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# Transport Phenomena

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An Informal Set of Notes

$$\rho \frac{\partial \mathbf{u}}{\partial t} + \rho \mathbf{u} \cdot \nabla \mathbf{u} = \mu \nabla^2 \mathbf{u} - \nabla P + \rho \mathbf{G}$$

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# Chapter 1

## The General Conservation Equation

### 1.1 Introduction

This document offers a brief mathematical view behind the main equations of differential analysis in transport phenomena. There are no numerical examples, but rather, the goal is to develop a theoretical understanding of differential conservation equations and *why* they have their form. Thus, motivated derivations are the main results of this document along with several methods of analyzing the resulting equations.

In this light, physical arguments will be used rather than full mathematical rigor. However, the math is still the forefront of the developments, so an adequate and intuitive knowledge of calculus is required (including vector calculus!). If you need a refresher on vector calculus notation, refer to Appendix 1 or this [video](#). The analysis is not simple, so you may be tempted to skip it, but by reading this document carefully and working through the arguments yourself, you should develop a reasonable intuition of the differential transport equations. This is not to say that every mathematical step must be understood line by line, but skipping to the end to memorize equations does not lead to good intuition. One cannot expect to be able to successfully perform calculations without a gut feeling for what the equations mean. Besides, in any practical applications of transport phenomena, computers are able to perform the math. Therefore, it is job of the engineer to *model* the system of interest and understand what certain terms mean and what mathematical operations will allow the correct simulation of the system. In short: good theory = good calculation.

In contrast, the appendices are completely optional to read and go into more mathematical detail than the main text. Generally, they do not add more intuition to the physical arguments, but they serve as justification for some of the advanced developments.

## 1.2 Gauss' Divergence Theorem

Remember this theorem from multivariable calculus? ... It's probably more likely that you remember asking yourself: "When will I ever use this?". The answer is still practically never, but conservation equations are a beautiful application of this theorem. As review, here are some nice YouTube videos giving intuitive explanations of the theorem: [Video 1 \(Shorter\)](#), [Video 2 \(Longer\)](#). A brief explanation is that for a differentiable vector field,  $\mathbf{F}$ , and a given control volume,  $V$ ,

$$\iiint_V \nabla \cdot \mathbf{F} dV = \iint_{\partial V} \mathbf{F} \cdot \mathbf{n} dA,$$

where  $\nabla \cdot$  is the divergence operator,  $\mathbf{n}$  is the normal vector to the boundary of the volume, and  $\partial V$  denotes the surface enclosing the volume (the boundary or control surface). Intuitively, the theorem states that the flux,  $\mathbf{F}$ , through the control surface is equal to the sum of the fluxes at every point (the divergence,  $\nabla \cdot \mathbf{F}$ ). Understanding of this theorem is crucial to a good understanding of the proceeding developments, so ensure that its meaning is well understood.

## 1.3 The Continuity Equation

To start with a familiar example, consider the mass conservation equation where we have a moving control volume (CV) and we are measuring the velocity from a fixed reference frame,

$$\begin{aligned} 0 &= \frac{d}{dt} \iiint_V \rho dV + \iint_{\partial V} \rho \mathbf{v} \cdot \mathbf{n} dA, \\ &= \iiint_V \frac{\partial \rho}{\partial t} dV + \iint_{\partial V} \rho (\mathbf{v} + \mathbf{v}_{CV}) \cdot \mathbf{n} dA, \end{aligned}$$

where,

$$\begin{aligned} &\text{Change of mass inside the CV} \\ &+ \text{Mass that enters/leaves the CV} \\ &\text{due to movement of the boundary} \end{aligned} = \frac{d}{dt} \iiint_V \rho dV,$$

$$\text{Mass flux due to fluid flow through the CV} = \iint_{\partial V} \rho \mathbf{v} \cdot \mathbf{n} dA,$$

$$\text{Only the change of mass inside the CV} = \iiint_V \frac{\partial \rho}{\partial t} dV,$$

$$\begin{aligned} &\text{Mass that enters/leaves the CV} \\ &\text{due to movement of the boundary} \end{aligned} = \iint_{\partial V} \rho \mathbf{v}_{CV} \cdot \mathbf{n} dA.$$

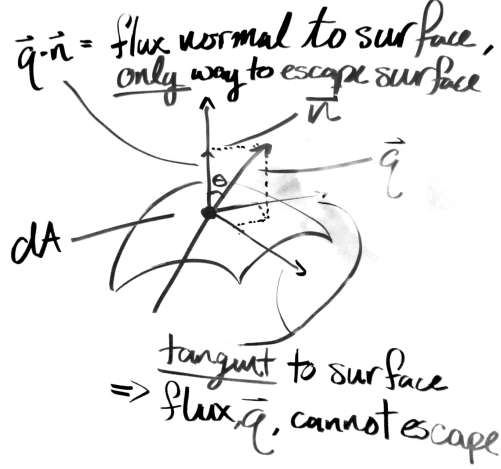


Figure 1.1: Visual representation of  $\rho \mathbf{v} \cdot \mathbf{n} dA$  term where  $\mathbf{q} = \rho \mathbf{v}$

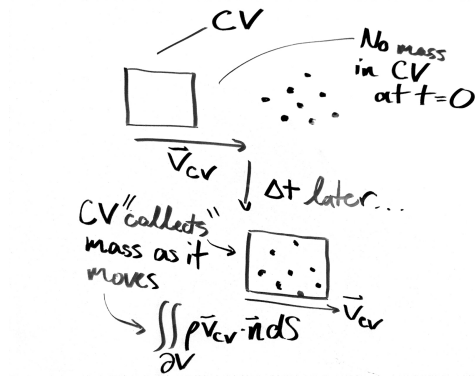


Figure 1.2: Visual representation of  $\rho \mathbf{v}_{CV} \cdot \mathbf{n} dA$  term

The total change in mass in the CV is the contribution of 3 terms: the mass flux due movement of the boundary, the local change in mass *inside* the CV, and the flux *through* the CV due to fluid flow. To avoid the inconvenience of the moving boundary altogether and simplify analysis, we can change to a reference frame where  $\mathbf{v}_{CV} = \mathbf{0}$ , or in other words, we attach our coordinate system to the CV and move its velocity. Mathematically, this assumption gives,

$$0 = \iiint_V \frac{\partial \rho}{\partial t} dV + \iint_{\partial V} \rho \mathbf{v} \cdot \mathbf{n} dA.$$

A key observation to make is that the second surface integral can be reexpressed using Gauss' divergence theorem with  $\mathbf{F} = \rho \mathbf{v}$ ,

$$0 = \iiint_V \frac{\partial \rho}{\partial t} dV + \iiint_V \nabla \cdot (\rho \mathbf{v}) dV,$$

or,

$$0 = \iiint_V \left[ \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) \right] dV.$$

Another observation is that the CV was arbitrary, thus, for the integral to be 0, the integrand *must* be 0. To see this, if the integrand was non-zero anywhere, it would be possible to take the CV as that region. The above relation would then be violated since the integral would be non-zero, meaning the only way for the above relation to hold is if the integrand is *identically* zero. This implies that at every point in the fluid flow,

$$0 = \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}),$$

which is exactly the statement of the continuity equation. Notice for an incompressible fluid,  $\rho$  is constant, giving,

$$\nabla \cdot \mathbf{v} = 0.$$

Physically, this means that if you draw box around *any* point in the velocity field, the amount of flux (velocity) coming in is equal to the amount of flux going out. A classical example of such a flow field is given in the following figure where the velocity field "swirls".

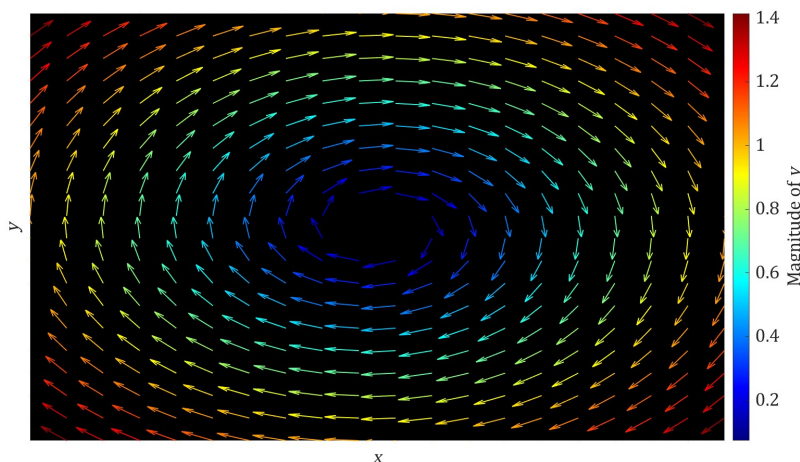


Figure 1.3: Velocity field where  $\nabla \cdot \mathbf{v} = 0$ ,  $\mathbf{v} = (y, -x)$

This local flux condition on the velocity is a core characteristic of incompressible flows and is fundamental to the kinds of solutions encountered.

Since this was a quick derivation, let's remind ourselves of what we have done. We considered a fluid parcel (CV) and moved along with the parcel. The key is that this parcel moves on a *fixed* path over time, so instead of considering the whole system of interest, we only look at a *single* path in the system: the parcel's center of mass. We then used the divergence

theorem to argue that the volume of the parcel was arbitrary, which allowed us to make the volume infinitesimally small and describe *any* point in the system along *any* path. This method of successive constraints allowed for the development of the differential continuity equation, but this method also holds in a more general context.

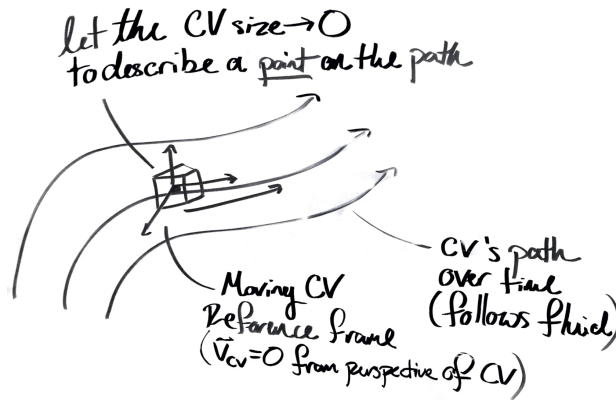


Figure 1.4: Moving fluid parcel with moving reference frame

## 1.4 Conservation Equations, A Unified Approach

The following is an abstract and mostly mathematical development of conservation equations. However, the benefit of this approach is that it presents the underlying principle of many governing equations: they are simply *glorified accounting*. Consider a general (integral) conservation equation with a moving control volume,

$$\{\text{Generation in CV}\} = \{\text{Accumulation in CV}\} - \{\text{Flux into CV}\} + \{\text{Flux out of CV}\}.$$

In mathematical terms, if we have *any* extensive quantity,  $\mathbf{B}$ , and associated intensive quantity,  $\mathbf{b}$  ( $\mathbf{B}$  per mass), then,

$$\underbrace{\iiint_V \rho \mathbf{g} dV}_{\text{Generation}} = \underbrace{\iint_{\partial V} \boldsymbol{\varphi} \cdot \mathbf{n} dA}_{\text{Non-Convective Flux}} + \underbrace{\iint_{\partial V} \mathbf{b} \rho (\mathbf{v} + \mathbf{v}_{CV}) \cdot \mathbf{n} dA}_{\text{Convective Flux + Boundary Flux}} + \underbrace{\iiint_V \frac{\partial(\rho \mathbf{b})}{\partial t} dV}_{\text{Accumulation}}.$$

where  $\mathbf{g}$  is the generation of  $\mathbf{B}$  per unit mass and  $\boldsymbol{\varphi}$  is the flux of  $\mathbf{B}$  not due to mass transport (convection) or movement of the boundary. Convective flux is the transport of  $\mathbf{B}$  as it is carried by the *moving fluid* through the control volume. It is beneficial to think of this term informally as  $(\rho v A) \mathbf{b} = \dot{m} \mathbf{b}$  which is interpreted as,

$$(\text{Mass flow rate}) \times (\mathbf{B} \text{ per mass}) = \text{Flow rate of } \mathbf{B} \text{ through CV}.$$



Or even more succinctly, it is the "out – in" term due to  $\mathbf{B}$  being transported by the fluid through the control volume. An alternative way to think of the three fluxes is that the convective flux represents the macroscopic transport of  $\mathbf{B}$  through bulk motion. Boundary flux represents the transport of  $\mathbf{B}$  due to the movement of the CV boundary. The non-convective flux represents the microscopic mechanisms for the transport of  $\mathbf{B}$ , which is often due to the random motion of molecules. This difference between macro and microscopic scales is the main reason we want to split up the flux term into convective and non-convective parts. These fluxes describe completely different physics, so we should expect they will have different mathematical forms.

Bearing with these abstract forms of flux, we will proceed in the same style as the continuity equation where we consider a moving reference frame where  $\mathbf{v}_{CV} = \mathbf{0}$ . Thus,

$$\iiint_V \rho \mathbf{g} dV = \iint_{\partial V} \boldsymbol{\varphi} \cdot \mathbf{n} dA + \iint_{\partial V} \rho \mathbf{b} \mathbf{v} \cdot \mathbf{n} dA + \iiint_V \frac{\partial(\rho \mathbf{b})}{\partial t} dV.$$

Applying the divergence theorem to the  $\rho \mathbf{b} \mathbf{v}$  and  $\boldsymbol{\varphi}$  terms,

$$\mathbf{0} = \iiint_V \left[ -\rho \mathbf{g} + \nabla \cdot (\boldsymbol{\varphi} + \rho \mathbf{b} \mathbf{v}) + \frac{\partial(\rho \mathbf{b})}{\partial t} \right] dV.$$

Again, by analogy with the continuity equation, the integrand must be  $\mathbf{0}$  since the size of the CV was arbitrary, giving,

$$\rho \mathbf{g} = \nabla \cdot (\boldsymbol{\varphi} + \rho \mathbf{b} \mathbf{v}) + \frac{\partial(\rho \mathbf{b})}{\partial t},$$

or by rearrangement,

$$\underbrace{\frac{\partial(\rho \mathbf{b})}{\partial t}}_{\text{Accumulation}} + \underbrace{\nabla \cdot (\rho \mathbf{b} \mathbf{v})}_{\text{Convection}} = \underbrace{-\nabla \cdot \boldsymbol{\varphi}}_{\text{Molecular Transport}} + \underbrace{\rho \mathbf{g}}_{\text{Generation}}$$

This equation holds for *any*  $\mathbf{b}$ , whether it be a scalar, vector, or even a tensor! So what makes conservation equations different (or similar)? The convection term and time derivative are present for any  $\mathbf{b}$  in a fluid, thus, it is the  $\mathbf{g}$  and  $\boldsymbol{\varphi}$  terms which capture the unique properties of transported quantities. Particularly, for  $\boldsymbol{\varphi}$  there are many so-called "constitutive relations". The following chapter will go over some of these terms for mass, momentum, and energy transport.

# Chapter 2

## Developing the Transport Equations

### 2.1 Flux Equations

It is important to remember that flux has to do with *movement*, so it is represented by a *vector* or *tensor* quantity which has magnitude and direction(s). The underlying principle for the following equations is the intuitive notion that nature *does not* like highly concentrated pockets of energy, so it finds mechanisms to distribute the energy. There are mathematically precise ways of defining how nature "does not like" high energy states, but this mathematical baggage will be abandoned by simply taking this preference of nature as a fundamental principle. For those who are interested, a mathematical overview of this principle is discussed in Appendix 4.

#### 2.1.1 Fick's Law of Diffusion (Mass Transport)

If we have a solution with some concentration,  $C$ , how can we quantify the way the mass distribute will itself throughout the system? We know that the system seeks to move towards equilibrium, which means that there is no net flux of concentration in the system. This must mean that the distribution of concentration is "smoothed out" and there are no local spots of high or low concentration. If we had a localized spot of high concentration, we should expect that the system would seek to move this spot to a region of lower concentration to achieve equilibrium. This movement is described by the flux,  $\mathbf{J}$ , of the concentration,  $C$ ,

$$\varphi = \mathbf{J} = -D\nabla C.$$

Recall that the gradient points in the direction of greatest increase and the negative gradient points in the steepest descent direction. Therefore, this simply states that the flux,  $\mathbf{J}$ , moves towards the steepest descent direction, or towards the lowest concentrations. Based on

what we previously argued, this is intuitive, the mass flows from high concentrations to low concentrations to achieve equilibrium.  $D$  simply measures the tendency for the mass to move based on how large the gradient is.

