Biological Transport Phenomena

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Chapter 1

Diffusion

1.1 Diffusion and Random Walk

1.1.1 One-Dimensional Diffusion

The basis of diffusion on a molecular scale, in dilute solutions, can be modeled as the movement of solute molecules throughout the medium via random trajectories. These random trajectories are mainly determined by collisions or interactions between solute and medium.

For the sake of simplicity, we must strip diffusion to its barest essentials and consider solute diffusion along one dimension. Suppose that N particles of solute are situated at position x = 0 at time t = 0. The following assumptions must be made.

- 1. After every τ seconds, each particle either moves to the right by one step $(+\delta)$ or to the left by one step $(-\delta)$.
- 2. The probabilities that the particle moves by $-\delta$ and that it moves by $+\delta$ are equal.
- 3. The particles do not collide with each other, and that random-walk diffusion is driven only by solute—solvent interactions. As a result, the present model for diffusion holds well only under dilute concentrations of solute.

In addition, the variable n is defined as the number of steps taken at the present time t. Symbolically,

$$t = n\tau, \tag{1.1}$$

and at every nth step, each ith particle moves from its previous position either to the left or to the right by a certain distance δ .

$$x_i(n) = x_i(n-1) \pm \delta \tag{1.2}$$

where i = 0, 1, ..., N - 1. It can be inferred by intuition and by mathematics that the mean displacement of particles is zero, as the equal probability of $\pm \delta$ ensures the distribution is symmetric.

$$\langle x(n) \rangle \equiv \frac{1}{N} \sum_{i} x_i(n)$$
 (1.3)

From Equation (1.2), the mean displacement is the same as it was one step ago. For large enough N, the mean value of $\pm \delta$ for all particles is equal to zero.

$$\langle x(n) \rangle = \frac{1}{N} \sum_{i} \left[x_i(n-1) \pm \delta \right] = \langle x(n-1) \rangle + \langle \pm \delta \rangle = \langle x(n-1) \rangle$$
 (1.4)

By the principle of mathematical induction, the mean displacement for every nth time step is zero, since all particles were initially set at position zero.

$$\langle x(n) \rangle = 0 \tag{1.5}$$

The mean squared displacement at the nth time step can be determined by the same approach,

$$\langle x^2(n)\rangle \equiv \frac{1}{N} \sum_i x_i^2(n),$$
 (1.6)

and since the squared displacement for each particle is

$$x_i^2(n) = [x_i(n-1) \pm \delta]^2$$
 (1.7a)

$$= x_i^2(n-1) \pm 2x_i(n-1)\delta + \delta^2$$
 (1.7b)

then, since the average of the middle term in Equation (1.7b) is zero due to the symmetry of the distribution,

$$\langle x^2(n)\rangle = \langle x^2(n-1)\rangle + \delta^2. \tag{1.8}$$

At time t=0, all particles are situated at x=0, so the initial mean squared displacement is zero,

$$\langle x^2(n)\rangle = \langle x^2(0)\rangle + n\delta^2 = n\delta^2. \tag{1.9}$$

Recalling Equation (1.1), that the step number is the ratio of the present time and the time taken per step ("diffusion time"), the mean squared displacement can be expressed in terms of the present time and diffusion time,

$$\langle x^2(n)\rangle = t\delta^2/\tau. \tag{1.10}$$

In the scope of one-dimensional random walk, one can state that, through different mediums, the solute particles can traverse different lengths δ for each step, depending on the solute–medium interactions. A diffusion constant can be defined to account for the variability in diffusive spread,

$$\boxed{D_{ij} \equiv \delta^2/(2\tau)} \tag{1.11}$$

which is called the (binary) **diffusion coefficient**, or **diffusivity**. The subscript notation for diffusivity denotes the solute as index i and the medium as index j. By this definition, Equation (1.10) becomes

$$\langle x^2 \rangle = 2D_{ij}t \tag{1.12}$$

Note that the diffusion coefficient is one-half of δ^2/τ ; the reason behind this multiple will become clear once Fick's laws of diffusion are explored.

