma_{ji} \frac{\partial u_i}{\partial x_j} + \frac{DP}{Dt} + P\Delta \qquad [1\text{-}50]$$

We can introduce the temperature, T, by using the general relationship between the thermodynamic internal energy (or the enthalpy) and other thermodynamic properties:

$$de = c_v dT - \left[\frac{T\beta_P}{\kappa_T} - P \right] \frac{d\rho}{\rho^2} \qquad [1\text{-}51]$$

$$dh = c_p dT + \left[1 - T\beta_P \right] \frac{dP}{\rho} \qquad [1\text{-}52]$$

The quantities β_P and κ_T are fluid properties giving the relative change in density at constant pressure and temperature, respectively. These are formally defined as follows:

$$\beta_P = -\frac{1}{\rho} \left(\frac{\partial \rho}{\partial T} \right)_P \qquad and \qquad \kappa_T = \frac{1}{\rho} \left(\frac{\partial \rho}{\partial P} \right)_T \qquad [1\text{-}53]$$

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For an ideal gas ($P = \rho RT$), $\beta_P = 1/T$, and $\kappa_T = 1/P$. In this case, equations [1-51] and [1-52] simplify to $de = c_v dT$ and $dh = c_p dT$.

Substituting equation [1-52] into equation [1-50] gives a differential equation for temperature that uses the constant pressure heat capacity, c_P.

$$\rho \frac{Dh}{Dt} = \rho \left(c_p \frac{DT}{Dt} + \frac{1 - \beta_P T}{\rho} \frac{DP}{Dt} \right) = -\frac{\partial q_i}{\partial x_i} + \sigma_{ji} \frac{\partial u_i}{\partial x_j} + \frac{DP}{Dt} + P\Delta \qquad [1\text{-}54]$$

Combining the DP/Dt terms gives the following result.

$$\rho c_p \frac{DT}{Dt} = -\frac{\partial q_i}{\partial x_i} + \sigma_{ji} \frac{\partial u_i}{\partial x_j} + \beta_P T \frac{DP}{Dt} + P\Delta \qquad [1\text{-}54]$$

We can also obtain an equation for the temperature that uses the constant volume heat capacity, c_v. This is done by substituting equation [1-51] into equation [1-46].

$$\rho \frac{\partial e}{\partial t} + \rho u_i \frac{\partial e}{\partial x_i} = \rho \frac{De}{Dt} = \rho \left[c_v \frac{DT}{Dt} + \frac{1}{\rho^2} \left(\frac{T\beta_P}{\kappa_T} - P \right) \frac{D\rho}{Dt} \right] = -\frac{\partial q_i}{\partial x_i} + \sigma_{ji} \frac{\partial u_i}{\partial x_j} \qquad [1\text{-}55]$$

We can use the result that $D\rho/Dt = -\rho\Delta$, from equation [1-49] to simplify equation [1-55].

$$\rho c_v \frac{DT}{Dt} = -\frac{\partial q_i}{\partial x_i} + \sigma_{ji} \frac{\partial u_i}{\partial x_j} + \left(\frac{T\beta_P}{\kappa_T} - P \right) \Delta \qquad [1\text{-}56]$$

We can write equation [1-50] for the enthalpy balance and equations [1-54] and [1-56] for the temperature in conservation form. These results are given below.

$$\frac{\partial \rho h}{\partial t} + \frac{\partial \rho u_i h}{\partial x_i} = -\frac{\partial q_i}{\partial x_i} + \sigma_{ji} \frac{\partial u_i}{\partial x_j} + \frac{DP}{Dt} + P\Delta \qquad [1\text{-}57]$$

$$c_p \left[\frac{\partial \rho T}{\partial t} + \frac{\partial \rho u_i T}{\partial x_i} \right] = -\frac{\partial q_i}{\partial x_i} + \sigma_{ji} \frac{\partial u_i}{\partial x_j} + \beta_P T \frac{DP}{Dt} + P\Delta \qquad [1\text{-}58]$$

$$c_v \left[\frac{\partial \rho T}{\partial t} + \frac{\partial \rho u_i T}{\partial x_i} \right] = -\frac{\partial q_i}{\partial x_i} + \sigma_{ji} \frac{\partial u_i}{\partial x_j} + \left(\frac{T\beta_P}{\kappa_T} - P \right) \Delta \qquad [1\text{-}59]$$

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Substitutions for Stresses and Heat Flux

Up to this point we have kept the equations completely general. In order to solve an energy equation we have to have some definition for the heat flux and the stress forces in terms of other fluid properties. For the stress terms, we will use the relations for a Newtonian fluid given by equation [1-29]. For the heat flux, we will use the Fourier relationship given in equation [1-33]. In more complex problems, particularly those involving high-temperature reacting flows, the usual Fourier heat flux may need to be augmented by one or more of the following:

- radiation heat flux,

- diffusion-thermo, i.e., a heat flux due to a temperature gradient, and

- enthalpy diffusion (a usually ignored term associated with the diffusion of species with different enthalpy values,

Using only the Fourier Law heat transfer, the source term involving the heat flux in the energy balance equation can be written as follows.

$$-\frac{\partial q_i}{\partial x_i} = -\frac{\partial}{\partial x_i}\left(-k\frac{\partial T}{\partial x_i}\right) = \frac{\partial}{\partial x_i}k\frac{\partial T}{\partial x_i} = \frac{\partial}{\partial x}k\frac{\partial T}{\partial x} + \frac{\partial}{\partial y}k\frac{\partial T}{\partial y} + \frac{\partial}{\partial z}k\frac{\partial T}{\partial z} \qquad [1\text{-}60]$$

Substituting equation [1-60] and equation [1-29] for the Newtonian stress relation into equation [1-47] for the thermodynamic internal energy balance, we obtain the following result.

$$\frac{\partial \rho e}{\partial t} + \frac{\partial \rho u_i e}{\partial x_i} = \frac{\partial}{\partial x_i}k\frac{\partial T}{\partial x_i} + \left[-P\delta_{ij} + \mu\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right) + (\kappa - \frac{2}{3}\mu)\Delta\delta_{ij}\right]\frac{\partial u_i}{\partial x_j} \quad [1\text{-}61]$$

From the definition of the Kroenecker delta, ($\delta_{ij} = 1$ if i = j and zero otherwise), and the definition of the dilatation, Δ, we can simplify the terms in this equation that involve δ_{ij} as follows.

$$\delta_{ij}\frac{\partial u_i}{\partial x_j} = \frac{\partial u_j}{\partial x_j} = \Delta \qquad [1\text{-}62]$$

With this simplification, equation [1-61] becomes.

$$\frac{\partial \rho e}{\partial t} + \frac{\partial \rho u_i e}{\partial x_i} = \frac{\partial}{\partial x_i} k \frac{\partial T}{\partial x_i} - P\Delta + \mu\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)\frac{\partial u_i}{\partial x_j} + (\kappa - \frac{2}{3}\mu)\Delta^2 \qquad [1\text{-}63]$$

The terms that are multiplied by the viscosity can be shown to be a sum of perfect squares, which must always be positive. These terms represent the dissipation of mechanical energy into heat. They are usually small except for high Mach number flows. These terms are defined as the dissipation and are usually given the symbol, Φ. In there notes we will use the symbol $\boldsymbol{\Phi_D}$ to represent the dissipation to avoid confusion with the general quantity in a balance equation. The dissipation is simply defined as all the terms in equation [1-63] that contain the viscosity.

$$\boldsymbol{\Phi_D} = \mu\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)\frac{\partial u_i}{\partial x_j} + (\kappa - \frac{2}{3}\mu)\Delta^2 \qquad [1\text{-}64]$$

With this definition, equation [1-63] may be simply written as follows.

$$\frac{\partial \rho e}{\partial t} + \frac{\partial \rho u_i e}{\partial x_i} = \frac{\partial}{\partial x_i} k \frac{\partial T}{\partial x_i} - P\Delta + \boldsymbol{\Phi_D} \qquad [1\text{-}65]$$

The temperature gradient in the Fourier law conduction term may also be written as a gradient of enthalpy or internal energy by using equations [1-51] or [1-52].

$$\frac{\partial T}{\partial x_i} = \frac{1}{c_v}\frac{\partial e}{\partial x_i} + \frac{1}{c_v}\left[\frac{T\beta_P}{\kappa_T} - P\right]\frac{1}{\rho^2}\frac{\partial \rho}{\partial x_i} \qquad [1\text{-}66]$$

$$\frac{\partial T}{\partial x_i} = \frac{1}{c_p}\frac{\partial h}{\partial x_i} - \frac{1 - T\beta_P}{\rho c_p}\frac{\partial P}{\partial x_i} \qquad [1\text{-}67]$$