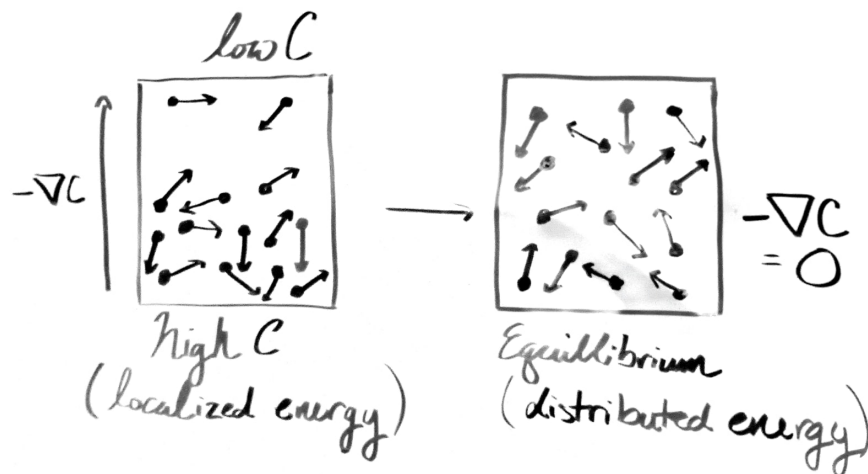


Figure 2.1: Microscopic transport of  $C$  due to a concentration gradient

Microscopically, high concentrations means that there are a lot of intermolecular forces acting in a concentrated area. This means there is a lot of kinetic and internal energy concentrated in one spot. By our underlying principle, nature wishes to avoid this concentrated energy and it distributes the energy to low concentration areas through the mechanism of random molecular motion.

To further this energy argument, Fick's Law can be recasted in terms of the chemical potential energy,  $\mu$ . First consider an ideal gas,

$$P = \frac{n}{V}RT,$$

using  $C = n/V$ ,

$$P = CRT.$$

Thus, Fick's Law becomes (at constant  $T$ ),

$$\mathbf{J} = -\frac{D}{RT}\nabla P.$$

Using the thermodynamic relation,

$$\begin{aligned}\nabla\mu &= RT\nabla\ln(P) \\ &= \frac{RT}{P}\nabla P \\ &= \frac{1}{C}\nabla P,\end{aligned}$$

we now have,

$$\mathbf{J} = -\frac{DC}{RT}\nabla\mu.$$

This states that the flux of a chemical species occurs due to the difference in chemical potential and the flux moves towards the regions of lowest chemical potential. Thus, equilibrium is achieved when there is no chemical potential gradient and the energy is distributed. While this derivation was for an ideal gas, this argument can be extended to a real gas by replacing  $P$  with the fugacity,  $f$ .

$$\mathbf{J} = -\frac{D}{RT}\nabla f.$$

### 2.1.2 Newton's Law of Viscosity (Momentum Transport)

Newton's Law of Viscosity states that the flux of momentum, which we call the stress,  $\boldsymbol{\tau}$ , is proportional to the velocity (momentum) gradient. Or in other words, for an incompressible fluid,

$$\text{1D:} \quad -\boldsymbol{\varphi} = \boldsymbol{\tau} = \mu \frac{du}{dy},$$

$$\text{General:} \quad -\boldsymbol{\varphi} = \boldsymbol{\tau} = \mu \left( \nabla \mathbf{u} + (\nabla \mathbf{u})^T \right) \quad (\text{Difficult!}),$$

where the negative sign for the flux is for convention. These relations seem more complicated, but they are saying the *same* thing as Fick's Law. Nature wishes to go from a state of high momentum to low momentum, thus the momentum flux,  $\boldsymbol{\varphi}$ , moves in the negative momentum gradient (steepest descent direction) to distribute the high momentum to lower momentum states. That's it! Nature does not like the concentrated kinetic energy when a lot of fluid particles with high momentum are concentrated in one area. Therefore, by random collision of the high momentum molecules with lower momentum molecules, the momentum transfers from high to low concentrations. The following figure is an example of this concept for laminar and circular pipe flow.

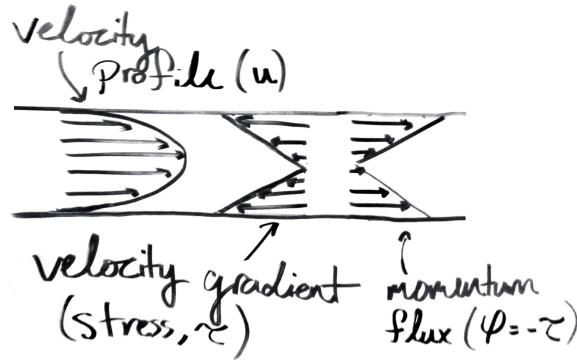


Figure 2.2: Velocity profile and velocity gradient in laminar pipe flow

Notice how the highest "concentration" of velocity occurs at the center of the pipe; this means the momentum flux is lowest at the center since the gradient is zero. Conversely, the velocity "concentration" is lowest at the pipe walls which corresponds to the flux being the highest there. An alternative way to see this is that the momentum flux being the highest at the wall means all of the velocity has "escaped" from the wall, leaving no velocity. The momentum flux being the lowest at the center means that there is no "escape" of velocity, thus giving rise to the maximum velocity. Alternatively, viewing this in terms of stress, there is the highest amount of stress at the wall and thus the most amount of friction. This gives rise to the lowest velocity; the opposite argument works for the center of the pipe which has the least amount of friction. It is nice to get a good grasp of momentum flux and stress; they are essentially the same thing since they are related by a negative sign, but sometimes it is more natural to think of one concept over the other.

For practical computations, it is best to organize the momentum flux using matrices. If you are not familiar with matrix notation, it is quick to learn through a Google search, here is a nice [video](#) to review. In Cartesian coordinates,

$$\nabla \mathbf{u} = \nabla \begin{pmatrix} u_x \\ u_y \\ u_z \end{pmatrix} = \begin{pmatrix} \nabla u_x \\ \nabla u_y \\ \nabla u_z \end{pmatrix} = \begin{pmatrix} \frac{\partial u_x}{\partial x} & \frac{\partial u_x}{\partial y} & \frac{\partial u_x}{\partial z} \\ \frac{\partial u_y}{\partial x} & \frac{\partial u_y}{\partial y} & \frac{\partial u_y}{\partial z} \\ \frac{\partial u_z}{\partial x} & \frac{\partial u_z}{\partial y} & \frac{\partial u_z}{\partial z} \end{pmatrix},$$

thus, adding this with the transpose of the  $\nabla \mathbf{u}$  matrix,

$$\boldsymbol{\tau} = \mu \begin{pmatrix} 2\frac{\partial u_x}{\partial x} & \left(\frac{\partial u_x}{\partial y} + \frac{\partial u_y}{\partial x}\right) & \left(\frac{\partial u_x}{\partial z} + \frac{\partial u_z}{\partial x}\right) \\ \left(\frac{\partial u_y}{\partial x} + \frac{\partial u_x}{\partial y}\right) & 2\frac{\partial u_y}{\partial y} & \left(\frac{\partial u_y}{\partial z} + \frac{\partial u_z}{\partial y}\right) \\ \left(\frac{\partial u_z}{\partial x} + \frac{\partial u_x}{\partial z}\right) & \left(\frac{\partial u_z}{\partial y} + \frac{\partial u_y}{\partial z}\right) & 2\frac{\partial u_z}{\partial z} \end{pmatrix},$$

or component-wise,

$$\tau_{ij} = \mu \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right), \quad \text{for } i, j = x, y, \text{ or } z$$

... a ghastly expression. Admittedly, the general case of Newton's Law of Viscosity requires a lot of mathematical development to fully justify. For those who are interested, this development is included in Appendix 3 and is based on a more classical derivation from continuum mechanics. For another classical derivation based on force balances, consider this [video](#), paired with 10 minutes into this [video](#). However, while these derivations are complete, the mathematical baggage gets in the way of the physical interpretation: that stress is simply the negative momentum flux. It is also important to remember the above argument only works for an incompressible and Newtonian fluid. For the compressible case, the  $\boldsymbol{\tau}$  matrix changes.

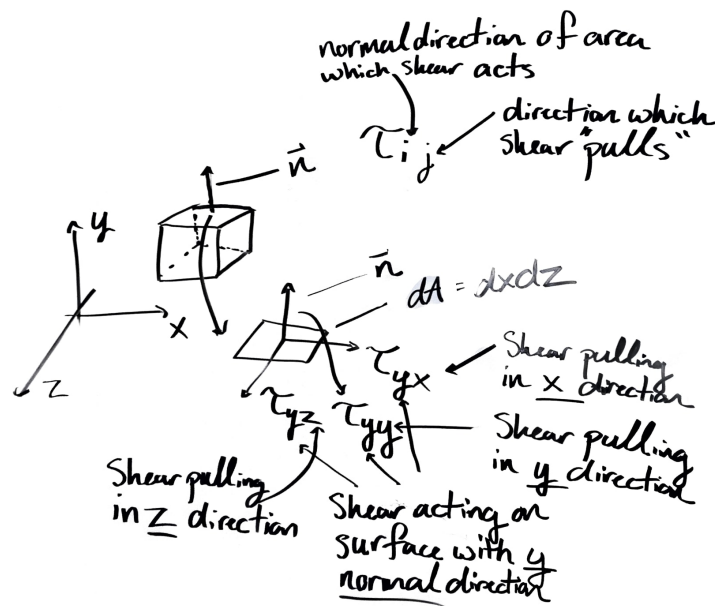


Figure 2.3: Index notation for  $\boldsymbol{\tau}$  matrix

### 2.1.3 Fourier's Law (Energy Transport)

For conservation of energy, we commonly describe the energy flux as heat flux,  $\mathbf{q}$ , through Fourier's Law,

$$\varphi = \mathbf{q} = -k\nabla T,$$

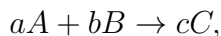
where  $T$  is the temperature of the medium. Development of this follows exactly the same argument as Fick's Law. We expect that heat will flow from high to low temperatures, meaning that the direction of heat flow is in the steepest descent direction: the negative gradient.  $k$  simply measures the tendency of the heat to flow due to the temperature difference. Again, this simply states that nature has a tendency to force highly concentrated energy states to lower, distributed energy states. Can you come up with an argument for *why* this distribution of energy happens on a microscopic scale?

## 2.2 Generation Equations

Generation equations are often much more unique to the specific system being studied. Thus, only a few examples will be discussed and keep in mind these examples are by no means comprehensive.

### 2.2.1 Chemical Reactions (Mass Transport)

Suppose we have a simple reaction,



where  $C$  is generated. A simple model for generation is then given by kinetics,

$$\rho_C \mathbf{g}_C = kA^a B^b,$$

where  $k$  is a rate constant. Notice that this will lead to a system of coupled equations between  $A$ ,  $B$ , and  $C$  since they are all changing in space and time and depend on each other. This is just one example of a reaction term, but other reactions often follow a similar structure by considering kinetics.

Another interesting example for mass transport is when one considers neutron diffusion in a nuclear reactor in which case the conserved quantity is the neutrons and the generation term becomes the neutron source.

### 2.2.2 Sum of Forces (Momentum Transport)

For momentum transport, the sum of forces acting at a point can be modeled as the generation of momentum. That is,

$$\rho \mathbf{g} = \sum \mathbf{F},$$

where  $\mathbf{F}$  represents the force per volume. Some examples of possible  $\mathbf{F}$ 's:

Pressure:  $\mathbf{F} = -\nabla P$

Gravity:  $\mathbf{F} = \rho \mathbf{G}$

Why do we consider the pressure gradient and not the absolute pressure? This is because the pressure acts in the normal direction,  $\mathbf{n}$ , to the control volume. Mathematically,

$$\begin{aligned} \text{Pressure Force} &= - \iint_{\partial V} P \mathbf{n} dA \\ &= - \iiint_V \nabla P dV. \end{aligned}$$

This simply states that the total pressure acting on the surface of the control volume (surface integral) is the sum (volume integral) of the *changes* in pressure inside the control volume. Or alternatively, the sum of *changes* in pressure inside the control volume cancel each other out and leave only the total pressure acting on the surface of the control volume. The volume integral is eventually what turns into the  $-\nabla P$  term.

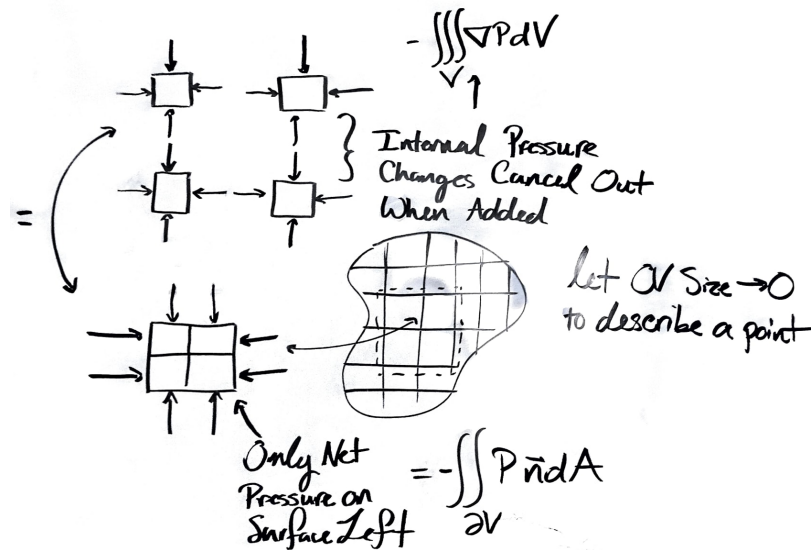


Figure 2.4: Net pressure acting on a fluid surface is the sum of internal changes in pressure of the fluid



### 2.2.3 Heat and Work (Energy Transport)

Suppose we are heating our system at given points,  $\mathbf{x}$ , and at given times,  $t$ , then the generation term simply becomes the heat source at those points,  $Q(\mathbf{x}, t)$ ,

$$\rho g_{heat} = Q(\mathbf{x}, t).$$

We also have the shaft,  $PV$  (flow), and shear work which can also be viewed as generation terms. It is best to first view these quantities in terms of their integral forms and convert them to their differential terms. In the case of the differential energy equation, the shaft work,  $W_S$ , is often taken as 0 since it does not make sense to do shaft work at a point. Thus, we are left with the flow and shear work, these terms arise from flow through or along the *boundary* of the CV, and thus they are represented by *surface* integrals. For the flow work,

$$\iint_{\partial V} W_{PV} dA = - \iint_{\partial V} \frac{P}{\rho} \rho \mathbf{v} \cdot \mathbf{n} dA,$$

where  $-P/\rho$  is the flow work per mass and the  $\rho \mathbf{v} \cdot \mathbf{n} dA$  is the differential mass flow rate through the control volume. For the shear work, we must consider the shear stress,  $\boldsymbol{\tau}$  developed previously. To get the shear work, we consider the shear force occurring at a differential area of the control surface,  $d\mathbf{F} = \boldsymbol{\tau} \cdot \mathbf{n} dA$ . Remember that work is a force times a distance, thus, to get the rate of work done (power), we must dot the force with the velocity (distance/time). Thus,

$$\mathbf{v} \cdot d\mathbf{F} = \mathbf{v} \cdot \boldsymbol{\tau} \cdot \mathbf{n} dA,$$

or by integrating,

$$\text{Shear Work} = \iint_{\partial V} (\mathbf{v} \cdot \boldsymbol{\tau}) \cdot \mathbf{n} dA.$$

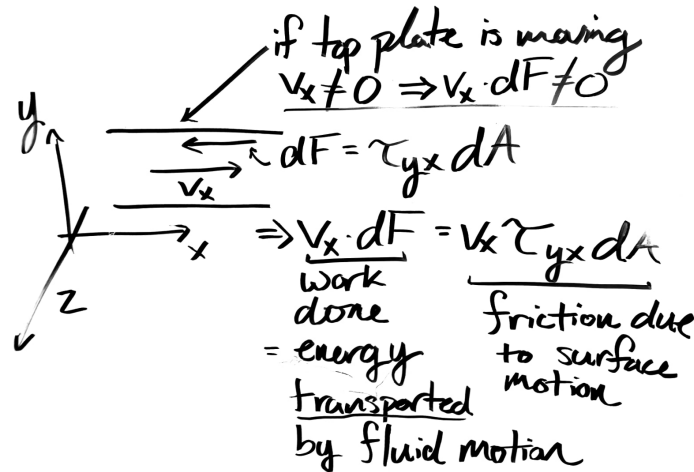


Figure 2.5: Shear work done by a fluid parcel due to a moving plate

By applying the divergence theorem to the integral work terms and letting the CV size go to 0, we get,

$$\begin{aligned}\text{Flow Work} &= -\nabla \cdot (\mathbf{v}P), \\ \text{Shear Work} &= \nabla \cdot (\mathbf{v} \cdot \boldsymbol{\tau}).\end{aligned}$$

For the sake of completeness and for those who are interested, for an incompressible Newtonian fluid,

$$\begin{aligned}\text{Shear Work} &= \mu \nabla \cdot (\mathbf{v} \cdot (\nabla \mathbf{v} + (\nabla \mathbf{v})^T)) \\ &= \text{trace}(\mu \nabla \mathbf{v} [\nabla \mathbf{v} + (\nabla \mathbf{v})^T]) + \mu \mathbf{v} \cdot \nabla^2 \mathbf{v},\end{aligned}$$

where we define the viscous dissipation function,  $\Phi$ , as,

$$\Phi = \text{trace}(\mu \nabla \mathbf{v} [\nabla \mathbf{v} + (\nabla \mathbf{v})^T]).$$

Thus, the shear work becomes,

$$\text{Shear Work} = \Phi + \mu \mathbf{v} \cdot \nabla^2 \mathbf{v}.$$

When solving the transport equations by hand, the dissipation function,  $\Phi$ , is often neglected as it is small and makes the equations considerably harder to solve. It is also a subject geared more towards an advanced continuum mechanics course and thus, for the purposes of this document, it can simply be interpreted as the frictional energy loss.