1.1.2 Random Walk Diffusion in Higher Dimensions

1.1.3 Estimations of the Diffusion Coefficient

The diffusion coefficient is a quantity that is ideally obtained via experiment, as it depends on temperature of the system, fluid viscosity, and molecular size (weight) of the solvent.

$$D_{ij} \sim D_{ij}(T, \mu, M) \tag{1.13}$$

There are assumptions, however, that simplify the solute's molecular structure as a sphere. The mean square displacement of a spherical solute particle in one dimension is

$$\langle x^2 \rangle = \frac{2k_{\rm B}T}{\overline{f}}t - \frac{2m_p k_{\rm B}T}{\overline{f}} \left(1 - e^{-\overline{f}t/m_p}\right),\tag{1.14}$$

where

$$\overline{f} = 6\pi\mu R,\tag{1.15}$$

is the drag coefficient, μ is the dynamic viscosity, R is the effective solute radius, T is the temperature, and $k_{\rm B}$ is the Boltzmann constant. After long enough times, the mean square coefficient is approximately equal to

$$\langle x^2 \rangle = \frac{2k_{\rm B}T}{6\pi\mu R}.\tag{1.16}$$

Applying Equation (1.12) to this equation, the diffusivity constant is then

$$D_{ij} = \frac{k_{\rm B}T}{6\pi\mu R} \,. \tag{1.17}$$

This is named the **Stokes–Einstein equation**.

The **Wilke–Chang correlation** is a semiempirical yet more accurate estimation of the diffusion coefficient,

$$D_{ij} = (7.4 \times 10^{-10}) \frac{T\sqrt{\phi M}}{\mu V_0^{0.6}}$$
(1.18)

where the quantities included above are in the following units,

$$[D_{ij}] = \text{cm}^2 \,\text{s}^{-1} \tag{1.19a}$$

$$[T] = K \tag{1.19b}$$

$$[\phi] = 1 \tag{1.19c}$$

$$[M] = g \operatorname{mol}^{-1} \tag{1.19d}$$

$$[\mu] = g \,\mathrm{cm}^{-1} \,\mathrm{s}^{-1}$$
 (1.19e)

$$[V_0] = \text{cm}^3 \,\text{mol}^{-1} \tag{1.19f}$$

1.2 Fick's Laws of Diffusion

1.3 Unsteady Diffusion in a Finite Medium

1.3.1 Unsteady Diffusion in the One-Dimensional Case

The assumption of unsteady diffusion supposes that the solute diffuses out of a one-dimensional chamber with an initial concentration of solute into a surrounding well-mixed bath, in an unsteady (i.e., time-dependent) manner.

Suppose the one-dimensional chamber has length 2L and is centered at the origin, having an initial concentration c_0 . By symmetry, the diffusion behavior of solute is equivalent to that of a chamber of length L with its left boundary at the origin. The governing equation is Fick's second law,

$$\frac{\partial c}{\partial t} = D\nabla^2 c \tag{1.20}$$

where c is the concentration, and D is the diffusion coefficient. In the one-dimensional case, the Laplace operator collapses down to the direction of diffusion.

$$\frac{\partial c}{\partial t} = D \frac{\partial^2 c}{\partial x^2} \tag{1.21}$$

Similar to diffusion under the semi-infinite assumption, Fick's second law can be expressed in terms of nondimensional quantities (Greek letters),

$$c - c_0 \rightarrow \theta(c_1 - c_0) \tag{1.22a}$$

$$x \to \eta L$$
 (1.22b)

$$x \to \eta L$$
 (1.22b)
 $t \to \tau t_{\text{diff}} = \tau(L^2/D)$ (1.22c)

where L is the characteristic length, and $t_{\text{diff}} = L^2/D$ is the characteristic diffusion time. Once Equations (1.22a) to (1.22c) are substituted into Equation (1.21), the differential equation becomes

$$\frac{\partial \theta}{\partial \tau} = \frac{\partial^2 \theta}{\partial \eta^2} \tag{1.23}$$

However, for the differential equation to be solvable via separation of variables, the boundary conditions must hold homogeneity. The boundary conditions require that the nondimensional quantity θ be equal to unity at x = 0 for all times. An additional substitution of

$$\Omega = 1 - \theta \tag{1.24}$$

solves this issue. Under this substitution, Equation (1.23) transforms into

$$\frac{\partial \Omega}{\partial \tau} = \frac{\partial^2 \Omega}{\partial \eta^2} \tag{1.25}$$

that is solvable by separation of variables.

