# Transport Phenomena II

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## Contents

# 1 Temperature Distributions with More Than One Independent Variable

## 1.1 The Microscopic Energy Balance

- The microscopic energy balance states that

$$\rho \hat{C}_p \left[ \frac{\partial T}{\partial t} + v \cdot \nabla T \right] = -\nabla \cdot q$$

  where $v$ and $q$ are vector quantities

- In the limit of no convection and applying Fourier's law,

$$\rho \hat{C}_p \frac{\partial T}{\partial t} = (\nabla \cdot k \nabla T)$$

  where Fourier's law is

$$q = -k \nabla T$$

  - This can be occasionally rewritten as $q = k \dfrac{\Delta T}{L}$

- Occasionally, $k$ can be assumed to be independent of temperature, which then makes the energy balance

$$\frac{\partial T}{\partial t} = \alpha \nabla^2 T$$

  where $\alpha$ is the thermal diffusivity defined as

$$\alpha = \frac{k}{\rho \hat{C}_P}$$

  - The units of $\alpha$ are length-squared per unit time
    * The units of $k$ are frequently watts per meter-kelvin=

- The heat flow is given as

$$Q = \int_A q \, dA$$

  which simplifies to the following if $q$ is assumed to be uniform over the area (e.g. if you use an average heat transfer coefficient, $\bar{h}$ to find $q$)

$$Q = qA = -Ak \nabla T$$

- The energy over a period of time can be given by

$$E = A \int_0^t q \, dt$$

## 1.2 Unsteady State Heat Conduction: Separation of Variables Technique

Before I begin this section, I'd like to point out that **Section 1.2** is not explore in full rigor, and you are not advised to try to understand the poor explanations I've included here. The takeaway points are how to use the technique of separation of variables and that we add the unsteady state term to the steady state term to get a true equation for the temperature profile.

Problem: Consider a rod of length $\ell$, initially at $T_0$, that is perfectly insulated except at the ends (such that there is 1-D flow of temperature). Find the steady-state temperature profile if the left side is held at a constant $T_L$ and the right side at a constant $T_R$

### 1.2.1   Introduction

1. Since we are not worrying about radial temperature, we shall use Cartesian coordinates

2. The boundary and initial conditions are

$$T(0, t) = T_L$$

$$T(\ell, t) = T_R$$

$$T(x, 0) = T_0$$

3. Try a solution of

$$T(x, t) = X(x)\,\hat{T}(t)$$

4. The microscopic energy balance is

$$\frac{\partial T}{\partial t} = \alpha \frac{\partial^2 T}{\partial x^2}$$

5. Therefore, plugging in the trial solution yields

$$X\hat{T}' = \alpha \hat{T} X''$$

which can be rewritten as

$$\frac{\hat{T}'}{\hat{T}} = \alpha \frac{X''}{X} = \text{Constant}$$

6. Now, we analyze the possible conditions

   (a) If the expression equals zero, it is the steady-state solution

   (b) If the expression equals a positive quantity, then the temperature would increase up to (positive or negative) infinity, so it is unphysical. This is shown below (where $C^2$ is some arbitrary positive constant):

$$\frac{\hat{T}'}{\hat{T}} = C^2 \rightarrow \frac{1}{\hat{T}}\frac{d\hat{T}}{dt} = C^2$$

   now rewriting this (temporarily) using the differential operator $D$ yields

$$D\hat{T} - C^2\hat{T} = 0 \rightarrow \hat{T}\left(D - C^2\right) = 0$$

   which has roots of

$$D = C^2$$

   such that the solution to the ODE is

$$\hat{T} = C_1 \exp\left(C^2 t\right)$$

   which approaches infinity if $C_1$ is positive and negative infinity if $C_1$ is negative

   (c) If the expression equals a negative quantity, then the temperature would be something that's feasible. The same mathematical progression would show that for a negative constant $(-C^2)$:

$$\hat{T} = C_1 \exp\left(-C^2 t\right)$$

   which decays to zero at infinite time. Since $t \rightarrow \infty$ is steady-state, the $\hat{T}(t)$ term should drop out (i.e. the transient term goes to zero), which it does. Therefore, a negative constant value is the unsteady state solution

7. Let's tackle this problem by addressing the steady-state solution, then the unsteady state solution, and finally adding them together

### 1.2.2   The Steady State Solution

1. If the expression equals zero (the steady state solution), then we can evaluate this as follows:

$$\frac{\hat{T}'}{\hat{T}} = 0 \rightarrow \hat{T} = C_1$$

$$\alpha \frac{X''}{X} = 0 \rightarrow X = C_2 X + C_3$$

such that

$$T(x,t) = C_1 (C_2 X + C_3)$$

and creating a new constant will yield

$$T(x,t) = C_4 X + C_5$$

which can be solved using the boundary and initial conditions to yield

$$T(0,t) = T_L = C_5$$

$$T(\ell,t) = T_R = C_4 \ell + C_5$$

so for the steady-state solution to heat conduction in a rod that is perfectly insulated except at the ends:

$$T(x,t) = \left(\frac{T_R - T_L}{\ell}\right) x + T_L$$

### 1.2.3   The Transient Solution (both steady and unsteady state)

1. If the expression equals a negative constant (i.e. $-C^2$), let's try the differential equation of

$$\frac{X''}{X} = -C^2$$

Rewriting this (temporarily) using the $D$ differential operator yields

$$D^2 X + C^2 X = 0 \rightarrow X \left(D^2 + C^2\right) = 0$$

which has roots of

$$D = \pm\sqrt{-C^2} = \pm i\sqrt{C^2} = \pm iC$$

such that the solution of the ODE is

$$X = C_{1,x,i} \cos\left(Cx\right) + C_{2,x,i} \sin\left(Cx\right)$$

2. Let's now try the other differential equation for a negative constant,

$$\frac{\hat{T}'}{\hat{T}} = -C^2$$

which can be solved, as earlier with $C^2$, to yield

$$\hat{T} = C_{3,x} \exp\left(-C^2 \alpha t\right)$$

3. Finally, we can write the solution as

$$T = X\hat{T} = C_{3,x} \exp\left(-C^2 \alpha t\right) \left[C_{1,x,i} \cos\left(Cx\right) + C_{2,x,i} \sin\left(Cx\right)\right]$$

which can be rewritten absorbing $C_{3,x}$ into the other constants to yield

$$T_{uss} = \exp\left(-C^2 \alpha t\right) \left[C_{1,x} \cos\left(Cx\right) + C_{2,x} \sin\left(Cx\right)\right]$$

