

**CHEMISTRY,
PHYSICS, AND
LIFE SCIENCE
PRINCIPLES**

**MICROFLUIDICS
AND NANOFUIDICS
HANDBOOK**

**CHEMISTRY,
PHYSICS, AND
LIFE SCIENCE
PRINCIPLES**

EDITED BY

**SUSHANTA K. MITRA
SUMAN CHAKRABORTY**



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Preface

Microfluidics has been an important research area for the last twenty years. A number of textbooks have been printed in the last couple of years because of demand in a large variety of practical engineering and science applications. When the publisher approached us with the task to generate a handbook for this multidisciplinary area of microfluidics and nanofluidics, we tried our best to ensure that it really captures the cross-disciplinary breadth of this subject encompassing biological sciences, chemistry, physics, and engineering applications. It is often a challenge, particularly for those with engineering backgrounds, to work in this area that requires fundamental knowledge of the basic sciences. We tried our best to fill in the knowledge gap that exists with available publications by pulling together key individuals, well known in their respective areas, to author chapters that will help graduate students, scientists, and practicing engineers to understand the overall area of microfluidics and nanofluidics.

This handbook is published in two volumes. This volume, Volume I, consists of a section on Physics and Transport Phenomena and a section on Life Sciences and Related Applications. Hopefully, Volume I will provide readers with the fundamental science background that is required for the study of microfluidics and nanofluidics. Volume II begins by focusing on topics related to Experimental and Numerical Methods before moving to another section on Fabrications and Other Applications, the chapters of which vary from aerospace to biological systems. The efforts have been to include as much interdisciplinary knowledge as possible, reflecting the inherent nature of this area.

Editing a handbook of this wide breadth is not possible without active help, mentorships, and support from a large number of individuals, which include all authors and reviewers who spent long hours going through the different chapters of this handbook. Dr. Mitra specifically acknowledges the mentorship he received from Dr. M. Yovanovich during this editorial process. He also thanks the support he received from his wife Jayeeta and son Neil, who never complained about him spending long hours on this handbook. Dr. Chakraborty acknowledges with gratitude the continuous moral support that he received from his parents and his wife, without which this project could not have been realized. He also dedicates this book to his son, who saw the light of the earth for the first time very recently. Both the editors are very thankful to Michael Slaughter, Jill Jurgensen, and the rest of the publishing team at CRC Press for their cooperation and support.

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More details on his research can be obtained from the following URLs:

http://www.iitkgp.ac.in/fac-profiles/showprofile.php?emocode=bTmVW&depts_name=ME
http://sites.google.com/site/suman_chakrabortymicrofluidics/home.

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Part I

Physics and Transport Phenomena

1

An Overview of Continuum Description of Fluid Flow and Transport Processes

Debapriya Chakraborty and Suman Chakraborty

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1.1 Introduction

Solution of problems in continuum transport stems from the considerations of basic governing principles as expressed in pertinent mathematical forms, in terms of differential equations, the corresponding integral expressions, or sometimes in integro-differential forms. Examples of such equations include the ones describing conservation of mass, momentum, energy, and species. Each of these equations considers certain physical quantities as dependent variables and may be derived by invoking the basic principles of balance that influence changes in those variables.

The physical laws that are traditionally used for describing the conservation principles pertinent to fluid dynamics applications are commonly expressed in terms of mathematical statements that are valid under continuum considerations. According to the continuum hypothesis, equations describing the flow characteristics may be formulated disregarding the details of underlying molecular behavior (provided that this hypothesis itself remains

valid; see subsequent discussions). This may be achieved by describing the concerned transport phenomena through macroscopic properties such as velocity, pressure density, temperature, and concentration and their suitable spatial and temporal derivatives. The corresponding mathematical expressions may be conceptually conceived to be representing the statistically averaged behavior of sufficiently large number of molecules, disregarding their discreteness. Moreover, these equations are often closed with the aid of suitable constitutive relationships, expressions that are intrinsic to the characteristic response of a material against a given stimulus.

The aim of the present chapter is to describe the basic conservation laws in continuum fluid mechanics in a generalized conservative framework. First, we discuss the basic postulates of the continuum hypothesis on which the validity of the derivation of the corresponding equations is inherently based. Subsequently, we describe a general integral form of the conservation equations by using the Reynolds transport theorem [1]. Using this general approach, we subsequently derive the corresponding differential forms of these equations and close those with suitable constitutive relationships for representative cases. Further, we give a detailed accounting of the various possible boundary conditions consistent with the pertinent conservation equations. We also outline possible deviations from the standard continuum hypothesis for cases characterized with strong local gradients in flow properties. Finally, we discuss the occurrence of situations, in which the continuum conservation equations in their standard forms may cease to be valid altogether and mesoscopic/molecular considerations need to be explicitly invoked.

1.2 Continuum Hypothesis

The definition of fluid properties over micron or submicron scales is not often free from ambiguities. Such ambiguities stem from the fact that traditional fluid mechanics is normally concerned with the behavior of matter over dimensions that are significantly larger as compared with the molecular length scales (may be characterized loosely by average intermolecular distances, or more rigorously, by the molecular mean free path). The behavior of fluids, under such conditions, may be idealized as if the fluid were a continuous medium (continuum description). The local fluid property at a point may then be defined as the average property of all the molecules occupying a “sensitive” elemental volume chosen in the neighborhood of the point under concern [2]. The sensitive volume should be small enough for the measurement to be local enough, so that further reduction in its size does not change the value of the property. Considering a large elemental volume would invariably include the variations associated with the spatial distribution of the property, as demonstrated in Figure 1.1, preventing the analyzer in capturing the trends in variations of properties over the system scale.

On the other hand, if the volume is considered to be too small to contain only a few molecules, then statistical fluctuations with regard to the relative occupancies of the molecules in the elemental volume may give rise to locally oscillating natures in the predicted fluid properties (see Figure 1.1). If the system length scale is itself of comparable extent as that of the characteristic length scales of these local oscillations, continuum considerations may not be applicable altogether. Summarizing the above discussions, we may simply reiterate the fundamental consideration that *fluid is said to be in a continuum when the measured fluid property is constant for sensitive elemental volumes that are small as compared with the system*

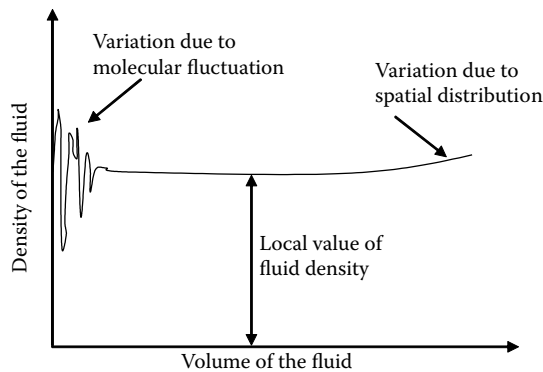


FIGURE 1.1
Variation of the density of the fluid on the volume considered.

scale but large as compared with the local scale. In the subsequent mathematical description, we would first consider this hypothesis to be valid and accordingly derive the integral and differential forms of the corresponding conservation principles.

1.3 Transport Phenomenon

1.3.1 General Concepts of Conservation

Any differential or integral equation governing transport phenomena essentially represents the principle of conservation of some physical quantity. This provides the corresponding mathematical description a concrete physical meaning. Dependent variables of different equations may represent specific properties (quantity per unit mass) pertinent to distinctive transport processes. To understand the generic form of a conservation equation of this kind, let us attempt to go through the basis of development of such an equation and describe any generic transport process in terms of variations in a scalar quantity, Φ , which may represent the pertinent dependent variable per unit mass [3]. We denote the flux of the transport variable, that is, time rate of transport per unit area normal to the direction of transport, by J . Flux of any quantity constitutes two parts—one due to the advection or the bulk motion of the molecules because of the flow, whereas other constitutes the diffusion or the gradient-based transport because of intermolecular interactions. For example, in the energy conservation equation, the diffusion or the gradient-based transport is nothing but the phenomenon of heat conduction.

Advection is the transport mechanism of a substance that is carried by the bulk motion of the medium. The flow in advection is described mathematically as a vector field. An example of advection is the transport of pollutants or silt in a river. Any substance or conserved property (such as heat) can be advected. In presence of a given flow field, the net advection flux of Φ is given by $\rho \vec{u} \Phi$, where ρ is the density of the fluid and \vec{u} is the local flow velocity. It should be noted that several authors refer to this quantity as the *convective flux*, which is not technically correct. Convection in general refers to the combined effects of both advection and diffusion.

Unlike the advection flux, the diffusion flux is independent of any bulk fluid motion. A physical perspective to the diffusion fluxes can be provided as follows. Molecules in a medium can randomly vibrate with respect to their mean positions in different directions depending on their respective degrees of freedom. These vibrations may transfer disturbances in momentum, energy, and so on from one molecule to the other, during their interactions, which can be a basic mechanism of diffusion transport (although diffusion transport is not necessarily restricted to this mechanism). A gradient of the cause (e.g., temperature gradient for the case of heat transfer) leads to the transfer of the effect (e.g., heat) from one location to another. Mathematically, the diffusion flux is proportional to the negative gradient of the scalar quantity Φ , and the proportionality constant is given by the diffusion coefficient, Γ . The diffusion flux is hence represented as $-\Gamma\nabla\Phi$ (the minus sign indicates that the flux occurs in a direction from higher value of Φ to lower value of Φ ; for example, heat conduction occurs from higher temperature to lower temperature). The net flux hence can be represented as

$$\vec{J} = \underbrace{\rho\vec{u}\Phi}_{\text{advection flux}} + \underbrace{-\Gamma\nabla\Phi}_{\text{diffusion flux}}. \quad (1.1)$$

For further analysis, let us consider a rectangular control volume (see Figure 1.2), across which the property changes smoothly (following continuum hypothesis). The control volume is essentially a specified region in space across which mass and energy can flow. Let the dimensions of the edges of the control volume be Δx , Δy , Δz , along the respective coordinate directions.