First, a substitution must be performed, assuming the function Ω is the product of two independent functions each dependent on a variable of Ω ,

$$\Omega(\eta, \tau) = H(\eta) T(\tau) \tag{1.26}$$

which transforms Equation (1.25), after some rearrangement, into

$$\frac{1}{T}\frac{dT}{d\tau} = \frac{1}{H}\frac{d^2H}{d\eta^2} \equiv -\lambda^2 \tag{1.27}$$

for some constant λ . This leads to the ansatz of

$$\Omega = HT = (A\cos\lambda\eta + B\sin\lambda\eta)Ce^{-\lambda^2\tau}$$
(1.28a)

$$= (E\cos\lambda\eta + F\sin\lambda\eta)e^{-\lambda^2\tau}$$
 (1.28b)

where A, B, and C are constants of integration, E = AC, and F = BC.

It can be assumed from the symmetry of the system that there is zero flux at the center of the chamber of length 2L,

$$0 = \frac{\partial \Omega}{\partial \eta} \bigg|_{\eta=0} = \lambda (F \cos \lambda \eta - E \sin \lambda \eta) e^{-\lambda^2 \tau} \bigg|_{\eta=0} = \lambda F e^{-\lambda^2 \tau}$$
 (1.29)

leading to F = 0.

It can also be assumed that the solute concentration at the boundaries of the chamber is equal to the concentration outside at all times,

$$0 = E e^{-\lambda^2 \tau} \cos \lambda \tag{1.30}$$

leading to $\cos \lambda = 0$ or, for integer n,

$$\lambda = \left(n + \frac{1}{2}\right)\pi\tag{1.31}$$

which, by the principle of superposition, transforms Equation (1.28b) to the following form

$$\Omega = \sum_{n} E_n \cos \left[\left(n + \frac{1}{2} \right) \pi \eta \right] \exp \left[-\left(n + \frac{1}{2} \right)^2 \pi^2 \tau \right]$$
(1.32)

The value of E_n can obtained via the initial condition ($\tau = 0$) that the concentration inside the chamber is equal to c_0 , which yields

$$1 = \sum_{n} E_n \cos \left[\left(n + \frac{1}{2} \right) \pi \eta \right] \tag{1.33}$$

An inner product can be defined over the space of real-valued functions continuous over domain

 $0 \le x \le 1$ as follows,

$$\int_0^1 \cos(m\pi\eta) \cos(n\pi\eta) \,\mathrm{d}\eta = \begin{cases} 1/2 & m = n\\ 0 & m \neq n \end{cases}$$
 (1.34)

where m is a nonnegative integer. Applying the inner product to Equation (1.33) allows E_n to be isolated,

$$\int_0^1 \cos \left[\left(m + \frac{1}{2} \right) \pi \eta \right] d\eta = \sum_n \int_0^1 E_n \cos \left[\left(m + \frac{1}{2} \right) \pi \eta \right] \cos \left[\left(n + \frac{1}{2} \right) \pi \eta \right] d\eta \tag{1.35}$$

$$\frac{\sin\left[(m+1/2)\pi\right]}{(m+1/2)\pi} = \frac{E_m}{2} \tag{1.36}$$

which, considering the integral value of n, yields

$$E_n = \frac{2(-1)^n}{(n+1/2)\pi} \tag{1.37}$$

Our final solution follows from Equations (1.22a), (1.24), (1.32) and (1.37),

$$c = c_0 + (c_1 - c_0)(1 - \Omega)$$
(1.38)

where

$$\Omega = \frac{2}{\pi} \sum_{n} \frac{(-1)^n}{(n+1/2)} \cos\left[\left(n + \frac{1}{2}\right)\pi\eta\right] \exp\left[-\left(n + \frac{1}{2}\right)^2\pi^2\tau\right]$$
(1.39)

1.3.2 Unsteady Diffusion in the Spherical Case

1.4 Quasi-steady State Diffusion

Suppose a membrane separates two finitely sized, well-mixed baths, each with a certain solute concentration. Under *quasi*-steady-state diffusion, the solute concentrations are *time-dependent*.

From Fick's first law of diffusion, the

Chapter 2

Flow

The study of the movement and deformation of fluids, known as fluid dynamics, is a key discipline in the general field of transport phenomena. Understanding fluid dynamics provides insight into transport behavior in physiological and synthetic biosystems, such as blood flow through a capillary, or fluid flow through a microfluidic channel. The mathematical framework behind fluid dynamics is derived from two governing principles, namely the conservation of mass and the conservation of momentum. Close analysis of these principles leads to two complex but important sets of equations, which are the continuity equation and the Navier–Stokes equations. Under carefully chosen assumptions about the fluid's behavior, the Navier–Stokes equation can be solved to yield certain analytic solutions.