## 2.3 Putting it All Together

We have developed flux and generation relations for mass, momentum, and energy transport. We also have a general conservation equation which relates these fluxes and generation terms, so let's put them together! To get started, an important definition is the so-called "Laplace operator" or "Laplacian", which is a generalization of the second derivative,

$$\nabla \cdot \nabla = \nabla^2 = \underbrace{\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}}_{\text{Cartesian}}.$$

Physically, this operator represents the diffusion or "spreading out" of the quantity it acts on. For example, the figure below represents the diffusion,  $\nabla^2 T$ , of temperature,  $T$ , over time in non-dimensionalized units.

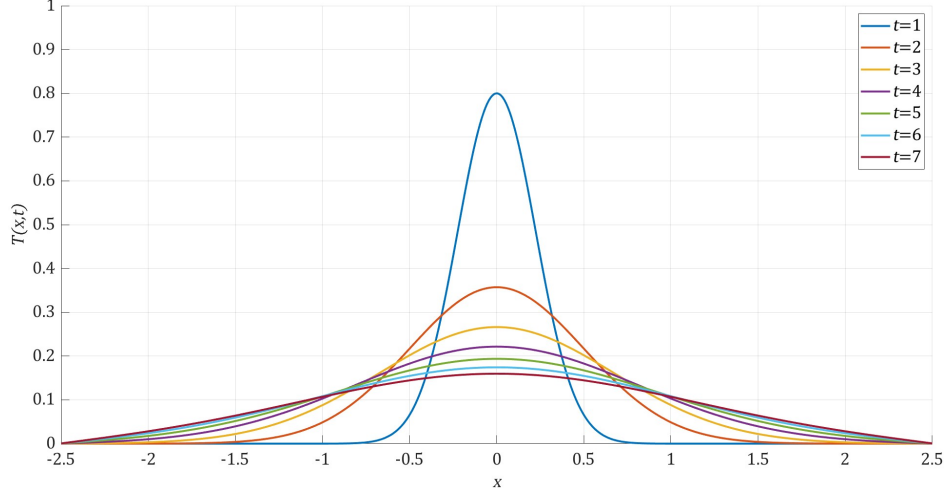


Figure 2.6: Diffusion of  $T$  simulated using the transient heat equation

We will see that diffusion has to do with microscopic transport and arises out of the non-convective flux terms from the conservation equations. Thus, diffusion captures our fundamental principle that nature seeks to spread out high energy states.

### 2.3.1 Mass Conservation Equation

Beyond this point, putting everything together is just mathematical manipulation. It is beneficial to see this once, but its not completely necessary to understand every mathematical step to understand the physical meaning of the equations. It is more important to note the assumptions in deriving the equations and *when* those assumptions are imposed. We'll start with the general mass conservation equation. Recall the general conservation equation,

$$\rho \mathbf{g} = \nabla \cdot (\boldsymbol{\varphi} + \rho \mathbf{b} \mathbf{v}) + \frac{\partial(\rho \mathbf{b})}{\partial t}.$$

Our conserved intensive quantity is the concentration,  $\rho \mathbf{b} = C$ . To avoid specific reaction (generation) terms, let  $R$  be the generation of a substance, with concentration,  $C$ , i.e.  $\rho \mathbf{g} = R$ . From Fick's Law, we also know  $\boldsymbol{\varphi} = -D \nabla C$ . Putting it all together,

$$R = \nabla \cdot (-D \nabla C + \mathbf{v} C) + \frac{\partial C}{\partial t}.$$

Expanding out the flux terms,

$$\underbrace{R}_{\text{Generation}} = \underbrace{-\nabla \cdot (D \nabla C)}_{\text{Diffusion}} + \underbrace{\nabla \cdot (\mathbf{v} C)}_{\text{Convective Flux}} + \underbrace{\frac{\partial C}{\partial t}}_{\text{Accumulation}}.$$

This is can also be written in terms of the material derivative defined as,

$$\frac{DC}{Dt} = \frac{\partial C}{\partial t} + \mathbf{v} \cdot \nabla C.$$

A more visual explanation of the material derivative is given in Appendix 1. With the material derivative, the general mass conservation equation becomes,

$$R = -\nabla \cdot (D\nabla C) + C\nabla \cdot \mathbf{v} + \frac{DC}{Dt}.$$

Often,  $D$  is constant, giving,

$$R = -D\nabla^2 C + C\nabla \cdot \mathbf{v} + \frac{DC}{Dt}.$$

If the fluid is assumed incompressible ( $\nabla \cdot \mathbf{v} = 0$ ), this gives,

$$R + D\nabla^2 C = \frac{DC}{Dt},$$

or,

$$\underbrace{\frac{\partial C}{\partial t}}_{\text{Accumulation}} + \underbrace{\mathbf{v} \cdot \nabla C}_{\text{Convection}} = \underbrace{D\nabla^2 C}_{\text{Diffusion}} + \underbrace{R}_{\text{Generation}}.$$

The differential equation has the same interpretation as the integral conservation equation but with the non-convective flux term replaced with diffusion; this is a common theme among transport equations. In other words, differential conservation equations often follow,

$$\{\text{Accumulation}\} + \{\text{Convection}\} = \{\text{Diffusion}\} + \{\text{Generation}\}.$$

The accumulation term can also be interpreted as the "local" change in time of the quantity of interest.

### 2.3.2 Momentum Conservation Equation

For momentum conservation,  $\mathbf{b} = \mathbf{u}$  and the fluid velocity is the convective velocity,  $\mathbf{v} = \mathbf{u}$ . The generation term is given by  $\rho \mathbf{g} = -\nabla P + \rho \mathbf{G}$ . The flux term is given by  $\boldsymbol{\varphi} = -\mu (\nabla \mathbf{u} + (\nabla \mathbf{u})^T)$ . Thus, we have

$$\frac{\partial(\rho \mathbf{u})}{\partial t} + \nabla \cdot (\rho \mathbf{u} \mathbf{u}) - \mu \nabla \cdot (\nabla \mathbf{u} + (\nabla \mathbf{u})^T) = -\nabla P + \rho \mathbf{G}.$$

For the convective flux term, we can apply the product rule,

$$\nabla \cdot (\rho \mathbf{u} \mathbf{u}) = \nabla \cdot (\rho \mathbf{u}) \mathbf{u} + (\rho \mathbf{u}) \cdot \nabla \mathbf{u}.$$

To see why this form of the product rule is true, see Appendix 2. Recall from the continuity equation,

$$\begin{aligned} 0 &= \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}), \\ \implies \nabla \cdot (\rho \mathbf{u}) &= -\frac{\partial \rho}{\partial t}, \\ \implies \nabla \cdot (\rho \mathbf{u}) \mathbf{u} &= -\mathbf{u} \frac{\partial \rho}{\partial t}. \end{aligned}$$

Using this, now consider the time derivative and convection terms together,

$$\begin{aligned} \frac{\partial(\rho \mathbf{u})}{\partial t} + \nabla \cdot (\rho \mathbf{u} \mathbf{u}) &= \rho \frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \frac{\partial \rho}{\partial t} - \mathbf{u} \frac{\partial \rho}{\partial t} + \rho \mathbf{u} \cdot \nabla \mathbf{u} \\ &= \rho \frac{\partial \mathbf{u}}{\partial t} + \rho \mathbf{u} \cdot \nabla \mathbf{u} \\ &= \rho \frac{D\mathbf{u}}{Dt}. \end{aligned}$$

The above is valid for compressible and incompressible flow. Now consider the diffusion term, the divergence of the stress, which we only developed for incompressible fluids,

$$\mu \nabla \cdot (\nabla \mathbf{u} + (\nabla \mathbf{u})^T) = \mu \nabla^2 \mathbf{u} + \mu \nabla \cdot (\nabla \mathbf{u})^T.$$

The second term of the above drops out for an incompressible fluid (see Appendix 2 if interested), leaving only,

$$\text{Diffusion} = \mu \nabla^2 \mathbf{u}.$$

Thus, for an incompressible fluid, combining all the terms we just developed,

$$\underbrace{\rho \frac{\partial \mathbf{u}}{\partial t}}_{\text{Accumulation}} + \underbrace{\rho \mathbf{u} \cdot \nabla \mathbf{u}}_{\text{Convection}} = \underbrace{\mu \nabla^2 \mathbf{u}}_{\text{Diffusion}} + \underbrace{-\nabla P + \rho \mathbf{G}}_{\text{Generation}}.$$

Notice that in the convection term, the momentum is convected by its own movement; this non-linear term makes these equations *extremely* hard to solve. Therefore, when doing solutions by hand, we often try to find arguments to get rid of this term such as through scaling analysis.

### 2.3.3 Energy Conservation Equation

As a warning, this is a longer derivation with a lot of assumptions and mathematical trickery to simplify the equation. To start, our conserved intensive quantity is the total energy of the system,  $e$ ,

$$\mathbf{b} = e = u + \frac{1}{2} \mathbf{v} \cdot \mathbf{v} + \mathbf{G} \cdot \mathbf{X},$$

where  $u$  is the internal energy,  $\mathbf{v}$  is the velocity of medium (kinetic energy),  $\mathbf{G}$  is the gravitational force, and  $\mathbf{X}$  is the position vector of the medium; in total  $\mathbf{G} \cdot \mathbf{X}$  simply represents the gravitational potential energy. For a constant volume process or an ideal gas,

$$du = C_v dT,$$

where  $C_v$  is the constant volume heat capacity. Furthermore, for a liquid or solid,  $C_v \approx C_p \approx \text{constant}$ . Thus,  $u$  may be replaced by  $C_p T$  in the following equations for a liquid or solid.

The generation term becomes the heat added to the system and the flow and shear work done by the system. Mathematically,

$$\rho \mathbf{g} = \underbrace{Q}_{\text{Heat}} - \underbrace{\nabla \cdot (\mathbf{v}P)}_{\text{Flow Work}} + \underbrace{\Phi + \mu \mathbf{u} \cdot \nabla^2 \mathbf{u}}_{\text{Shear Work}}.$$

The non-convective flux term comes from Fourier's Law,

$$\boldsymbol{\varphi} = \mathbf{q} = -k \nabla T.$$

Putting it all together,

$$\frac{\partial(\rho e)}{\partial t} + \nabla \cdot (\rho \mathbf{v} e) - \nabla \cdot (k \nabla T) = Q - \nabla \cdot (\mathbf{v}P) + \Phi + \mu \mathbf{v} \cdot \nabla^2 \mathbf{v}.$$

Consider the accumulation and convection terms together,

$$\begin{aligned} \frac{\partial(\rho e)}{\partial t} + \nabla \cdot (\rho \mathbf{v} e) &= \rho \frac{\partial e}{\partial t} + e \frac{\partial \rho}{\partial t} + e \nabla \cdot (\rho \mathbf{v}) + (\rho \mathbf{v}) \cdot \nabla e \\ &= \rho \frac{\partial e}{\partial t} + \rho \mathbf{v} \cdot \nabla e + e \left( \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) \right). \end{aligned}$$

The second term is 0 by the continuity equation, thus,

$$\frac{\partial(\rho e)}{\partial t} + \nabla \cdot (\rho \mathbf{v} e) = \rho \frac{\partial e}{\partial t} + \rho \mathbf{v} \cdot \nabla e = \rho \frac{De}{Dt}.$$

This is valid for an both compressible and incompressible flows, but the following developments only consider an incompressible and Newtonian fluid. First considering the time derivative,

$$\begin{aligned} \rho \frac{\partial e}{\partial t} &= \rho \left( C_p \frac{\partial T}{\partial t} + \frac{1}{2} \frac{\partial}{\partial t} (\mathbf{v} \cdot \mathbf{v}) + \frac{\partial}{\partial t} (\mathbf{G} \cdot \mathbf{X}) \right) \\ &= \rho C_p \frac{\partial T}{\partial t} + \rho \mathbf{v} \cdot \frac{\partial \mathbf{v}}{\partial t} + \rho \mathbf{v} \cdot \mathbf{G}, \end{aligned}$$

where the kinetic energy term comes from application of the product rule and the potential energy term comes from the fact that  $\mathbf{G}$  is a constant vector and the time derivative of the position vector,  $\mathbf{X}$ , is the velocity vector,  $\mathbf{v}$ . Now for the convection term,

$$\begin{aligned}\rho \mathbf{v} \cdot \nabla e &= \rho C_p \mathbf{v} \cdot \nabla T + \frac{1}{2} \rho \mathbf{v} \cdot \nabla (\mathbf{v} \cdot \mathbf{v}) + \rho \mathbf{v} \cdot \nabla (\mathbf{G} \cdot \mathbf{X}) \\ &= \rho C_p \mathbf{v} \cdot \nabla T + \rho \mathbf{v} \cdot \mathbf{v} \cdot \nabla \mathbf{v} + \rho \mathbf{v} \cdot \mathbf{G} \cdot \nabla \mathbf{X},\end{aligned}$$

where the kinetic energy term comes from the product rule and and potential energy term arises because  $\mathbf{G}$  is a constant vector. By recombining the accumulation and convection terms,

$$\frac{\partial(\rho e)}{\partial t} + \nabla \cdot (\rho \mathbf{v} e) = \rho C_p \left( \frac{\partial T}{\partial t} + \mathbf{v} \cdot \nabla T \right) + \rho \mathbf{v} \cdot \left( \frac{\partial \mathbf{v}}{\partial t} + \mathbf{v} \cdot \nabla \mathbf{v} \right) + \rho \mathbf{v} \cdot \mathbf{G} + \rho \mathbf{v} \cdot \mathbf{G} \cdot \nabla \mathbf{X}.$$

By the Navier-Stokes equations, we have,

$$\rho \mathbf{v} \cdot \left( \frac{\partial \mathbf{v}}{\partial t} + \mathbf{v} \cdot \nabla \mathbf{v} \right) = \mathbf{v} \cdot \mu \nabla^2 \mathbf{v} - \mathbf{v} \cdot \nabla P + \rho \mathbf{v} \cdot \mathbf{G}.$$

This allows us to rewrite the accumulation and convection terms as,

$$\frac{\partial(\rho e)}{\partial t} + \nabla \cdot (\rho \mathbf{v} e) = \rho C_p \left( \frac{\partial T}{\partial t} + \mathbf{v} \cdot \nabla T \right) + \mathbf{v} \cdot \mu \nabla^2 \mathbf{v} - \mathbf{v} \cdot \nabla P + 2\rho \mathbf{v} \cdot \mathbf{G} + \rho \mathbf{v} \cdot \mathbf{G} \cdot \nabla \mathbf{X}.$$

Plugging this back into the main conservation equation,

$$\begin{aligned}\rho C_p \left( \frac{\partial T}{\partial t} + \mathbf{v} \cdot \nabla T \right) + \cancel{\mu \mathbf{v} \cdot \nabla^2 \mathbf{v}} - \cancel{\mathbf{v} \cdot \nabla P} + 2\rho \mathbf{v} \cdot \mathbf{G} + \rho \mathbf{v} \cdot \mathbf{G} \cdot \nabla \mathbf{X} - \nabla \cdot (k \nabla T) \\ = Q - \cancel{\mathbf{v} \cdot \nabla P} + \Phi + \cancel{\mu \mathbf{v} \cdot \nabla^2 \mathbf{v}}.\end{aligned}$$

Assuming constant  $k$  and cancelling terms,

$$\rho C_p \left( \frac{\partial T}{\partial t} + \mathbf{v} \cdot \nabla T \right) + (2\rho \mathbf{v} \cdot \mathbf{G} + \rho \mathbf{v} \cdot \mathbf{G} \cdot \nabla \mathbf{X}) = k \nabla^2 T + Q + \Phi.$$

Assuming that the fluid does not gain a considerable amount of gravitational potential energy, we take  $\mathbf{G} = \mathbf{0}$ , giving,

$$\underbrace{\rho C_p \frac{\partial T}{\partial t}}_{\text{Accumulation}} + \underbrace{\rho C_p \mathbf{v} \cdot \nabla T}_{\text{Convection}} = \underbrace{k \nabla^2 T}_{\text{Diffusion}} + \underbrace{Q + \Phi}_{\text{Generation}}.$$

This is a practical form of the energy equation for an incompressible and Newtonian liquid

that gains negligible gravitational energy. To describe heat conduction in a solid, take  $\mathbf{v} = \mathbf{0}$  and  $\Phi = 0$ . To describe an ideal gas that is approximately incompressible, replace  $C_p$  with  $C_v$ .