4. Since we defined the problem to be at steady state at $x = 0$ and $x = \ell$, it is clear that $T_{uss} = 0$ at these values. Therefore, $C_{1,x} = 0$ and $C_{2,x} = \exp\left(-C^2 \alpha t\right) B \sin\left(C\ell\right)$

5. Since we just stated that $T_{uss} = 0$ at $x = \ell$, we have an issue. We can have $B = 0$, but that means $T_{uss} = 0$ for all $x$ and $t$. Clearly that's not possible. There are no parameters to alter in $\exp\left(-C^2 \alpha t\right)$ either. This leaves us with forcing the $\sin\left(C\ell\right)$ term to zero. To do this, we can state that $C_n = \dfrac{n\pi}{\ell}$ where $n$ is an integer greater than or equal to 1. Rewriting our expression for the unsteady state temperature yields $T_{uss} = \exp\left(-\dfrac{n^2 \pi^2 \alpha t}{\ell^2}\right) B_n \sin\left(\dfrac{n\pi x}{\ell}\right)$

6. After a lot of math and applying the half-range sine expansion in addition to the initial conditions, we find that for the case of $T_R = 100$, $T_L = 50$, and $T(x,0) = 100$ that $B_n = \dfrac{100}{n\pi}$ and

$$T(x, \ell) = 50\left(\frac{x}{\ell} + 1\right) + \frac{100}{\pi} \sum_{n=1}^{\infty} \left[\frac{1}{n} \sin\left(\frac{n\pi x}{\ell}\right) \exp\left(\frac{-\pi^2 n^2 \alpha t}{\ell^2}\right)\right]$$

for both steady and unsteady state

## 1.3 Heating a Semi-Infinite Solid

Problem: Consider a solid material occupying the space from $y = 0$ to $y = \infty$ that is initially at temperature $T_0$. At time $t = 0$, the surface at $y = 0$ is suddenly raised to temperature $T_1$ and maintained at that temperature for $t > 0$. Find the time-dependent temperature profiles $T(y, t)$. Assume a constant $k$.

Solution:

1. The microscopic energy balance in the $y$ direction states that

$$\frac{\partial T}{\partial t} = \alpha \frac{\partial^2 T}{\partial y^2}$$

2. We can introduce a dimensionless variable of

$$\Theta = \frac{T - T_0}{T_1 - T_0}$$

to simplify the calculations such that

$$\frac{\partial \Theta}{\partial t} = \alpha \frac{\partial^2 \Theta}{\partial y}$$

3. The boundary and initial conditions state that:

$$\Theta(y, 0) = 0$$

$$\Theta(0, t) = 1$$

$$\Theta(\infty, t) = 0$$

4. Since $\Theta$ is dimensionless, it must be related to $\dfrac{y}{\sqrt{\alpha t}}$ since this (or multiplicative scale factors of it) is the only possible dimensionless group from the given variables. Therefore,

$$\Theta = \Theta(\eta)$$

where

$$\eta = \frac{y}{\sqrt{4\alpha t}}$$

(a) The $\sqrt{4}$ term in the denominator is included for mathematical simplicity during the derivation

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5. The differential equation in Step 2 can be broken down from a PDE to an ODE

   (a) First,
   $$\frac{\partial \Theta}{\partial t} = \frac{\partial \Theta}{\partial \eta} \frac{\partial \eta}{\partial t}$$

   The value for $\frac{\partial \eta}{\partial t}$ can be found from taking the derivative of $\eta$ with respect to $t$. This yields
   $$\frac{\partial \Theta}{\partial t} = -\frac{d\Theta}{d\eta} \frac{1}{2} \frac{\eta}{t}$$

   (b) Next,
   $$\frac{\partial \Theta}{\partial y} = \frac{\partial \Theta}{\partial \eta} \frac{\partial \eta}{\partial y}$$

   The value for $\frac{\partial \eta}{\partial y}$ can be found from taking the derivative of $\eta$ with respect to $y$. This yields
   $$\frac{\partial \Theta}{\partial y} = \frac{d\Theta}{d\eta} \frac{1}{\sqrt{4\alpha t}}$$

   i. We want $\frac{\partial^2 \Theta}{\partial y^2}$ though, so
   $$\frac{\partial^2 \Theta}{\partial y^2} = \frac{\partial}{\partial y} \left( \frac{\partial \Theta}{\partial y} \right) = \frac{d^2 \Theta}{d\eta^2} \frac{1}{4\alpha t}$$

   (c) Therefore,
   $$\frac{d^2 \Theta}{d\eta^2} + 2\eta \frac{d\Theta}{d\eta} = 0$$

6. A new set of boundary conditions are needed for $\eta$

   (a) At $\eta = 0$, $\Theta = 1$ since this is when $y = 0$, and it was stated earlier that $\Theta(0, t) = 1$

   (b) At $\eta = \infty$, $\Theta = 0$ since this is when $y = \infty$, and it was stated earlier that $\Theta(\infty, t) = 0$

7. To solve this differential equation, introduce $\psi = \frac{d\Theta}{d\eta}$ to make the equation
   $$\frac{d\psi}{d\eta} + 2\eta\psi = 0$$

   (a) This yields,
   $$\psi = C_1 \exp\left(-\eta^2\right)$$

8. Integrating $\psi$ yields,
   $$\Theta = C_1 \int_0^\eta \exp\left(-\bar{\eta}^2\right) d\bar{\eta} + C_2$$

9. The boundary conditions of $\Theta = 0$ and $\Theta = 1$ can be used here to find $C_1$ and $C_2$, which produces the equation
   $$\Theta(\eta) = 1 - \operatorname{erf}(\eta)$$

   which corresponds to the following solution for the heating of a semi-infinite slab[1]:
   $$\boxed{\Theta = \frac{T(y, t) - T_0}{T_1 - T_0} = 1 - \operatorname{erf}\left(\frac{y}{\sqrt{4\alpha t}}\right)}$$

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[1]$T_0$ is the initial temperature, $T_1$ is the surface temperature, and $T$ is the temperature at a point in space and time afterwards

(a) **Important Point:** The above expression tells you about the temperature at some point along the semi-infinite axis. If you have a semi-infinite object, but you want to find the temperature somewhere on the finite axis, then this is not the equation for you.