The remainder of this chapter aims to first introduce the behavioral régimes of fluid flow based on the comparison between the inertial forces (i.e. forces that originate from momentum) and viscous forces (i.e. forces that originate from the shear stress between two flowing packets of fluids). Several fluid flow situations are then surveyed for their possible analytic solutions. Under further observations of fluid behaviors, it may be observed that either the inertial forces and viscous forces dominate over one another. Accounting for the dominant force in transport leads to simplified forms of the Navier–Stokes equations that hold practical, analytic use in transport phenomena.

2.1 Describing Fluid Flow

2.1.1 Flow Régimes and the Reynolds Number

Describing the flow of fluid requires determining the relation between the inertial forces driving such flow and the viscous forces, due to the fluid's viscosity. To achieve this, a dimensionless quantity called the **Reynolds number** is defined,

$$Re \equiv \frac{\rho v^2}{\mu v/L} = \frac{Lv}{\mu},\tag{2.1}$$

where v is the magnitude of flow velocity field v, μ is the **dynamic viscosity** of the fluid of interest, and L is the characteristic length of the system. The choice of "characteristic length" is

later discussed in Section 2.1.2.

2.1.2 Characteristic Length and Time

The "characteristic length" of the system is technically arbitrary, but

2.2 The Definition of a Newtonian Fluid

Before the governing equations of fluid momentum transport can be derived, the notion of a Newtonian fluid must be properly defined. A body of flowing fluid that experiences outside body forces can be viewed as a collection of differential elements, each experiencing a force from the surrounding fluid elements. These forces cause the element to undergo gradual deformation.

2.2.1 Stress and Rate of Deformation

The deformation of such a differential element is induced by a (small) force that is applied over a particular face of the element. If one considers the differential force dF applied over a differential face with area dA, then the stress is defined as

$$\tau = \frac{dF}{dA} \tag{2.2}$$

This definition is inadequate, as there can be multiple stresses over the differential element depending on: (1) the direction of the force component, and (2) which face of the element the force component acts. To account for all configurations of face and direction, the (Cauchy) stress tensor, denoted by τ , is defined as

$$\tau_{ij} = \frac{dF_j}{dA_i} \tag{2.3}$$

where i is the direction perpendicular to the area of interest, and j is the direction of the force component of interest.

The deformation that the differential element goes through can also be considered. Assuming the deformation is small, one can approximate the deformation behavior using the infinitesimal stress tensor, denoted by ε , defined via

$$\varepsilon_{ij} = \frac{1}{2} \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \tag{2.4}$$

where u is the displacement, and i and j follow the same conventions as described in Equation (2.3). Using this definition, the stress tensor can be more succinctly expressed in terms of the deformation gradient,

$$\varepsilon = \frac{1}{2} \left[\nabla u + (\nabla u)^T \right]$$
 (2.5)

2.2.2 The Constitutive Relations for Newtonian Flow

A fluid is called a **Newtonian fluid** if there exists an accurately linear relation between the deviatoric stress tensor τ and the rate-of-strain tensor ε^* ,

$$\tau_{ij} = c_{ijkl} \varepsilon_{kl}^* \tag{2.6}$$

where c_{ijkl} is a fourth-order tensor coefficient. It is described in books on Cartesian tensor analysis that even-order isotropic tensors can be written as the sum of products of Kronecker delta tensors, and therefore

$$c_{ijkl} = \mu \delta_{ik} \delta_{jl} + \mu \delta_{il} \delta_{jk} + \lambda \delta_{ij} \delta_{kl}$$
(2.7)

where μ is called the dynamic viscosity and λ the second viscosity. Equations (2.6) and (2.7) may be observed to have corresponding similarities to the general Hookean behaviors of linear, elastic, and isotropic solids, with the two viscosities in replacement of the Young modulus and Poisson ratio of elasticity, and the rate-of-strain tensor in replacement of the strain tensor itself.¹

The substitution of the isotropic tensor in Equation (2.6) by Equation (2.7) results in the following,

$$\tau_{ij} = \lambda \delta_{ij} \varepsilon_{kk}^* + 2\mu \varepsilon_{ij}^* \tag{2.8}$$

or, in tensor form,

$$\tau = \lambda(\nabla \cdot v) + 2\mu \varepsilon^* \tag{2.9a}$$

$$= \lambda(\nabla \cdot v) + \mu \left[\nabla v + (\nabla v)^T \right]$$
 (2.9b)

where v is the velocity field describing the fluid's motion. For Newtonian fluids with incompressible flow, the term associated with the second viscosity is zero, as the velocity field is divergenceless. However, in the case of compressible flow, the divergence of the velocity field may not be zero, which implicates the need to assume a model of the second viscosity.