From physical considerations, it may be appreciated that the time rate of change of the quantity inside the control volume is nothing but equal to the rate of change of quantity crossing the control surface (as manifested through the flux in minus flux out) plus the rate of the quantity generated inside the control volume. The net rate of change due to the flux across the control surface may be represented as

$$\Delta J = (J_x - J_{x+\Delta x})\Delta y\Delta z + (J_y - J_{y+\Delta y})\Delta x\Delta z + (J_z - J_{z+\Delta z})\Delta x\Delta y, \quad (1.2)$$

where J_x represents the flux coming in through the surface x and $J_x + \Delta x$ represents the flux going out through the surface located at $x + \Delta x$, $\Delta y\Delta z$ being the surface areas of the corresponding faces. Similarly, changes in other directions (y , z) are also added to get the net

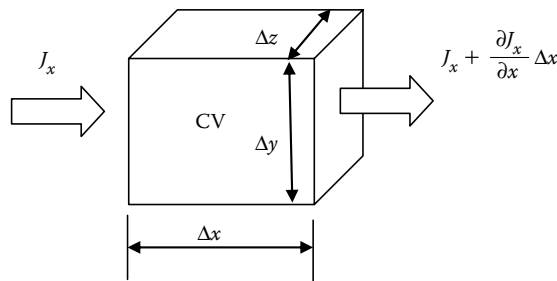


FIGURE 1.2

The flux (J_x) is entering into the control volume and $J_x + (\partial J_x/\partial x) \Delta x$ is coming out of the control volume along the direction x .

rate of transport across the control surface. Further, we may use the Taylor's series expansion to express the change of the flux J_x in the x -direction, to obtain

$$J_{x+\Delta x} - J_x = \frac{\partial J_x}{\partial x} \Delta x + O(\Delta x). \quad (1.3)$$

Using Equation 1.3 and similar forms for other two directions, Equation 1.2 may be rewritten as

$$\Delta J = (\nabla \cdot \vec{J}) \Delta x \Delta y \Delta z. \quad (1.4)$$

Finally, to complete the control volume balance, we consider a mathematical representation of the time rate of change of the conserved quantity within the control volume. To do that, we first note that the product $\rho\Phi$, of the density ρ and the specific quantity Φ , denotes the net property contained per unit volume within the control volume. The rate of change of the property per unit volume, within the control volume, is thus given by $\partial(\rho\Phi)/\partial t$. We assume that the generation (or the source) in the control volume per unit volume is S . Assembling all the components of the control volume balance (by noting that "flux in minus flux out plus generation equals the net change in flux"), we obtain the general equation for control volume conservation, as follows:

$$\frac{\partial(\rho\Phi)}{\partial t} + \nabla \cdot (\rho\vec{u}\Phi) = \nabla \cdot (\Gamma\nabla\Phi) + S. \quad (1.5)$$

We will revisit this general form again later in this chapter, by referring to the special cases of conservation of mass, momentum, and energy. It is also important to appreciate at this stage that Equation 1.5 is essentially a differential form of the general conservation statement. The same principle, nevertheless, may be expressed in suitable integral forms as well, to be described subsequently. Through the corresponding illustrations, we will also demonstrate the interchangeable manners in which the differential and integral forms may be derived from one another. This may be achieved in an elegant manner through the use of a very powerful mathematical paradigm known as Reynolds transport theorem, which we describe below.

1.3.2 Reynolds Transport Theorem

Classical laws of mechanics and thermodynamics are expressed in terms of the changes in system of fixed mass and identity. However, for situations involving fluid flow, analysis is traditionally made by referring to a specified region of space, across which mass and energy can flow. This region is commonly known as control volume, as mentioned earlier. In other words, there is a shift of paradigm from Lagrangian or particle tracking approach to Eulerian or control volume approach in fluid flow analysis because fluid is a continuously deformable medium and it may get prohibitively tedious to track individual particles during fluid motion [1,4]. Hence, it may be convenient to formulate a generalized transformation rule that can express the control mass or system-based physical principles in terms of corresponding control-volume-based physical principles, which may also imply a transformation from Lagrangian to Eulerian framework. This is achieved by invoking a theorem called Reynolds transport theorem. We would designate a generic

symbol A , which represents any arbitrary extensive property (mass, momentum, angular momentum, energy, or entropy, for example) of a system to be conserved and an associated symbol a , denoting the corresponding intensive property (extensive property per unit mass) related to A by

$$A = \int_{cv} \rho a \, d\forall, \quad (1.6)$$

where $d\forall$ is an element of the control volume \forall . In control volume formulation, the basic laws, expressed as the rate of change of A , need to be expressed in terms of the variation of the property associated with the control volume. The variation in A associated with the control volume may involve a net advective flux across the control surface. To account for this advective flux, two different configurations of the system as conceptualized over a very short time interval may be considered, so that the system coincides with the control volume in the limit as the time interval tends to zero [1]. In this limiting condition, the rate of change in the overlapped region (the intersection of the domains of the two systems at two different instants of time, which is essentially the control volume) and the flux across the regions surrounding the control volume give the net rate of change associated with the system. To elucidate this fact, we consider a system in space relative to the fixed coordinate system xyz at two different instants of time t and $t + \Delta t$ as shown in Figure 1.3.

The extensive property of the system assumes a value A_t at the time instant t , which comprises the value of the property in region I and region II, as denoted by $(A_I)_t$ and $(A_{II})_t$, respectively. The property has a value of $A_t + \Delta_t$ at the time instant $t + \Delta t$, which comprises the value of the property in region II and region III, as denoted by $(A_{II})_{t+\Delta t}$ and $(A_{III})_{t+\Delta t}$, respectively. Thus, one may write

$$A_t = (A_I)_t + (A_{II})_t \quad (1.7a)$$

$$A_{t+\Delta t} = (A_{II})_{t+\Delta t} + (A_{III})_{t+\Delta t}. \quad (1.7b)$$

From the first principle, the derivative may be expressed as the rate of change of the variable, given as

$$\left. \frac{dA}{dt} \right|_{\text{sys}} = \text{Lt}_{\Delta t \rightarrow 0} \frac{A_{t+\Delta t} - A_t}{\Delta t}. \quad (1.8)$$

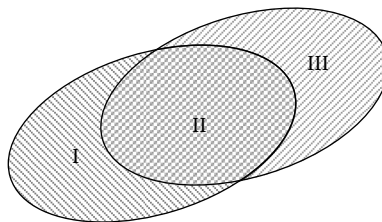


FIGURE 1.3

The system at time t and $t + \Delta t$ are the regions (I + II) and (II + III), respectively, with the overlapped region II designated as the control volume.

Substituting Equations 1.7a and 1.7b into Equation 1.8, we obtain

$$\left. \frac{dA}{dt} \right|_{\text{sys}} = \lim_{\Delta t \rightarrow 0} \frac{(A_{\text{II}})_{t+\Delta t} - (A_{\text{II}})_t}{\Delta t} + \lim_{\Delta t \rightarrow 0} \frac{(A_{\text{III}})_{t+\Delta t} - (A_{\text{I}})_t}{\Delta t}. \quad (1.9)$$

In the limit $\Delta t \rightarrow 0$, the overlapped region II of the system approaches the control volume. The first term in the right-hand side of Equation 1.9 is, accordingly, the rate of change as perceived from the control volume. The second term in the right-hand side represents the net rate of change of the quantity as it is advected across the control volume boundaries in this limit considered, or in other words may be expressed as the net rate of advective transport through the control surface, which may be expressed in an integral form as $\int_{\text{cs}} \rho a \bar{v}_r \cdot \hat{n} dS$, where \bar{v}_r represents the velocity of the fluid relative to an elemental area dS on the control surface having a unit outward normal vector as \hat{n} . Equation 1.9 may accordingly be expressed as [1]:

$$\left. \frac{DA}{Dt} \right|_{\text{sys}} = \frac{\partial}{\partial t} \int_{\text{cv}} \rho a d\forall + \int_{\text{cs}} \rho a \bar{v}_r \cdot \hat{n} dS. \quad (1.10)$$

Equation 1.10 is a mathematical statement of the Reynolds transport theorem. Different conservation equations like conservation of mass, momentum, and energy may be derived with the help of Equation 1.10 and will be illustrated in the subsequent discussions.

1.4 Conservation of Mass

Total mass of a system is conserved which leads to the fact that the rate of change of mass of a system is zero and symbolically represented by $Dm/Dt|_{\text{sys}} = 0$. The statement of conservation of mass may be obtained from the Reynolds transport theorem by considering $A = m$ (total mass of the system) and $a = 1$. Using Gauss divergence theorem, a surface integral over the control surface may be converted into an equivalent volume integral over the control volume, so that mathematically one can write $\int_{\text{cs}} \rho a \bar{v}_r \cdot \hat{n} dS = \int_{\text{cv}} \nabla \cdot (\rho a \bar{v}_r) d\forall$. Further, considering a nondeformable control volume (so that the partial time derivative may be taken inside and outside the integral interchangeably) and stationary control volume (so that relative and absolute flow velocities are identical, i.e., $\bar{v}_r = \bar{u}$), Equation 1.10 may be represented in the form [1,4]

$$\int_{\text{cv}} \left(\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \bar{u}) \right) d\forall = 0, \quad (1.11)$$

where \bar{u} is the velocity of flow. For further simplification, a mathematical rule known as the Dubois–Raymond lemma is used, which says $\int_{\text{cv}} f d\forall = 0$ always implies $f = 0$ if the control volume is arbitrary and f is continuous. Accordingly, from Equation 1.11, the differential form of the equation for conservation of mass, which is commonly known as the continuity equation, may be written as

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \bar{u}) = 0. \quad (1.12)$$

As an alternative, Equation 1.12 may also be written in Cartesian index notation as $(\partial\rho/\partial t) + (\partial/\partial x_j)(\rho u_j) = 0$. Importantly, for an incompressible flow, $D\rho/Dt = 0$. Using this fact, Equation 1.12 may be rearranged to obtain $\nabla \cdot \vec{u} = 0$, which is the condition for incompressibility of a fluid flow.

1.5 Conservation of Momentum

In a manner similar to the conservation of mass, one may also apply the Reynolds transport theorem for the balance of linear momentum. Assuming a stationary and nondeformable control volume and considering $A = m\vec{u}$ (so that $a = \vec{u}$), the linear momentum conservation principle (essentially, Newton's second law extended to control volumes) yields

$$\sum \vec{F}_{\text{ext}} = \frac{\partial}{\partial t} \int_{\text{cv}} \rho \vec{u} dV + \int_{\text{cs}} \rho \vec{u} \vec{v}_r \cdot \hat{n} dS, \quad (1.13)$$

where $\sum \vec{F}_{\text{ext}}$ represents the net external force acting on a control volume, which may be described using the summation of surface and body forces.