10. If the heat flux is desired at the wall (i.e. surface)[2],

$$\boxed{q_s = q_y\big|_{y=0} = -k\frac{\partial T}{\partial y}\bigg|_{y=0} = \frac{k}{\sqrt{\pi \alpha t}}\left(T_1 - T_0\right)}$$

since

$$\frac{d}{dx}\left(\text{erf}\left(u\right)\right) = \frac{2}{\sqrt{\pi}}\exp\left(u^2\right)\frac{du}{dx}$$

- As a side-note, the thermal penetration thickness, $\delta_T$, is defined as the value of $\eta$ when $\text{erf}\left(\eta\right) = 0.99$ (such that there is a 1% change in $\Theta$). This occurs close to $\eta = 2$, so

$$\boxed{\delta_T = 4\sqrt{\alpha t}}$$

## 1.4    Heating a Finite Slab

Problem: A solid slab occupying the space between $y = -b$ and $y = b$ is initially at temperature $T_0$. At time $t = 0$, the surfaces at $y = \pm b$ are suddenly raised to $T_1$ and maintained there. Find $T(y, t)$. Assume a constant $k$.

Solution:

1. The microscopic energy balance in the $y$-direction states that

$$\frac{\partial T}{\partial t} = \alpha\frac{\partial^2 T}{\partial y^2}$$

2. We can introduce the following dimensionless variables to simplify the math:

$$\Theta = \frac{T_1 - T}{T_1 - T_0}$$

$$\eta = \frac{y}{b}$$

$$\tau = \frac{\alpha t}{b^2}$$

(a) It should be noted that the steady state solution goes to zero because at $t = \infty$, $T = T_1$ such that $\Theta = 0$ for all $\tau > 0$

3. This makes the microscopic energy balance now read

$$\frac{\partial \Theta}{\partial \tau} = \frac{\partial^2 \Theta}{\partial \eta^2}$$

4. The initial and boundary conditions are now:

(a) At $\tau = 0$, $\Theta = 1$

(b) At $\eta = \pm 1$, $\Theta = 0$ for $\tau > 0$

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[2]Additional expressions: $q_s = \frac{\sqrt{k\rho C_P}}{\sqrt{\pi t}}\left(T_1 - T_0\right)$. At constant $\Delta T$ and $\Delta t$, $\frac{q_{s,2}}{q_{s,1}} = \frac{\sqrt{k_2 \rho_2 C_{P,2}}}{\sqrt{k_1 \rho_1 C_{P,1}}}$. The energy (J/m$^2$) over a period of time is $E = \int_0^t q_s \, dt = \frac{2k\sqrt{t}\left(T_1 - T_0\right)}{\sqrt{\pi \alpha}}$.

5. We can implement the method of separation of variables by stating

$$\Theta\left(\eta, \tau\right) = f\left(\eta\right) g\left(\tau\right)$$

6. Substituting the trial solution for $\Theta$ yields

$$f g' = g f''$$

7. Dividing by $fg$ yields

$$\frac{1}{g}\frac{dg}{d\tau} = \frac{1}{f}\frac{d^2 f}{d\eta^2}$$

8. If the left side is a function of only $\tau$, and the right side is a function of only $\eta$, then both must be equal to some constant. The constant will be chosen as $-c^2$ solely to simplify the math. Therefore,

$$\frac{dg}{d\tau} = -c^2 g$$

$$\frac{d^2 f}{d\eta^2} = -c^2 f$$

9. Integrating the above equations yields

$$g = A\exp\left(-c^2\tau\right)$$

$$f = B\sin\left(c\eta\right) + C\cos\left(c\eta\right)$$

10. The integration constant $B$ must equal zero since $\Theta\left(\eta, \tau\right)$ must equal $\Theta\left(-\eta, \tau\right)$ due to symmetry about the $xz$-plane. Applying the boundary conditions then yields

$$C\cos\left(c\right) = 0$$

(a) If $C = 0$, then the temperature profile is always zero, which cannot be the case. Other solutions exist as follows:

$$c = \left(n + \frac{1}{2}\right)\pi$$

where

$$n = 0, \pm 1, \pm 2, ..., \pm\infty$$

11. Therefore,

$$\Theta_n = A_n\exp\left(-\left(n + \frac{1}{2}\right)^2\pi^2\tau\right) C_n\cos\left(n + \frac{1}{2}\right)\pi\eta$$

12. Since $\Theta$ is the sum of all $\Theta_n$,

$$\Theta = \sum_{n=0}^{\infty} D_n\exp\left(-\left(n + \frac{1}{2}\right)^2\pi^2\tau\right)\cos\left(n + \frac{1}{2}\right)\pi\eta$$

where

$$D_n = A_n C_n + A_{-(n+1)}C_{-(n+1)}$$

13. Applying the initial condition yields

$$1 = \sum_{n=0}^{\infty} D_n\cos\left(n + \frac{1}{2}\right)\pi\eta$$

14. The solution for $D_n$ is the following (see BSL for more details)

$$D_n = \frac{2\left(-1\right)^n}{\left(n + \dfrac{1}{2}\right)\pi}$$

15. Plugging $D_n$ into the equation for $\Theta$ in Step 12 yields

$$\frac{T_1 - T}{T_1 - T_0} = 2\sum_{n=0}^{\infty} \frac{(-1)^n}{\left(n + \dfrac{1}{2}\right)\pi} \exp\left(-\left(n + \frac{1}{2}\right)^2 \pi^2 \frac{\alpha t}{b^2}\right) \cos\left(n + \frac{1}{2}\right)\pi\frac{y}{b}$$

(a) The solution to this equation (as well as the analogous equations for cylindrical and spherical systems) is graphically shown in BSL Figures 12.1-1, 12.1-2, and 12.1-3

16. For a cube-like solid,

$$\boxed{\frac{T_1 - T}{T_1 - T_0} = \Theta\left(\frac{x}{a}, \frac{\alpha t}{a^2}\right)\Theta\left(\frac{y}{b}, \frac{\alpha t}{b^2}\right)\Theta\left(\frac{z}{c}, \frac{\alpha t}{c^2}\right) = \Theta_x\Theta_y\Theta_z}$$

where each side is $2a$, $2b$, and $2c$

(a) **Important Note**: You multiply the $\Theta$ of every finite dimension you have. For a semi-infinite cylinder, you would just use $\Theta_r$, but for a finite cylinder, you'd have to do $\Theta_r\Theta_z$.