## 2.4 Multicomponent Mass Transfer

### 2.4.1 Component Transport Equations

This section is addendum to the mass conservation equation to account for mass transfer when multiple components are involved. Implicitly, we only considered one species in a solution or mixture and arrived at the equation,

$$\frac{\partial C}{\partial t} + \nabla \cdot (\mathbf{v}C) = D\nabla^2 C + R,$$

where we assumed a constant diffusion coefficient,  $D$ . However, this equation generalizes to each component in the system. Physically, nothing changes, however, the mathematical notation becomes much more delicate. Suppose we have an  $N$  component system and we consider the  $i$ th species. By the general conservation equation for the  $i$ th species, we can conclude,

$$\frac{\partial C_i}{\partial t} + \nabla \cdot (\mathbf{v}C_i) = D_i \nabla^2 C_i + R_i,$$

where  $C_i$  is the concentration of the  $i$ th species,  $D_i$  is the diffusion constant of the  $i$ th species, and  $R_i$  is the generation or consumption of the  $i$ th species. If we sum over all of the  $N$  species, we find,

$$C = \sum_{i=1}^N C_i, \quad R = \sum_{i=1}^N R_i,$$

where  $C$  is the total concentration of the system and  $R$  is the total generation of the system. Thus, the system conservation equation becomes,

$$\frac{\partial C}{\partial t} + \sum_{i=1}^N (\nabla \cdot (\mathbf{v}C_i)) = \sum_{i=1}^N (D_i \nabla^2 C_i) + R,$$

or equivalently,

$$\frac{\partial C}{\partial t} + \nabla \cdot \left( \mathbf{v} \sum_{i=1}^N C_i \right) = \sum_{i=1}^N (D_i \nabla^2 C_i) + R,$$

thus,

$$\frac{\partial C}{\partial t} + \nabla \cdot (\mathbf{v}C) = \sum_{i=1}^N (D_i \nabla^2 C_i) + R.$$



This is a nice relation, but it doesn't tell us anything new. We'll see soon that we can simplify the above to get rid of the last summation. A better form of the above equation comes from considering the mass (density) of each component instead of the concentration. Using the relation,  $\rho_i = C_i M_i$ , where  $M_i$  is the molar mass of the  $i$ th component, we have,

$$\frac{1}{M_i} \frac{\partial \rho_i}{\partial t} + \frac{1}{M_i} \nabla \cdot (\rho_i \mathbf{v}) = \frac{D_i}{M_i} \nabla^2 \rho_i + R_i,$$

or equivalently,

$$\frac{\partial \rho_i}{\partial t} + \nabla \cdot (\rho_i \mathbf{v}) = D_i \nabla^2 \rho_i + M_i R_i.$$

We again sum over all components to find,

$$\rho = \sum_{i=1}^N \rho_i, \quad MR = \sum_{i=1}^N M_i R_i,$$

where  $\rho$  is the total density and  $MR$  is the total mass generation of the system. For most processes, mass is not generated and thus,  $MR = 0$ , giving,

$$\frac{\partial \rho}{\partial t} + \sum_{i=1}^N (\nabla \cdot (\rho_i \mathbf{v})) = \sum_{i=1}^N (D_i \nabla^2 \rho_i).$$

or,

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \left( \mathbf{v} \sum_{i=1}^N \rho_i \right) = \sum_{i=1}^N (D_i \nabla^2 \rho_i),$$

which becomes,

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = \sum_{i=1}^N (D_i \nabla^2 \rho_i).$$

However, since we are analyzing the total mass of the system, we can apply the continuity equation to the total system,

$$0 = \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}).$$

Thus, we have,

$$\sum_{i=1}^N (D_i \nabla^2 \rho_i) = 0.$$

Physically, this means that the total mass diffusion in a system is 0. That is, diffusion in one component will be made up for by diffusion in another component.

### 2.4.2 Common Notations for Multicomponent Systems

In addition to the differential equations, there is some important (and confusing) notation to become accustomed to. Often, we define total the concentration flux,  $\mathbf{N}_i$ , as the sum of the non-convective and convective flux,

$$\mathbf{N}_i := \mathbf{J}_i + \mathbf{v}C_i := \mathbf{v}_iC_i,$$

where  $\mathbf{J}_i$  comes from Fick's Law of Diffusion,

$$\mathbf{J}_i = -D_i \nabla C_i,$$

and we have defined the average component velocity,  $\mathbf{v}_i$ . We can rearrange the above equations as,

$$-D_i \nabla C_i = C_i (\mathbf{v}_i - \mathbf{v}),$$

if we consider a stationary fluid with  $\mathbf{v} = \mathbf{0}$ , then,

$$-D_i \nabla C_i = C_i \mathbf{v}_i,$$

Physically, this tells us that diffusion is due to microscopic transport of particles with component velocity  $\mathbf{v}_i$ . This tells us that an individual component of solution can diffuse with a velocity  $\mathbf{v}_i$  while the solution as a whole remains stationary. If we further define the bulk velocity,  $\mathbf{v}$ , as,

$$\mathbf{v}C := \sum_{i=1}^N \mathbf{v}_i C_i,$$

then we can sum over the component flux relations to get,

$$\sum_{i=1}^N \mathbf{v}_i C_i = - \sum_{i=1}^N (D_i \nabla C_i) + \mathbf{v} \sum_{i=1}^N C_i,$$

giving,

$$\mathbf{v}C = - \sum_{i=1}^N (D_i \nabla C_i) + \mathbf{v}C,$$

or,

$$\sum_{i=1}^N (D_i \nabla C_i) = 0.$$

If we plug this back into the summed concentration equation,

$$\frac{\partial C}{\partial t} + \nabla \cdot \sum_{i=1}^N (\mathbf{v}_i C_i) = R,$$

or written in terms of the total component fluxes,  $\mathbf{N}_i$ ,

$$\frac{\partial C}{\partial t} + \nabla \cdot \sum_{i=1}^N \mathbf{N}_i = R,$$

or even more simply,

$$\frac{\partial C}{\partial t} + \nabla \cdot (\mathbf{v}C) = R.$$

We can also express any concentrations in terms of mole fractions,  $x_i$  for a liquid and  $y_i$  for a vapor. For example, for a liquid,

$$x_i = \frac{C_i}{C},$$

with the condition that over all  $N$  components,

$$\sum_{i=1}^N x_i = 1.$$

To summarize all the notation,

$$\begin{aligned} \mathbf{N}_i &= \mathbf{v}_i C_i = \mathbf{J}_i + \mathbf{v} C_i \\ &= -D_i \nabla C_i + \mathbf{v} C_i \\ &= -D_i \nabla C_i + x_i \sum_{i=1}^N \mathbf{v}_i C_i \\ &= -D_i \nabla C_i + x_i \sum_{i=1}^N \mathbf{N}_i. \end{aligned}$$

When we consider the density instead of the concentration, we define the total mass flux,  $\mathbf{n}_i$ ,

$$\mathbf{n}_i := \mathbf{j}_i + \rho_i \mathbf{v} := \rho_i \mathbf{v}_i,$$

where,

$$\mathbf{j}_i = -D_i \nabla \rho_i.$$

By the same arguments used in the concentration equation, we find that for the entire system,

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \sum_{i=1}^N \mathbf{n}_i = 0,$$

where the reaction term is 0 since the total mass is conserved. Again, we can express any of the mass relations this in terms of mass fractions,  $w_i$ ,

$$w_i = \frac{\rho_i}{\rho},$$

with the condition that over all  $N$  components,

$$\sum_{i=1}^N w_i = 1.$$

To summarize all the notation,

$$\begin{aligned} \mathbf{n}_i &= \rho_i \mathbf{v}_i = \dot{\mathbf{j}}_i + \rho_i \mathbf{v} \\ &= -D_i \nabla \rho_i + \rho_i \mathbf{v} \\ &= -D_i \nabla \rho_i + w_i \sum_{i=1}^N \rho_i \mathbf{v}_i \\ &= -D_i \nabla \rho_i + w_i \sum_{i=1}^N \mathbf{n}_i. \end{aligned}$$

# Chapter 3

## Analyzing the Transport Equations

### 3.1 Non-Dimensional Forms of the Transport Equations

The following section is an aside for the main developments in this document and may be skipped, however, it offers an explanation of the seemingly random definitions of common dimensionless numbers. We often define dimensionless numbers to help us analyze the properties of differential equations without actually solving them, in essence, they tell us what terms are important and which terms can be ignored. The disadvantage is that it takes quite a bit of mathematical trickery to arrive at the results. However, by bearing with this, we may arrive at very general and rigorous methods of analyzing transport equations.

#### 3.1.1 Momentum Conservation Equation

The momentum conservation equation gives rise to perhaps the most important dimensionless number in transport equations - the Reynolds number. The main idea behind non-dimensionalization is to measure the main variables of the equation on a "natural" scale. What "natural" means depends on the problem, but generally, we take the natural scale to be any quantity that we can readily measure. Mathematically, this means we multiply our variables by constants to turn them into dimensionless numbers. For example, if we want to non-dimensionalize the velocity,  $\mathbf{u}$ , we would divide the velocity by a natural velocity,  $U$ . We may take  $U$  to be an average velocity or a free stream velocity, but most importantly, it is a velocity that we can readily measure. Ultimately, this measurability will allow us to simplify analysis. Let us define the non-dimensional velocity,  $\mathbf{u}^*$ , as,

$$\mathbf{u}^* = \frac{\mathbf{u}}{U},$$

or,

$$U\mathbf{u}^* = \mathbf{u}.$$

Similarly, let's define a natural length,  $L$ , and non-dimensionalize the spatial variables,

$$L \begin{pmatrix} x^* \\ y^* \\ z^* \end{pmatrix} = \begin{pmatrix} x \\ y \\ z \end{pmatrix}.$$

Notice that this rescaling of the spatial variables implies that the gradient becomes,

$$\frac{1}{L}\nabla^* = \nabla,$$

because,

$$\frac{\partial}{\partial x^*} = \frac{\partial}{\partial (x/L)} = L \frac{\partial}{\partial x},$$

which can be generalized to the other spatial variables. To non-dimensionalize time,  $t$ , there is often not an easily measurable time scale, so we *define* a time scale by dividing the natural length by the natural velocity. In other words, the non-dimensionalized time,  $t^*$ , becomes,

$$\frac{L}{U}t^* = t,$$

which implies,

$$\frac{U}{L} \frac{\partial}{\partial t^*} = \frac{\partial}{\partial t}.$$

We also turn the  $\mathbf{G}$  vector into the magnitude of gravity,  $g$ , times the unit direction vector  $\mathbf{G}^*$ ,

$$g\mathbf{G}^* = \mathbf{G}.$$

Similarly, for the pressure, we select a natural pressure drop (can be the pressure drop from an inlet to an outlet),  $\Delta p$ , with the corresponding non-dimensionalized pressure,  $P^*$ ,

$$\Delta p P^* = P.$$

With these definitions, we can finally non-dimensionalize the Navier-Stokes equations. Recall that the equations can be written as,

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} = \nu \nabla^2 \mathbf{u} + \mathbf{G} - \frac{1}{\rho} \nabla P,$$

where  $\nu = \mu/\rho$  is the kinematic viscosity or "momentum diffusivity". Plugging in all of the non-dimensional equivalent variables,

$$\frac{U^2}{L} \frac{\partial \mathbf{u}^*}{\partial t^*} + \frac{U^2}{L} \mathbf{u}^* \cdot \nabla^* \mathbf{u}^* = \nu \frac{U}{L^2} \nabla^{*2} \mathbf{u}^* + g \mathbf{G}^* - \frac{\Delta p}{\rho L} \nabla^* P^*.$$

Multiplying the entire equation by  $L/U^2$ ,

$$\frac{\partial \mathbf{u}^*}{\partial t^*} + \mathbf{u}^* \cdot \nabla^* \mathbf{u}^* = \frac{\nu}{UL} \nabla^{*2} \mathbf{u}^* + \frac{gL}{U^2} \mathbf{G}^* - \frac{\Delta p}{\rho U^2} \nabla^* P^*.$$

This is where we now define some common dimensionless numbers. First, the famous Reynolds number,  $Re$ ,

$$Re = \frac{\text{Inertia Force}}{\text{Viscous Force}} = \frac{\rho U^2 L^2}{\mu (U/L) L^2} = \frac{\rho U L}{\mu} = \frac{UL}{\nu}.$$

The Froude number,  $Fr$ ,

$$Fr = \sqrt{\frac{\text{Inertia Force}}{\text{Gravitational Force}}} = \sqrt{\frac{\rho U^2 L^2}{\rho g L^3}} = \frac{U}{\sqrt{gL}}.$$

The Euler number,  $Eu$ ,

$$Eu = \frac{\text{Pressure Force}}{\text{Inertia Force}} = \frac{\Delta p L^2}{\rho U^2 L^2} = \frac{\Delta p}{\rho U^2}.$$

Using these definitions, the Navier-Stokes equations become,

$$\frac{\partial \mathbf{u}^*}{\partial t^*} + \mathbf{u}^* \cdot \nabla^* \mathbf{u}^* = \frac{1}{Re} \nabla^{*2} \mathbf{u}^* + \frac{1}{Fr^2} \mathbf{G}^* - Eu \nabla^* P^*.$$

It may seem that we have done nothing to simplify the equations, but here is where the measurability of the natural variables becomes important. Since the dimensionless numbers are in terms of measurable variables, we know  $Re$ ,  $Fr$ , and  $Eu$  for a given system. Thus, we can input information about the system into the differential equation without solving it. For example, if we know  $U$  is large, then the inertial forces will be large, implying  $Re$  and  $Fr$  will be large. This allows us to ignore the diffusion and gravity terms,

$$\frac{\partial \mathbf{u}^*}{\partial t^*} + \mathbf{u}^* \cdot \nabla^* \mathbf{u}^* = \cancel{\frac{1}{Re} \nabla^{*2} \mathbf{u}^*} + \cancel{\frac{1}{Fr^2} \mathbf{G}^*} - Eu \nabla^* P^*,$$

$$\frac{\partial \mathbf{u}^*}{\partial t^*} + \mathbf{u}^* \cdot \nabla^* \mathbf{u}^* = -Eu \nabla^* P^*.$$

Notice we cannot necessarily ignore the pressure term, while  $Eu$  is small due to high interial forces, the pressure gradient,  $\nabla^* P^*$ , may be large, which makes the pressure term on the same order of magnitude as the other terms. Alternatively, if we have a highly viscous flow (high  $\nu$ ) with small interial forces (small  $U$ ), then ,

$$Re \left( \frac{\partial \mathbf{u}^*}{\partial t^*} + \mathbf{u}^* \cdot \nabla^* \mathbf{u}^* \right) = \nabla^{*2} \mathbf{u}^* + \frac{Re}{Fr^2} \mathbf{G}^* - Re Eu \nabla^* P^*.$$

Since  $Re$  is known to be small based on our assumptions, we can cancel any terms with  $Re$ , giving,

$$\nabla^{*2} \mathbf{u}^* = Re Eu \nabla^* P^*,$$

where the pressure term again cannot be ignored since the pressure gradient may be high. These scaling arguments are the main idea behind non-dimensionalizing variables, it allows us to argue which terms in a differential equation are important based on ratios of quantities we know. We will see that  $Re$  also shows up in the other transport equations where it serves as a measure of the convection in the equations.