We first define here a few terminologies to describe the surface forces. The stress field is the distribution of internal "tractions" that balances a given set of external tractions [1,2,4]. Traction vector \vec{T}^n represents the force per unit area acting at a given location on the body's surface. It is a *bound vector*, which implies that it cannot slide along its line of action or translate to another location and keep the same meaning. In other words, a traction vector cannot be fully described unless both the force and the surface (where the force acts on) have been specified. It is defined mathematically as $\vec{T}^n = \text{Lim}_{\Delta s \rightarrow 0} \Delta \vec{F} / \Delta s$; where both ΔF and Δs are shown in Figure 1.4. The specification of \vec{T}^n , importantly, depends on the orientation of Δs as specified by its outward normal vector \hat{n} so that the traction vector is usually associated with a superscript n (\vec{T}^n), indicating the direction normal of the surface based on which the traction vector is calculated. In Cartesian index notation, the i th component of the traction vector is represented as T_i^n . Interestingly, the traction vector on a plane with arbitrary orientation may be expressed in terms of traction vector components oriented along special planes that are the Cartesian principal planes. The corresponding components of the traction vector are known as the Cartesian stress tensor components,

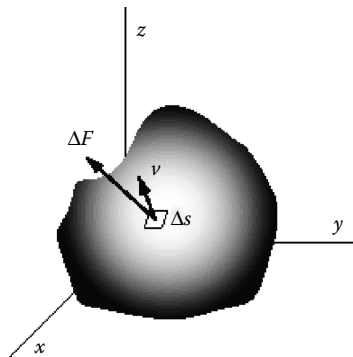


FIGURE 1.4

The traction vector is represented by the force ΔF and the area Δs on a surface with unit normal \hat{v} .

in terms of which the traction vector may be expressed, by invoking a theorem known as Cauchy’s theorem, to be illustrated subsequently.

To illustrate the Cauchy’s theorem, we first note that the components of the stress tensor are denoted in standard notation by τ_{ij} , where i is the direction normal to the face on which it is acting and j represents the direction of action of the stress (consistent with its vector sense). A representation of the stress tensor acting on a rectangular box with the unit vectors along x_1, x_2 , and x_3 is shown in Figure 1.5a. We will now attempt to find out the relation between the traction vector on any arbitrary surface and the stress tensor components. To do that, we consider a tetrahedron OABC, with three surfaces having direction normals along the principal directions and the fourth surface oriented along an arbitrary fashion. For illustration, we consider the following surfaces of the tetrahedron (Figure 1.5b): OAB (of surface area S_3) with surface normal along x_3 , OBC (of surface area S_2) with surface normal along x_2 , OAC (of surface area S_1) with surface normal along x_1 , and ABC (of surface area S) with surface normal along \hat{n} (given by $\hat{n} = n_1\hat{i} + n_2\hat{j} + n_3\hat{k}$). Under dynamic equilibrium, one can write, for the tetrahedron OABC [1]

$$F_1 = -\tau_{11}S_1 - \tau_{21}S_2 - \tau_{31}S_3 - T_1^n S + \frac{1}{3}Shb_1 = \rho \frac{1}{3}Sha_1, \tag{1.14}$$

where \bar{b} (b_1, b_2, b_3) is the body force per unit volume, \bar{a} (a_1, a_2, a_3) is the acceleration, and h is the perpendicular distance from O to ABC. Using $S_1 = Sn_1$ and taking h to be tending to zero (so that the entire tetrahedron shrinks to the point O), we obtain the generalized relation between the traction vector and the stress tensor components, which is commonly known as Cauchy’s theorem and is given by

$$T_i^n = \bar{\tau}_i \cdot \hat{n} = \tau_{ij}n_j, \tag{1.15}$$

where i th component of $\bar{\tau}$ is given by $\tau_i = \tau_{i1}\hat{i} + \tau_{i2}\hat{j} + \tau_{i3}\hat{k}$. The stress tensor is symmetric in nature. This fact may be easily derived from the considerations of the conservation of the angular momentum. Let us consider the angular momentum in the xy plane. The first moment of the stresses about the center of the bounding box is given as $\tau_{12}\Delta y\Delta x - \tau_{21}\Delta x\Delta y$

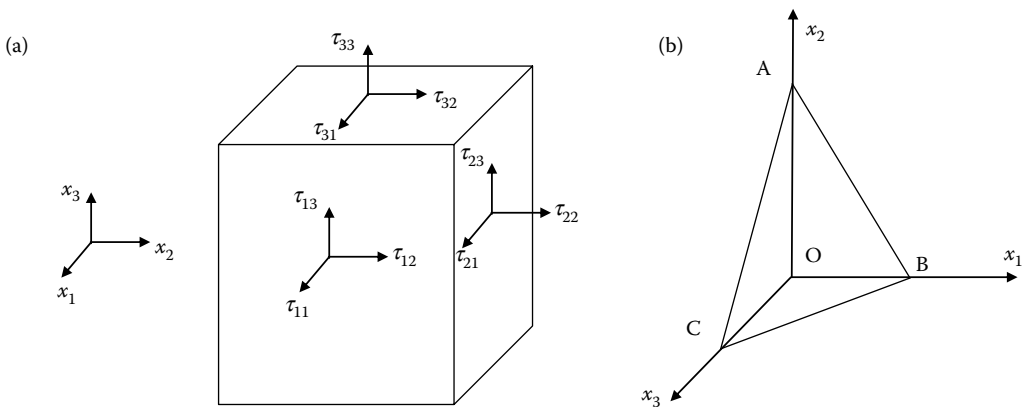


FIGURE 1.5 Representation of stress tensor. (a) The stress tensor components acting on the different surfaces of a rectangular elemental volume is shown. (b) An arbitrary tetrahedral volume (OABC) in three-dimensional space with the projections OAB, OBC, and OAC along three perpendicular planes with normal along x_1, x_2 , and x_3 .

(where Δx and Δy are the extents of the control volume box in consideration), which should be equal to moment of inertia $K\rho\Delta x\Delta y(\Delta x^2 + \Delta y^2)$ (where K is a constant) times the angular velocity ω . Now, the size of the box considered is small enough implying $\Delta x, \Delta y \rightarrow 0$, which finally leads to the symmetrical form of the stress tensor given as $\tau_{12} = \tau_{21}$, or in general $\tau_{ij} = \tau_{ji}$. Importantly, this fact holds true only when there is no net body couple present.

The net surface force on a control volume may be calculated by integrating the traction vector along the surfaces of the control volume [1,2,4,5]. Using the Cauchy's theorem along with the Gauss divergence theorem, the same may be represented in the form $\int_{cs} \bar{\tau}_i \cdot \hat{n} dS = \int_{cv} \nabla \cdot \bar{\tau}_i dV$. If b_i represents the body force per unit volume in i th direction, then the external body force along that direction can be denoted in terms of the volume integral as $\int_{cv} b_i dV$. Hence, Equation 1.10, for a stationary and nondeformable control volume, may be expressed as (using $\sum \bar{F}_{ext} = \int_{cv} (\nabla \cdot \bar{\tau}_i + b_i) dV$, $\partial/\partial t \int_{cv} \rho u_i dV = \int_{cv} (\partial(\rho u_i)/\partial t) dV$ and $\int_{cs} \rho u_i \bar{v}_r \cdot \hat{n} dS = \int_{cv} \nabla \cdot (\rho u_i \bar{v}_r) dV = \int_{cv} \nabla \cdot (\rho u_i \bar{u}) dV$):

$$\frac{\partial}{\partial t} (\rho u_i) + \frac{\partial}{\partial x_j} (\rho u_i u_j) = \frac{\partial \tau_{ij}}{\partial x_j} + b_i. \quad (1.16)$$

Equation 1.16 is known as the Navier equation of equilibrium. The above equation is essentially a general differential representation of the dynamics of a fluid, irrespective of its constitutive behavior. It is the constitutive relationship by virtue of which the final forms of the fluid flow equations differ from one another. It is also important to mention in this context that the constitutive relationships are also necessary from a pure mathematical perspective, in an effort to close the system of fluid flow equations with a matching number of unknowns.

To close the Navier equation with appropriate constitutive relationships, we first note that the stress tensor may be decomposed into two components, namely, the hydrostatic and deviatoric components. The deviatoric component is a function of the rate of deformation tensor (and hence related to the deformation of the fluid), whereas the hydrostatic part takes care of the stress tensor component that is solely dependent on the fluid pressure (which is pertinent even for a nondeforming fluid, that is, fluid at rest). The constitutive relation between the stress and strain rate for fluids is accordingly expressed as

$$\tau_{ij} = -p\delta_{ij} + \tau_{ij}^{dev}, \quad (1.17)$$

where p is the thermodynamic pressure, δ_{ij} is the Kronecker delta symbol, and τ_{ij}^{dev} is the deviatoric component of the stress vector. For Newtonian fluids, the deviatoric stress varies linearly with the strain rate (rate of deformation), which is mathematically depicted as [2]

$$\tau_{ij}^{dev} = C_{ijkl} e_{kl}, \quad (1.18)$$

where e_{kl} is the rate of deformation tensor which may be expressed in terms of the velocity gradients as $1/2((\partial u_k/\partial x_l) + (\partial u_l/\partial x_k))$, the later being the symmetric part of the strain rate tensor $(\partial u_i/\partial x_j)$. C_{ijkl} is essentially a linear transformation that maps the stress tensor (of second order) to another second-order tensor—the rate of deformation. Each index can take three values corresponding to the three Cartesian coordinate directions in space, which implies that C_{ijkl} contains 81 coefficients. Considerations of homogeneity and isotropy, as given by the Stokes postulates, lead to the reduction in number of coefficients. To achieve that reduction, we first note that because four indices are involved in C_{ijkl} , quantities

involving the repetition of these four indices need to be conjugated with C_{ijkl} to render the result an isotropic scalar (say, s). We may choose these quantities as four vectors \vec{A} , \vec{B} , \vec{C} , and \vec{D} , so that one may write [2]

$$s = C_{ijkl}A_iB_jC_kD_l. \quad (1.19)$$

If the scalar s is isotropic in nature, then it is independent of the rotation of the coordinate axes and hence is independent on the absolute orientations of the vectors chosen but is dependent only on the angle between the vectors taken two at a time (which is invariant with rotation). Because three such pairwise combinations with four vectors may be possible, one may express s as the linear combination of the product of the angles between them (as represented by dot products) taken two at a time, so that one may write

$$s = \alpha(\vec{A} \cdot \vec{B})(\vec{C} \cdot \vec{D}) + \beta(\vec{A} \cdot \vec{C})(\vec{B} \cdot \vec{D}) + \gamma(\vec{A} \cdot \vec{D})(\vec{B} \cdot \vec{C}), \quad (1.20)$$

where α , β , γ are three position-independent and direction-independent coefficients. Equation 1.20 may be written alternatively in Cartesian index notation as

$$s = A_iB_jC_kD_l(\alpha\delta_{ij}\delta_{kl} + \beta\delta_{ik}\delta_{jl} + \gamma\delta_{il}\delta_{jk}). \quad (1.21)$$