(b) **Important Note**: The middle is $0$ since the top is $a$ and the bottom is $-a$

## 1.5 Complexification

### 1.5.1 Background

- Recall that

$$e^{i\theta} = \cos\theta + i\sin\theta$$

- The approach to complexification is to translate a real system to a complex one, solve the system, and extract the real part of the solution (frequently used with periodic conditions)

### 1.5.2 Unsteady Heat Conduction near a Wall with Sinusoidal Heat Flux

Problem: A solid body occupying the space from $y = 0$ to $y = \infty$ is initially at temperature $T_0$. Beginning at time $t = 0$, a periodic heat flux is given by

$$q_y = q_0\cos\left(\omega t\right) = q_0\mathbb{R}\left[e^{i\omega t}\right]$$

is imposed at $y = 0$. Here, $q_0$ is the amplitude of the heat flux oscillations, and $\omega$ is the frequency. It is desired to find the temperature in this system, $T(y, t)$, in the periodic steady steady state. Assume a constant $k$.

Solution:

1. The microscopic energy balance in the $y$-direction states that

$$\frac{\partial T}{\partial t} = \alpha\frac{\partial^2 T}{\partial y^2}$$

2. If both sides are multiplied by $-k$ and both sides are acted on by the operator $\dfrac{\partial}{\partial y}$ then with a little rearrangement,

$$\frac{\partial}{\partial t}\left(-k\frac{\partial T}{\partial y}\right) = \alpha\frac{\partial^2}{\partial y^2}\left(-k\frac{\partial T}{\partial y}\right)$$

3. The definition of heat flux can then be used such that

$$\frac{\partial q_y}{\partial t} = \alpha \frac{\partial^2 q_y}{\partial y^2}$$

4. The boundary conditions are:

   (a) At $y = 0$, $q_y = q_0 \mathbb{R}\left[e^{i\omega t}\right]$
   (b) At $y = \infty$, $q_y = 0$

5. We postulate an oscillatory solution of the form

$$q_y = \mathbb{R}\left[q^\circ e^{i\omega t}\right]$$

   where $q^\circ$ of a complex function of $y$

6. Substituting the trial solution into the equation in Step 3 yields

$$\mathbb{R}\left[q^\circ i\omega e^{-i\omega t}\right] = \alpha \mathbb{R}\left[\frac{d^2 q^\circ}{dy^2} e^{i\omega t}\right]$$

   where $q^\circ$ means complex $q$

7. The above expression is mathematically equivalent to

$$\frac{d^2 q^\circ}{dy^2} - \left(\frac{i\omega}{\alpha}\right) q^\circ = 0$$

8. The new boundary conditions are:

   (a) At $y = 0$, $q^\circ = q_y$
   (b) At $y = \infty$, $q^\circ = 0$

9. The differential equation has the solution of

$$q^\circ = C_1 \exp\left(y\sqrt{\frac{i\omega}{\alpha}}\right) + C_2 \exp\left(-(1+i)y\sqrt{\frac{i\omega}{2\alpha}}\right)$$

10. Since $\sqrt{i} = \pm\left(\frac{1}{\sqrt{2}}\right)(1+i)$,

$$q^\circ = C_1 \exp\left((1+i)y\sqrt{\frac{\omega}{2\alpha}}\right) + C_2 \exp\left(-(1+i)y\sqrt{\frac{\omega}{2\alpha}}\right)$$

11. The second boundary condition requires that $C_1 = 0$, and the first boundary condition requires that $C_2 = q_0$. Therefore,

$$q^\circ = q_0 \exp\left(-(1+i)y\sqrt{\frac{\omega}{2\alpha}}\right)$$

12. As such,

$$q_y = \mathbb{R}\left[q_0 \exp\left(-(1+i)y\sqrt{\frac{\omega}{2\alpha}}\right)e^{i\omega t}\right] = q_0 \exp\left(-y\sqrt{\frac{\omega}{2\alpha}}\right)\mathbb{R}\left[\exp\left(-i\left(y\sqrt{\frac{\omega}{2\alpha}} - \omega t\right)\right)\right]$$

13. The above expression is equivalent to

$$q_y = q_0 \exp\left(-y\sqrt{\frac{\omega}{2\alpha}}\right)\cos\left(\omega t - y\sqrt{\frac{\omega}{2\alpha}}\right)$$

14. Integrating Fourier's law yields

$$-k \int_T^{T_0} d\bar{T} = \int_y^\infty q_{\bar{y}} d\bar{y}$$

15. The above expression simplifies to

$$T - T_0 = \frac{q_0}{k} \sqrt{\frac{\alpha}{\omega}} \exp\left(-y\sqrt{\frac{\omega}{2\alpha}}\right) \cos\left(\omega t - y\sqrt{\frac{\omega}{2\alpha}} - \frac{\pi}{4}\right)$$

## 1.6   Laplace Transforms

### 1.6.1   General Definitions

- The Laplace Transform, a linear operator, is defined as

$$F(s) = \int_0^\infty e^{-st} f(t) \, dt$$

- We write the Laplace transform as

$$F(s) = \mathscr{L}\left[f(t)\right]$$

- If $F(s) = \mathscr{L}\left[f(t)\right]$, then we say that $f(t)$ is the inverse Laplace transform, written as

$$f(t) = \mathscr{L}^{-1}\left[F(s)\right]$$

- The First Shift Formula states that

$$\mathscr{L}\left[e^{at} f(t)\right] = F\left(s - a\right)$$

where $F(s) = \mathscr{L}\left[f(t)\right]$

- Equivalently,

$$\mathscr{L}^{-1}\left[F(s)\right] = e^{at} \mathscr{L}^{-1}\left[F(s + a)\right]$$