Talk about Stokes' hypothesis over here.

2.2.3 The Viscosity of Non-Newtonian Fluids

In real life, most fluids are certainly not able to conform to the Newtonian model (Equation (2.6)), especially when placed under high enough stresses. In other words, the relationship between viscous stress and rate of deformation is not linear, and the dynamic viscosity may vary due to different material- or time-dependent parameters.

2.3 The Navier–Stokes Equations

2.3.1 The Acceleration of a Fluid

A moving particle within a fluid at position $\boldsymbol{x}=(x,y,z)$ at time t can be characterized by its velocity vector

$$v = \frac{dx}{dt} = \frac{dx}{dt}\hat{x} + \frac{dy}{dt}\hat{y} + \frac{dz}{dt}\hat{z}$$
 (2.10)

which, differentiated again with respect to time, returns the acceleration vector

$$\boldsymbol{a} \equiv \frac{d\boldsymbol{v}}{dt} = \frac{dv_x}{dt}\hat{\boldsymbol{x}} + \frac{dv_y}{dt}\hat{\boldsymbol{y}} + \frac{dv_z}{dt}\hat{\boldsymbol{z}}$$
(2.11)

The acceleration vector can alternatively determined as the total derivative of $\mathbf{v} = \mathbf{v}(x, y, z, t)$ in the form of (2.10), which yields the following by the multivariate chain rule,

$$a_{i} = \frac{dv_{i}}{dt} = \frac{\partial v_{i}}{\partial t}\frac{dt}{dt} + \frac{\partial v_{i}}{\partial x}\frac{dx}{dt} + \frac{\partial v_{i}}{\partial y}\frac{dy}{dt} + \frac{\partial v_{i}}{\partial z}\frac{dz}{dt}$$
(2.12)

or, in terms of \boldsymbol{v} ,

$$\mathbf{a} = \frac{\partial \mathbf{v}}{\partial t} + v_x \frac{\partial \mathbf{v}}{\partial x} + v_y \frac{\partial \mathbf{v}}{\partial y} + v_z \frac{\partial \mathbf{v}}{\partial z}$$
(2.13)

which can be simplified further with the advection operator $v \cdot \nabla$.

$$\boldsymbol{a} = \frac{\partial \boldsymbol{v}}{\partial t} + (\boldsymbol{v} \cdot \boldsymbol{\nabla}) \boldsymbol{v} \tag{2.14}$$

The partial derivative of the velocity field with respect to time t (or $\partial \boldsymbol{v}/\partial t$) is known as the **local acceleration**, and the advection operator applied to \boldsymbol{v} (or $(\boldsymbol{v} \cdot \nabla)\boldsymbol{v}$) returns what is named the **convective acceleration**.

This formulation of a appears in the left-hand side of the Navier–Stokes equations. In the régime of steady-state fluid flow, the velocity field is defined to have no local acceleration, or $\partial v/\partial t = 0$.

2.3.2 The Forces Acting on a Fluid

The forces acting on a differential element of a fluid involve both stress-induced forces due to the surrounding fluid and the outside body forces on the fluid, such as those induced by gravitational acceleration.

$$F = F_{\text{surf}} + F_{\text{body}} \tag{2.15}$$

Each component of $F_{\rm surf}$ depends on the normal and shear stresses in one direction,

$$F_{\text{surf},x} = -\sigma_{xx}dydz + \left(\sigma_{xx} + \frac{\partial\sigma_{xx}}{\partial x}dx\right)dydz - \sigma_{yx}dydz + \left(\sigma_{yx} + \frac{\partial\sigma_{xy}}{\partial y}dy\right)dxdz - \sigma_{zx}dxdy + \left(\sigma_{zx} + \frac{\partial\sigma_{zx}}{\partial z}dz\right)dxdy \quad (2.16a)$$

$$F_{\text{surf},x} = \left(\frac{\partial \sigma_{xx}}{\partial x} + \frac{\partial \sigma_{yx}}{\partial y} + \frac{\partial \sigma_{zx}}{\partial z}\right) dx dy dz$$
 (2.16b)

and by symmetry,

$$F_{\text{surf},y} = \left(\frac{\partial \sigma_{xy}}{\partial x} + \frac{\partial \sigma_{yy}}{\partial y} + \frac{\partial \sigma_{zy}}{\partial z}\right) dx dy dz \tag{2.17}$$

$$F_{\text{surf},z} = \left(\frac{\partial \sigma_{xz}}{\partial x} + \frac{\partial \sigma_{yz}}{\partial y} + \frac{\partial \sigma_{zz}}{\partial z}\right) dx dy dz$$
 (2.18)