On comparing Equation 1.19 with Equation 1.21, we get

$$C_{ijkl} = \alpha\delta_{ij}\delta_{kl} + \beta\delta_{ik}\delta_{jl} + \gamma\delta_{il}\delta_{jk}. \quad (1.22)$$

Using symmetry of the stress tensor given by $\tau_{ij} = \tau_{ji}$, from Equations 1.18 and 1.22, we may easily obtain $\beta = \gamma$. Thus, using Equation 1.18, the deviatoric component of stress may be expressed as

$$\tau_{ij}^{\text{dev}} = \alpha e_{kk}\delta_{ij} + 2\beta e_{ij}. \quad (1.23)$$

Physically, the coefficient α is related to the volumetric deformation (because $e_{kk} = \partial u_k / \partial x_k$) of the fluid and is known as the volumetric dilation coefficient (commonly represented by the symbol λ in standard texts). The coefficient β is related to the shear deformation (because e_{ij} is related to the rate of deformation) of the fluid and is known as dynamic viscosity or simply viscosity (commonly represented by the symbol μ in standard texts). For homogeneous, isotropic, and Newtonian fluids, the resultant stress tensor thus assumes the following form (using Equations 1.17 and 1.23)

$$\tau_{ij} = -p\delta_{ij} + \lambda \frac{\partial u_k}{\partial x_k} \delta_{ij} + \mu \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right). \quad (1.24)$$

It needs to be noted here that the thermodynamic pressure, p , as appearing in Equation 1.24, is conceptually different from the mechanical pressure, p_m (which is negative of the arithmetic mean of the normal stress components). These two pressures are related by

$$-p_m = -p + \kappa \frac{\partial u_k}{\partial x_k}, \quad (1.25)$$

where $\kappa (= \lambda + \frac{2}{3}\mu)$ is known as the bulk viscosity. It may be hypothesized that p_m and p are equal when κ is equal to zero (yielding $\lambda = -\frac{2}{3}\mu$); this is known as the Stokes hypothesis. This hypothesis holds true when the characteristic time scales in the system are large compared with the molecular relaxation time (which is true for most cases). Fundamentally, the mechanical pressure accounts for the translational degrees of freedom of the molecules only, whereas the thermodynamic pressure accounts for the combination of translational, rotational, and vibrational degrees of freedom. For a dilute monoatomic gas, there is no vibrational and rotational degree of freedom, so that the mechanical pressure is identically equal to the thermodynamic pressure without any approximation. The equality of these two pressures is also valid when the flow is incompressible ($\partial u_k / \partial x_k = 0$). The Stokes hypothesis may be violated for typical cases in which the system undergoes transients that are characteristically much more rapid than the timescales over which the system may equilibrate or relax. For example, one may cite the cases of alternating rapid expansions and contractions of bubbles under an external stimulus at a rate more rapid than molecular relaxation rates. However, in most other practical cases, such effects are not prominent, and one may safely use the Stokes hypothesis without incurring errors. In such cases, combining Equations 1.12, 1.16, 1.24, and 1.25, one may obtain the celebrated Navier–Stokes equation, as follows:

$$\rho \left(\frac{\partial u_i}{\partial t} + u_j \frac{\partial u_i}{\partial x_j} \right) = -\frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j} \left(\mu \frac{\partial u_i}{\partial x_j} \right) + \frac{\partial}{\partial x_k} \left(\frac{\mu}{3} \frac{\partial u_k}{\partial x_k} \right) + b_i. \quad (1.26)$$

It needs to be remembered that Equation 1.26 is valid only for a homogeneous, isotropic, Newtonian, and Stokesian fluid (i.e., a fluid that obeys Stokes hypothesis). For a non-Stokesian fluid, the coefficient $\mu/3$ appearing in Equation 1.26 needs to be replaced with the bulk viscosity, κ . In general, a limit on the value of κ may be arrived at by noting the following thermodynamic relationship, $T ds = di + p dv$ (where s is the specific entropy, i is the specific internal energy, and v is the specific volume), and the first law of thermodynamics for a system, $\delta q = di + p_m dv$ (where q is the specific heat transfer). Because $\delta q \leq T ds$ (Clausius inequality), it follows $p - p_m \geq 0$, that is, $\kappa \geq 0$.

1.5.1 Non-Newtonian Fluids

Until this stage, we have considered fluids having linear stress–strain rate characteristics passing through the origin. However, in many practical situations, we come across different types of fluids that do not conform to such constitutive behavior [4,5]. Such fluids are termed as non-Newtonian fluids. Some of the common fluids that we use in daily life such as ketchup, tooth paste, starch suspensions, paint, blood, shampoo, and molten polymers fall in the category of non-Newtonian fluids. Although the concept of viscosity (apparent viscosity, to be more specific) is commonly used to characterize these materials, it can be inadequate to describe the mechanical behavior of a substance. These are best studied through several other rheological properties that relate the relations between the stress and the strain rate tensors under many different flow conditions, such as oscillatory shear, or extensional flow that is measured using different devices known as rheometers. The properties are better studied using tensor-valued constitutive equations, which are common in the field of continuum mechanics.

Some non-Newtonian fluids may have a linear stress–strain rate relationship, but unlike Newtonian fluids, these require a finite yield stress before showing their ability to flow.

Such fluids, known as Bingham plastics, have shear stress versus shear strain rate curves characterized with an offset from the origin. Examples of such fluids are clay suspensions, toothpaste, mayonnaise, chocolate, mustard, and ketchup. Another example of non-Newtonian behavior is the suspension of starch (e.g., corn flour) in water. Sudden application of force, for example, by stabbing the surface with a finger, or rapidly inverting the container holding it, leads to the fluid behaving like a solid rather than a liquid. Such fluids possess “shear thickening” property, that is, they tend to lose their fluidity (flowing ability) under the application of shear stress. Shear thickening (or dilatant) fluids are also used in wheel drive systems where a viscous coupling unit is used for power transmission. The increment of apparent viscosity with increases in the shear rate for dilatant fluids may be due to the shift of a closely packed particulate system to a more open arrangement under shear, which may entrap some of the liquid. In contrast to this behavior, some of the fluids become more fluidic (“shear thinning,” or “pseudoplastic”) only when a shear is applied. The most common example refers to paints that flow off readily when it is applied to a surface, although it does not drip from the surface when the shear is removed. The reason for which the apparent viscosity of a pseudoplastic fluid decreases with increase in the shear rate may be qualitatively attributed to a breakdown of loosely bonded aggregates by the shearing effect of flow. Biofluids like blood typically fall in this category and may be modeled as a power law fluid with the stress varies as n th power of the strain rate, where $0 < n < 1$. Fluids belonging to the category of Hershel–Buckley are also special types of non-Newtonian fluids (more general versions of Bingham plastics and pseudoplastics), possessing a yield stress beyond which they become pseudoplastic. For graphical representations of shear stress versus rate of deformation for typical non-Newtonian fluids, Figure 1.6 may be referred to.

There are fluids whose strain rates vary with time. Figure 1.7 shows flow curves for two common classes of purely viscous time-dependent non-Newtonian fluids. It is seen that such fluids have a hysteresis loop or memory whose shape depends on the time-dependent rate at which the shear stress is applied. Curve (a) illustrates a pseudoplastic time-dependent fluid and curve (b) represents a dilatant time-dependent fluid. These are called, respectively, as thixotropic and rheopectic fluids. Apparent viscosity of a thixotropic fluid decreases with time under constant shear because of particle agglomeration.

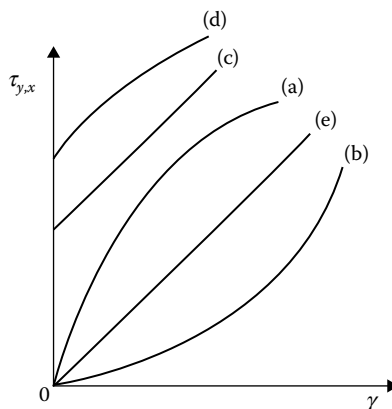


FIGURE 1.6

Flow curves for viscous, time-dependent fluids: (a) pseudoplastic, (b) dilatant, (c) Bingham plastic, (d) Hershel–Buckley, and (e) Newtonian.

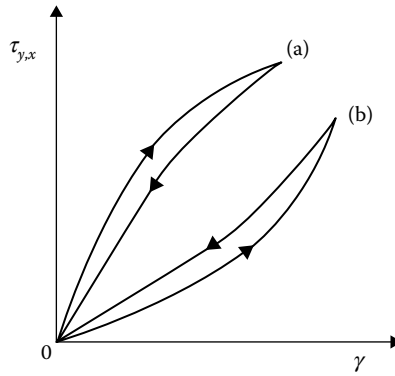


FIGURE 1.7
Flow curves for viscous, time-dependent fluids: (a) thixotropic and (b) rheopectic.

Classical example is water suspension in bentonitic clay, which is a typical drilling fluid used in the petroleum industry. Fluids for which the apparent viscosity decreases with increase in time for a given shear rate are called as rheopectic fluids. Examples of rheopectic fluids include gypsum pastes and printers inks.

The study of non-Newtonian fluid is a vast chapter in itself, and hence further elucidation of this topic is not considered in this chapter. Interested readers are asked to refer to Astarita and Marrucci [6].