- The Second Differentiation Formula states that

$$\mathscr{L}\left[t^n f(t)\right] = (-1)^n \frac{d^n}{ds^n} \mathscr{L}\left[f(t)\right]$$

- While the Laplace and inverse Laplace operators are linear, they have analogous properties with integrals, so $\mathscr{L}\left[A \cdot B\right] \neq \mathscr{L}\left[A\right] \cdot \mathscr{L}\left[B\right]$

### 1.6.2   Common Transforms

- The following is a list of basic transforms and inverse transforms:

$$\mathscr{L}\left[e^{\lambda t}\right] = \frac{1}{s - \lambda} \quad \text{and} \quad \mathscr{L}^{-1}\left[\frac{1}{s - \lambda}\right] = e^{\lambda t}$$

$$\mathscr{L}\left[1\right] = \frac{1}{s} \quad \text{and} \quad \mathscr{L}^{-1}\left[\frac{1}{s}\right] = 1$$

$$\mathscr{L}\left[t^n\right] = \frac{n!}{s^{n+1}} \quad \text{and} \quad \mathscr{L}^{-1}\left[\frac{1}{s^n}\right] = \frac{t^{n-1}}{(n-1)!}$$

$$\mathscr{L}\left[\cos(\beta t)\right] = \frac{s}{s^2 + \beta^2} \quad \text{and} \quad \mathscr{L}^{-1}\left[\frac{s}{s^2 + \beta^2}\right] = \cos(\beta t)$$

$$\mathscr{L}\left[\sin(\beta t)\right] = \frac{\beta}{s^2 + \beta^2} \quad \text{and} \quad \mathscr{L}^{-1}\left[\frac{1}{s^2 + \beta^2}\right] = \frac{1}{\beta} \sin(\beta t)$$

### 1.6.3 Using the Laplace Transform to Solve Initial-Value Problems

1. Transform both sides of the differential equation, incorporating the initial data by means of the first differentiation formula,

$$\mathscr{L}\left[D^k x\right] = s^k \mathscr{L}\left[x\right] - s^{k-1}x(0) - s^{k-2}x'(0) - \ldots - x^{(k-1)}(0)$$

where $D \equiv \dfrac{d}{dt}$

2. Solve algebraically for $\mathscr{L}\left[x\right]$ in terms of $s$

3. Obtain $x$ as the inverse Laplace transform of the equation found in Step 2

### 1.6.4 Reworking the Semi-Infinite Slab

- First, realize that Laplace transforms convert the $t$ to $s$ such that

$$\mathscr{L}\left[\Theta\left(x,t\right)\right] \equiv \bar{\Theta}\left(x,s\right)$$

- Recall that

$$\Theta\left(x,0\right) = 0$$
$$\Theta\left(0,t\right) = 1$$
$$\Theta\left(\infty,t\right) = 0$$

- The differential equation that applies for this system (if we consider the $x$ direction) is

$$\frac{\partial\Theta}{\partial t} = \alpha\frac{\partial^2\Theta}{\partial x^2}$$

- Taking the Laplace transform of both sides yields the following once the first differentiation formula is used,

$$s\mathscr{L}\left(\Theta\right) - 0 = \alpha\mathscr{L}\left[\frac{\partial^2\Theta}{\partial x^2}\right]$$

- Since we said that $\mathscr{L}\left[\Theta\right] = \bar{\Theta}$,

$$s\bar{\Theta} = \alpha\frac{\partial^2\bar{\Theta}}{\partial x^2}$$

- Rewriting this with more familiar notation yields

$$\bar{\Theta}'' = \frac{s}{\alpha}\bar{\Theta}$$

- The boundary conditions can be rewritten using the Laplace transform as

$$\bar{\Theta}\left(0,s\right) = \frac{1}{s}$$

$$\bar{\Theta}\left(\infty,s\right) = 0$$

- Recall that this second-order homogeneous differential equation can be solved as

$$D^2\bar{\Theta} - \frac{s}{\alpha}\bar{\Theta} = 0 \rightarrow \bar{\Theta}\left(D^2 - \frac{s}{\alpha}\right) = 0$$

such that the roots are

$$D = \pm\sqrt{\frac{s}{\alpha}}$$

which means that the solution is

$$\bar{\Theta} \quad = \quad C_1\exp\left(x\sqrt{\frac{s}{\alpha}}\right) + C_2\exp\left(-x\sqrt{\frac{s}{\alpha}}\right)$$

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- Applying the second boundary condition yields $C_1 = 0$ such that

$$\bar{\Theta} = C_2 \exp\left(-x\sqrt{\frac{s}{\alpha}}\right)$$

- The second boundary condition yields $C_2 = \dfrac{1}{s}$ such that

$$\bar{\Theta} = \frac{1}{s} \exp\left(-x\sqrt{\frac{s}{a}}\right)$$

- This Laplace transform is tabulated and can be readily found to be

$$\Theta = 1 - \operatorname{erf}\left(\frac{x}{\sqrt{4\alpha t}}\right)$$

# 2 Boundary Layer Theory for Nonisothermal Flow

## 2.1 Velocity Boundary Layer

- The local friction coefficient is defined as

$$\boxed{C_f \equiv \frac{2\tau_s}{\rho u_\infty^2}}$$

  - Don't forget that $\tau_s$ is evaluated at $y = 0$

- The boundary layer thickness for a velocity boundary is where $u = 0.99 u_\infty$

- Recall that the shear stress is given by

$$\boxed{\tau_s = \mu \frac{\partial u}{\partial y}\bigg|_{y=0}}$$

## 2.2 Thermal Boundary Layer

- The thermal boundary layer looks like the following (for $T_s > T_\infty$)
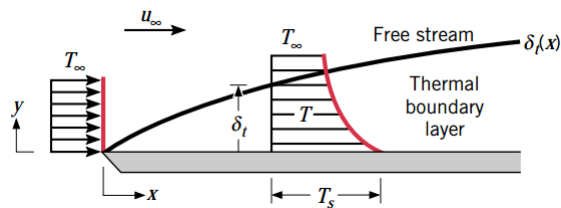