The total surface force can be succinctly expressed as the divergence of the stress tensor over a differential volume,

$$F_{\text{surf}} = (\nabla \cdot \boldsymbol{\sigma})dV \tag{2.19}$$

where dV = dxdydz. Likewise, the total body force over the differential element is equal to the acceleration over its differential mass,

$$\mathbf{F}_{\text{body}} = \rho \mathbf{g} \, dx dy dz = \rho \mathbf{g} \, dV \tag{2.20}$$

leading to the key component of the Navier-Stokes equations

$$\mathbf{F} = (\nabla \cdot \boldsymbol{\sigma} + \rho \mathbf{g}) \, dV \tag{2.21}$$

In the case of incompressible flow, the stress tensor can be divided into the hydrostatic stress tensor and the deviatoric stress tensor τ ,

$$\sigma = -pI + \tau \tag{2.22}$$

for pressure p and identity tensor I. Note the negative sign attached in front of p to account for the inward direction of pressure. Thus, from Equation (2.21),

$$\mathbf{F} = \left[\nabla \cdot (-p\mathbf{I} + \boldsymbol{\tau}) + \rho \mathbf{g} \right] dV \tag{2.23}$$

2.3.3 The Navier–Stokes Equations

The general Navier-Stokes equations (NSE) are based on the momentum conservation principle,

$$m\frac{d\mathbf{v}}{dt} = \mathbf{F} \tag{2.24}$$

for any resultant force F acting on the fluid.

The previous results (Equations (2.14) and (2.23)) imply that the momentum is the result of local and advective acceleration, and the resultant force on the fluid involves hydrostatic pressure, deviatoric stress, and acceleration from body forces, such as gravitational acceleration,

$$\rho dV \left(\frac{\partial \boldsymbol{v}}{\partial t} + (\boldsymbol{v} \cdot \boldsymbol{\nabla}) \boldsymbol{v} \right) = \left[\boldsymbol{\nabla} \cdot (-p\boldsymbol{I} + \boldsymbol{\tau}) + \rho \boldsymbol{g} \right] dV, \tag{2.25}$$

which is more simply expressed

$$\rho \frac{\partial \boldsymbol{v}}{\partial t} + \rho(\boldsymbol{v} \cdot \boldsymbol{\nabla}) \boldsymbol{v} = -\boldsymbol{\nabla} p + \boldsymbol{\nabla} \cdot \boldsymbol{\tau} + \rho \boldsymbol{g}, \tag{2.26}$$

where the deviatoric stress tensor for Newtonian fluids is

$$\tau = \lambda(\nabla \cdot v) + \mu \Big[\nabla v + (\nabla v)^T \Big], \tag{2.27}$$

given dynamic viscosity coefficient μ and second viscosity coefficient λ . In the incompressible case, the continity equation implies that the velocity field be divergenceless, yielding

$$\nabla \cdot \boldsymbol{\tau} = \mu \nabla^2 \boldsymbol{v}. \tag{2.28}$$

Thus, the NSE, assuming the fluid is Newtonian and incompressible, is

$$\rho \frac{\partial \boldsymbol{v}}{\partial t} + \rho(\boldsymbol{v} \cdot \boldsymbol{\nabla})\boldsymbol{v} = -\boldsymbol{\nabla}p + \mu \nabla^2 \boldsymbol{v} + \rho \boldsymbol{g}$$
(2.29)

2.4 Stokes Flow

2.4.1 The Stokes Equation

The NSE for an incompressible Newtonian fluid may be non-dimensionalized using the following parametric conversions,

$$t \to \tau t^*,$$
 (2.30a)

$$v \to Uv^*$$
, (2.30b)

$$x_i \to Lx_i^*$$
, (2.30c)

$$p \to \left(\frac{\mu U}{L}\right) p^*,$$
 (2.30d)

$$g \to gg^*,$$
 (2.30e)

where U, L, and τ are the characteristic velocity, length and time, respectively. Additionally, we define non-dimensionalized del operators

$$\nabla \to \nabla^* / L,$$
 (2.30f)