Substituting equation [1-67] into equation [1-65] gives the following result.

$$\frac{\partial \rho e}{\partial t} + \frac{\partial \rho u_i e}{\partial x_i} = \frac{\partial}{\partial x_i}\frac{k}{c_v}\frac{\partial e}{\partial x_i} - P\Delta + \boldsymbol{\Phi_D} + \frac{\partial}{\partial x_i}\frac{1}{c_v}\left[\frac{T\beta_P}{\kappa_T} - P\right]\frac{1}{\rho^2}\frac{\partial \rho}{\partial x_i} \qquad [1\text{-}68]$$

In the deriving equation [1-68], we started with the energy balance equation for the thermodynamic internal energy and took the following steps: (1) substituted the Fourier Law expression for the heat flux, (2) substituted the Newtonian fluid stress relations, (3) did some simplifications and defined a dissipation term, and (4) substituted an energy gradient for a temperature gradient. If we started with equation [1-57] for the enthalpy balance and took the same steps we would obtain the following result.

$$\frac{\partial \rho h}{\partial t} + \frac{\partial \rho u_i h}{\partial x_i} = \frac{\partial}{\partial x_i} \frac{k}{c_p} \frac{\partial h}{\partial x_i} + \boldsymbol{\Phi_D} + \frac{\partial}{\partial x_i} \left[\frac{1 - T\beta_P}{\rho c_p} \right] \frac{\partial P}{\partial x_i} + \frac{DP}{Dt} \qquad [1\text{-}69]$$

If we started with the temperature equations [1-58] or [1-59], involving c_v or c_p, respectively, and repeated the process outlined in the paragraph above equation [1-69] we would obtain the equations shown below. (In these cases, we keep the temperature gradient in the final equations instead of substituting an energy or enthalpy gradient.)

$$c_p \left[\frac{\partial \rho T}{\partial t} + \frac{\partial \rho u_i T}{\partial x_i} \right] = \frac{\partial}{\partial x_i} k \frac{\partial T}{\partial x_i} + \boldsymbol{\Phi_D} + \beta_P T \frac{DP}{Dt} \qquad [1\text{-}70]$$

$$c_v \left[\frac{\partial \rho T}{\partial t} + \frac{\partial \rho u_i T}{\partial x_i} \right] = \frac{\partial}{\partial x_i} k \frac{\partial T}{\partial x_i} + \boldsymbol{\Phi_D} + \frac{T\beta_P}{\kappa_T} \Delta \qquad [1\text{-}71]$$

The Species Balance Equation

For this equation, φ is the mass fraction of species K, $W^{(K)}$. (The mass fraction symbol $W^{(K)}$ – for weight fraction, which is the same as mass fraction – to avoid confusion with the w velocity component and the mass, m. A superscript is used for the species index to avoid confusion with the coordinate subscripts.) The source term is due to the diffusive flux and the species production by chemical reaction. In a multicomponent mixture, the different species will move at different velocities as they mix. (If a fully mixed system, all species move with the same velocity.) The velocity component of species K in the ith direction is called the particular velocity of species K (in direction i) and is given the symbol $u_i^{(K)}$. The usual velocity component that was used in our balance equations, u_j, is called the mass-average velocity, when dealing with mixtures. This mass-average velocity is given by the following equation.

$$u_i = \sum_K W^{(k)} u_i^{(K)} \qquad\qquad [1\text{-}72]$$

The diffusive flux of species K, in the ith direction, has the symbol, $j_i^{(K)}$, and is given by Fick's Law, shown in the following equation.

$$j_i^{(K)} = \rho W^{(K)}(u_i^{(K)} - u_i) \qquad\qquad [1\text{-}73]$$

If we look at the inflow and outflow of species K, with its particular velocity component, $u_i^{(K)}$, across the various faces of a control volume, we can write a balance equation by noting that the net storage and outflow must be balanced by the chemical production of species K, $r^{(K)}$. This gives the following balance equation.

$$\frac{\partial \rho W^{(K)}}{\partial t} + \frac{\partial \rho W^{(K)} u_i^{(K)}}{\partial x_i} = r^{(K)} \qquad\qquad [1\text{-}74]$$

Substituting equation [1-73] into equation [1-74] gives the following result.

$$\frac{\partial \rho W^{(K)}}{\partial t} + \frac{\partial \rho W^{(K)} u_i}{\partial x_i} = -\frac{\partial j_i^{(K)}}{\partial x_i} + r^{(K)} \qquad\qquad [1\text{-}75]$$

This is the basic species balance equation. In order to proceed further with the solution of this equation we need to relate the diffusive flux to fluid properties. For an isothermal, binary system the diffusive flux is given by Fick's Law. This defines a property known as the binary diffusion coefficient; for the diffusion of two species, A and B, this coefficient is written as $\mathbf{D}_{AB}$. Fick's law is then written as follows.

$$j_i^{(A)} = -\rho \mathbf{D}_{AB} \frac{\partial W^{(A)}}{\partial x_i} \qquad\qquad [1\text{-}76]$$

A full consideration of the relationship between diffusive fluxes and flow properties would have to consider many additional effects that can contribute to a diffusive flux. These other effects include thermal diffusion, pressure diffusion, body force diffusion, and the diffusion of one species due to concentration gradients in other species. An accurate picture of diffusion in multicomponent mixtures may not be helpful when turbulent flows are involved. In such cases, a simple picture of the laminar diffusion

process will suffice since that process will usually be overwhelmed by the turbulent diffusion. In this simple picture, an average diffusion coefficient for the individual species in the mixture will be assumed and the diffusive flux for any individual species will be assumed to follow Fick's law. For simplification we assume that we can define an average diffusion coefficient for a species K in a mixture, $\mathbf{D}_{K,Mix}$, by one of the following equations.

$$\mathbf{D}_{K,Mix} = \sum_L W^{(L)}\mathbf{D}_{K\mathbf{L}} \qquad or \qquad \frac{1}{\mathbf{D}_{K,Mix}} = \sum_L \frac{W^{(L)}}{\mathbf{D}_{K\mathbf{L}}} \qquad [1\text{-}77]$$

With this definition of an average diffusion coefficient, we can write the diffusive flux, for a mixture with any number of components by the following approximate equation.

$$j_i^{(K)} = -\rho\mathbf{D}_{K,Mix}\frac{\partial W^{(K)}}{\partial x_i} \qquad [1\text{-}78]$$

If we substitute this equation for the diffusive flux into the species balance given by equation [1-75], we obtain the following result.

$$\frac{\partial \rho W^{(K)}}{\partial t} + \frac{\partial \rho W^{(K)} u_i}{\partial x_i} = \frac{\partial}{\partial x_i}\rho\mathbf{D}_{K,Mix}\frac{\partial W^{(K)}}{\partial x_i} + r^{(K)} \qquad [1\text{-}79]$$

This is our general species balance equation.

The General Equation

All the equations derived in the previous section have the following kinds of terms

- A transient term given by a time derivative
- A set of convection terms involving first order derivatives in the three coordinate directions and the velocity components in those directions
- A "diffusive" term that involves a second derivative in all space dimensions of the per-unit-mass quantity in the balance equation. All such terms involve coefficients such as viscosity, thermal conductivity, or the diffusion coefficient.

They are associated with irreversible processes that tend to smooth out gradients in flows.

- Other terms, including source terms for the quantity in the balance equation

This can be most clearly seen in the species balance equation that we just derived. We can identify the four kinds of terms in equation [1-79] as shown below.

$$\underbrace{\frac{\partial \rho W^{(K)}}{\partial t}}_{Transient} + \underbrace{\frac{\partial \rho W^{(K)} u_i}{\partial x_i}}_{Convective} = \underbrace{\frac{\partial}{\partial x_i} \mathbf{D}_{K,Mix} \frac{\partial W^{(K)}}{\partial x_i}}_{Diffusive} + \underbrace{r^{(K)}}_{Source} \qquad [1\text{-}80]$$

Here we have identified the second-derivative terms as representing a diffusive process. In the other equations that we have seen the second derivative terms represented viscous stresses and heat conduction. All of these processes have similarities at a molecular level and we can loosely use the name of diffusive for the second derivative terms in all the other balance equations that we have seen.