1.5.2 Considerations of Rotating Reference Frame

In the preceding discussions, we have formulated the conservation equations for a control volume without considering any control volume rotation. However, in addition to a rectilinear motion, a control volume may have rotational motion as well. To extend the preceding formulation toward that case, we revisit the Newton's laws of motion in a stationary or fixed reference frame, given by

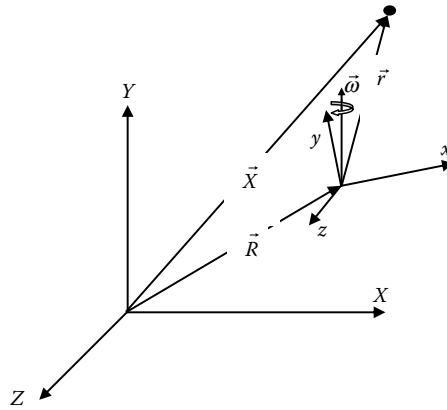
$$\vec{F} = \int_{\text{sys}} \vec{a}_{XYZ} dm, \quad (1.27)$$

where \vec{a}_{XYZ} is the acceleration with respect to the stationary reference XYZ , which has to be related to \vec{a}_{xyz} , the acceleration with respect to a rotating reference frame xyz . The origin of xyz is located at a position vector \vec{R} relative to XYZ . Further, xyz rotates at an angular velocity $\vec{\omega}$ (see Figure 1.8).

Thus, the position \vec{X} of a particle relative to XYZ may be related to the position of the same particle having a position of \vec{r} with respect to xyz as $\vec{X} = \vec{R} + \vec{r}$. The velocity of the particle in stationary reference frame is denoted by $\vec{V}_{XYZ} = d\vec{X}/dt$ and is related to the velocity in the rotating frame as [1]

$$\vec{V}_{XYZ} = \vec{V}_R + \frac{d\vec{r}}{dt}, \quad (1.28)$$

where $\vec{V}_R (=d\vec{R}/dt)$ is the velocity of the rotating reference frame with respect to the stationary frame of reference. The term $d\vec{r}/dt$ may be related to the velocity in rotating frame


FIGURE 1.8

The position of a particle from the stationary reference frame (XYZ) and rotating reference frame (xyz).

using simple vector algebra to obtain

$$\frac{d\vec{r}}{dt} = \vec{V}_{xyz} + \vec{\omega} \times \vec{r}. \quad (1.29)$$

Substituting Equation 1.29 in Equation 1.28, we obtain an expression relating the velocity in these two frames as

$$\vec{V}_{XYZ} = \vec{V}_R + \vec{V}_{xyz} + \vec{\omega} \times \vec{r}. \quad (1.30)$$

We differentiate each of these terms in Equation 1.30 to get

$$\frac{d\vec{V}_{XYZ}}{dt} = \vec{a}_{XYZ}; \quad \frac{d\vec{V}_R}{dt} = \vec{a}_R \quad (1.31a)$$

$$\frac{d\vec{V}_{xyz}}{dt} = \vec{a}_{xyz} + \vec{\omega} \times \vec{V}_{xyz} \quad (1.31b)$$

$$\frac{d(\vec{\omega} \times \vec{r})}{dt} = \dot{\vec{\omega}} \times \vec{r} + \vec{\omega} \times (\vec{V}_{xyz} + \vec{\omega} \times \vec{r}) \quad (1.31c)$$

Assembling the terms, we obtain an expression for the acceleration as [1]

$$\vec{a}_{XYZ} = \vec{a}_R + \vec{a}_{xyz} + 2\vec{\omega} \times \vec{V}_{xyz} + \vec{\omega} \times (\vec{\omega} \times \vec{r}) + \dot{\vec{\omega}} \times \vec{r}. \quad (1.32)$$

Physically, \vec{a}_{XYZ} represents the rectilinear acceleration of a particle relative to fixed reference frame XYZ , \vec{a}_R represents the rectilinear acceleration of the origin of moving frame of reference xyz from the fixed frame XYZ , \vec{a}_{xyz} represents the rectilinear acceleration of a particle relative to moving reference frame xyz (in rotating frame), $2\vec{\omega} \times \vec{V}_{xyz}$ is the Coriolis component of acceleration of the particle experienced in a noninertial frame of reference, $\vec{\omega} \times (\vec{\omega} \times \vec{r})$ is the centripetal acceleration due to the rotation of the moving frame xyz , and

$\dot{\vec{\omega}} \times \vec{r}$ is the tangential component of acceleration due to angular acceleration of moving reference frame xyz . From Newton's law, the force acting on a system may be related to the mass of the system (M) and acceleration by $\vec{F}_{\text{sys}} = \int_{M(\text{system})} \vec{a}_{xyz} dm$. In the rotating reference frame, the external force \vec{F} is the sum of net surface forces (\vec{F}_S) and the net body force (\vec{F}_B) acting on a control volume, which may be represented in terms of volume integrations using $dm = \rho dV$ as

$$\vec{F}_S + \vec{F}_B - \int_{V(\text{system})} (\vec{a}_R + 2\vec{\omega} \times \vec{V}_{xyz} + \vec{\omega} \times (\vec{\omega} \times \vec{r}) + \dot{\vec{\omega}} \times \vec{r}) \rho dV = \int_{V(\text{system})} \vec{a}_{xyz} \rho dV. \quad (1.33)$$

The right-hand side of Equation 1.33 is the rate of change of momentum \vec{P}_{xyz} of the system measured relative to the frame xyz . Using the Reynolds transport theorem, with $A = \vec{P}_{xyz}$ and $a = \vec{V}_{xyz}$, Equation 1.33 may be rewritten as

$$\vec{F}_S + \vec{F}_B - \int_{CV} (\vec{a}_R + 2\vec{\omega} \times \vec{V}_{xyz} + \vec{\omega} \times (\vec{\omega} \times \vec{r}) + \dot{\vec{\omega}} \times \vec{r}) \rho dV = \frac{\partial}{\partial t} \int_{CV} \vec{V}_{xyz} \rho dV + \int_{CS} \vec{V}_{xyz} \rho \vec{V}_{xyz} \cdot d\vec{A}. \quad (1.34)$$

These effects of the rotating reference frame may be accounted in Navier–Stokes equation (Equation 1.26) with three additional terms in body force

$$b_i = -\rho(\vec{a}_R + 2\vec{\omega} \times \vec{V}_{xyz} + \vec{\omega} \times (\vec{\omega} \times \vec{r}) + \dot{\vec{\omega}} \times \vec{r}). \quad (1.35)$$

1.6 Conservation of Energy

The statement of conservation of energy may be derived from the Reynolds transport theorem by considering $A = E$, where E is the total energy of the system, comprising the internal energy (mi), the kinetic energy ($mv^2/2$), and the potential energy (mgz), where m is the mass of the system. To begin with, we express Equation 1.10 with $a = e$, where e is E (energy) per unit mass (or in other words, the specific energy), to yield [3]

$$\left. \frac{dE}{dt} \right|_{\text{sys}} = \frac{\partial}{\partial t} \int_{CV} (\rho e) dV + \int_{CS} \rho e (\vec{v}_r \cdot \hat{n}) dS \quad (1.36)$$

Using the consideration of nondeformable control volume, using Gauss divergence theorem along with the continuity Equation 1.12, right-hand side of Equation 1.36 may be written as $\int_{CV} \rho (De/Dt) dV$. From the first law of thermodynamics, the rate of change of total energy of a system (left-hand side of Equation 1.36) may be expressed as the difference of the rate of heat transfer from a system and the rate of work done (with the sign convention that work done by the system and heat transfer to the system are positive).

In a small time interval, the changes in system may be conceived as the corresponding ones in the control volume. The net heat transfer associated with a control volume is a combined consequence of the heat generated inside the control volume and the heat

transferred across the control surface, which may be expressed mathematically as [7]

$$\dot{Q}_{cv} = \int_{cv} Q''' dV - \int_{cs} \vec{q}'' \cdot \hat{n} dS, \quad (1.37)$$

where Q''' is the volumetric heat generation per unit volume and \vec{q}'' is the net heat flux out of the control surface (the negative sign stems from the fact that heat transfer to the control volume is taken to be positive by sign convention). Using Gauss divergence theorem, Equation 1.37 may be expressed as

$$\dot{Q}_{cv} = \int_{cv} \left[Q''' - \frac{\partial q_i}{\partial x_i} \right] dV. \quad (1.38)$$

The work done associated with the control volume is a combined consequence of the work done by the body force, b_i (per unit volume), given by $\int_{cv} b_i u_i dV$, and the work done by the surface forces as given by $\int_{cs} (T_i^n u_i) dS$. The net rate of work done associated with the control volume may be expressed by using the Gauss divergence theorem, to yield:

$$\dot{W}_{cv} = \int_{cv} \left[b_i u_i + \frac{\partial(\tau_{ij} u_i)}{\partial x_j} \right] dV. \quad (1.39)$$

For any arbitrary choice of control volume, Equations 1.36, 1.38, and 1.39, combined together, yield

$$\rho \frac{De}{Dt} = Q''' - \frac{\partial q_i}{\partial x_i} + b_i u_i + \frac{\partial(\tau_{ij} u_i)}{\partial x_j}. \quad (1.40)$$

Equation 1.40 represents the statement of conservation of total energy—mechanical and thermal. At this stage, we are interested in the statement of conservation for the thermal energy, an expression for which may be obtained by subtracting the equation for mechanical energy (obtained by multiplying u_i with Equation 1.26) from the equation of total energy (Equation 1.40), so that one gets

$$\rho \frac{Di}{Dt} = Q''' - \frac{\partial q_j}{\partial x_j} + \tau_{ij} \frac{\partial u_i}{\partial x_j}. \quad (1.41)$$

The product $\tau_{ij} \partial u_i / \partial x_j$ for homogeneous, isotropic, Newtonian, and Stokesian fluid may be obtained by multiplying the expression given by Equation 1.24 with $\partial u_i / \partial x_j$ to obtain

$$\tau_{ij} \frac{\partial u_i}{\partial x_j} = -p \nabla \cdot V + \mu \Phi, \quad (1.42)$$

where $\mu \Phi$ represents the viscous dissipation term (physically accounting for an irreversible of work done to overcome viscous shear effects into intermolecular forms of energy),

given by [7]

$$\Phi = \frac{2}{3} \left[\left(\frac{\partial u_1}{\partial x_1} - \frac{\partial u_2}{\partial x_2} \right)^2 + \left(\frac{\partial u_1}{\partial x_1} - \frac{\partial u_3}{\partial x_3} \right)^2 + \left(\frac{\partial u_2}{\partial x_2} - \frac{\partial u_3}{\partial x_3} \right)^2 \right] + \left[\left(\frac{\partial u_1}{\partial x_2} + \frac{\partial u_2}{\partial x_1} \right)^2 + \left(\frac{\partial u_1}{\partial x_3} + \frac{\partial u_3}{\partial x_1} \right)^2 + \left(\frac{\partial u_2}{\partial x_3} + \frac{\partial u_3}{\partial x_2} \right)^2 \right]. \quad (1.43)$$