### 3.1.2 Mass Conservation Equation

The non-dimensionalization of the mass conservation equation follows a similar start as the momentum equations. We define the natural velocity,  $U$ , natural length,  $L$ , and natural time,  $L/U$ , and their corresponding non-dimensional variables,

$$U \mathbf{v}^* = \mathbf{v}, \quad L \begin{pmatrix} x^* \\ y^* \\ z^* \end{pmatrix} = \begin{pmatrix} x \\ y \\ z \end{pmatrix}, \quad \frac{L}{U} t^* = t.$$

To non-dimensionalize the concentration,  $C$ , we follow a similar procedure by defining a reference concentration,  $C_0$ ,

$$C_0 C^* = C,$$

where we often take  $C_0$  to be based on concentrations known on the boundary of the domain of interest. Using these definitions, we can take the mass conservation equation,

$$\frac{\partial C}{\partial t} + \nabla \cdot (\mathbf{v}C) = D \nabla^2 C + R,$$

and plug in the equivalent non-dimensional variables,

$$\frac{UC_0}{L} \frac{\partial C^*}{\partial t^*} + \frac{UC_0}{L} \nabla^* \cdot (\mathbf{v}^* C^*) = D \frac{C_0}{L^2} \nabla^{*2} C^* + R.$$



Multiplying the entire equation by  $L/UC_0$ ,

$$\frac{\partial C^*}{\partial t^*} + \nabla^* \cdot (\mathbf{v}^* C^*) = \frac{D}{UL} \nabla^{*2} C^* + \frac{L}{UC_0} R,$$

by multiplying the diffusion term by  $\nu/\nu$ ,

$$\frac{\partial C^*}{\partial t^*} + \nabla^* \cdot (\mathbf{v}^* C^*) = \frac{D}{\nu} \frac{\nu}{UL} \nabla^{*2} C^* + \frac{L}{UC_0} R,$$

we arrive at,

$$\frac{\partial C^*}{\partial t^*} + \nabla^* \cdot (\mathbf{v}^* C^*) = \frac{1}{Sc} \frac{1}{Re} \nabla^{*2} C^* + \frac{L}{UC_0} R.$$

Where we define the Schmidt number,  $Sc$ , as,

$$Sc = \frac{\text{Momentum Diffusivity}}{\text{Mass Diffusivity}} = \frac{\nu}{D}.$$

Alternatively, it is sometimes useful to define the Péclet number,  $Pe$ , as,

$$Pe = \frac{\text{Mass Convection Rate}}{\text{Mass Diffusion Rate}} = \frac{UL}{D} = Sc \cdot Re.$$

From the presence of  $Re$ , we see that if  $U$  is large,  $Re$  will be large, indicating that convective transport dominates and diffusion is negligible,

$$\frac{\partial C^*}{\partial t^*} + \nabla^* \cdot (\mathbf{v}^* C^*) = \frac{1}{\cancel{Sc}} \frac{1}{Re} \cancel{\nabla^{*2} C^*} + \frac{L}{UC_0} R.$$

Similarly, if  $Re$  is moderate while there is a high mass diffusivity,  $D$ , (small  $Sc$ ), then,

$$Re \left( \frac{\partial C^*}{\partial t^*} + \nabla^* \cdot (\mathbf{v}^* C^*) \right) = \frac{1}{Sc} \nabla^{*2} C^* + Re \frac{L}{UC_0} R.$$

Assuming  $Re \ll 1/Sc$ , then we have,

$$0 = \frac{1}{Sc} \nabla^{*2} C^* + Re \frac{L}{UC_0} R,$$

where we cannot necessarily ignore the reaction term since it may be large. What this means is that at small flow rates (low convection), diffusion dominates and is the main mode of transport, which is quite intuitive. Again, we see that by using natural variables to define dimensionless numbers, we can develop intuitive and more rigorous arguments to simplify our analysis of transport equations.

### 3.1.3 Energy Conservation Equation

The energy conservation equation follows the exact same steps as the mass conservation equation but instead of a reference concentration, we select a reference temperature,  $T_0$ . Explicitly, our non-dimensional variables are,

$$U\mathbf{v}^* = \mathbf{v}, \quad L \begin{pmatrix} x^* \\ y^* \\ z^* \end{pmatrix} = \begin{pmatrix} x \\ y \\ z \end{pmatrix}, \quad \frac{L}{U} t^* = t, \quad T_0 T^* = T.$$

The energy equation,

$$\rho C_p \frac{\partial T}{\partial t} + \rho C_p \mathbf{v} \cdot \nabla T = k \nabla^2 T + Q + \Phi,$$

can be written as,

$$\begin{aligned} \frac{\partial T}{\partial t} + \mathbf{v} \cdot \nabla T &= \frac{k}{\rho C_p} \nabla^2 T + \frac{1}{\rho C_p} (Q + \Phi) \\ &= \alpha \nabla^2 T + \frac{1}{\rho C_p} (Q + \Phi) \end{aligned}$$

where we define the thermal diffusivity,  $\alpha$ , as  $\alpha = k/\rho C_p$ . Plugging in the non-dimensional variables into this form of the energy equation,

$$\frac{UT_0}{L} \frac{\partial T^*}{\partial t^*} + \frac{UT_0}{L} \mathbf{v}^* \cdot \nabla^* T^* = \alpha \frac{T_0}{L^2} \nabla^{*2} T^* + \frac{1}{\rho C_p} (Q + \Phi),$$

and multiplying the entire equation by  $L/UT_0$ ,

$$\frac{\partial T^*}{\partial t^*} + \mathbf{v}^* \cdot \nabla^* T^* = \frac{\alpha}{UL} \nabla^{*2} T^* + \frac{L}{\rho C_p UT_0} (Q + \Phi).$$

If we multiply the diffusion term by  $\nu/\nu$ ,

$$\frac{\partial T^*}{\partial t^*} + \mathbf{v}^* \cdot \nabla^* T^* = \frac{\alpha}{\nu} \frac{\nu}{UL} \nabla^{*2} T^* + \frac{L}{\rho C_p UT_0} (Q + \Phi),$$

we arrive at,

$$\frac{\partial T^*}{\partial t^*} + \mathbf{v}^* \cdot \nabla^* T^* = \frac{1}{Pr} \frac{1}{Re} \nabla^{*2} T^* + \frac{L}{\rho C_p UT_0} (Q + \Phi).$$

Where we define the Prandtl number,  $Pr$ , as,

$$Pr = \frac{\text{Momentum Diffusivity}}{\text{Thermal Diffusivity}} = \frac{\nu}{\alpha}.$$

Using these definitions, can you come up arguments for simplifications of the energy equation? What happens when  $Re$  is large? What happens when  $Pr$  is large? What do these mean physically? What are the main modes of transport in each case?

### 3.1.4 Transport Equation Analogies

Using the same reasoning as we used in the previous sections, we can see that all of the non dimensionalized transport equations have the form <sup>1</sup>,

$$\frac{\partial \mathbf{b}^*}{\partial t^*} + \mathbf{v}^* \cdot \nabla^* \mathbf{b}^* = \frac{1}{\beta} \frac{1}{Re} \nabla^{*2} \mathbf{b}^* + \mathbf{g}^*,$$

where  $\mathbf{g}^*$  is the non dimensionalized generation term and  $\beta$  is a dimensionless number defined as,

$$\beta = \frac{\text{Momentum Diffusivity}}{\text{Diffusivity of } \mathbf{b}} = \frac{\nu}{\gamma}.$$

$\gamma$  is the measure of diffusivity of  $\mathbf{b}$ , for example, for energy transport  $\gamma = \alpha$  and for momentum transport  $\gamma = \nu$ . We observe that since  $\beta$  is dimensionless,  $\gamma$  must have units of  $L^2/T$ . Thus, using this general structure, we may summarize all of the dimensionless transport equations in a single table.

**Table 1: Summary of Dimensionless Transport Equations**

Transported Quantity	$\mathbf{b}^*$	$\beta$
Momentum	$\mathbf{u}^*$	1
Mass	$C^*, \rho^*$	$Sc = \nu/D$
Energy	$T^*$	$Pr = \nu/\alpha$

Using the same reasoning we previously developed, we see that in convection dominated situations,  $Re$  is large and the diffusion of  $\mathbf{b}$  is negligible ( $Re \gg 1/\beta$ ). If  $Re \ll 1/\beta$ , then diffusive forces dominate and the convection term can be ignored. It is easy to see that all of the transport equations have the *same* mathematical form. What changes is the physical interpretation of the equations and particularly the assumptions and boundary conditions that are needed to solve the equations.

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<sup>1</sup>To get this analogy to work for the mass and concentration equations, it is assumed the system as a whole is incompressible ( $\nabla^* \cdot \mathbf{v}^* = 0$ ). Physically, this arises in a well mixed tank ( $\nabla \rho = \mathbf{0}$ ) and when the mass to volume ratio remains constant in time ( $\partial \rho / \partial t = 0$ ). If these assumptions do not hold, replace  $\mathbf{v}^* \cdot \nabla^* \mathbf{b}^*$  with  $\nabla^* \cdot (\mathbf{b}^* \mathbf{v}^*)$ .

## 3.2 Common Assumptions

This section offers alternative methods for simplifying transport equations. These methods are a little less rigorous than non-dimensionalization, but they offer a quicker way to eliminate a lot of terms for simple situations.

### 3.2.1 Steady State

A very common assumption when solving transport equations by hand is to only consider steady state problems, mathematically, this means,

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

Physically, this assumption states that the fluxes in or out of the control volume are due solely to generation.

$$\cancel{\frac{\partial(\rho\mathbf{b})}{\partial t}} + \nabla \cdot (\varphi + \rho\mathbf{b}\mathbf{v}) = \rho\mathbf{g}.$$

Moreover, if there is no convection, then there is only molecular transport through diffusion driven by the generation term.

$$\nabla \cdot (\varphi + \cancel{\rho\mathbf{b}\mathbf{v}}) = \rho\mathbf{g},$$

$$\underbrace{\nabla \cdot \varphi}_{\text{Molecular Transport}} = \underbrace{\rho\mathbf{g}}_{\text{Generation}}$$

In other words, the generation term will cause the system to diffuse into a steady state profile that remains constant in time. In contrast, to see just how messy solutions can get for transient problems, consider reading Appendix 5.

### 3.2.2 Symmetry

Often, when working in cylindrical or spherical coordinates, we assume that the system is radially symmetric, which means,

$$\frac{\partial}{\partial \theta} = \frac{\partial}{\partial \varphi} = 0.$$

This means the solution will only be a function of the radius,  $r$ , in spherical coordinates or  $r$  and  $z$  in cylindrical coordinates. That is, for any function,  $f$ ,

$$f = f(r) \quad (\text{Spherical}),$$

$$f = f(r, z) \quad (\text{Cylindrical}),$$

Physically, for pipe flow, this often a reasonable assumption since it does not make sense for there to be a preferred radial direction unless there are generation terms to *force* a preferred

direction.

### 3.2.3 Scaling Analysis

Here is perhaps the most important method in simplifying the transport equations: scaling analysis. The idea is similar to non-dimensionalization in that we replace the variables in the equation by "natural" or "characteristic" constants that are measurable. This method is most readily applicable for momentum transport since there are many velocity and length variables that can be simplified. To further explain this, we first replace our real variables by characteristic variables, represented by capital letters,

$$\begin{pmatrix} x \\ y \\ z \end{pmatrix} \rightarrow \begin{pmatrix} X \\ Y \\ Z \end{pmatrix}, \quad \begin{pmatrix} u \\ v \\ w \end{pmatrix} \rightarrow \begin{pmatrix} U \\ V \\ W \end{pmatrix}, \quad \frac{\partial}{\partial x} \rightarrow \frac{1}{X} \dots$$

Since it is often hard to measure a time scale, we *define* characteristic time scales. We may do this by dividing the characteristic velocities by the length scales,

$$\frac{\partial}{\partial t} \begin{pmatrix} u \\ v \\ w \end{pmatrix} \rightarrow \begin{pmatrix} U/(X/U) \\ V/(Y/V) \\ W/(Z/W) \end{pmatrix} = \begin{pmatrix} U^2/X \\ V^2/Y \\ W^2/Z \end{pmatrix}.$$

The idea is to now get an order of magnitude estimation of the equations using these characteristic variables. For example, suppose we want to derive the boundary layer equation for  $x$  momentum along a large  $X \times Z$  flat plate. If we consider the continuity and  $x$  momentum equations with characteristic variables,

$$\begin{aligned} \frac{U}{X} + \frac{V}{Y} + \frac{W}{Z} &\sim 0, \\ \rho \frac{U^2}{X} + \rho \left( U \frac{U}{X} + V \frac{U}{Y} + W \frac{U}{Z} \right) &\sim \mu \left( \frac{U}{X^2} + \frac{U}{Y^2} + \frac{U}{Z^2} \right) + \rho g - \frac{P}{X}. \end{aligned}$$

We know there is nearly no flow in the  $Z$  direction since  $X, Y \ll Z$ , meaning  $W/Z \rightarrow 0$  in the limit that the plate width,  $Z$ , becomes infinitely large. From this, we can rearrange the continuity equation as,

$$V \sim Y \frac{U}{X},$$

plugging this into the  $x$  momentum equation and using  $W/Z \rightarrow 0$ ,

$$\rho \frac{U^2}{X} + \rho \left( U \frac{U}{X} + Y \frac{U}{X} \frac{U}{Y} \right) \sim \mu \left( \frac{U}{X^2} + \frac{U}{Y^2} + \frac{U}{Z^2} \right) + \rho g - \frac{P}{X}.$$

From this, we clearly see that,

$$\mathcal{O}\left(U\frac{U}{X}\right) = \mathcal{O}\left(Y\frac{U}{X}\frac{U}{Y}\right),$$

meaning,

$$\mathcal{O}\left(u\frac{\partial u}{\partial x}\right) = \mathcal{O}\left(v\frac{\partial u}{\partial y}\right),$$

where  $\mathcal{O}(\cdot)$  denotes the order of magnitude. This means that these terms are roughly the same size and are both important. If we further impose steady flow and no gravity in the  $x$  direction (horizontal flow), then the  $x$  momentum equation becomes,

$$\rho\left(u\frac{\partial u}{\partial x} + v\frac{\partial v}{\partial y}\right) = \mu\left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}\right) - \frac{\partial P}{\partial x}.$$

We also know  $X$  is much larger than  $Y$  since we are considering a very long plate such that the  $Y$  direction can be considered small. Using this in the characteristic variable equation,

$$\rho\left(U\frac{U}{X} + Y\frac{U}{X}\frac{U}{Y}\right) \sim \mu\left(\frac{U}{X^2} + \frac{U}{Y^2}\right) - \frac{P}{X}.$$

Suppose we *choose* to only consider terms on the order of magnitude of  $U/X$  or larger, then  $U/X^2 \ll U/X \ll U/Y^2$ , meaning,

$$\frac{\partial^2 u}{\partial x^2} \sim 0.$$

Therefore, our  $x$  momentum equation becomes,

$$\rho\left(u\frac{\partial u}{\partial x} + v\frac{\partial u}{\partial y}\right) = \mu\frac{\partial^2 u}{\partial y^2} - \frac{\partial P}{\partial x},$$

or,

$$u\frac{\partial u}{\partial x} + v\frac{\partial u}{\partial y} = \nu\frac{\partial^2 u}{\partial y^2} - \frac{1}{\rho}\frac{\partial P}{\partial x},$$

which is the  $x$  momentum boundary layer equation. Furthermore, if we know more information such as in the case of no pressure gradient, the equation reduces to,

$$u\frac{\partial u}{\partial x} + v\frac{\partial u}{\partial y} = \nu\frac{\partial^2 u}{\partial y^2},$$

which physically tells us that the convective and diffusive forces balance in the boundary layer. It also tells us that there is a non-negligible amount of  $x$  momentum being transported

in the vertical direction by the,

$$v \frac{\partial u}{\partial y},$$

term. This term is the main reason for the "boundary layer thickness", which is related to the vertical transfer the  $x$  momentum by pretending that the momentum is carried upwards by the presence of a wall formed by the boundary layer.