In expanding the nomenclature we have written above to other equations, we will rewrite equation [1-80] in the more general form shown below.

$$c \underbrace{\left[\frac{\partial \rho \phi}{\partial t} + \frac{\partial \rho u_i \varphi}{\partial x_i} \right]}_{Transient \quad Convective} = \underbrace{\frac{\partial}{\partial x_i} \Gamma^{(\varphi)} \frac{\partial \varphi}{\partial x_i}}_{Diffusive} + \underbrace{S^{(\varphi)}}_{Source} \qquad [1\text{-}81]$$

In this equation c = 1 in all equations except for the temperature-based energy equations where c may represent c_P or c_v; $\Gamma^{(\varphi)}$ represents some transport property such as the viscosity or thermal conductivity divided by heat capacity. It will generally have dimensions of mass/(length times time). In SI units, the typical $\Gamma^{(\varphi)}$ will be measured in kg/m-s. The "Source" term is a combination of true source terms, such as the production of species by chemical reactions and other terms that do not fit into the classification of transient, convection and diffusive.

In this formulation, we can represent the equation as follows.

$$\textit{\textbf{STORAGE}} + \textit{\textbf{CONVECTION}} = \textit{\textbf{"DIFFUSION"}} + \textit{\textbf{"SOURCE"}} \qquad [1\text{-}82]$$

The words transient and convection accurately describe the terms in the general equation. The second-derivative term is truly diffusion only in the species balance equation. However, in all the other equations, these terms represent some sort of transport (momentum, heat, or mass) that is driven by a gradient term. As noted above, the "Source" term will contain terms that arise from phenomena other that true source terms. In many cases, these other terms may be negligible, especially in cases where properties are constant or in the case of ideal gases.

When we derive the numerical analysis equations for the differential equations representing balance phenomena, we will start with equation [1-81]. The numerical algorithms that we derive for this equation can be applied to any balance equation. We do need to keep in mind the actual meaning of the different terms in equation [1-81] for the various balance equations. These terms are shown in Table 1-2. The derivation of these source terms is outlined below.

The basic momentum balance in equation in the jth direction is given by equation [1-31], which is copied below.

$$\frac{\partial \rho u_j}{\partial t} + \frac{\partial \rho u_i u_j}{\partial x_i} = -\frac{\partial P}{\partial x_j} + \frac{\partial}{\partial x_i}\left[\mu\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)\right] + \frac{\partial}{\partial x_j}\left[(\kappa - \frac{2}{3}\mu)\Delta\right] + \rho B_j \quad j = 1, \text{K } 3 \text{ [1-31]}$$

This equation may be rearranged as follows

$$\frac{\partial \rho u_j}{\partial t} + \frac{\partial \rho u_i u_j}{\partial x_i} = -\frac{\partial P}{\partial x_j} + \frac{\partial}{\partial x_i}\mu\frac{\partial u_j}{\partial x_i} + \frac{\partial}{\partial x_i}\mu\frac{\partial u_i}{\partial x_j} + \frac{\partial}{\partial x_j}\left[(\kappa - \frac{2}{3}\mu)\Delta\right] + \rho B_j \quad \text{[1-83]}$$

We can identify the transient, convective, and diffusive terms. All the remaining terms are considered the "Source" term. Thus, we define the "Source" term for the momentum in the jth direction as follows.

$$S^{(j)} = -\frac{\partial P}{\partial x_j} + \frac{\partial}{\partial x_i}\mu\frac{\partial u_i}{\partial x_j} + \frac{\partial}{\partial x_j}\left[(\kappa - \frac{2}{3}\mu)\Delta\right] + \rho B_j \quad \text{[1-84]}$$

With this definition, the general form for the momentum balance equation in direction j can be written as follows.

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$$\frac{\partial \rho u_j}{\partial t} + \frac{\partial \rho u_i u_j}{\partial x_i} = \frac{\partial}{\partial x_i} \mu \frac{\partial u_j}{\partial x_i} + S^{(j)}$$ [1-85]

For many numerical methods, it will be useful to address the pressure term in the momentum as a part of the solution algorithm. We consider the subdivision of the source term into a pressure gradient term and the remaining terms in equation [1-85] in the text following Table 1-2.

We can get a special case of the momentum equation for no body force terms and constant properties. For no body forces, $B_j = 0$. For constant density, $\Delta = 0$. For constant viscosity, we can bring μ outside the derivative. When we do all these three things, we get the equation below that we can manipulate in steps. First, we change the order of differentiation in the mixed second derivatives that are multiplied by the viscosity. When we do this, we obtain the dilatation, Δ, which is zero for a constant density fluid. Thus, for the simplest case considered here (constant density and viscosity and zero body force terms) the source term in the momentum equation is simply the pressure gradient.

$$S^{(j)} = -\frac{\partial P}{\partial x_j} + \mu \frac{\partial}{\partial x_i} \frac{\partial u_i}{\partial x_j} = -\frac{\partial P}{\partial x_j} + \mu \frac{\partial}{\partial x_j} \frac{\partial u_i}{\partial x_i} = -\frac{\partial p}{\partial x_i} + \mu \frac{\partial \Delta}{\partial x_j} = -\frac{\partial P}{\partial x_j}$$ [1-86]

The source terms in the various energy equations are simply found by inspection of equations [1-68] through [1-71] which are copied below. In each of these equations, the transient and convective terms are on the left-hand side and the diffusive term is the first term on the right-hand side. All the remaining terms on the right-hand side, for each of these, equations, is the source term. The source term for each of these equations is shown in Table 1-2.

$$\frac{\partial \rho e}{\partial t} + \frac{\partial \rho u_i e}{\partial x_i} = \frac{\partial}{\partial x_i} \frac{k}{c_v} \frac{\partial e}{\partial x_i} - P\Delta + \boldsymbol{\Phi_D} + \frac{\partial}{\partial x_i} \frac{1}{c_v} \left[\frac{T\beta_P}{\kappa_T} - P \right] \frac{1}{\rho^2} \frac{\partial \rho}{\partial x_i}$$ [1-68]

$$\frac{\partial \rho h}{\partial t} + \frac{\partial \rho u_i h}{\partial x_i} = \frac{\partial}{\partial x_i} \frac{k}{c_p} \frac{\partial h}{\partial x_i} + \boldsymbol{\Phi_D} + \frac{\partial}{\partial x_i} \left[\frac{1 - T\beta_P}{\rho c_p} \right] \frac{\partial P}{\partial x_i} + \frac{DP}{Dt}$$ [1-69]

27

$$c_p \left[\frac{\partial \rho T}{\partial t} + \frac{\partial \rho u_i T}{\partial x_i} \right] = \frac{\partial}{\partial x_i} k \frac{\partial T}{\partial x_i} + \boldsymbol{\Phi_D} + \beta_P T \frac{DP}{Dt}$$

[1-70]

$$c_v \left[\frac{\partial \rho T}{\partial t} + \frac{\partial \rho u_i T}{\partial x_i} \right] = \frac{\partial}{\partial x_i} k \frac{\partial T}{\partial x_i} + \boldsymbol{\Phi_D} + \frac{T\beta_P}{\kappa_T} \Delta$$

[1-71]

The various forms of the energy equation may be simplified in the following cases:

- For low Mach number flows, the dissipation is very small and can be ignored

- For constant density flows, the dilatation, Δ, is zero as are any other density derivatives.

- For ideal gases, $\beta_P = 1/T$, $\kappa_T = 1/P$

For low-Mach-number, constant density flows, the source terms in the energy equation and the temperature equation involving c_v are zero. There is a difference between an incompressible flow and a constant density flow. A constant density flow is one in which the density is constant. An incompressible flow is one in which the Mach number is nearly zero. In an incompressible flow the density may change because of temperature, but the effect of pressure on density may be ignored. Thus, a furnace may be analyzed as an incompressible flow. The large temperature variation in the furnace leads to large density variations. However, the pressure changes in the furnace that are used in the momentum equation are very small compared to the average pressure. Such a flow may be analyzed as an incompressible flow, but it is not a constant density flow.