$$\nabla^2 \to \nabla^2 / L^2. \tag{2.30g}$$

The non-dimensionalized NSE is, in turn,

$$ReSt\frac{\partial \boldsymbol{v}}{\partial t^*} + Re(\boldsymbol{v}^* \cdot \boldsymbol{\nabla}^* \boldsymbol{v}^*) = -\boldsymbol{\nabla}^* p^* + \boldsymbol{\nabla}^{*2} \boldsymbol{v} + \frac{Re}{Fr^2} \boldsymbol{g}^*$$
(2.31)

where

$$St \equiv (L/U)/\tau, \tag{2.32a}$$

$$Re \equiv (\rho UL)/\mu,$$
 (2.32b)

$$Fr \equiv U/\sqrt{gL},$$
 (2.32c)

are the Strouhal, Reynolds, and Froude numbers, respectively. In the régime of Stokes flow, the Reynolds number is extremely miniscule ($Re \ll 1$). Upon the additional assumptions of approximately steady-state flow ($St \ll 1$) and negligible gravitational potential ($Fr \gg 1$), Equation (2.31) becomes the Stokes equation,

$$\boxed{\boldsymbol{\nabla}p = \nabla^2 \boldsymbol{v}} \tag{2.33}$$

upon redimensionalization.

2.4.2 Solutions to the Stokes Equation

2.4.3 The Stokes–Einstein Equation

2.5 Inviscid Flow and the Bernoulli Equation

2.5.1 The Euler Equations

The non-dimensionalization approach applied to the NSE for incompressible Newtonian fluids can be repeated under the assumption of inviscid flow. **Inviscid flow** is defined to be flow in which the inertial forces of a fluid dominate over viscous forces,

$$\rho U^2 \gg \mu U/L \tag{2.34}$$

or in which the Reynolds number is extremely high. Therefore, in the régime of inviscid flow, the fluid can be modeled to have negligible viscosity.

Under inviscid flow, the NSE for an incompressible Newtonian fluid is non-dimensionalized using parametric conversions to non-dimensional quantities (marked by an asterisk),

$$t \to \tau t^*,$$
 (2.35a)

$$v \to Uv$$
, (2.35b)

$$x_i \to Lx_i^*$$
, (2.35c)

$$p \to (\rho U^2) p^*, \tag{2.35d}$$

$$g \to gg^*,$$
 (2.35e)

and the associated del operators are

$$\nabla \to \nabla^* / L,$$
 (2.35f)

$$\nabla^2 \to \nabla^2 / L^2. \tag{2.35g}$$

Applying the aforementioned non-dimensionalization, the NSE becomes

$$St\frac{\partial \boldsymbol{v}^*}{\partial t^*} + \boldsymbol{v}^* \cdot \boldsymbol{\nabla}^* \boldsymbol{v}^* = -\boldsymbol{\nabla}^* p^* + \frac{1}{Re} \boldsymbol{\nabla}^{*2} \boldsymbol{v}^* + \frac{1}{Fr^2} \boldsymbol{g}^*$$
(2.36)

for Strouhal number St, Reynolds number Re, and Froude number Fr. One can assume approximately steady flow ($St \ll 1$), but the inverse of the Reynolds number must be taken as zero due to the prioritization of inertial forces. Unlike the Stokes flow régime, the gravitational potential must be accounted for. The NSE transforms into

$$\rho(\boldsymbol{v} \cdot \boldsymbol{\nabla} \boldsymbol{v}) = -\boldsymbol{\nabla} p + \rho \boldsymbol{g}$$
(2.37)

upon redimensionalization. Equation (2.37), dubbed the **Euler equations**, is the simplified form of the NSE assuming that viscous forces are negligible compared to inertial forces.

2.5.2 The Bernoulli Equation

The Bernoulli equation,

$$\frac{1}{2}\rho v^2 + p + \rho gz = \text{constant}, \tag{2.38}$$

for velocity v, pressure p, and height z at a certain position within a fluid streamline, is a consequence of the Euler equations, which describe the behavior of inviscid flow. The Euler equations state, for an incompressible Newtonian fluid,

$$\rho(\boldsymbol{v} \cdot \boldsymbol{\nabla} \boldsymbol{v}) = -\boldsymbol{\nabla} p + \rho \boldsymbol{g}. \tag{2.39}$$