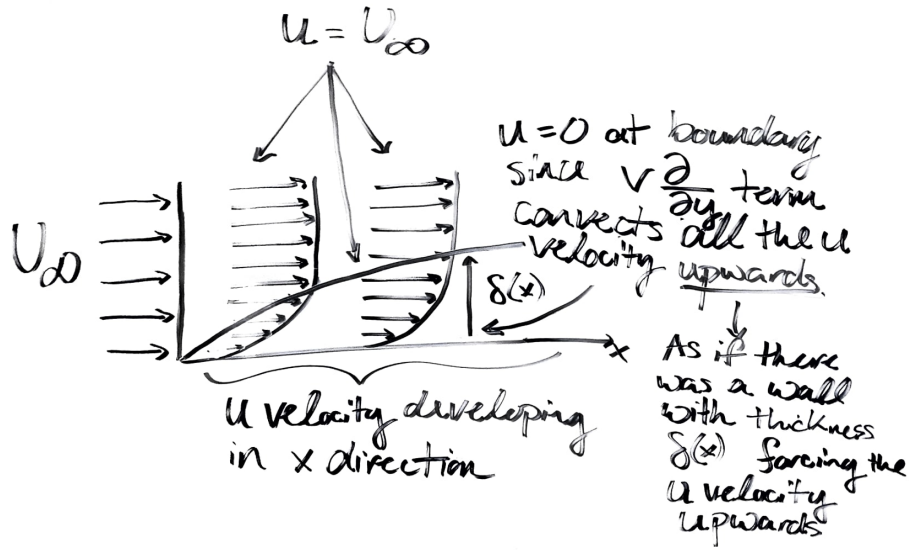


Figure 3.1: Boundary layer over a flat plate

Remember that we derived most of this equation and interpretation using only considerations of the relative magnitude of  $X$ ,  $Y$ , and  $Z$ . We can therefore see the importance scaling arguments in simplifying the full Navier-Stokes equations to a simpler problem that captures the physics we want to describe while being at the scale we want to observe. In the case of the boundary layer equation, we chose a scale such that we still have a (difficult!) partial differential equation to solve.

When solving transport equations by hand, we can often only easily solve 1D equations. This means that we implicitly need that one of the length variables is much smaller than the others such as  $Y \ll X, Z$  for Cartesian problems. If we further impose a steady problem with  $V/Y, W/Z \rightarrow 0$ , then,

$$\frac{U}{X} + \frac{V}{Y} + \frac{W}{Z} \sim 0,$$

meaning,

$$\frac{U}{X} \sim 0,$$

further implying,

$$\cancel{\rho \frac{U^2}{X}} + \rho \left( \cancel{\frac{U}{X}} + \cancel{\frac{V}{Y}} + \cancel{\frac{W}{Z}} \right) \sim \mu \left( \cancel{\frac{U}{X^2}} + \frac{U}{Y^2} + \cancel{\frac{U}{Z^2}} \right) + \rho g_x - \frac{P}{X}.$$

This reduces our equation to,

$$\mu \frac{d^2 v}{dy^2} + \rho g_x - \frac{\partial P}{\partial x} = 0,$$

which is the general form of a 1D Navier-Stokes problem in Cartesian coordinates. Similarly, by considering radial symmetry and scaling analysis together, one can arrive at a general form of the 1D cylindrical Navier-Stokes problem,

$$\frac{\mu}{r} \frac{d}{dr} \left( r \frac{du_z}{dr} \right) + \rho g_z - \frac{\partial P}{\partial z} = 0.$$

Scaling arguments can be extended to mass and energy conservation problems in a similar fashion as momentum transport. In fact, scaling analysis is often easier to apply to mass and energy transport equations since they are scalar equations with less variables.

### 3.3 Common Boundary Conditions

Now that our differential transport equations are developed, we need conditions on the equations to solve them. These are done through so-called "boundary conditions" where we impose information we know on the system boundaries. From the theory of partial differential equations, there are *many* kinds of boundary conditions and even seemingly simple conditions can lead to *very* complex behavior. We will only consider a few types of (common) boundary conditions and provide physical interpretations of them.

#### 3.3.1 Mathematical Forms of Boundary Conditions

The first condition is the "fixed" or "Dirichlet" boundary condition as it is commonly called in mathematics. This simply states the transported variable such as  $C$ ,  $\mathbf{u}$ , or  $T$ , takes on a certain value on the boundaries. Mathematically, we denote this as,

$$\mathbf{b}|_{\partial V} = f,$$

where  $\mathbf{b}$  is the transported quantity,  $\partial V$  denotes evaluation on the boundary, and  $f$  is some number or function.

The second condition is the "flux" or "Neumann" boundary condition. This states that



the non-convective flux of the transported variable is fixed or prescribed at the boundaries. Mathematically,

$$\varphi|_{\partial V} \cdot \mathbf{n} = f,$$

where  $\mathbf{n}$  is the normal vector to the control surface and  $f$  is a number or function. The dot product with  $\mathbf{n}$  is included as we only care about the flux leaving the surface and only the normal component of the flux can leave the surface.

A less common boundary condition is the "finiteness" or "regularity" condition. This states that in certain limits, the solution should remain finite. For example, in the derivation of laminar flow in a pipe, eventually, one divides by the pipe radius,  $r$ , which means dividing by 0 at  $r = 0$ . Since we know the stress is finite at  $r = 0$ , any constants connected to the  $1/r$  term must be set to 0 if  $r = 0$  is in the domain. This condition is more common when working in cylindrical or spherical coordinates.

Symmetry conditions also often arise in cylindrical or spherical coordinates. For example, if  $\mathbf{u}(r, \theta, z)$  is the velocity in a circular pipe, then,

$$\begin{cases} \mathbf{u}(r, \theta, z) = \mathbf{u}(r, \theta + 2\pi, z) \\ \frac{\partial}{\partial \theta} \mathbf{u}(r, \theta, z) = \frac{\partial}{\partial \theta} \mathbf{u}(r, \theta + 2\pi, z) \end{cases},$$

which states that the values of the velocity agree and the values of flux agree when one full revolution around the pipe is made. Or in other words,  $\theta$  and  $\theta + 2\pi$  correspond to the same points.

### 3.3.2 Momentum Transport

For momentum transport, there is the "no-slip" boundary condition which states that when a fluid and solid meet, the fluid does not slip or slide along the solid interface. Thus, the velocity of the fluid must coincide with the wall or interface velocity,

$$\mathbf{u}|_{\partial V} = \mathbf{v}_{wall}.$$

There is also the no flux boundary condition which states that there is no momentum flux (no fluid flow) through the boundary of the control volume. This is equivalent to saying that the shear stress at the boundary is fixed. That is,

$$\boldsymbol{\tau} \cdot \mathbf{n} = \mu \left( \nabla \mathbf{u} + (\nabla \mathbf{u})^T \right) \Big|_{\partial V} \cdot \mathbf{n} = \mathbf{0}.$$

Often, this general expression can be simplified greatly, but that is specific to the problem at hand.

### 3.3.3 Energy Transport

For energy transport, the fixed boundary condition simply means that the temperature,  $T$ , is known at the boundary. For example, if one end of a metal rod is placed in a furnace with a temperature,  $f$ , and allowed to heat up, then,

$$T|_{\partial V} = T|_{rod\ end} = f.$$

A more common boundary condition for energy transport is the non-convective flux condition. This simply states that the heat flux,  $\mathbf{q}$ , is known at the boundary. Mathematically,

$$\mathbf{q} \cdot \mathbf{n}|_{\partial V} = -k \nabla T|_{\partial V} \cdot \mathbf{n} = f.$$

Physically, this means there is a known amount of energy put into the system at the boundaries. This arises from a heat source and conduction through the boundary. For example, an electric stovetop outputs a known amount of energy and conducts heat through a metal pan. The heat flux into the pan can be calculated since the energy outputted by the stovetop is related to the heat conduction through the pan's bottom boundary. Conversely, if there is insulation at the boundary, then the heat cannot penetrate and thus  $f = 0$  since there is no flux.

Another important condition is convective heat transfer at a boundary due to Newton's Law of Cooling,

$$\mathbf{q} \cdot \mathbf{n} = -k \nabla T|_{\partial V} \cdot \mathbf{n} = h (T|_{\partial V} - T_{\infty}),$$

where  $h$  is the convective heat transfer coefficient and  $T_{\infty}$  is the surrounding temperature. This simply states that the conduction through the surface of the control volume is proportional to the temperature difference with its surroundings. Notice if we non-dimensionalize the above equation with a new temperature and length scale,

$$T^* = \frac{T - T_{\infty}}{T_0}, \quad \frac{1}{L} \nabla^* = \nabla,$$

we get,

$$\begin{aligned} -\nabla^* T^*|_{\partial V} \cdot \mathbf{n} &= \frac{hL}{k} \cdot T^*|_{\partial V} \\ &= Nu \cdot T^*|_{\partial V} \end{aligned}$$

where  $Nu$  is the Nusselt number, the ratio of heat transport through convection to conduction. Since  $Re$  relates to convection and  $Pr$  relates to conduction (diffusion), it is reasonable to see that  $Nu = f(Re, Pr)$ . This explains why there exists so many correlations between  $Nu$ ,  $Re$ , and  $Pr$ . Generally, these correlations are derived by solving the non-dimensionalized

momentum and energy equations and applying this boundary condition.

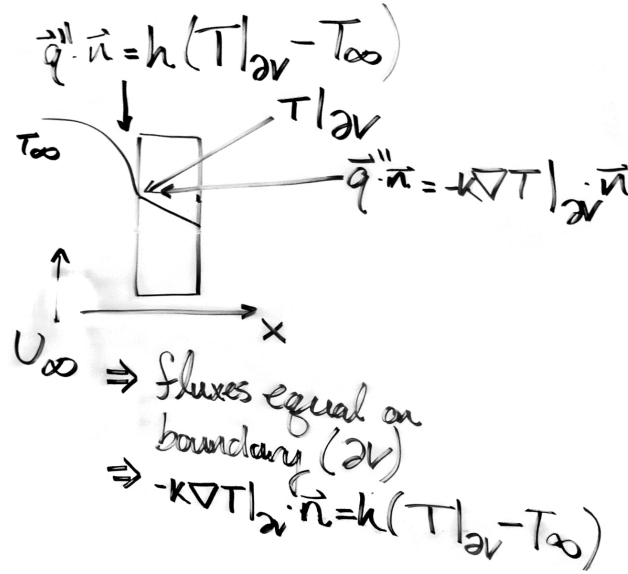


Figure 3.2: Energy convective boundary condition

### 3.3.4 Mass Transport

Mass transport contains the exact same boundary conditions as energy transport but with  $T \rightarrow C$  and the units of the proportionality constants changed appropriately. The fixed boundary condition denotes a known concentration,  $f$ , on the boundary,

$$C|_{\partial V} = f.$$

An example of this is if we have a volume of liquid with its vapor above it. We know by Raoult's Law that the vapor pressure is proportional to the mole fraction of the substance in the liquid,

$$P_i = x_i P_i^{sat}.$$

Since  $P_i = C_i RT$  for an ideal gas,

$$C_i|_{\partial V} = \frac{x_i P_i^{sat}}{RT},$$

which means that the concentration of the vapor touching the liquid is known if the concentration of the liquid solution is known.

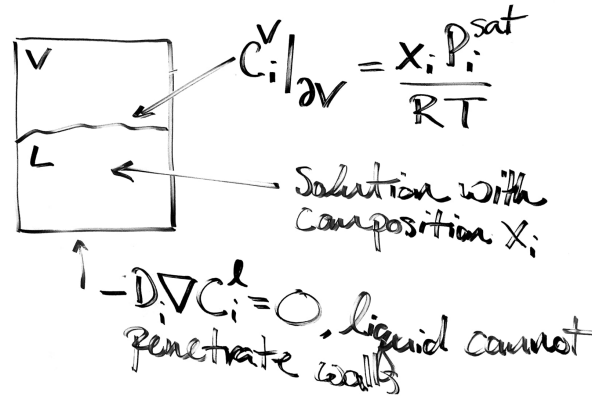


Figure 3.3: Vapor-liquid and no flux boundary conditions

Another example is if a fluid with a known concentration,  $C$ , is allowed to flow through the boundary of the system, then we may assume there is a fixed concentration at the boundary.

Another common condition is that the diffusive flux is known at the boundary. Mathematically, from Fick's Law of Diffusion,

$$\boldsymbol{\varphi} \cdot \mathbf{n} = \mathbf{J}|_{\partial V} \cdot \mathbf{n} = -D \nabla C|_{\partial V} \cdot \mathbf{n} = f.$$

It is most common that we take  $f = 0$ , meaning there is no diffusion at the boundary of the domain, this is commonly referred to as an impermeable surface. Often times, this condition applies at the walls of a glass or metal container since mass cannot penetrate the walls, meaning there is no flux.

The final condition is the convective boundary condition which is analogous to the convective condition from energy transport. Mathematically,

$$-D \nabla C|_{\partial V} \cdot \mathbf{n} = k_c (C|_{\partial V} - C_\infty),$$

where  $k_c$  is the convective mass transfer coefficient. Physically, this condition may arise when there is a vapor with a concentration,  $C_\infty$ , flowing over a liquid with concentration,  $C$ . The amount of diffusion of the substance into the liquid is proportional to the difference in concentration between the liquid and vapour. This condition may also occur at a liquid-solid or vapor-solid interface if there is flow past a permeable membrane. This is analogous to heat conduction through a solid boundary due to a fluid at one temperature flowing over surface with a different temperature. To strengthen this analogy, let's consider the non-dimensional

form of convective boundary condition. First, defining a new concentration and length scale,

$$C^* = \frac{C - C_\infty}{C_0}, \quad \frac{1}{L} \nabla^* = \nabla.$$

Plugging this into the boundary condition,

$$-\frac{C_0 D}{L} \nabla C^*|_{\partial V} \cdot \mathbf{n} = C_0 k_c C^*|_{\partial V},$$

rearranging,

$$-\nabla C^*|_{\partial V} \cdot \mathbf{n} = \frac{k_c L}{D} C^*|_{\partial V}.$$

We define the Sherwood number,  $Sh$ , as,

$$Sh = \frac{\text{Convective Mass Transfer}}{\text{Diffusive Mass Transfer}} = \frac{k_c L}{D}.$$

Thus, we have,

$$-\nabla C^*|_{\partial V} \cdot \mathbf{n} = Sh \cdot C^*|_{\partial V},$$

recall the energy transport equivalent,

$$-\nabla^* T^*|_{\partial V} \cdot \mathbf{n} = Nu \cdot T^*|_{\partial V}.$$

From this, it is clear that  $C^* \iff T^*$  and  $Sh \iff Nu$ . One may wonder that if  $Nu = f(Re, Pr)$ , then is  $Sh = f(Re, Sc)$ ? Amazingly, the analogy between these two boundary conditions is so strong that, by using convective correlations for  $Nu$ , one can simply replace  $Nu$  with  $Sh$  and  $Pr$  with  $Sc$ . For example, the Dittus Boelter equation for convective heat transfer in a pipe,

$$Nu = 0.023 Re^{0.8} Pr^{0.4},$$

becomes,

$$Sh = 0.023 Re^{0.8} Sc^{0.4},$$

from which we can estimate the convective mass transfer coefficient. Physically, this kind of correlation would arise with fluid flow through a permeable pipe, such as blood diffusing nutrients through a capillary tube.