Table 1-2 – Identification of Terms in the General Balance Equation

φ	c	$\Gamma^{(\varphi)}$	$S^{(\varphi)}$
1	1	0	0
$u = u_x = u_1$	1	μ	$-\dfrac{\partial P}{\partial x}+\dfrac{\partial}{\partial x}\mu\dfrac{\partial u}{\partial x}+\dfrac{\partial}{\partial y}\mu\dfrac{\partial v}{\partial x}+\dfrac{\partial}{\partial z}\mu\dfrac{\partial w}{\partial x}+\dfrac{\partial}{\partial x}\left[(\kappa-\dfrac{2}{3}\mu)\Delta\right]+\rho B_x$
$v = u_y = u_2$	1	μ	$-\dfrac{\partial P}{\partial y}+\dfrac{\partial}{\partial x}\mu\dfrac{\partial u}{\partial y}+\dfrac{\partial}{\partial y}\mu\dfrac{\partial v}{\partial y}+\dfrac{\partial}{\partial z}\mu\dfrac{\partial w}{\partial y}+\dfrac{\partial}{\partial y}\left[(\kappa-\dfrac{2}{3}\mu)\Delta\right]+\rho B_y$
$w = u_z = u_3$	1	μ	$-\dfrac{\partial P}{\partial z}+\dfrac{\partial}{\partial x}\mu\dfrac{\partial u}{\partial z}+\dfrac{\partial}{\partial y}\mu\dfrac{\partial v}{\partial z}+\dfrac{\partial}{\partial z}\mu\dfrac{\partial w}{\partial z}+\dfrac{\partial}{\partial z}\left[(\kappa-\dfrac{2}{3}\mu)\Delta\right]+\rho B_z$
e	1	k/c_v	$-P\Delta+\boldsymbol{\Phi_D}+\dfrac{\partial}{\partial x_i}\dfrac{1}{c_v}\left[\dfrac{T\beta_P}{\kappa_T}-P\right]\dfrac{1}{\rho^2}\dfrac{\partial\rho}{\partial x_i}$
h	1	k/c_P	$\boldsymbol{\Phi_D}+\dfrac{\partial}{\partial x_i}\left[\dfrac{1-T\beta_P}{\rho c_p}\right]\dfrac{\partial P}{\partial x_i}+\dfrac{DP}{Dt}$
T	c_P	k	$\boldsymbol{\Phi_D}+\beta_P T\dfrac{DP}{Dt}$
T	c_v	k	$\boldsymbol{\Phi_D}+\dfrac{T\beta_P}{\kappa_T}\Delta$
$W^{(K)}$	1	$\rho D_{K,Mix}$	$r^{(K)}$

Pressure in the momentum equations

CFD solutions must determine the pressure as well as the velocity components. Because of this, it is necessary to explicitly treat the pressure term, which is listed as part of the source term in Table 1-2. To do this, we define a new source term for the momentum equations, $S*^{(j)}$, which is the same as the source term in Table 1-2, except that the pressure term is removed. To do this we rewrite the general momentum equation [1-85] as follows.

$$\frac{\partial\rho u_j}{\partial t}+\frac{\partial\rho u_i u_j}{\partial x_i}=\frac{\partial}{\partial x_i}\mu\frac{\partial u_j}{\partial x_i}+S^{(j)}=-\frac{\partial P}{\partial x_i}+\frac{\partial}{\partial x_i}\mu\frac{\partial u_j}{\partial x_i}+S*^{(j)} \qquad [1\text{-}87]$$

The new source terms for equation [1-87] are shown in Table 1-3.

Table 1-3 – Identification of Terms in the General Momentum Equation			
φ	c	$\Gamma^{(\varphi)}$	$S^{*(\varphi)}$
1	1	0	0
$u = u_x = u_1$	1	μ	$\dfrac{\partial}{\partial x}\mu\dfrac{\partial u}{\partial x} + \dfrac{\partial}{\partial y}\mu\dfrac{\partial v}{\partial x} + \dfrac{\partial}{\partial z}\mu\dfrac{\partial w}{\partial x} + \dfrac{\partial}{\partial x}\left[(\kappa - \dfrac{2}{3}\mu)\Delta\right] + \rho B_x$
$v = u_y = u_2$	1	μ	$+\dfrac{\partial}{\partial x}\mu\dfrac{\partial u}{\partial y} + \dfrac{\partial}{\partial y}\mu\dfrac{\partial v}{\partial y} + \dfrac{\partial}{\partial z}\mu\dfrac{\partial w}{\partial y} + \dfrac{\partial}{\partial y}\left[(\kappa - \dfrac{2}{3}\mu)\Delta\right] + \rho B_y$
$w = u_z = u_3$	1	μ	$\dfrac{\partial}{\partial x}\mu\dfrac{\partial u}{\partial z} + \dfrac{\partial}{\partial y}\mu\dfrac{\partial v}{\partial z} + \dfrac{\partial}{\partial z}\mu\dfrac{\partial w}{\partial z} + \dfrac{\partial}{\partial z}\left[(\kappa - \dfrac{2}{3}\mu)\Delta\right] + \rho B_z$

Note that the general momentum equation [1-87] has the same form as the general transport equation [1-81], except for the addition of the pressure gradient term. This allows differencing schemes developed for the general transport equation to be applied to the momentum equation with additional steps required to handle the pressure terms.

Time derivative approach

An alternative approach to the treatment of pressure, often used in compressible flows and in some finite-element approaches, uses first-order, time-derivative equations. In this approach the various flux terms and their constitutive relations are treated as separate equations in the numerical algorithms. In these approaches the total stress term, σ_{ij}, is written as the sum of the pressure, $p\,\delta_{ij}$, and the viscous stress, τ_{ij}.

$$\sigma_{ij} = -P\delta_{ij} + \tau_{ij} \tag{1-88}$$

Comparing this equation with equation [1-29] for σ_{ij} shows that the viscous stress term is given by the following equation.

$$\tau_{ij} = \mu\left[\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right] + (\kappa - \frac{2}{3}\mu)\Delta\delta_{ij} \tag{1-89}$$

Over overall momentum balance, in of the stress, was given by equation [1-28], which is copied below.

$$\frac{\partial \rho u_j}{\partial t} + \frac{\partial \rho u_i u_j}{\partial x_i} = \frac{\partial \sigma_{ij}}{\partial x_i} + \rho B_j \qquad j = 1, \text{K } 3 \qquad \text{[1-28]}$$

Using equation [1-88] we can rewrite this general momentum balance equation as follows

$$\frac{\partial \rho u_j}{\partial t} + \frac{\partial \rho u_i u_j}{\partial x_i} = -\frac{\partial p}{\partial x_j} + \frac{\partial \tau_{ij}}{\partial x_i} + \rho B_j \qquad j = 1, \text{K } 3 \qquad \text{[1-90]}$$

Recall that the summation convention over repeated indices means that the term $\frac{\partial \tau_{ij}}{\partial x_i}$ is actually the sum of three different terms. (When equation [1-88] was substituted into equation [1-28] there was a term $-\frac{\partial p \delta_{ij}}{\partial x_i}$. However, this term may be written as $-\frac{\partial p}{\partial x_j}$, since $\delta_{ij} = 0$ if i is not equal to j.)

Equation [1-90] uses only first order derivatives, but it is necessary to use equation [1-89] to compute the viscous stress terms, τ_{ij}, in this equation. (Because the viscous stress terms are symmetric – i.e., $\tau_{ij} = \tau_{ji}$ – it is in only necessary to compute six of the nine different τ_{ij} terms.)

The solution of CFD equations, using differential equations that have only first derivatives, also uses equations [1-18], [1-41], and [1-75], copied below, for mass, energy, and species balance.

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_i}{\partial x_i} = 0 \qquad \text{[1-18]}$$

$$\frac{\partial \rho (e + \mathbf{V}^2/2)}{\partial t} + \frac{\partial \rho u_i (e + \mathbf{V}^2/2)}{\partial x_i} = -\frac{\partial q_i}{\partial x_i} + \frac{\partial u_i \sigma_{ji}}{\partial x_j} + \rho u_i B_i \qquad \text{[1-41]}$$

$$\frac{\partial \rho W^{(K)}}{\partial t} + \frac{\partial \rho W^{(K)} u_i}{\partial x_i} = -\frac{\partial j_i^{(K)}}{\partial x_i} + r^{(K)} \qquad \text{[1-75]}$$

We can use equation [1-88] to replace σ_{ij}, in the energy balance equation by the pressure and the viscous stress, τ_{ij}. Doing this and using the fact that $\delta_{ij} = 0$ if i is not equal to j, allows us to rewrite the energy balance equation as follows:

$$\frac{\partial \rho(e + \mathbf{V}^2/2)}{\partial t} + \frac{\partial \rho u_i(e + \mathbf{V}^2/2)}{\partial x_i} = -\frac{\partial q_i}{\partial x_i} + \frac{\partial P u_j}{\partial x_j} + \frac{\partial u_i \tau_{ji}}{\partial x_j} + \rho u_i B_i \qquad [1\text{-}91]$$

Since the subscripts are used as summation indices, we can replace i by j on the convection term and the heat flux gradient term without changing the result. Doing this allows us to rewrite equation [1-91] as follows

$$\frac{\partial \rho(e + \mathbf{V}^2/2)}{\partial t} + \frac{\partial \rho u_j(e + \mathbf{V}^2/2)}{\partial x_j} = -\frac{\partial q_j}{\partial x_j} + \frac{\partial P u_j}{\partial x_j} + \frac{\partial u_i \tau_{ji}}{\partial x_j} + \rho u_i B_i \qquad [1\text{-}92]$$