- For a thermal boundary layer, the boundary layer thickness is the position where $\dfrac{T_s - T}{T_s - T_\infty} = 0.99$

- The local surface heat flux can be obtained by

$$\boxed{q_s|_{y=0} = -k_f \frac{\partial T}{\partial y}\bigg|_{y=0} = h(T_s - T_\infty)}$$

such that

$$h = \frac{-k_f \dfrac{\partial T}{\partial y}\bigg|_{y=0}}{T_s - T_\infty}$$

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- Also,

$$Q = \int q \, dA_s = (T_s - T_\infty) \int h \, dA_s$$

which is equivalent to

$$\boxed{Q = \bar{h} A_s \, (T_s - T_\infty)}$$

where $\bar{h}$ is the average convection coefficient for the entire surface

  - For a sphere, $A_s = 4\pi r^2 = \pi D^2$
  - For a cylinder, $A_s = 2\pi r L = \pi D L$
  - If it's a 1-D characteristic length (such that $Q$ has units of W/m) for a cylinder or sphere, then it's $L = 2\pi r = \pi D$

- It follows that

$$\bar{h} = \frac{1}{A} \int h \, dA_s$$

  - For 1D heat transfer of a flat plate[3],

$$\boxed{\bar{h} = \frac{1}{L} \int_0^L h \, dx}$$

## 2.3 Laminar and Turbulent Velocity Boundary Layers
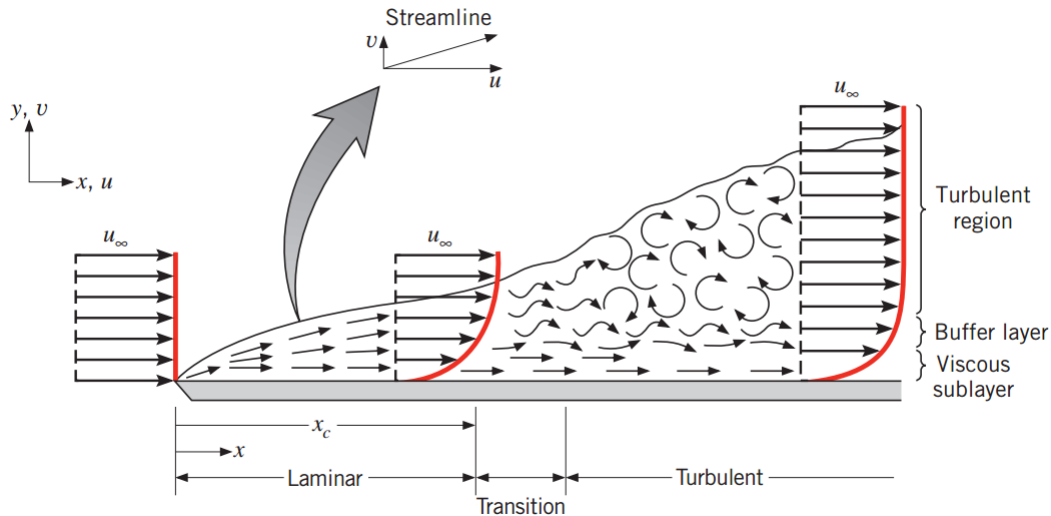


- The term $x_c$ marks the transition between the laminar and turbulent regions

- The turbulence brings in fluid from the undisturbed main stream closer to the plate

---

[3] $\bar{h}_{turb} = \frac{1}{x} \left[ \int_0^{x_c} h_{lam}(x) \, dx + \int_{x_c}^x h_{turb}(x) \, dx \right]$

$$\left.\frac{\partial u}{\partial y}\right|_{y=0,\ \text{lam}} < \left.\frac{\partial \bar{u}}{\partial y}\right|_{y=0,\ \text{turb}}$$



Laminar        Turbulent

- The Reynolds number is defined as[4]

$$Re_x = \frac{\rho u_\infty x}{\mu} = \frac{u_\infty x}{\nu}$$

where

$$\nu \equiv \frac{\mu}{\rho}$$

- The critical Reynolds number that marks the transition from the laminar to turbulent regions is approximated as the following for a flat-plate

$$Re_{x,c} = 5 \times 10^5$$

- Differences in the thickness of the velocity and thermal boundary layers tend to be much smaller in turbulent flow than in laminar flow since turbulence causing mixing that reduces the importance of conduction in determining the thermal boundary layer thickness

## 2.4 The Momentum and Energy Balance

- The assumptions that shall be used here include: steady state, incompressible fluid, no body forces (ignore $g$), constant properties (e.g. $\mu$, $\rho$), and continuity (i.e. no mass accumulation)

- Recall that the momentum balance states that

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

- For the system we are describing, this simplifies to

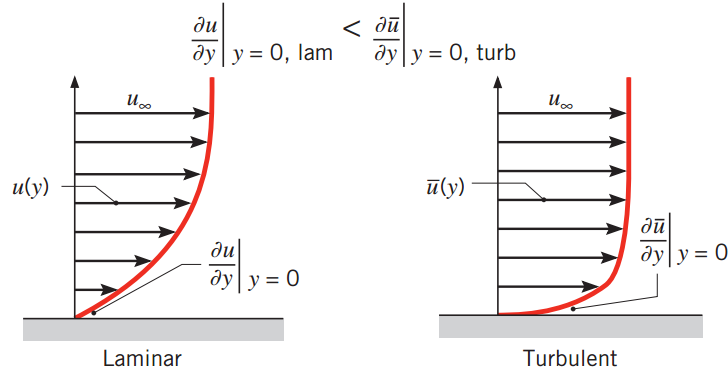$$\rho \left( \vec{v} \cdot \nabla \vec{v} \right) = -\nabla P + \mu \nabla^2 \vec{v}$$

- If we state that $u = v_x$ and $v = v_y$, the $x$-momentum equation is

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

- The full energy balance is given by

$$\rho C_p \left( \vec{v} \cdot \nabla T \right) = k \nabla^2 T + \mu \Phi$$

where $\mu \Phi$ is the viscous dissipation term

---

[4]Additional expression: $\dfrac{Re_{x,c}}{Re_L} = \dfrac{x_c}{L}$

## 2.5   The Boundary Layer Equations

- The additional assumptions for boundary layer theory is the gradients perpendicular to the surface are much greater than the gradients parallel to the surface and that $P_\infty$ changes slowly with $x$ such that

$$\frac{\partial P}{\partial x} \approx \frac{dP_\infty}{dx}$$

where $P$ is the pressure gradient within the boundary layer and $P_\infty$ is the pressure gradient of the free stream