In a chemical engineering context, the convective mass transfer boundary condition often arises from considering adsorption columns by passing vapor bubbles with concentration  $C$  through a tank of a solution with concentration  $C_\infty$ . By integrating the convective boundary condition, we can get an estimate for the amount of the solute absorbed by the gas.

### 3.3.5 General Advice

*Do not* ignore studying boundary conditions. They may seem like an afterthought when solving the differential equation, but they are *extremely* important to study and misinterpreting these conditions can lead to very different behavior for the solution. They can also give clues to which terms in the transport equation can be ignored or not. For example, in 1D problems, if there are 2 boundary conditions, there *must* be a second derivative term to impose those 2 conditions.

# Chapter 4

## Concluding Remarks and Summary

### 4.1 "Cookbook Recipe" to Conservation Equations

The following section is easier said than done, but it gives a general thought process for deriving and solving transport equations by hand. If you have made it this far in chemical engineering, you have probably figured most of this process out, in which case, the following section is just a list to formalize that process. The only way to truly build intuition is to practice a *lot* of problems. Understanding the transport equations is only one part of the process, but equally as important is understanding how to simplify the problem and impose the correct conditions.

A general problem solving process may follow:

- Draw a *good* diagram of the system of interest
  - DO NOT skip this step, it helps in building intuition and identifying boundary conditions
  - Clearly label all of the variables used in the diagram and note what is known
  - Select a coordinate system
- Identify relevant terms in the conservation equation
  - What are the generation terms?
  - What is the form of the flux?
  - Is there convection (fluid flow)?
  - Apply assumptions, i.e. steady state, fully developed flow, etc.
  - Can some terms be assumed constant?

- Scaling analysis – What is large? What does not vary a lot in space?
- Are more equations required? i.e. Continuity equation, sum of mole fractions, etc.
- Identify boundary conditions – No flux? Fixed value? Convection?
- Solve the differential equation(s)
- Does the answer make sense? Does it match intuition? What are the units of the answer?
- Are there "special cases" to try? Ex: setting certain terms to 0, taking limits at  $\infty$ , etc.

## 4.2 Other Remarks

There are countless other applications of the general conservation equations beyond transport systems. A quite important example left out is the conservation of charge; this leads to Maxwell's equations which are fundamental in the understanding of electricity. Perhaps a more surprising example is found in a quantum mechanics course where one may learn that the probability density,  $|\Psi|^2$ , associated with a wavefunction,  $\Psi$ , is conserved. This has fundamental consequences on the evolution of molecular systems.

Despite all of this great generality, there are great costs – conservation equations are *hard* to solve. Many times these equations are only numerically solvable and require considerable computational costs. In fact, the conservation of momentum equation or the "Navier-Stokes" equations are so important and difficult to solve that mathematicians have offered a \$1,000,000 "[Millennium Prize](#)" to prove certain properties of the equations.

For practical computations in [COMSOL](#), [OpenFoam](#), [MOOSE](#), or other multiphysics (transport) simulation software, the user often specifies what terms in the transport equation they want from certain "modules". This is why the focus of this document was on identifying specific terms for generation, flux, diffusion, boundary conditions, etc. as this is what you would practically do in a computation. This identification and modeling of mathematical terms is an important skill to develop if you are interested in computational work or if you want to communicate with somebody who performs these simulations. In short, the take-away from transport phenomena should not necessarily be on how to solve equations, but rather understanding *modeling* and converting physical problems to mathematics.



## 4.3 Summary of the Main Transport Equations

The following section is a summary of the differential transport equations for mass, momentum, and energy assuming constant  $D$ ,  $\mu$ , and  $k$ . Additionally, for the momentum and energy equations, it is assumed the fluid is incompressible and Newtonian.

### General Conservation Equation

$$\underbrace{\frac{\partial(\rho \mathbf{b})}{\partial t}}_{\text{Accumulation}} + \underbrace{\nabla \cdot (\rho \mathbf{b} \mathbf{v})}_{\text{Convection}} = \underbrace{-\nabla \cdot \boldsymbol{\varphi}}_{\text{Diffusion}} + \underbrace{\rho \mathbf{g}}_{\text{Generation}}$$

### Mass Conservation Equation

#### Concentration Form

$$\underbrace{\frac{\partial C_i}{\partial t}}_{\text{Accumulation}} + \underbrace{\nabla \cdot (\mathbf{v} C_i)}_{\text{Convection}} = \underbrace{D_i \nabla^2 C_i}_{\text{Diffusion}} + \underbrace{R_i}_{\text{Generation}}$$

$$C = \sum_{i=1}^N C_i, \quad \sum_{i=1}^N (D_i \nabla C_i) = 0, \quad R = \sum_{i=1}^N R_i$$

$$\frac{\partial C}{\partial t} + \nabla \cdot (\mathbf{v} C) = R$$

#### Density Form

$$\underbrace{\frac{\partial \rho_i}{\partial t}}_{\text{Accumulation}} + \underbrace{\nabla \cdot (\rho_i \mathbf{v})}_{\text{Convection}} = \underbrace{D_i \nabla^2 \rho_i}_{\text{Diffusion}} + \underbrace{M_i R_i}_{\text{Generation}}.$$

$$\rho = \sum_{i=1}^N \rho_i, \quad \sum_{i=1}^N (D_i \nabla^2 \rho_i) = 0, \quad \sum_{i=1}^N M_i R_i = 0$$

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0$$

### Momentum Conservation Equation

$$\underbrace{\rho \frac{\partial \mathbf{u}}{\partial t}}_{\text{Accumulation}} + \underbrace{\rho \mathbf{u} \cdot \nabla \mathbf{u}}_{\text{Convection}} = \underbrace{\mu \nabla^2 \mathbf{u}}_{\text{Diffusion}} + \underbrace{-\nabla P + \rho \mathbf{G}}_{\text{Generation}}$$

### Energy Conservation Equation

$$\underbrace{\rho C_p \frac{\partial T}{\partial t}}_{\text{Accumulation}} + \underbrace{\rho C_p \mathbf{v} \cdot \nabla T}_{\text{Convection}} = \underbrace{k \nabla^2 T}_{\text{Diffusion}} + \underbrace{Q + \Phi}_{\text{Generation}}$$

## Common Assumptions

$$\text{Steady State : } \frac{\partial}{\partial t} = 0$$

$$\text{Radial Symmetry : } \frac{\partial}{\partial \theta} = \frac{\partial}{\partial \varphi} = 0$$

$$\text{Scaling Analysis : } u \rightarrow U, \frac{\partial}{\partial x} \rightarrow \frac{1}{X} \dots \text{etc.}$$

(What order of magnitude do we care about?)

## Common Boundary Conditions

$$\text{Fixed : } \mathbf{b}|_{\partial V} = f$$

$$\text{Flux : } \boldsymbol{\varphi}|_{\partial V} \cdot \mathbf{n} = f$$

$$\text{Finite : } \mathbf{b} \not\rightarrow \infty \text{ or } \boldsymbol{\varphi} \cdot \mathbf{n} \not\rightarrow \infty$$

$$\text{Symmetry : } \mathbf{b}(r, \theta, z) = \mathbf{b}(r, \theta + 2\pi, z)$$

$$\frac{\partial}{\partial \theta} \mathbf{b}(r, \theta, z) = \frac{\partial}{\partial \theta} \mathbf{b}(r, \theta + 2\pi, z)$$

... or similar conditions

$$\text{Convection : } -D\nabla C|_{\partial V} \cdot \mathbf{n} = k_c (C|_{\partial V} - C_\infty)$$

$$-k\nabla T|_{\partial V} \cdot \mathbf{n} = h (T|_{\partial V} - T_\infty)$$

## 4.4 Summary of Dimensionless Numbers

Table 2: Dimensionless Numbers for Transport Equations

Name	Symbol	Ratio	Expression
Reynolds	$Re$	$\frac{\text{Inertia Force}}{\text{Viscous Force}}$	$\frac{\rho U L}{\mu} = \frac{U L}{\nu}$
Froude	$Fr$	$\sqrt{\frac{\text{Inertia Force}}{\text{Gravitational Force}}}$	$\frac{U}{\sqrt{gL}}$
Euler	$Eu$	$\frac{\text{Pressure Force}}{\text{Inertia Force}}$	$\frac{\Delta p}{\rho U^2}$
Schmidt	$Sc$	$\frac{\text{Momentum Diffusivity}}{\text{Mass Diffusivity}}$	$\frac{\nu}{D}$
Sherwood	$Sh$	$\frac{\text{Convective Mass Transfer}}{\text{Diffusive Mass Transfer}}$	$\frac{k_c L}{D}$
Prandtl	$Pr$	$\frac{\text{Momentum Diffusivity}}{\text{Thermal Diffusivity}}$	$\frac{\nu}{\alpha} = \frac{\mu C_p}{k}$
Nusselt	$Nu$	$\frac{\text{Convective Heat Transfer}}{\text{Diffusive Heat Transfer}}$	$\frac{h L}{k}$
Lewis	$Le$	$\frac{\text{Thermal Diffusivity}}{\text{Mass Diffusivity}}$	$\frac{\alpha}{D}$

# Appendices

## 4.5 Appendix 1: Mathematical Operators in Cartesian Coordinates

### Vector Calculus Review

The following a quick review of common operations from multivariable calculus which are useful in deriving conservation equations. We will only consider Cartesian coordinates as operators in cylindrical and spherical coordinates become *much* more complex. We let  $f$  be any function,  $\mathbf{a}$  and  $\mathbf{b}$  be vectors,  $\mathbf{F}$  be a vector field, and  $\mathbf{P}$  be any differentiable quantity,

$$f = f(x, y, z), \quad \mathbf{a} = \begin{pmatrix} a_1 \\ a_2 \\ a_3 \end{pmatrix}, \quad \mathbf{b} = \begin{pmatrix} b_1 \\ b_2 \\ b_3 \end{pmatrix}, \quad \mathbf{F} = \begin{pmatrix} f(x, y, z) \\ g(x, y, z) \\ h(x, y, z) \end{pmatrix}.$$

The dot product between two vectors  $\mathbf{a}$  and  $\mathbf{b}$ , denoted as  $\mathbf{a} \cdot \mathbf{b}$ , is defined as,

$$\mathbf{a} \cdot \mathbf{b} := |\mathbf{a}| |\mathbf{b}| \cos(\theta) = a_1 b_1 + a_2 b_2 + a_3 b_3.$$

Geometrically, the dot product is the projection, or amount of one vector in the direction of another vector. Two vectors are said to be perpendicular (orthogonal) when  $\mathbf{a} \cdot \mathbf{b} = 0$  since  $\cos(\theta) = 0$  when  $\theta = \pi/2$ .

The gradient of a function,  $f$ , denoted as  $\nabla f$ , is defined as,

$$\nabla f := \begin{pmatrix} \frac{\partial f}{\partial x} \\ \frac{\partial f}{\partial y} \\ \frac{\partial f}{\partial z} \end{pmatrix}.$$

Geometrically, the gradient is normal to curves of constant  $f$ , that is, if  $\mathbf{dx}$  is a small change in position such that the output of  $f$  remains constant, then,

$$\nabla f \cdot \mathbf{dx} = 0.$$

Conversely, let  $\mathbf{v}$  be any unit vector ( $|\mathbf{v}| = 1$ ), then, the directional derivative is defined as,

$$\nabla f \cdot \mathbf{v} := |\nabla f| |\mathbf{v}| \cos(\theta) = |\nabla f| \cos(\theta).$$

The directional derivative measures the change of a function when moving in a direction,  $\mathbf{v}$ . This quantity is maximized when  $\theta = 0$  where cosine is equal to 1. This means that if  $\mathbf{v}$  points in the gradient direction, then the directional derivative, or the change in  $f$ , is the greatest. This is often stated as the gradient vector points in the steepest ascent direction. By using the same line of reasoning when  $\theta = \pi$ , we see that the negative gradient points in the steepest descent direction.

The divergence of a vector field,  $\mathbf{F}$ , denoted as  $\nabla \cdot \mathbf{F}$ , is defined as,

$$\nabla \cdot \mathbf{F} := \frac{\partial f}{\partial x} + \frac{\partial g}{\partial y} + \frac{\partial h}{\partial z} = \left( \frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z} \right) \cdot (f, g, h).$$

Physically, the divergence represents the flux of  $\mathbf{F}$  at a point or how much of  $\mathbf{F}$  is coming in or out of a point. To see this, draw a box with side lengths  $\Delta x$ ,  $\Delta y$ , and  $\Delta z$ , then the flux of  $\mathbf{F}$ , denoted as  $\varphi$ , can be evaluated as,

$$\varphi \Delta x \Delta y \Delta z = (f|_{x+\Delta x} - f|_x) \Delta y \Delta z + (g|_{y+\Delta y} - g|_y) \Delta x \Delta z + (h|_{z+\Delta z} - h|_z) \Delta x \Delta y,$$

dividing by  $\Delta x \Delta y \Delta z$ ,

$$\varphi = \frac{f|_{x+\Delta x} - f|_x}{\Delta x} + \frac{g|_{y+\Delta y} - g|_y}{\Delta y} + \frac{h|_{z+\Delta z} - h|_z}{\Delta z},$$

letting  $\Delta x$ ,  $\Delta y$ , and  $\Delta z$  approach 0, we get,

$$\varphi = \frac{\partial f}{\partial x} + \frac{\partial g}{\partial y} + \frac{\partial h}{\partial z}.$$

## The Laplacian

The Laplacian is defined as,

$$\nabla^2 \mathbf{P} := \nabla \cdot \nabla \mathbf{P} = \frac{\partial^2 \mathbf{P}}{\partial x^2} + \frac{\partial^2 \mathbf{P}}{\partial y^2} + \frac{\partial^2 \mathbf{P}}{\partial z^2}.$$

## The Convective Derivative

The convective derivative is defined as,

$$\mathbf{u} \cdot \nabla \mathbf{P} := u_x \frac{\partial \mathbf{P}}{\partial x} + u_y \frac{\partial \mathbf{P}}{\partial y} + u_z \frac{\partial \mathbf{P}}{\partial z},$$

where  $\mathbf{u}$  is the velocity of the fluid carrying the quantity  $\mathbf{P}$ .

## The Material Derivative

The material derivative is defined as,

$$\begin{aligned} \frac{D\mathbf{P}}{Dt} &:= \frac{\partial \mathbf{P}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{P} \\ &= \frac{\partial \mathbf{P}}{\partial t} + u_x \frac{\partial \mathbf{P}}{\partial x} + u_y \frac{\partial \mathbf{P}}{\partial y} + u_z \frac{\partial \mathbf{P}}{\partial z} \\ &= \frac{\partial \mathbf{P}}{\partial t} + \frac{dx}{dt} \frac{\partial \mathbf{P}}{\partial x} + \frac{dy}{dt} \frac{\partial \mathbf{P}}{\partial y} + \frac{dz}{dt} \frac{\partial \mathbf{P}}{\partial z}. \end{aligned}$$

The first 10 minutes of this [video](#) has a classical explanation of the material derivative using temperature,  $T$ , as the variable of interest. The video also has some great explanations for different forms of the Navier-Stokes equations for those interested in CFD, so it is worth a watch.

## 4.6 Appendix 2: Mathematical Operations in the Navier-Stokes Equations

In the following development, we let  $i$  and  $j$  indices represent  $x$ ,  $y$ , or  $z$ . We claim,

$$\nabla \cdot (\rho \mathbf{u} \mathbf{u}) = \nabla \cdot (\rho \mathbf{u}) \mathbf{u} + (\rho \mathbf{u}) \cdot \nabla \mathbf{u}.$$

To see this, consider and verify the Cartesian definition of the divergence and the gradient,

$$\nabla \cdot \mathbf{u} = \sum_i \frac{\partial u_i}{\partial x_i} \text{ (Scalar)}, \quad \nabla \mathbf{u} = \frac{\partial u_j}{\partial x_i} \mathbf{e}_i \mathbf{e}_j \text{ (Matrix)},$$

where the  $\mathbf{e}$ 's represent the Cartesian basis vectors. The  $\rho \mathbf{u} \mathbf{u}$  term is also a matrix (tensor) which can be written as,

$$\rho \mathbf{u} \mathbf{u} = \rho u_i u_j \mathbf{e}_i \mathbf{e}_j.$$

Remember that matrices are represented by two *different* indices, the above expression runs through all  $(i, j)$  pairs. If we take the divergence of the above and apply the standard product

rule,

$$\frac{\partial(\rho u_i u_j \mathbf{e}_i \mathbf{e}_j)}{\partial x_i} = \left( \frac{\partial(\rho u_i)}{\partial x_i} u_j + \rho u_i \frac{\partial u_j}{\partial x_i} \right) \mathbf{e}_i \mathbf{e}_j,$$

or in vector calculus notation,

$$\nabla \cdot (\rho \mathbf{u} \mathbf{u}) = \nabla \cdot (\rho \mathbf{u}) \mathbf{u} + (\rho \mathbf{u}) \cdot \nabla \mathbf{u}.$$

The vector calculus expression actually holds in all coordinate systems, but this requires more advanced tensor calculus to prove.