CFD practitioners who use the first-derivative approach derive a general algorithm from writing a vector form of the equation. This form summarizes the continuity equation [1-18], the three momentum equations implied in equation [1-90], the energy equation of equation [1-92] and the species balance of equation [1-75]. The equation they use is written as follows.

$$\frac{\partial \mathbf{U}}{\partial t} + \frac{\partial \mathbf{E}}{\partial x} + \frac{\partial \mathbf{F}}{\partial y} + \frac{\partial \mathbf{G}}{\partial z} = \mathbf{H} \qquad [1\text{-}93]$$

Where the terms $\mathbf{U}$, $\mathbf{E}$, $\mathbf{F}$, $\mathbf{G}$, and $\mathbf{H}$ are vectors (one-dimensional column matrices) defined by the following equations:

$$\mathbf{U} = \begin{bmatrix} \rho \\ \rho u \\ \rho v \\ \rho w \\ \rho(e + V^2/2) \\ \rho W^{(K)} \end{bmatrix} = \begin{bmatrix} U_1 \\ U_2 \\ U_3 \\ U_4 \\ U_5 \\ U_6 \end{bmatrix} \qquad \mathbf{H} = \begin{bmatrix} 0 \\ \rho B_x \\ \rho B_y \\ \rho B_z \\ \rho(u B_x + v B_y + w B_z) \\ r^{(K)} \end{bmatrix} = \begin{bmatrix} h_1 \\ h_2 \\ h_3 \\ h_4 \\ h_5 \\ h_6 \end{bmatrix} \qquad [1\text{-}94]$$

$$\mathbf{E} = \begin{bmatrix} \rho u \\ \rho uu + p - \tau_{xx} \\ \rho vu - \tau_{xy} \\ \rho wu - \tau_{xz} \\ u[\rho(e + V^2/2) + p]) - u\tau_{xx} - v\tau_{xy} - w\tau_{xz} - q_x \\ \rho u W^{(K)} + j_x^{(K)} \end{bmatrix} = \begin{bmatrix} e_1 \\ e_2 \\ e_3 \\ e_4 \\ e_5 \\ e_6 \end{bmatrix} \qquad [1\text{-}95]$$

$$\mathbf{F} = \begin{bmatrix} \rho v \\ \rho uv - \tau_{yx} \\ \rho vv + p - \tau_{yy} \\ \rho wv - \tau_{yz} \\ v[\rho(e + V^2/2) + p] - u\tau_{yx} - v\tau_{yy} - w\tau_{yz} - q_y \\ \rho v W^{(K)} + j_y^{(K)} \end{bmatrix} = \begin{bmatrix} f_1 \\ f_2 \\ f_3 \\ f_4 \\ f_5 \\ f_6 \end{bmatrix} \qquad [1\text{-}96]$$

$$\mathbf{G} = \begin{bmatrix} \rho w \\ \rho uw - \tau_{zx} \\ \rho vw - \tau_{zy} \\ \rho ww + p - \tau_{zz} \\ w[\rho(e + V^2/2) + p] - u\tau_{zx} - v\tau_{zy} - w\tau_{zz} - q_z \\ \rho w W^{(K)} + j_z^{(K)} \end{bmatrix} = \begin{bmatrix} g_1 \\ g_2 \\ g_3 \\ g_4 \\ g_5 \\ g_6 \end{bmatrix} \qquad [1\text{-}97]$$

The algorithms that use this format typically solve for the **U** matrix components. (In equations [1-94] and [1-98], the U_i terms refer to the components of the **U** vector, not to velocity components, u_i.)

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UNIT – II – Computational Fluid Dynamics – SCHA1403

II.   Turbulence and its Modelling

Turbulence

Whenever turbulence is present in a certain flow it appears to be the dominant over all other flow phenomena. That is why successful modeling of turbulence greatly increases the quality of numerical simulations.

All analytical and semi-analytical solutions to simple flow cases were already known by the end of 1940s. On the other hand there are still many open questions on modeling turbulence and properties of turbulence it-self. No universal turbulence model exists yet.

Ideal turbulence model

Solving CFD problem usually consists of four main components: geometry and grid generation, setting-up a physical model, solving it and post-processing the computed data. The way geometry and grid are generated, the set problem is computed and the way acquired data is presented is very well known. Precise theory is available. Unfortunately, that is not true for setting-up a physical model for turbulence flows.

The problem is that one tries to model very complex phenomena with a model as simple as possible.

Therefore an ideal model should introduce the minimum amount of complexity into the modeling equations, while capturing the essence of the relevant physics.

Complexity of the turbulence model

Complexity of different turbulence models may vary strongly depends on the details one wants to observe and investigate by carrying out such numerical simulations. Complexity is due to the nature of Navier-Stokes equation (N-S equation). N-S equation is inherently nonlinear, time-dependent, three-dimensional PDE.

Turbulence could be thought of as instability of laminar flow that occurs at

high Reynolds numbers (Re). Such instabilities origin form interactions between non- linear inertial terms and viscous terms in N-S equation. These interactions are rotational, fully time-dependent and fully three-dimensional. Rotational and three- dimensional interactions are mutually connected via vortex stretching. Vortex stretching is not possible in two dimensional space. That is also why no satisfactory two-dimensional approximations for turbulent phenomena are available.

Classification of turbulent models

Nowadays turbulent flows may be computed using several different approaches. Either by solving the Reynolds-averaged Navier-Stokes equations with suitable models for turbulent quantities or by computing them directly. The main approaches are summarized below.

Reynolds-Averaged Navier-Stokes (RANS) Models

- **Eddy-viscosity models (EVM)**

    One assumes that the turbulent stress is proportional to the mean rate of strain. Further more eddy viscosity is derived from turbulent transport equations (usually k + one other quantity).

- **Non-linear eddy-viscosity models (NLEVM)**

    Turbulent stress is modelled as a non-linear function of mean velocity gradients. Turbulent scales are determined by solving transport equations (usually k + one other quantity). Model is set to mimic response of turbulence to certain important types of strain.

- **Differential stress models (DSM)**

    This category consists of Reynolds-stress transport models (RSTM) or second-order closure models (SOC). One is required to solve transport equations for all turbulent stresses.

Computation of fluctuating quantities

- **Large-eddy simulation (LES)**

  One computes time-varying flow, but models sub-grid-scale motions.

- **Direct numerical simulation (DNS)**

  No modelling what so ever is applied. One is required to resolve the smallest scales of the flow as well.

Extend of modelling for certain CFD approach is illustrated in the following figure Figure 2.1. It is clearly seen, that models computing fluctuation quantities resolve shorter length scales than models solving RANS equations. Hence they have the ability to provide better results. However they have a demand of much greater computer power than those models applying RANS methods.
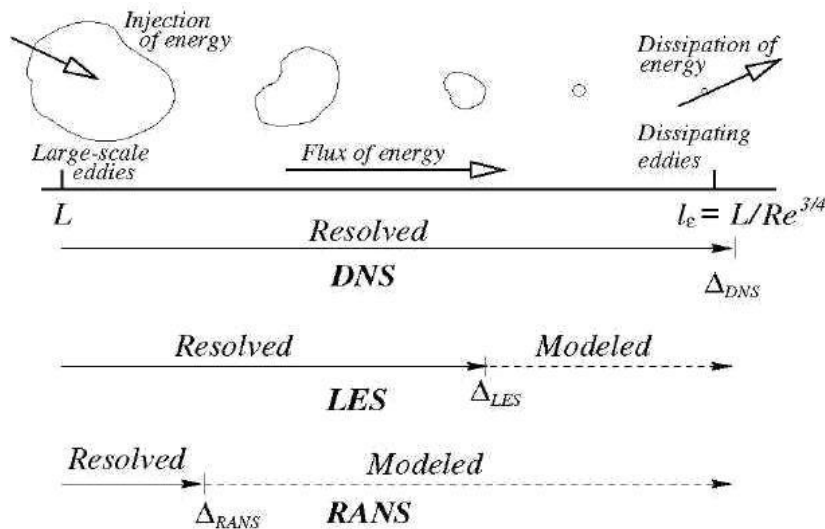

Figure 2.1 Extend of modelling for certain types of turbulent models

REYNOLDS-AVERAGED NAVIER-STOKES MODELS

The following chapter deals with the concept of Reynolds's decomposition or Further on methods how to include these ideas into certain numerical

models are presented.

Equations describing instantaneous fluid motion

For easier understanding of certain mathematical ideas it is convenient to briefly revise N-S equations describing instantaneous fluid motion at the beginning. All variables describing instantaneous flow are marked with a tilde.