It is important to note that the viscous dissipation term is always positive. Equation 1.41 may also be expressed in terms of the specific enthalpy by using the property relation: $\rho i = \rho h - p$, where h is the specific enthalpy. Accordingly, Equation 1.41 along with Equation 1.42 may be expressed as [7]

$$\rho \frac{Dh}{Dt} + \frac{Dp}{Dt} = Q''' - \frac{\partial q_j}{\partial x_j} + \mu \Phi. \quad (1.44)$$

For a simple compressible pure substance without phase change, h is a function of temperature (T) and pressure (p). From thermodynamic considerations, these may be related as

$$dh = \left. \frac{\partial h}{\partial T} \right|_p dT + \left. \frac{\partial h}{\partial p} \right|_T dp = C_p dT + \left. \frac{\partial h}{\partial p} \right|_T dp, \quad (1.45)$$

where C_p is the specific heat at constant pressure. From the property relationship, h may be expressed as

$$dh = T ds + v dp, \quad (1.46)$$

where s is the specific entropy. Because entropy is a state function, it may be represented as

$$ds = \left. \frac{\partial s}{\partial T} \right|_p dT + \left. \frac{\partial s}{\partial p} \right|_T dp. \quad (1.47)$$

The entropy is not a measurable quantity and hence we use the Maxwell relationship to express it in terms of other measurable parameters: $\left. \frac{\partial s}{\partial p} \right|_T = -\left. \frac{\partial v}{\partial T} \right|_p$. Substituting Equation 1.47 in Equation 1.46 and using the Maxwell relationship along with the definition of the compressibility factor: $\beta = (1/v)(dv/dT)|_p$, one gets

$$\frac{Dh}{Dt} = C_p \frac{DT}{Dt} + v(1-\beta T) \frac{Dp}{Dt}. \quad (1.48)$$

Using Equation 1.48 along with Equation 1.45 and considering the Fourier law of heat conduction to be valid ($\vec{q}'' = -k\nabla T$), the governing equation for the temperature variation is given by

$$\rho C_p \frac{DT}{Dt} = \beta T \frac{Dp}{Dt} + Q''' + \nabla(k\nabla T) + \mu \Phi. \quad (1.49)$$

1.7 Entropy Generation

The statement of second law is indicative of a property called *entropy*, which measures the degree of disorder or randomness of a system. The entropy of universe always increases, and the difference in the entropy of initial and final states of a system is known as entropy generation, which is positive for any physical system [4,7]. The change in entropy is related to the change of internal energy i for a simple compressible pure substance without any phase change:

$$T dS = di + p dv, \quad (1.50)$$

where S is the entropy of the system and v is the specific volume. The rate of change of entropy is expressed by taking the derivatives with respect to time and substituting specific volume v as inverse of the density ($=1/\rho$), resulting in

$$T \frac{dS}{dt} = \frac{Di}{Dt} - \frac{p}{\rho^2} \frac{D\rho}{dt}. \quad (1.51)$$

Substituting internal energy equation given by Equation 1.41 along with Equation 1.42 and continuity equation $D\rho/Dt = -\rho \nabla \cdot \mathbf{V}$ in Equation 1.51 yields

$$\rho T \frac{DS}{Dt} = Q''' - \frac{\partial q_j}{\partial x_j} + \mu \Phi. \quad (1.52)$$

The entropy balance equation may be derived using the Reynolds transport theorem Equation 1.10 by considering $A = S$ with $a = s$, where s is the specific entropy for a stationary control volume to give

$$\left. \frac{dS}{dt} \right|_{\text{sys}} = \frac{\partial}{\partial t} \int_{\text{cv}} \rho s dV + \int_{\text{cs}} \rho s (\bar{\mathbf{V}} \cdot d\bar{\mathbf{A}}). \quad (1.53)$$

Using the Gauss divergence theorem ($\int_{\text{cs}} \rho s (\bar{\mathbf{V}} \cdot d\bar{\mathbf{A}}) = \int_{\text{cv}} \nabla \cdot (\rho s \bar{\mathbf{V}}) dV$) along with the continuity equation, Equation 1.53 may be expressed as

$$\left. \frac{dS}{dt} \right|_{\text{sys}} = \int_{\text{cv}} \rho \frac{Ds}{Dt} dV. \quad (1.54)$$

For a reversible process, the change in entropy of a system is given by the heat transferred through that process per unit temperature. However, any arbitrary process involves entropy generation (S_{gen}), and the balance in entropy is expressed through

$$(S_2 - S_1)_{\text{sys}} = \int \frac{\delta Q}{T} + S_{\text{gen}}. \quad (1.55)$$

Dividing Equation 1.55 by Δt and in the limit $\Delta t \rightarrow 0$, we obtain

$$\left. \frac{dS}{dt} \right|_{\text{sys}} = \frac{\dot{Q}_{\text{cv}}}{T} + \dot{S}_{\text{gen}}. \quad (1.56)$$

Expressing in terms of the volume integral and using Equation 1.38

$$\left. \frac{dS}{dt} \right|_{\text{sys}} = \int_{\text{cv}} \left(-\nabla \cdot \left(\frac{\bar{q}''}{T} \right) + \frac{Q'''}{T} + S''_{\text{gen}} \right) dV. \quad (1.57)$$

Comparing Equation 1.57 with Equation 1.54 gives

$$\rho \frac{ds}{dt} = -\nabla \cdot \left(\frac{\bar{q}''}{T} \right) + \frac{Q'''}{T} + S''_{\text{gen}}. \quad (1.58)$$

Assuming Fourier's law of heat conduction to be valid, multiplying Equation 1.58 with T and equating it with Equation 1.52 yields the expression for the entropy generation as [4]

$$S''_{\text{gen}} = \frac{\mu \Phi}{T} + k \frac{(\nabla T)^2}{T^2}. \quad (1.59)$$

The viscous dissipation Φ is always positive. An explicit analysis of second law is not required for most of the commonly encountered fluids, where μ and k are both considered positive. For the case of inviscid and nonheat conducting flows, the entropy is preserved along the particle paths.

1.8 General Equation of Conservation

We have derived separate equations for mass, momentum, and energy conservation, starting from the Reynolds transport theorem. Interestingly, all these equations may be cast in the general conservative form as depicted by Equation 1.5. The generalized conservation equation [3], accordingly, can represent the equations for conservation of mass momentum and the energy by modifying the scalar variable, the diffusion coefficient, and the source term, as represented in Table 1.1.

1.9 Boundary Conditions

The differential equations are incomplete without the specification of boundary conditions. The boundary conditions are specified in different forms—by specification of the value of the dependent variable, by specification of the gradient of the dependent variable, or by specifying the dependent variable as a function of its gradient. Such conditions are termed as Dirichlet, Neumann, and mixed boundary conditions, respectively. In case there is a periodicity in the problem description, periodic boundary conditions may also be used. Periodic boundary conditions are used to simulate domain of interest that is replicated to infinity by rigid translation in all the three Cartesian directions, completely filling the system space. These domains are known as the primary cells and the tiled copies of these primary cells are known as image cells. Description of the above types of boundary

TABLE 1.1

Different Values of the Scalar Variable Φ , the Diffusion Coefficient Γ , and the Source Term S for the Generalized Conservation Equation to Represent Specific Equations of Mass, Momentum, and Energy

Φ	Γ	S	Equation
1	0	0	Continuity
u	μ	$-\frac{\partial P}{\partial x} + \frac{\mu}{3} \frac{\partial(\nabla \cdot \bar{V})}{\partial x} + b_x$	x -momentum
v	μ	$-\frac{\partial P}{\partial y} + \frac{\mu}{3} \frac{\partial(\nabla \cdot \bar{V})}{\partial y} + b_y$	y -momentum
w	μ	$-\frac{\partial P}{\partial z} + \frac{\mu}{3} \frac{\partial(\nabla \cdot \bar{V})}{\partial z} + b_z$	z -momentum
T	k/C_p	$\frac{\beta}{C_p} T \frac{Dp}{Dt} + \frac{\mu\Phi}{C_p} + \frac{\dot{q}_{gen}}{C_p}$	Energy

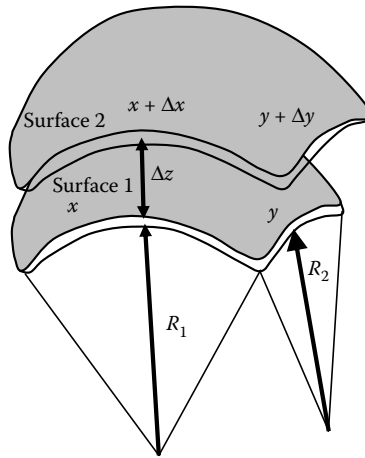


FIGURE 1.9
Virtual displacement Δz of a surface from 1 to 2.

conditions is relatively straight forward and is available in standard texts of continuum mechanics.

In continuum fluid mechanics, one important issue is to describe the boundary condition at the interface between two fluids. For illustration, let us consider a boundary or an interface between mediums 1 and 2. Imagine a cylinder [4] drawn through the interface separating the mediums, as shown in the Figure 1.10. dA_1 and dA_2 are the face areas directed toward the outward normal in mediums 1 and 2, respectively. The cylinder is of height l . As $l \rightarrow 0$, all the volume integrals in Equation 1.10 tend to zero. The surface integrals over the cylindrical surface are proportional to l , and hence they also turn out to be zero. If the mediums 1 and 2 are immiscible, no mass flows across the boundary. In case the interface is stationary, the mass conservation equation yields $\rho_1 \mathbf{u}_1 \cdot \mathbf{n} = \rho_2 \mathbf{u}_2 \cdot \mathbf{n}$. At each point on the interface in the limiting case, the face area of the cylinder tends to zero. In a special case, when medium 2 represents stationary solid, $\mathbf{u}_1 \cdot \mathbf{n} = 0$, which is also known as no penetration boundary condition.

The interface between the two fluids, in addition, may also experience surface tension, which may give rise to an interfacial curvature [2]. This is manifested in terms of the pressure difference on either sides of the meniscus, leading to the development of net normal force (pressure difference times the projected surface area). This normal force acting on the meniscus is balanced by the surface tension force in equilibrium, leading to a curved meniscus.