- The $x$-momentum equation simplifies to the following inside the boundary layer

$$u\frac{\partial u}{\partial x} + v\frac{\partial u}{\partial y} = -\frac{1}{\rho}\frac{dP_\infty}{dx} + \nu\frac{\partial^2 u}{\partial y^2}$$

since $\dfrac{\partial^2 u}{\partial x^2} \ll \dfrac{\partial^2 u}{\partial y^2}$ in the boundary layer (i.e. gradients normal to the object's surface are much larger than those along the surface)

- The energy equation simplifies to the following as well

$$u\frac{\partial T}{\partial x} + v\frac{\partial T}{\partial y} = \alpha\frac{\partial^2 T}{\partial y^2} + \frac{\nu}{C_P}\left(\frac{\partial u}{\partial y}\right)^2$$

since

$$\frac{\partial^2 T}{\partial x^2} \ll \frac{\partial^2 T}{\partial y^2}$$

- With no viscous dissipation

$$u\frac{\partial T}{\partial x} + v\frac{\partial T}{\partial y} = \alpha\frac{\partial^2 T}{\partial y^2}$$

## 2.6   Boundary Layer Similarity

- To non-dimensionalize our equations, we introduce the following variables:

$$x^* \equiv \frac{x}{L}$$

$$y^* \equiv \frac{y}{L}$$

$$u^* \equiv \frac{u}{V}$$

$$v^* \equiv \frac{v}{V}$$

$$T^* \equiv \frac{T - T_s}{T_\infty - T_s}$$

$$P^* \equiv \frac{P_\infty}{\rho V^2}$$

- The shear stress can be expressed equivalently as

$$\tau_s = \mu\frac{\partial u}{\partial y}\bigg|_{y=0} = \left(\frac{\mu V}{L}\right)\frac{\partial u^*}{\partial y^*}\bigg|_{y^*=0}$$

such that

$$C_f = \frac{2\tau_s}{\rho V^2} = \frac{2}{Re_L}\frac{\partial u^*}{\partial y^*}\bigg|_{y^*=0}$$

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- The non-dimensionalized $x$-momentum equation states that

$$u^* \frac{\partial u^*}{\partial x^*} + v^* \frac{\partial u^*}{\partial y^*} = \frac{dP^*}{dx^*} + \frac{1}{Re_L} \frac{\partial^2 P^*}{\partial y^{*2}}$$

  - The boundary condition at the wall is $u^*(x^*, 0) = 0$ and for the free stream is $u^*(x^*, \infty) = \frac{u_\infty(x^*)}{V}$
  - The similarity parameter used is

$$\boxed{Re_L = \frac{uL}{\nu}}$$

- The non-dimensionalized $x$-thermal equation states that

$$u^* \frac{\partial T^*}{\partial x^*} + v^* \frac{\partial T^*}{\partial y^*} = \frac{1}{Re_L Pr} \frac{\partial^2 T^*}{\partial y^{*2}}$$

  - The boundary condition at the wall is $T^*(x^*, 0) = 0$ and for the free stream is $T^*(x^*, \infty) = 1$
  - The similarity parameter used is

$$\boxed{Pr = \frac{\nu}{\alpha} = \frac{\text{momentum}}{\text{thermal}}}$$

- We expect that $u^* = f\left(x^*, y^*, \frac{dP^*}{dx^*}, Re_L\right)$ and $T^* = f\left(x^*, y^*, \frac{dP^*}{dx^*}, Re_L, Pr\right)$

- The heat transfer coefficient can be expressed similarly as

$$h = \frac{k_f}{L} \frac{\partial T^*}{\partial y^*}\Big|_{y^*=0}$$

- The Nusselt number is defined as

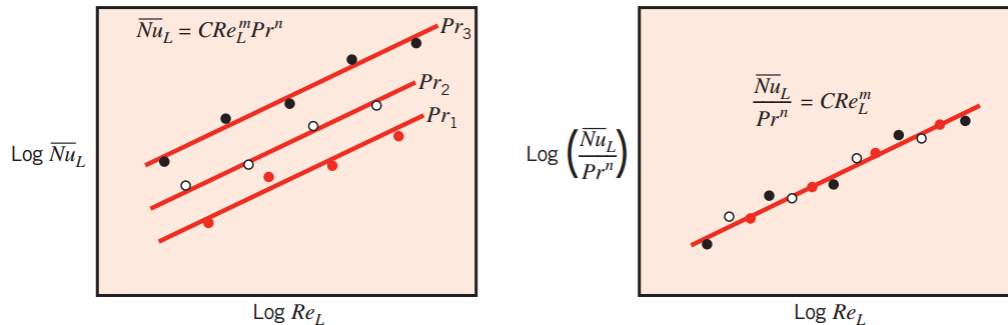$$\boxed{Nu \equiv \frac{hL}{k_f} = \frac{\partial T^*}{\partial y^*}\Big|_{y^*=0} = f(x^*, Re_L, Pr)}$$

$$\boxed{\overline{Nu} \equiv \frac{\bar{h}L}{k_f} = f(Re_L, Pr)}$$

- It is also true that

$$\overline{Nu} = CRe_L^m Pr^n$$

so the following plots are true

- Thermophysical quantities are frequently measured at the film temperature, which is defined as

$$\boxed{T_f = \frac{T_s + T_\infty}{2}}$$

  - Unless otherwise stated, evaluate thermophysical quantities at the film temperature. An exception to this would be evaluating the heat flux at a surface. Since you're evaluating it at the surface, you'd use the thermophysical properties at the surface temperature and not the film temperature

# 3 External Flow

## 3.1 Flat Plate in Parallel Flow

### 3.1.1 Hydrodynamic Solutions

- The Blasius solution states the following (it ignores $P$)