Reynolds averaging

The concept of Reynolds averaging was introduced by Reynolds in 1895. One may consider Reynolds averaging in many different ways. There are three most common perceptions of this term: time averaging, space averaging or ensemble averaging.Time averaging is appropriate when considering a stationary turbulence. That is when the flow does not vary on the average in time. In such cases time average is defined by:

The closure problem

One could pretend that Reynolds stress is indeed a stress and try to write constitutive relations similar to those for viscous stress. However there is an important difference among these two stresses. Viscous stress is a property of a fluid. That is why separate experiments can be carried out in order to determine corresponding constitutive relations. These relations are valid then whenever a flow in that particular fluid is observed. On the other hand Reynolds stress is a property of the flow. Hence it is dependent on the flow variables them-selves. That is the reason why it changes from flow to flow and no general constitutive relations are available.

Laminar flow, infinitesimal fluctuations and superposition

One solution to the closure problem is to treat the flow as a laminar flow with fluctuations superimposed. One subtracts the averaged momentum equation from equation describing instantaneous motion. The result for fluctuating motion reads:

$$\frac{\partial u}{} \quad \frac{\partial u}{} = -\frac{\partial p}{\partial x_i} \quad \frac{\partial \tau_{ij}^{(v)}}{\partial x_j} - \rho u_j \quad \frac{\partial U}{\partial x}_{j}{}_i - \rho u_j \quad \frac{\partial u}{\partial x_j}^{r} - \left\langle u_j \frac{\partial u}{\partial x_j^r} \right\rangle$$

$$\rho \quad {}_{\partial}{}^{i} + \underset{\partial}{U}j \quad x^{i} \quad +$$

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UNIT – III – Computational Fluid Dynamics – SCHA1403

III. Finite Volume Method

Heat Conduction, Convection And Diffusion

CFD provides the solution to the governing equations of the flow subject to a particular initial and boundary conditions. These equations are highly nonlinear and very difficult to solve even numerically. In applying these equations to a particular problem, some of the terms may disappear or be negligible which makes the solution much simpler. Various numerical techniques are developed for each of the particular application of the general flow equations and their simplified forms. In order to introduce various computational techniques we will first consider a simple form of the momentum equation, and then discretize various forms of that equation. The momentum equation (2) for a 1 - dimensional, incompressible flow with no body force, and constant properties reduces to

The first term in equation is the transient term, the second is the convective term, the third is the diffusive term, and the fourth is the pressure term. We will consider various combinations of the terms in this equation and discuss the methods to solve them.

Transient-Diffusive Terms

Consider only the 1st and the 3rd terms in the above equation and, to further simplify, assume $v=1$:

This is the transient diffusion equation which consists of a first derivative in the time direction t and a second derivative in the space direction x . This is a parabolic partial

differential equation that can be used to model the temporal changes in the diffusion of some quantity through a medium. For instance, the transient diffusion of heat (conduction) in a solid. We will solve this equation using both a finite difference and a finite element approach.

First we will describe the domain of the problem. Lets assume the diffusion occurs along a zone with thickness L. The time is usually started from $t=0$ and it is extended in the positive direction. Once we have identified the range of this domain, we place points throughout this domain.. The spacings in the x and t directions can be the same or they may be different. Each point is labeled using i for special discretization and n for temporal discretization.
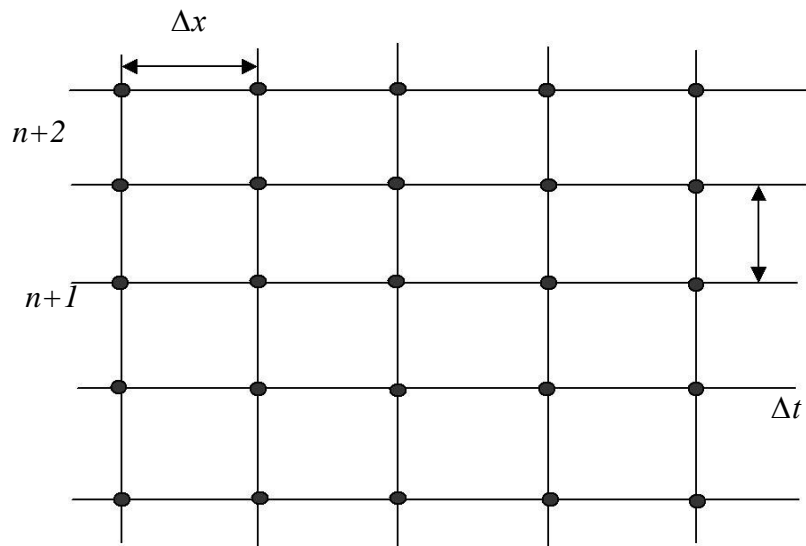
This procedure is referred to as the grid generation. Once the grid is generated one of the differencing scheme can be used to discretize the governing equation of the problem, equation (38). The type of differencing scheme used depends on the particular problem. It is mainly through testing that one may find the accuracy and efficiency of one scheme over another. One simple method to discretized the diffusion equation is to use a forward difference formula for the time derivative and a central difference formula for the spatial derivative. The discretized equation will then be

Note that the velocity at position i and time $n+1$ depends on the three values at the time level n. Thus by knowing the values of u at time level n, its value at the next time level $n+1$ can be calculated. Therefore, to start the calculation, values of u in all the domain, e.g. all the x locations, should be known. These known values at $t=0$ are known as the initial conditions.

We can generate other differencing equations. For instance, the left hand side of equation can be discretized based on the next time level $n+1$:

When a direct computation of the dependent variables can be made in terms of known quantities, the computation is said to be explicit. Some common explicit methods for parabolic partial differential equations (e.g., equation 38) are:

(1) **The Forward Time/Central Space (FTCS) method** which is represented by equation and it is stable for $\Delta t/\Delta x \leq 1/2$.

(2) **The Richardson method**, where central difference is used for both time and space and it is unconditionally unstable with no practical value:

(3) **The DuFort-Frankel Method**, which also uses central difference for both time and space, but u_i^n in the diffusion term is replace by $(u_i^{n+1} + u_i^{n-1})/2$. This modification makes the difference equations unconditionally stable.

The truncation error for DuFort-Frankel method is order of $O[(\Delta t)^2, (\Delta x)^2, (\Delta t/\Delta x)^2]$. In equation (43) the only unknown variable is u_i^{n+1}, therefore, it is explicit.

In equation , several unknown variables are related to the several known variables. This is referred to as an implicit equation. When the dependent variables are defined by coupled sets of equations, and either a matrix or iterative technique is needed to obtain the solution, the numerical method is said to be implicit. Some common implicit methods for parabolic partial differential equations are:

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UNIT – IV – Computational Fluid Dynamics – SCHA1403

IV.   CFD Methods

(1) Euler Explicit Method: An explicit differencing of equation results in the following formulation:

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} + c\frac{u_{i+1}^n - u_i^n}{\Delta x} = 0 \tag{1}$$

This is an explicit equation since only one unknown, u_i^{n+}, appears in the equation. This method is referred to as Euler Explicit Method and, unfortunately, it is unconditionally unstable and will not work for solving the wave equation. This method is first-order since the lowest-order term in the truncation error is first order, i.e., Δt, and Δx.

(2) First-Order Upwind Method: The Euler method can be made stable by using a backward difference instead of a forward difference for a positive wave speed:

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} + c\frac{u_i^n - u_{i-1}^n}{\Delta x} = 0 \tag{2}$$

 This method is stable for $0 \leq c\Delta t/\Delta x \leq 1$,   where $c\Delta t/\Delta x$ is referred to as the CFL (**Courant-Friedrichs-Lewy**) number. This method is referred to as the First-Order Upwind Method.

For discretized transport problems, the CFL number determines how many mesh cells, a fluid element passes during a timestep. For compressible flow, the definition is different. Here, the CFL number determines how many cells are passed by a propagating

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Perturbation. Hence, the wave-speed, i.e., fluid speed plus the sound speed, is employed. For explicit time-stepping schemes, such as Runge-Kutta, the CFL number must be less than the stability limit for the actual scheme to converge. For implicit and semi-implicit schemes, the CFL limit does not constitute a stability limit. On the other hand, the range of parameters in which these schemes converge may often be characterized by the CFL number.

(3) Lax Method: Another method of making the Euler equation stable is by using an average value for u_i^n based on the two neighboring points:

$$\frac{u_i^{n+1} - (u_i^n{}_{+1} + u_i^n{}_{-1})/2}{\Delta t} + c\,\frac{u_i^n{}_{+1} - u_i^n{}_{-1}}{2\Delta x} = 0 \tag{3}$$

This is referred to the Lax Method which is stable for CFL ≤ 1.

(4) Euler Implict Methods are another way of solving Euler equation:

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} + c\,\frac{u_i^n{}_{+1}{}^{+1} - u_i^n{}_{-1}{}^{+1}}{2\Delta x} = 0 \tag{4}$$

These methods are unconditionally stable for all time steps, however, a system of equations must be solved for each time level.