A simple approach to quantify the pressure difference across the two sides of the interface is by the method of virtual work. We consider surface 1 with dimensions x and y and having area $A(=xy)$ with the radii of curvatures as R_1 and R_2 (as shown in Figure 1.9). A small virtual displacement of Δz normal to the surface modifies the surface to a new configuration (surface 2) with area $A + \Delta A$, given by $(x + \Delta x)(y + \Delta y)$. From similarity considerations, it may be shown that $R_1/(R_1 + \Delta z) = x/(x + \Delta x)$ and $R_2/(R_2 + \Delta z) = y/(y + \Delta y)$, which imply

$$R_1 = \Delta z \frac{x}{\Delta x} \quad \text{and} \quad R_2 = \Delta z \frac{y}{\Delta y}. \quad (1.60)$$

The work done by the pressure in displacing interface from position 1 to 2 is given by ΔP ($A\Delta z$), which is equivalent to the work done in stretching the interface by overcoming surface tension: $\gamma\Delta A$. This fact leads a relationship between the pressure difference (ΔP) and the curvature along two principle radii (R_1 and R_2), which is known as the Young–Laplace equation, and using Equation 1.60, it results in

$$\Delta P = \gamma \left(\frac{1}{R_1} + \frac{1}{R_2} \right). \quad (1.61)$$

Equation 1.61 is a statement of static equilibrium of normal forces acting across the interface. The statement of dynamic equilibrium may be obtained from the integral form of the momentum balance Equation 1.13, which gives the resultant force per unit area on the surface ($n_i \tau_{ij}$). If the normal and tangential components of stresses are denoted by τ_n and τ_t , the balance of the stresses at the interface yields:

$$\tau_{t1} - \tau_{t2} = \nabla \gamma \quad (1.62a)$$

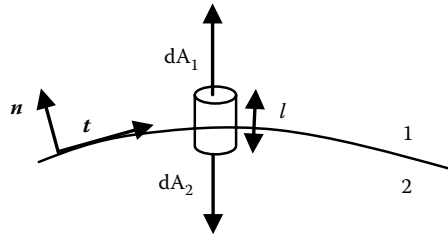
$$\tau_{n1} - \tau_{n2} = \gamma \kappa, \quad (1.62b)$$

where γ may be the function of temperature, concentration, or electric field and κ is the local curvature of the interface. The normal and the tangential stresses (τ_n and τ_t) may be evaluated from the general stress tensor using $\mathbf{n} \cdot \boldsymbol{\tau} \cdot \mathbf{n}$ and $\mathbf{t} \cdot \boldsymbol{\tau} \cdot \mathbf{n}$, where \mathbf{n} and \mathbf{t} are the normal and tangent vectors of the surface with $\boldsymbol{\tau} = -p\mathbf{I} + \mu(\nabla \mathbf{v} + (\nabla \mathbf{v})^T)$. In the limit of hydrostatic equilibrium, Equation 1.62b transforms to Equation 1.61.

The boundary condition encountered in gas–liquid flows or free surface flows is known as dynamic or kinematic boundary condition. If the interface is represented as $z = \eta(x, y, t)$, there must be equality of the velocity component of the either phase to maintain a continuity of the phases, which leads to

$$V_{liq} = V_{gas} = \frac{D\eta}{Dt} = \frac{\partial \eta}{\partial t} + \mathbf{V} \cdot \nabla \eta. \quad (1.63)$$

Interfacial boundary conditions are also critical to prescribe in heat transfer problems. For illustration, we again consider a boundary or an interface between mediums 1 and 2. Imagine a cylinder [4] drawn through the interface separating the mediums, as shown in


FIGURE 1.10

Interface between mediums 1 and 2, with the normal and tangent vectors \mathbf{n} and \mathbf{t} , respectively. A pillbox of length l is drawn with surface areas dA_1 and dA_2 .

the Figure 1.10. The integral form of the energy conservation Equation 1.36 may be applied on this cylinder of infinitesimal height l , to yield that $-k\partial T/\partial n$ (heat flux) is continuous at the interface, which also implies that interface cannot store heat. For cases in which change of phase occurs at the interface, these considerations should be augmented to accommodate the absorption/evolution of latent heat.

1.10 Extended Navier–Stokes Equation

In the earlier sections, we have seen that continuum description of fluid flow, heat transfer, and other transport process involves various constitutive relationships. The governing equations for Newtonian and Stokesian fluids obeying the Fourier’s law of heat conduction are known as the Navier–Stokes–Fourier equations. Although these equations have been widely used to solve problems of thermofluid mechanics, their applicability has been recently questioned by many researchers, particularly considering flows with strong local density and/or temperature gradients. Brenner suggested a modification of the Newton’s law of viscosity by distinguishing fluid’s mass velocity (i.e., velocity featuring in the continuity equation) from the fluid’s volume velocity (i.e., fluid’s volumetric flux density). He also pointed out that without considering a “boundary slip,” the classical mass-velocity-based formalism of the Navier–Stokes–Fourier equations might fail to predict the existence of thermophoresis, a phenomenon often observed during experimentation with highly compressible flow systems. Accordingly, fundamental modification of the Newton’s viscosity law was suggested by Brenner in the following form:

$$\tau_{ij} = \mu \left(\frac{\partial(U_j)_v}{\partial x_i} + \frac{\partial(U_i)_v}{\partial x_j} \right) + \lambda \delta_{ij} \frac{\partial(U_k)_v}{\partial x_k}, \quad (1.64)$$

where $(U_j)_v$ is the volume velocity (which physically represents a Eulerian flux density of volume, as a combined effect of the local advective and diffusive mechanisms). Brenner also indicated the conjecture that from a purely kinematic viewpoint [8–10], the volume velocity of flow becomes equal to the fluid’s tracer or Lagrangian velocity. With the arguments of distinctive mass velocities and volume velocities, Brenner postulated a modification in the Fourier law in a compressible limit, as

$$q_i'' = -k \frac{\partial T}{\partial x_i} - p(U_i)_v. \quad (1.65)$$

These constitutive arguments have been critically argued upon by various researchers. Alternatively, an extended Navier–Stokes has been proposed [11] from the upscaled analogy of molecular transport considerations. It considers the transport coefficient of diffusion as the gross volume averaged manifestations of the transport phenomenon occurring in the subcontinuum length scales. The continuum representation of velocity at a point may be discerning when strong local gradients of density or temperature are present because of the presence of discrete molecules of fluid (along with empty spaces in between them). Referring to fluxes instead of velocities is an alternate way to relate the continuum description of fluid flow equations with a “mesoscopic” interpretation. With respect to a Eulerian control volume, the velocity is interpreted as an advective flux density of mass across an element of the concerned control surface. Superimposed on this advective flux, phoretic or diffusive transport of mass across the control surface is also possible, which can be actuated by local gradients of density and/or temperature, independent of the action of any equivalent macroscopically resolvable pressure gradient. A classical example of phoretic transport is the phenomenon of thermophoresis. Thermophoresis, also called thermomigration, thermodiffusion, or Sorét effect, or the Ludwig–Soret effect, is a phenomenon observed when heat conducting and force- and torque-free particles move from hotter to colder regions in the fluid (usually, a gas), against an externally imposed temperature gradient. Considerations from the kinetic theory for ideal gases, net diffusive mass flux (over a spatial length scale of l surrounding a location x_i across which gradients of density or temperature occur in the flow domain) may be expressed as $\dot{m}_i = (1/6) [\rho|_{x_i-l} \bar{u}_i|_{x_i-l} - \rho|_{x_i+l} \bar{u}_i|_{x_i+l}]$ (where \bar{u}_i is the mean molecular speed). Expanding the expression for \dot{m}_i in the Taylor series and retaining only up to the linear terms in the first-order derivatives, one may obtain $\dot{m}_i = -(l/3)[\bar{u}_m(\partial\rho/\partial x_i) + \rho(\partial\bar{u}_m/\partial x_i)]$, where $\bar{u}_m = \bar{u}_i|_{x_i-l} = \bar{u}_i|_{x_i+l}$ represents the statistically averaged fluid-particle (group of fluid molecules) velocities. From the kinetic theory of gases, the velocity u_m may take a form analogous to $\sqrt{8k_B T / \pi m_M}$, where k_B is the Boltzmann constant, T is the absolute temperature, and m_M is the molecular mass. One can hence express velocity as a sole function of temperature as [12]:

$$\rho u_i = C_1 \left[\frac{\partial \rho}{\partial x_i} + \frac{1}{2T} \frac{\partial T}{\partial x_i} \right], \quad (1.66)$$

where C_1 is a phenomenological coefficient, which, for the case of ideal gases, can be described as $D\rho$, where D is the so-called *self-diffusion coefficient*. For an ideal gas, (with Prandtl and Schmidt numbers of unity), this becomes $(1/3)l\bar{u}_m$, where l is the microscopic mixing length (analogous to the mean free path of an ideal gas), \bar{u}_m is the mean thermal speed predicted from molecular-level considerations, and ρ is the fluid density. Further simplifications may be obtained by considering the equation of state for ideal gases ($P = \rho RT$) under local equilibrium conditions to obtain

$$u_i = \frac{C_1}{2\rho} \frac{\partial(\ln \rho)}{\partial x_i}. \quad (1.67)$$

Fundamentally, the shear stress (or, equivalently, momentum flux), τ_{ij} has contribution from three separate contributions, namely, τ_{ij}^I , τ_{ij}^{II} , and τ_{ij}^{III} . τ_{ij}^I represents the transfer of molecular momentum that originates from the interaction between the normalized advective flux components U_j and U_i . An additional contribution in τ_{ij}^I comes from an exchange

of momentum between the i th component of the velocity of the “phoretic” group of fluid particles in phoretic transport and the j th component of the normalized bulk advective flux density. By drawing analogies from the mass transport considerations, the momentum may be expressed as

$$\tau_{ij}^I = \frac{1}{6} \left[\rho \Big|_{x_i-l} \bar{u}_i \Big|_{x_i-l} U_j \Big|_{x_i-l} - \rho \Big|_{x_i+l} \bar{u}_i \Big|_{x_i+l} U_j \Big|_{x_i+l} \right]. \quad (1.68)$$