We also claimed,

$$\mu \nabla \cdot (\nabla \mathbf{u})^T = \mathbf{0}.$$

We again only consider Cartesian coordinates, giving,

$$\begin{aligned} \mu \nabla \cdot (\nabla \mathbf{u})^T &= \mu \frac{\partial}{\partial x_i} \left( \frac{\partial u_i}{\partial x_j} \mathbf{e}_i \mathbf{e}_j \right) \\ &= \mu \frac{\partial}{\partial x_j} \left( \frac{\partial u_i}{\partial x_i} \right) \mathbf{e}_i \mathbf{e}_j \\ &= \mu \nabla (\nabla \cdot \mathbf{u}) \\ &= \mathbf{0}. \end{aligned}$$

Where the last equality is because the fluid is incompressible.

## 4.7 Appendix 3: Development of the Stress Tensor

The following is an advanced development of the stress tensor by considering the symmetries of a fluid. The following derivation assumes knowledge of tensor calculus and Einstein notation for tensors. If these are not known, this section may be skipped.

### 4.7.1 Displacement Gradient

For a deformed volume, let  $\mathbf{X}$  denote the vector of a point in a material from its original position to its new, deformed position. We define the displacement gradient as,

$$\nabla_j X_i,$$

where  $\nabla_j$  denotes the covariant derivative and  $X_i$  denotes the components of the covariant position vector. This gives a second order tensor which accounts for how far point in a material moves as it is deformed by a differential amount. This tensor is commonly analyzed

by decomposing it into symmetric and anti-symmetric parts,

$$\nabla_j X_i = \frac{1}{2} (\nabla_j X_i + \nabla_i X_j) + \frac{1}{2} (\nabla_j X_i - \nabla_i X_j),$$

where we introduce the strain tensor,

$$\varepsilon_{ij} = \frac{1}{2} (\nabla_j X_i + \nabla_i X_j),$$

and the vorticity tensor,

$$\omega_{ij} = \frac{1}{2} (\nabla_j X_i - \nabla_i X_j).$$

Thus, the displacement gradient can be written as,

$$\nabla_j X_i = \varepsilon_{ij} + \omega_{ij}.$$

$\varepsilon_{ij}$  accounts for pure deformation while  $\omega_{ij}$  accounts for pure rotation (notice its similarity to the 3D curl). To analyze the stress tensor, we only need to account for  $\varepsilon_{ij}$  since we are interested in pure deformation in the absence of rotation.

## 4.7.2 General Stress Tensor

If we postulate the stress tensor,  $\tau$ , is linearly proportional to the strain,  $\varepsilon$ , then we get the following tensor relation,

$$\tau^{ij} = C^{ijkl} \varepsilon_{kl},$$

where  $C^{ijkl}$  is a 4th order tensor called the elasticity tensor. It can be shown that  $\tau^{ij}$  is symmetric in its indices and by considering the elastic potential energy,  $U$ , and using the definition of stress in Cartesian coordinates,

$$\tau^{ij} = \frac{\partial U}{\partial \varepsilon_{ij}}.$$

Thus,

$$C^{ijkl} = \frac{\partial^2 U}{\partial \varepsilon_{ij} \partial \varepsilon_{kl}},$$

which is symmetric in the index pairs  $ij$  and  $kl$ .

Another constraint is that fluids are isotropic, thus any rotation upon  $C^{ijkl}$  leaves it unchanged. A general infinitesimal rotation is described by the operator  $R_s^i$ ,

$$R_s^i = g^{ir} \epsilon_{rst} \nabla^t,$$

where  $\epsilon_{rst}$  is the Levi-Civita tensor. If  $C^{ijkl}$  is isotropic, then it should commute with  $R_s^i$  for



any index, giving for example,

$$g^{ir} \epsilon_{rst} (C^{sjkl} \nabla^t - \nabla^t C^{sjkl}) = 0,$$

to commute with the covariant derivative in every index,  $C^{ijkl}$  must be proportional to the metrics. One possible combination of this is,

$$C^{ijkl} = c_1 g^{ij} g^{kl} + c_2 g^{ik} g^{jl} + c_3 g^{il} g^{jk},$$

which accounts for all cases due to the symmetry of the metric tensor. There is an additional symmetry constraint,  $C^{ijkl} = C^{jikl}$ , that results from the symmetry of the stress tensor. This gives,

$$\begin{aligned} 0 &= c_1 (g^{ij} g^{kl} - g^{ji} g^{kl}) + c_2 (g^{ik} g^{jl} - g^{jk} g^{il}) + c_3 (g^{il} g^{jk} - g^{jl} g^{ik}), \\ \implies c_2 (g^{ik} g^{jl} - g^{jk} g^{il}) &= c_3 (g^{ik} g^{jl} - g^{jk} g^{il}), \\ \implies c_2 &= c_3. \end{aligned}$$

Often,  $c_1$  is denoted by  $\lambda$  and  $c_2$  is denoted by  $\mu$  which gives,

$$C^{ijkl} = \lambda g^{ij} g^{kl} + \mu (g^{ik} g^{jl} + g^{il} g^{jk}).$$

Using the definition of  $\epsilon_{kl}$ ,

$$\begin{aligned} \tau^{ij} &= \lambda g^{ij} g^{kl} \epsilon_{kl} + \mu (g^{ik} g^{jl} + g^{il} g^{jk}) \epsilon_{kl} \\ &= \lambda g^{ij} \epsilon_k^k + \mu (\epsilon^{ij} + \epsilon^{ji}) \\ &= \lambda g^{ij} \epsilon_k^k + 2\mu \epsilon^{ij} \\ &= \lambda g^{ij} \nabla_k X^k + \mu (\nabla^i X^j + \nabla^j X^i). \end{aligned}$$

In fluid mechanics, we are often interested in the divergence of the stress tensor which is achieved by contracting the above relation with a covariant derivative. We also take the time derivative of  $X$  since we are interested in the velocity field instead of the displacement field. Thus we replace  $X \rightarrow u$  and take a covariant derivative, giving,

$$\nabla_i \tau^{ij} = \lambda \nabla^j \nabla_k u^k + \mu \nabla_i \nabla^i u^j + \mu \nabla^j \nabla_i u^i.$$

In vector calculus notation,

$$\nabla \cdot \boldsymbol{\tau} = \lambda \nabla (\nabla \cdot \mathbf{u}) + \mu \nabla^2 \mathbf{u} + \mu \nabla (\nabla \cdot \mathbf{u}).$$

For an incompressible fluid,  $\nabla \cdot \mathbf{u} = 0$ , thus,

$$\nabla_i \tau^{ij} = \mu \nabla_i \nabla^i u^j,$$

$$\nabla \cdot \boldsymbol{\tau} = \mu \nabla^2 \mathbf{u}.$$

In the context of the incompressible Navier-Stokes equations we have,

$$\rho \partial_t u^i + \rho u^j \nabla_j u^i = -\nabla^i p + \rho f^i + \mu \nabla_j \nabla^j u^i.$$

### 4.7.3 Viscous Shear Work

To get the expression for the viscous shear work, we contract the stress tensor with the velocity vector,  $u_i$ ,

$$u_i \tau^{ij} = \lambda u^j \nabla_k u^k + \mu u_i [\nabla^i u^j + \nabla^j u^i].$$

We then take the divergence of this quantity by contracting with a covariant derivative and applying the product rule,

$$\begin{aligned} \nabla_j (u_i \tau^{ij}) &= \lambda \nabla_j (u^j \nabla_k u^k) + \mu \nabla_j (u_i [\nabla^i u^j + \nabla^j u^i]) \\ &= \lambda \nabla_j (u^j \nabla_k u^k) + \mu \nabla_j u_i [\nabla^i u^j + \nabla^j u^i] + \mu u_i \nabla_j [\nabla^i u^j + \nabla^j u^i] \\ &= \lambda \nabla_j (u^j \nabla_k u^k) + \mu \nabla_j u_i [\nabla^i u^j + \nabla^j u^i] + \mu u_i \nabla^i (\nabla_j u^j) + \mu u_i \nabla_j \nabla^j u^i. \end{aligned}$$

In vector calculus notation,

$$\nabla \cdot (\mathbf{u} \cdot \boldsymbol{\tau}) = \lambda \nabla \cdot [\mathbf{u} (\nabla \cdot \mathbf{u})] + \text{trace} (\mu \nabla \mathbf{u} [\nabla \mathbf{u} + (\nabla \mathbf{u})^T]) + \mu \mathbf{u} \cdot \nabla (\nabla \cdot \mathbf{u}) + \mu \mathbf{u} \cdot \nabla^2 \mathbf{u}.$$

For an incompressible fluid,  $\nabla \cdot \mathbf{u} = 0$ , thus,

$$\nabla \cdot (\mathbf{u} \cdot \boldsymbol{\tau}) = \text{trace} (\mu \nabla \mathbf{u} [\nabla \mathbf{u} + (\nabla \mathbf{u})^T]) + \mu \mathbf{u} \cdot \nabla^2 \mathbf{u}.$$

## 4.8 Appendix 4: Flux Through Energy Minimization

The following describes the one argument for energy minimization for flux terms. This has extensively been studied by mathematicians through the so-called "Dirichlet energy". To start, suppose we have a control volume,  $V$ , where we are given information about what is happening on the boundary and we want to find a function,  $u$ , that interpolates the data. To get distributed energy, we want an interpolation function that does not rapidly change over the volume or in other words, we want that the function is "smoothed" out. A way of quantifying this is to integrate (sum) the gradient of  $u$  over the domain; this gives a global

quantifier for the "change" in  $u$  over  $V$ . Therefore, we define the Dirichlet energy,  $E$ ,

$$E(u) := \frac{1}{2} \iiint_V |\nabla u|^2 dV.$$

Notice if the function changes rapidly in parts of the control volume, the gradient will be large and thus the integral and energy will be large. To get a smoothed out function, we want that globally (over the entire volume), the energy should be *minimized*, or the change in  $u$  at every point should be as small as possible. Physically,  $\nabla u$  is the generalized force acting on the system while  $u$  is the potential energy. We want to find a potential energy function,  $u$ , that minimizes the Dirichlet energy. This entails introducing a "functional derivative" so that we can speak of minimization. We define the functional derivative as,

$$\frac{\delta E}{\delta v} := \lim_{\varepsilon \rightarrow 0} \frac{E(u + \varepsilon v) - E(u)}{\varepsilon}.$$

Notice its resemblance to the directional derivative from vector calculus,

$$\nabla E \cdot \mathbf{v} := \lim_{\varepsilon \rightarrow 0} \frac{E(\mathbf{u} + \varepsilon \mathbf{v}) - E(\mathbf{u})}{\varepsilon}.$$

These are interpreted as a measure of how  $E$  changes as the input,  $u$ , changes by a little amount  $\varepsilon v$ .  $u$  and  $v$  are any "nice" functions, but we often choose the variation function,  $v$ , such that,

$$\|v\|^2 := \iiint_V v^2 dV = 1,$$

which means the "norm" or size of  $v$  is 1. Now to minimize the Dirichlet energy, we take the functional derivative and set it equal to 0 and use  $|\nabla u|^2 = \nabla u \cdot \nabla u$ ,

$$\begin{aligned} \frac{\delta E}{\delta v} &= \lim_{\varepsilon \rightarrow 0} \frac{1}{2\varepsilon} \iiint_V \left[ \nabla(u + \varepsilon v) \cdot \nabla(u + \varepsilon v) - \nabla u \cdot \nabla u \right] dV \\ &= \lim_{\varepsilon \rightarrow 0} \frac{1}{2\varepsilon} \iiint_V \left[ \cancel{\nabla u \cdot \nabla u} + 2\varepsilon \nabla u \cdot \nabla v + \varepsilon^2 \nabla v \cdot \nabla v - \cancel{\nabla u \cdot \nabla u} \right] dV \\ &= \lim_{\varepsilon \rightarrow 0} \frac{1}{2} \iiint_V \left[ 2\nabla u \cdot \nabla v + \cancel{\varepsilon \nabla v \cdot \nabla v} \right] dV \\ &= \iiint_V \nabla u \cdot \nabla v dV. \end{aligned}$$

Integration by parts gives,

$$\iiint_V \nabla u \cdot \nabla v dV = \iiint_{\partial V} v \nabla u \cdot \mathbf{n} dA \overset{0}{\rightarrow} - \iiint_V v \nabla^2 u dV.$$

Where we assume that  $v \equiv 0$  on  $\partial V$  since we know information on the boundary and thus there must be no variation on the boundary. Thus we now have,

$$- \iiint_V v \nabla^2 u \, dV = 0,$$

which implies that for the above equation to hold for any variation,  $v$ ,

$$-\nabla^2 u = 0,$$

which is Laplace's equation. This states that solutions to Laplace's equation, "harmonic" functions, are the minimizers of the Dirichlet energy. Physically, this states that diffusion minimizes the generalized potential energy,  $u$ , and minimizes the local change of energy. Thus, we now have some justification for why diffusion and flux capture nature's tendency to minimize energy.

As an aside for those interested in computational work, the integration by parts step suggests an alternative formulation of Laplace's equation as

$$\iiint_V \nabla u \cdot \nabla v \, dV = 0,$$

which requires that  $u$  only be once differentiable instead of twice differentiable as in the classical form of Laplace's equation. This is an important observation that this most commonly exploited in finite element methods that often use linear approximations of  $u$  for reduced computational costs. For more information, research the "Galerkin Method" and "Lagrange Polynomials".

## 4.9 Appendix 5: An Example of the Transient Energy Equation

The following is an example of just how complicated solutions become when transient transport is considered. For the sake of the example, consider a 1D metal rod that is insulated at both ends (no flux), and is heated to an initial temperature profile,  $f(x)$ . We also allow a heat source,  $Q(x, t)$ , to input energy into the rod. Mathematically, these conditions give,

$$\begin{cases} \frac{\partial T}{\partial t} = \alpha \frac{\partial^2 T}{\partial x^2} + Q(x, t) \\ \frac{\partial T}{\partial x}(0, t) = 0 = \frac{\partial T}{\partial x}(L, t) \\ T(x, 0) = f(x) \end{cases}$$

... a relatively tame transport equation. The solution is given by,

$$T(x, t) = \frac{1}{L} \int_0^L \left[ f(y) + \int_0^t Q(y, \tau) d\tau \right] dy$$

$$+ \frac{2}{L} \int_0^L \sum_{n=1}^{\infty} \left[ \left( f(y) e^{-\alpha \left( \frac{n\pi}{L} \right)^2 t} + \int_0^t Q(y, \tau) e^{-\alpha \left( \frac{n\pi}{L} \right)^2 (t-\tau)} d\tau \right) \cos \left( \frac{n\pi x}{L} \right) \cos \left( \frac{n\pi y}{L} \right) \right] dy.$$

It becomes easy to see why numerical methods are needed for even slightly more complex problems since the analytical solutions become so unwieldy.

## References

- [1] Bird, R., Stewart, W., Lightfoot, E.; *Transport Phenomena*. 2nd Ed., John Wiley and Sons, New York.
- [2] Geankoplis, C. J.; *Transport Processes and Unit Operations*, 3rd Ed., Prentice Hall, 2003.
- [3] Welty, J., Rorrer G. L., Foster D. G.; *Fundamentals of Momentum, Heat, and Mass Transfer*, 6th Ed., Wiley Global Education US, 2013.