The above methods are all first-order accurate. More accurate second-order methods are developed to solve the PDEs describing the flow. The commonly used methods are:

(5) Leap Frog Method

$$\frac{u_i^{n+1} - u_i^{n-1}}{2\Delta t} + c\,\frac{u_{i+1}^{n+1} - u_{i-1}^{n+1}}{2\Delta x} = 0 \tag{5}$$

(6) Lax-Wendroff Method[19]

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} + c\,\frac{u_i^n{}_{+1} - u_i^n{}_{-1}}{2\Delta x} = c^2\,\frac{\Delta t}{2(\Delta x)^2}\left(u_{i+1}^n - 2u_i^n + u_i^n{}_{-1}\right) \tag{6}$$

(7) MacCormack Method[20]
This is an explicit, predictor-corrector method which is written in the following form.

$$\text{Predictor:}\qquad (u_i^{n+1})^* = u_i^n - c\,\frac{\Delta t}{\Delta x}(u_i^n{}_{+1} - u_i^n) \tag{7}$$

$$^{n+1}\quad \frac{1}{} \quad n \qquad ^{n+1}\;\; * \qquad \frac{\Delta t}{} \quad ^{n+1}\;\; * \qquad ^{n+1} \qquad *$$

49

2 Δx

Here, $(u_i^{n+1})^*$ is the predicted value for u at point i and time level $n+1$. The forward and

backward differencing used in the above equations can be changed depending on the particular problem.

(8) Second-Order Upwind Method

This is a modification of the MacCormack method where upwind (backward) differences are used in both predictor and corrector.

Predictor: $$(u_i^{n+1})^* = u_i^n - c\frac{\Delta t}{\Delta x}(u_i^n - u_i^n{}_{-1})\tag{9}$$

Corrector: $$u_i^{n+1} = \frac{1}{2}u_i^n + (u_i^{n+1})^* - c\frac{\Delta t}{\Delta x}\left[(u_i^{n+1})^* - (u_{i-1}^{n+1})^*\right] - c\frac{\Delta t}{\Delta x}\left(u_i^n - 2u_{i-1} + u_{i-2}^n\right)\tag{10}$$

The fluid dynamics of inviscid flows are governed by Euler equations. These equations may have different character for various flow regimes. For time-dependent flows, the equations are hyperbolic for all Mach numbers. Therefore, a time-marching method can be used to obtain the solution. In steady inviscid flows, the Euler equations are elliptic for subsonic conditions, and hyperbolic for supersonic conditions. Several simplified form of the Euler equations are used for inviscid flows. For instance, if the flow is incompressible, by consider the flow is irrotational as well; a solution to the Laplace's equation for the velocity potential or stream function can describe the flow field. The traditional method of solving hyperbolic PDEs are by the method of characteristics. Alternatively, there are numerous FDM based solution schemes for such flows.

The following options for the discretization of the convection operator.

(1)   Upwind Schemes:

In an upwind (UW) scheme the convection term is formed using a first-order accurate difference equation equating the velocity derivative to the values at the reference point and its nearest neighbor taken in the upstream direction. This can give very inaccurate solutions but they are easy to obtain as they converge readily. For compressible flows, UW is viewed in a different light. Here, instead of the primitive variables, a set of characteristic variables is often used. The governing equations for the characteristic variables are locally hyperbolic. Hence, their solutions are wavelike and upwind differences are the correct treatment. UW here appears under designations such as flux splitting, flux difference splitting, fluctuation splitting etc.

(2)   Hybrid Schemes:

A hybrid scheme, where the upwind scheme is used if the Reynolds number is greater than two, and central differences are used if the Reynolds number is two or less. This is more accurate than the upwind scheme but does not converge on some grids of points.

(3)   QUICK Upwind Schemes:

The quadratic upstream interpolation for convective kinetics (QUICK) scheme[31] is a quadratic upwind scheme used mainly in the finite volume formulation and is more accurate than the two schemes described above. This scheme uses a three-point upstream-weighted quadratic interpolation for cell face values. In the QUICK scheme, one adds one point in each direction and calculates the derivative using the cubic polynomial drawn through the four involved points. Local truncation error analysis shows third order accuracy. The QUICK scheme is unconditionally bounded up to cell Reynold numbers of 5. Beyond this limit, it may become unbounded. The QUICK scheme is normally applied as a correction to the donor cell scheme. In situations with unboundedness, the correction may locally be limited, thus reverting to the donor cell scheme. The QUICK scheme has a somewhat different form in finite volume contexts, since here the differences rather than the derivatives are of interest.

(4) **Power-Law Schemes:** Power-law schemes are derivatives of QUICK but are more accurate.

4.5   *Incompressible Navier-Stokes Equations*

When considering all the terms in equation a special difficulty arises due to the weak coupling of the velocity and pressure fields. For the incompressible fluids, the continuity equation is only function of velocity and not a function of pressure. Only the momentum equations contain pressure terms. Since most of the terms in the momentum equations are functions of the velocity components it is natural to use these equations to produce the solutions for the velocity components. Then, the problem is how to obtain the pressure solution, since continuity does not contain pressure. A direct method is to discretize all the equations, i.e., continuity and momentum, and solve them simultaneously. This results in a very large solution vector that contains all variables and consequently very large computational effort. There are two commonly used methods to resolve this problem: (1) pressure-based methods, and (2) methods based on the concept of artificial compressibility (also known as pseudo-compressibility).

4.5.1 *Pressure-Based Methods*

In the pressure-based method (PBM), (also known as pressure correction, uncoupled, or segregated methods) a Poisson equation for pressure corrections is formulated, and then it is updated for the pressure and velocity fields until a divergence-free velocity field is obtained. There are numerous variety of this method, some of the more popular ones are

the marker-and-cell (MAC) method, SIMPLE and SIMPLER methods, the fractional-step method, and the pressure-implicit with splitting of operators (PISO) method.

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# UNIT –V – Computational Fluid Dynamics – SCHA1403

V. Grid Generation

Building a Mesh

One of the most cumbersome and time consuming part of the CFD is the mesh generation. Although for very simple flows, mesh generation is easy, it becomes very complex when the problem has many cavities and passages. Mesh generation is basically the discretization of the computational domain. The mesh in finite difference methods consists of a set of points, which are called nodes. The finite volume method considers points that form a set of volumes which are called cells. The finite element methods use sub-volumes called elements which have nodes where the variables are defined. Values of the dependent variables, such as velocity, pressure, temperature, etc. will be described for each element.

Element Form

Various forms of elements can be used. However, the most common type in CFD programs is a hexahedron with eight nodes, one at each corner, and this is known as a brick element or volume. For two-dimensional applications the equivalent element is a four-noded quadrilateral. Some finite volume programs have now been released which have the ability to use tetrahedral in three dimensions or triangles in two dimensions. Most finite element CFD codes will allow these elements to be used together with a small range of other element types. Figure 12 shows some of the commonly used sub-domains.

3-noded triangle   4-noded triangle   square

4-noded tetrahedral   6-noded prism   8-noded hexahedral
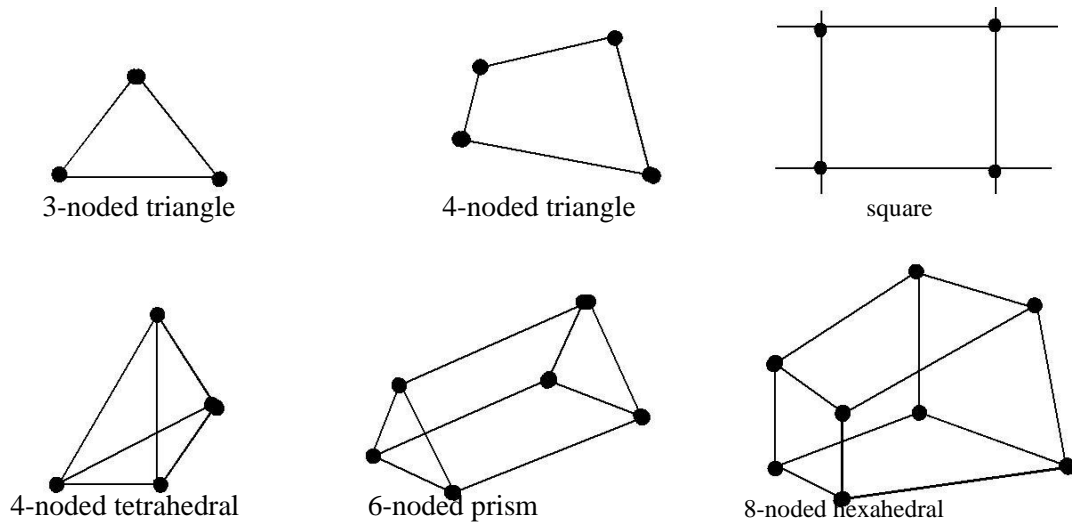
Typical computational elements.