The advection term can be rewritten using the vector relation

$$\mathbf{v} \cdot \nabla \mathbf{v} = \frac{1}{2} \nabla (\mathbf{v} \cdot \mathbf{v}) - \mathbf{v} \times (\mathbf{v} \times \nabla \mathbf{v}),$$
 (2.40)

and the gravitation term can be rewritten as the negative gradient of the gravitational potential,

$$\mathbf{g} = -\nabla\Phi. \tag{2.41}$$

An additional assumption can be made that the system occurs on the Earth's surface so that the gravitational potential is approximately constant in magnitude,

$$-\nabla\Phi \approx -g\hat{z} = -g\nabla z \tag{2.42}$$

transforming Equation (2.39) to the following form,

$$\frac{1}{2}\rho\nabla(\boldsymbol{v}\cdot\boldsymbol{v}) + \nabla p + \rho g\nabla z = \rho\boldsymbol{v} \times (\boldsymbol{v} \times \nabla \boldsymbol{v}). \tag{2.43}$$

Equation (2.43) can be applied along a streamline \mathcal{S} of inviscid fluid. A differential vector ds

tangent to the streamline can be applied to the current relation by taking the dot product,

$$\frac{1}{2}\rho\nabla(\boldsymbol{v}\cdot\boldsymbol{v})\cdot d\boldsymbol{s} + \nabla p\cdot d\boldsymbol{s} + \rho g\nabla z\cdot d\boldsymbol{s} = \rho\boldsymbol{v}\times(\boldsymbol{v}\times\nabla\boldsymbol{v})\cdot d\boldsymbol{s}. \tag{2.44}$$

Recognizing that $v^2 = \boldsymbol{v} \cdot \boldsymbol{v}$ and $\boldsymbol{v} \times (\boldsymbol{v} \times \boldsymbol{\nabla} \boldsymbol{v}) \cdot d\boldsymbol{s} = 0$, the relation can be massively simplified to

$$\frac{1}{2}\rho \nabla v^2 \cdot d\mathbf{s} + \nabla p \cdot d\mathbf{s} + \rho g \nabla z \cdot d\mathbf{s} = 0. \tag{2.45}$$

The gradient theorem states that the line integral of Equation (2.45) over the streamline yields the difference between the values of v^2 , pressure, and height at the two endpoints of the streamline.

$$\int_{\mathcal{S}} \frac{1}{2} \rho \nabla v^2 \cdot d\mathbf{s} + \nabla p \cdot d\mathbf{s} + \rho g \nabla z \cdot d\mathbf{s} = 0$$
 (2.46)

$$\int_{\mathcal{S}} \frac{1}{2} \rho \nabla v^2 \cdot d\mathbf{s} + \nabla p \cdot d\mathbf{s} + \rho g \nabla z \cdot d\mathbf{s} = 0$$

$$\boxed{\frac{1}{2} \rho (v_2^2 - v_1^2) + (p_2 - p_1) + \rho g (z_2 - z_1) = 0}$$
(2.46)

Equation (2.47) is the explicit form of the Bernoulli equation, which is only applicable for situations of fluid flow in which the inertial forces strongly dominate over viscous forces.

Most introductory problems involving inviscid flow through a pipe cannot be solved solely with the Bernoulli equation. For incompressible flow, the continuity equation implies that the velocity field of flow is divergenceless, i.e.

$$\nabla \cdot \boldsymbol{v} = 0. \tag{2.48}$$

Suppose the fluid streamline changes from a cross-sectional area A_1 to a second cross-sectional area A_2 . Letting \mathcal{V} be the volume of the streamline between the cross-sectional areas, we can rewrite the continuity equation using the divergence theorem,

$$0 = \int_{\mathcal{V}} (\nabla \cdot \boldsymbol{v}) dV = \int_{\partial \mathcal{V}} \boldsymbol{v} \cdot d\boldsymbol{a}, \tag{2.49}$$

where $\partial \mathcal{V}$ is the surface enclosing \mathcal{V} . The total volumetric flow rate depends on the flow rate through the two cross-sectional areas,

$$0 = -\int_{A_1} \boldsymbol{v} \cdot d\boldsymbol{a} + \int_{A_2} \boldsymbol{v} \cdot d\boldsymbol{a}, \qquad (2.50)$$

or equivalently,

$$v_1 A_1 = v_2 A_2 \tag{2.51}$$

assuming that v has norm v_1 where A_1 is located and norm v_2 where A_2 is located. Equation (2.51) is the continuity equation for a laminar inviscid streamline of incompressible fluid.

2.5.3Applications of Inviscid Flow

Appendix A

Newtonian Behavior in the General Case

Bibliography

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