Expanding Equation 1.68 using Taylor series and expressing in terms of the phoretic velocity component u_i given in Equation 1.67 and the momentum diffusion coefficient μ (given by $(1/3) l \bar{u}_m \rho$), one obtains [11]

$$\tau_{ij}^I = \mu \frac{\partial U_j}{\partial x_i} + \rho U_j u_i. \quad (1.69)$$

The phoretic transport results. exchange of momentum between the j th component of the phoretic velocity and the i th component of the normalized bulk advective flux density in an additional contribution τ_{ij}^{II} because of

$$\tau_{ij}^{II} = \mu \frac{\partial U_i}{\partial x_j} + \rho U_i u_j. \quad (1.70)$$

The term τ_{ij}^{III} is related to the volumetric dilation of the fluid elements is given by

$$\tau_{ij}^{III} = \lambda \delta_{ij} \frac{1}{\rho} \frac{\partial(\rho U_k)}{\partial x_k}. \quad (1.71)$$

The derivative in Equation 1.71 may also be written as

$$\tau_{ij}^{III} = \lambda \delta_{ij} \frac{\partial U_k}{\partial x_k} + \lambda \delta_{ij} U_k \frac{\partial(\ln \rho)}{\partial x_k}. \quad (1.72)$$

Using Equation 1.67, the previous equation can be simplified to obtain

$$\tau_{ij}^{III} = -\lambda \delta_{ij} \frac{\partial U_k}{\partial x_k} + \lambda \delta_{ij} \frac{2\rho}{\mu} U_k u_k. \quad (1.73)$$

The presence of the terms involving the product of advective and phoretic flux densities render the constitutive relationships nonlinear in nature. The linearization may be performed by considering an equivalent hypothetical pure diffusive flux of u_n , giving rise to same effective mass flux, or in other words, one can write $\rho U_m u_n = \mu' (\partial u_n / \partial x_m)$, (for $m \neq n$), where μ' is a diffusive momentum transport coefficient. Drawing analogies from the kinetic theory, the scale for the diffusional exchange of momentum between phoretic and the advective fluxes may be represented as $\mu' = (1/3) \rho l \bar{u}_m$, which also implies that

$\mu' \approx \mu$. Adopting the abovementioned linearization strategie, the expressions for shear stress components may be written as [11],

$$\tau_{ij} = \mu \left(\frac{\partial U_j}{\partial x_i} + \frac{\partial U_i}{\partial x_j} \right) + \lambda \delta_{ij} \frac{\partial U_k}{\partial x_k} + \mu \left(\frac{\partial u_j}{\partial x_i} + \frac{\partial u_i}{\partial x_j} \right) + \lambda \delta_{ij} \frac{\partial u_k}{\partial x_k}. \quad (1.74)$$

Alternatively, Equation 1.74 can be written as

$$\tau_{ij} = \mu \left(\frac{\partial u_{net,j}}{\partial x_i} + \frac{\partial u_{net,i}}{\partial x_j} \right) + \lambda \delta_{ij} \frac{\partial u_{net,k}}{\partial x_k}. \quad (1.75)$$

Equation 1.75 is analogous to Newton's law of viscosity, but with a modified reference velocity of $u_{net} = U + u$.

The heat flux under potentially strong gradients of density and/or temperature can be estimated similarly by expressing heat flux similar to the mass flux as described previously:

$$q_i'' = \frac{1}{6} \left[\rho \Big|_{x_i-l} \bar{u}_i \Big|_{x_i-l} h \Big|_{x_i-l} - \rho \Big|_{x_i+l} h \Big|_{x_i+l} \right]. \quad (1.76)$$

Using Equation 1.76, the definition of the thermal diffusivity along with the definition of the phoretic velocity component and with considerations of the equation of state for ideal gases, one obtains

$$q_i'' = -k \frac{\partial T}{\partial x_i} + p \frac{C_p}{R} u_i, \quad (1.77)$$

by noting that $dh = C_p dT$ for ideal gases.

Continuum conservation equations for fluid flow and heat transfer can be mathematically closed with the constitutive forms of Equations 1.75 and 1.77 and the modified reference velocity $u_{net} = U + u$, the continuum conservation equations for fluid flow and heat transfer can be mathematically closed. The additional terms appearing in these equations results from the considerations of phoretic transport mechanisms associated with strong local gradients of density and/or temperature within the flow domain.

1.11 Noncontinuum Simulations and Concept of Ensemble

Fundamentally, the macroscopic properties such as pressure and velocity are obtained by averaging over all the particles in an infinitesimal control volume around the point of interest. When the system length scales become smaller than a threshold limit (typically, comparable with the molecular mean free path) or the interest of any physical problem approaches the molecular dimensions, then the group behavior or the statistical behavior of a property described by a group of molecules expressed in the form of continuum approach may fail. The continuum hypothesis expects that this region will contain sufficient number of molecules to ensure good continuity and differentiability of these macroscopic properties over space and time. Typically for gas flows [12–15], Knudsen number (Kn) demarcates different regimes of

flow. The Knudsen number is representative of the ratio of the molecular mean free path to the system length scale. At low Knudsen numbers (typically less than 0.1), the numbers of molecular collisions are sufficient to ensure smooth gradients in the flow properties and hence continuum model works (except for physically induced jump discontinuities such as shock waves). For high Knudsen numbers, the number of molecules in the elemental volume may be reduced, so that there are insufficient numbers of molecules to give a meaningful average. Thus, the value of the macroscopic properties will fluctuate significantly over space and time. Continuum conservation equations often do not work for high Knudsen numbers. This, however, does not mean that the conservation equations are not valid in this regime. The reason for the failure of these equations is because the gradients in these equations become too steep or fluctuate too much, which may not be captured with adequate resolution disregarding the discreteness of the underlying molecular picture. The continuum mathematical descriptions with the standard gradient terms may fail to capture the variations in field variables under these conditions, and mesoscopic or molecular models may need to be invoked.

From molecular considerations, microscopic properties may be obtained by using the trajectories of individual elemental particles like atoms or molecules, using Lagrangian descriptions. These microscopic properties are summed up to be described through physically realizable properties of the microscale. The simulation may yield different configurations of the phase space and hence averaging is required by taking all possible conformations of the system as the initial state. In this respect, it is important to describe a term called ensemble. An ensemble is a collection of points in phase space satisfying the conditions of a particular thermodynamic state. Different ensembles are commonly used with different constraints [12]:

1. The NPT ensemble is obtained by a fixed number of atoms, N , at a fixed pressure, p , and a fixed temperature, T .
2. The microcanonical ensemble (NVE) has a thermodynamic state characterized by a fixed number of atoms, N , a fixed volume, V , and a fixed energy, E .
3. The canonical ensemble (NVT) is a set of all systems whose thermodynamic state is characterized by a fixed number of atoms, N , a fixed volume, V , and a fixed temperature, T .
4. The grand canonical ensemble (μVT) has a thermodynamic state characterized by a fixed chemical potential, μ , a fixed volume, V , and a fixed temperature, T .

There are few properties of a good ensemble. The chosen probability measure in a phase space should be a Gibbs state of the ensemble, that is, it should be invariant under time evolution. This provides a good representative of the ensembles of a quantity or property. Another good measure is the requirement of the *ergodicity*, which states that the ensemble average coincides with the time average. Physically, when a system fails to be ergodic, we may infer that there is more macroscopically discoverable information available about the microscopic state of the system than what we might have thought. In turn, this may be used to create a better-conditioned ensemble.

The molecular dynamics (MD) is a molecular/atomistic simulation method suitable for simulating very small volumes of liquid flow, with typical linear dimensions of the order of less than 10 nm and for time intervals of a few nanoseconds [14]. It is, however, relatively less accurate for simulating gas microflows because large intermolecular distances may demand prohibitively large domain sizes. In MD, the fundamental equation governing the trajectory of particles is the Newton's second law—the rate of change of momentum of the particles

is equal to the net external force exerted on them. The external forces come from different interactions of the system and the former is related as the negative of the gradient of the later. The Newton's law is hence solved numerically to generate the position and velocity of particles as a function of times which belong to the same ensemble and correspond to the different conformations of the system. The whole region is divided into different compartments called bins and the number of molecules in the bins gives the density of the fluid in that location represented by each bin. The positions and velocities of the particles are to be related to the macroscopic properties of the system by averaging over each bin.

MD is typically applied to systems of a few hundred to thousand atoms. Such small systems are usually dominated by surface effects or the boundaries of the cells. If we want to simulate the bulk liquid, the surface effects are removed using periodic boundary conditions. If N molecules are confined to a volume V (which is called the primary cell), we imagine that it is surrounded by exact replicas of itself (image cells)—this is commonly known as periodic boundary condition. Hence, we need not follow the trajectories of the image molecules because they can be easily computed, when needed. Each molecule in the primary cell interacts with all the $N - 1$ other molecules. If a molecule moves into the image cell, the image from the opposite cell moves into the primary cell.

Gas microflows are simulated more efficiently using the Direct Simulation Monte Carlo method [15]. This is a statistically based approach in which the details of a system are compromised with the help of "simulated" molecules that does not exactly follow the motion of the real molecules but effectively captures the physical behavior of the system. The Direct Simulation Monte Carlo strategy is implemented by splitting of the molecular motion and intermolecular collisions by choosing a time step smaller than the mean collision time and tracking the evolution of this molecular process in space and time.

It is important to mention in this context that molecular and microscopic (statistical) simulations are restricted only to relatively short spatiotemporal scales because of their large computation requirements in comparison with continuum-based modeling approaches. Multiscale modeling approaches, in practice, may be used to overcome such constraints by coupling these two levels of simulations. For example, the coupling of MD with Navier–Stokes equations extends the range of applicability of both approaches and provides a unifying description of flows from molecular to system scales. This not only imparts a computational tractability to a problem involving multiple physical scales but also improves the computational economy by reducing the simulation complexities for subdomains over which molecular simulations render to be overkills. For details of these coupling strategies, readers are requested to refer to Bejan [7].

1.12 Conclusion

In this chapter, we have described the equations of conservation of mass, momentum, and energy in a generalized continuum-based framework, both in integral as well as differential forms. We have also delineated possible extensions in the continuum framework for cases characterized with strong local gradients of flow variables, using the analogy of the upscaled molecular transport. In the last section, we have outlined the necessity of molecular simulations when the continuum equations are no longer applicable. We have also indicated the needs of multiscale modeling for problems involving multiple physical scales as an effective compromise between computational accuracy and simulation economy.

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