Before generating the mesh, we should know something about the flow behavior. For

instance, where in the flow field we have boundary layers, vortices, large gradients in pressure or velocity, etc. The mesh size and shape should be such that it can capture the proper physical conditions that occur in the flow. For regions where large gradients exist,

large number of points within the mesh is needed. This is due to using very simple variation of the parameter, usually, linear, within the each element. Thus the mesh should be small enough so that a linear approximation between two points is valid.

This is depicted in Fig. 13, were the variation of function u is given along the coordinate x. We will use a linear variation between the points of a numerical solution. If a coarse mesh (Δx_L) is used for the numerical calculation of the curve, the results would be far from the actual variation. However, a fine mesh (Δx_S) can produce results which are close to the actual points. The linear approximation results in large errors where the gradient of u along x is large.
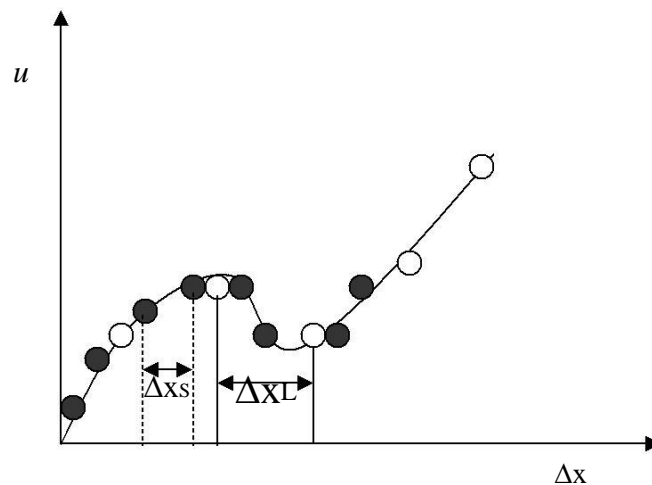
Coarse and fine mesh representation of function u.

One of the main difficulties of mesh generation is that, in many cases we do not know where the large gradients are. Usually, along the solid surfaces, where the boundary layer is developed, we need to put more points close to the surface in the direction normal to the surface. Another example is the large pressure changes close to a shock wave in compressible flows. Grid refinement is needed to resolve important flow details. Adaptive grid generation is the solution for complex physical and geometrical problems in which the location of large gradients is not predictable or varies with time, but this is beyond the scope of this text. Generally, refinement is needed near walls, stagnation points, in separation regions, and in wake regions. By increasing number of nodes better accuracy is achieved. Solution should always (if possible) be based on grid independence tests with same style and mesh arrangement.

Grid generation can be assigned to two distinct categories, structured or unstructured grids. Relating the mesh structure to the numerical method; finite difference programs require a mesh to have a regular structure and finite element programs can use a mesh

with an irregular structure. In theory finite volume programs could use a mesh with an irregular structure, but many implementations insist that the mesh has a regular structure. When a mesh with a regular structure is used there is an advantage in that the solver program should run faster than if a mesh with an irregular structure is used. This is due to the implicit relationship that exists between the number of a cell or a point and the number of its neighbors in a regular mesh, which enables data to be found easily. No such relationship occurs for meshes that have an irregular structure and so when trying to find the values of flow variables in neighboring volumes there must be a computational overhead. This often takes the form of a look-up table which relates the faces to the cells or the nodes to the elements.

Structured Grid

The main objective of generating a structured grid is to determine the coordinates transformation that maps the body fitted non-uniform non-orthogonal physical space (x,y,z) into the transformed orthogonal computational space (ξ,η,ζ).

Physical domain   Computational domain
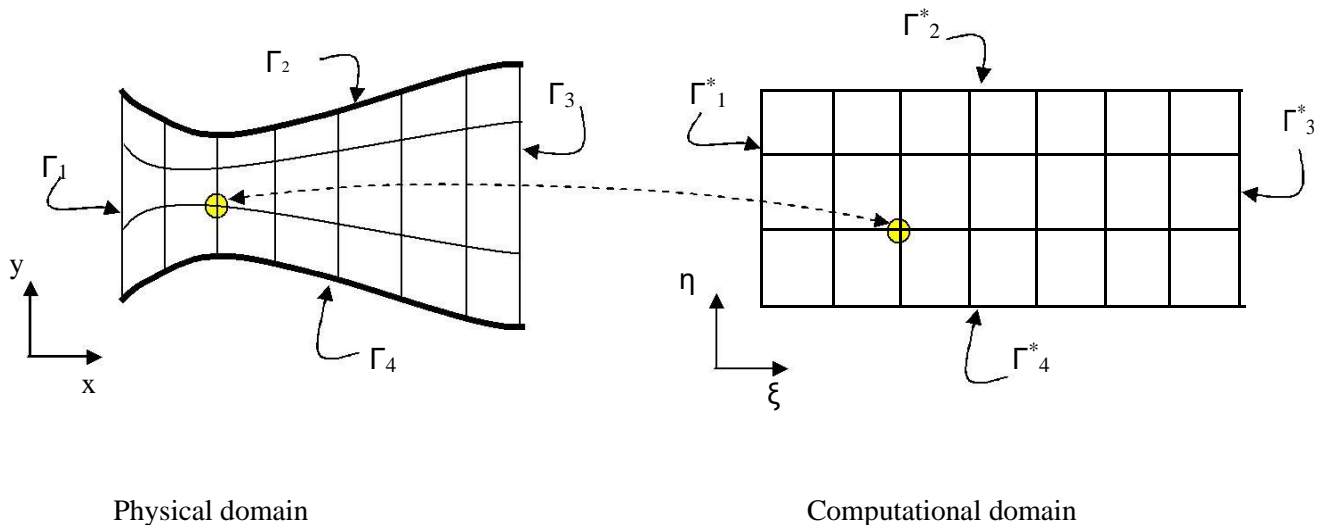
The Transformed Computational Domain

There are two steps in generating a structured grid: a) specification of the boundary point distribution, b) determination of the interior point distribution. The three popular methods for generating structured grids are:

Conformal mapping method

In a conformal mapping the angles between grid lines in computational and physical domains are the same. This is the most accurate method, but the application of this method is limited to two-dimensional problems with simple geometries.

Algebraic method

This is one of the most common methods used in commercial codes appropriate for several engineering applications. Clustering and stretching of grid elements using algebraic method can be done by different functions such as: polynomial, trigonometric, logarithmic, and geometric functions. Using the algebraic grid generation results in a good control over the grid structure and is relatively simple to apply.

Differential equation method

The partial differential equations used to generate a grid can be of elliptic, parabolic, or hyperbolic type. The most applied one is the elliptic type. In this case we want to have control over the followings:
   a) Grid point distribution on the boundaries,
   b) The angle between the boundaries and the gridlines, and
   c) The spacing between the gridlines.

Block-structured method

When the geometry is complex, it is very difficult to generate a single zone grid with adequate control on the distribution of the mesh points using structured grids. There are three main types of domain decomposition. These are patched zones, overlapped zones, and overlaid zones. Patched zones have a common boundary line (see Fig. 15). The mesh lines across the boundaries may be continuous or discontinuous[49]. In the second technique, an overlap region exists between the zones. The extent of that region may be from one up to several mesh points. In the third technique, which is also known as the Chimera method. Smaller zones are defined on top of a base grid. Inter-zone data transfer is accomplished by interpolation.

The application of block-structured grid with an algebraic grid generation for each block is explained by the following example:

Unstructured grid

Unstructured grids have the advantage of generality in that they can be made to conform to nearly any desired geometry. This generality, however, comes with a price. The grid

generation process is not completely automatic and may require considerable user interaction to produce grids with acceptable degrees of local resolution while at the same time having a minimum of element distortion. Unstructured grids require more information to be stored and recovered than structured grids (e.g., the neighbor connectivity list), and changing element types and sizes can increase numerical approximation errors.

A popular type of unstructured grid consists of tetrahedral elements (Fig. 15). These grids tend to be easier to generate than those composed of hexahedral elements, but they generally have poorer numerical accuracy. For example, it is difficult to construct approximations that maintain an accurate propagation of one-dimensional flow disturbances because tetrahedral grid elements have no parallel faces.

In summary, the best choice for a grid system depends on several factors: convenience in generation, memory requirements, numerical accuracy, flexibility to conform to complex geometries and flexibility for localized regions of high or low resolution.

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