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

- The thermal boundary layer distance scales as

$$\delta_v \sim \sqrt{\frac{\nu x}{u_\infty}}$$

and

$$\frac{u_\infty^2}{x} \sim \frac{\nu u_\infty}{\delta_v^2}$$

- The stream function is defined as

$$\boxed{u = \frac{\partial \psi}{\partial y}}$$

and

$$\boxed{v = -\frac{\partial \psi}{\partial x}}$$

  - Note that the signs are reversed for $u$ and $v$ in BSL

- We will then define

$$f(\eta) = \frac{\psi}{u_\infty\sqrt{\frac{\nu x}{u_\infty}}} \rightarrow \boxed{\psi = u_\infty f(\eta)\sqrt{\frac{\nu x}{u_\infty}}}$$

and

$$\boxed{\eta = y\sqrt{\frac{u_\infty}{\nu x}}}$$

- It turns out that[5]

$$\frac{u}{u_\infty} = \frac{df}{d\eta}$$

$$\frac{\partial u}{\partial x} = -\frac{u_\infty}{2x}\eta\frac{d^2 f}{d\eta^2}$$

$$\frac{\partial u}{\partial y} = u_\infty\sqrt{\frac{u_\infty}{\nu x}}\frac{d^2 f}{d\eta^2}$$

$$\frac{\partial^2 u}{\partial y^2} = \frac{u_\infty^2}{\nu x}\frac{d^3 f}{d\eta^3}$$

---

[5]I am now writing $f(\eta)$ as simply $f$

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- These equations can be combined with the momentum balance to yield (see BSL 4.3, 4.4)

$$2\frac{d^3 f}{d\eta^3} + f\frac{d^2 f}{d\eta^2} = 0$$

whose values are tabulated in Table 7.1 of Incropera

### 3.1.2 Laminar Flow Equations

- See Incropera Section 7.2 for the math, but

$$\boxed{\delta_v = \frac{5}{\sqrt{\dfrac{u_\infty}{\nu x}}} = \frac{5x}{\sqrt{Re_x}}}$$

since $\dfrac{u}{u_\infty} = 0.99$ for $\eta = 5$

- The shear stress at the wall may be expressed as

$$\tau_s = \mu\frac{\partial u}{\partial y}\bigg|_{y=0} = \mu u_\infty\sqrt{\frac{u_\infty}{\nu x}}\frac{d^2 f}{d\eta^2}\bigg|_{\eta=0}$$

so

$$\boxed{\tau_s = 0.332 u_\infty\sqrt{\frac{\rho\mu u_\infty}{x}} = \frac{0.664\rho u_\infty^2}{2\sqrt{Re_x}}}$$

  - Note that the unit of shear stress is $\mathrm{N/m^2}$ or, equivalently, $\dfrac{\mathrm{kg}}{\mathrm{m}\cdot\mathrm{s}^2}$

- At the boundary layer (i.e. $\eta = 5$), the local friction coefficient is

$$\boxed{C_{f,x} = \frac{2\tau_{s,x}}{\rho u_\infty^2} = \frac{0.664}{\sqrt{Re_x}}}$$

### 3.1.3 Heat Transfer Solution (Laminar)

- The energy equation in the boundary layer without viscous dissipation can be rewritten as the following when the dimensionless temperature is introduced and a similarity solution of the form $T^* = T^*(\eta)$ is assumed:

$$\frac{d^2 T^*}{d\eta^2} + \frac{Pr}{2}f\frac{dT^*}{d\eta} = 0$$

with boundary conditions of $T^*(0) = 0$ and $T^*(\infty) = 1$

- For $Pr > 0.6$, the surface temperature gradient is given as

$$\frac{dT^*}{d\eta}\bigg|_{\eta=0} = 0.332 Pr^{1/3}$$

- The local convection coefficient can be expressed as

$$h_x = \frac{q_s}{T_s - T_\infty} = \frac{-(T_\infty - T_s)}{T_s - T_\infty}k\frac{\partial T^*}{\partial y}\bigg|_{y=0} = k\left(\frac{u_\infty}{\nu x}\right)^{1/2}\frac{dT^*}{d\eta}\bigg|_{\eta=0}$$

- From this, we can state that (for $Pr > 0.6$)

$$\boxed{Nu_x = \frac{h_x x}{k} = 0.332 Re_x^{1/2} Pr^{1/3}}$$

which means that

$$\boxed{\frac{\delta_v}{\delta_t} = Pr^{1/3}}$$

### 3.1.4   Average Boundary Layer Parameters (Laminar)

- The average boundary layer parameters are

$$\bar{C}_{f,x} = \frac{1.328}{\sqrt{Re_x}}$$

and

$$\overline{Nu_x} = \frac{\bar{h}_x x}{k} = 0.664 Re_x^{1/2} Pr^{1/3}$$

for $Pr > 0.6$ since

$$\bar{h}_x = 2h_x$$

### 3.1.5   Turbulent Flow

- The equations for turbulent flow over a flat plate, the local friction coefficient is approximately

$$C_{f,x} = 0.0592 Re_x^{-1.5}$$

for Reynolds numbers between $R_{x,c} \approx 5 \times 10^5$ and $10^8$

- Also, the velocity boundary layer thickness is

$$\boxed{\delta = 0.37 x Re_x^{-1/5}}$$

- The local Nusselt number for a Prandtl number between 0.6 and 60 is

$$\boxed{Nu_x = 0.0296 Re_x^{4/5} Pr^{1/3}}$$

## 3.2   Cylindrical and Spherical Systems in Cross Flow

- At the leading edge ($\theta = 0$),

$$Nu_D = 1.15 Re_D^{1/2} Pr^{1/3}$$

- For a cylinder, Hilpert's relation states that

$$\boxed{\overline{Nu_D} = \frac{\bar{h} D}{k} = C Re_D^m Pr^{1/3}}$$

for $Pr > 0.7$

TABLE 7.2   Constants of Equation 7.52 for the circular cylinder in cross flow [11, 12]

| $Re_D$ | $C$ | $m$ |
|---|---|---|
| 0.4–4 | 0.989 | 0.330 |
| 4–40 | 0.911 | 0.385 |
| 40–4000 | 0.683 | 0.466 |
| 4000–40,000 | 0.193 | 0.618 |
| 40,000–400,000 | 0.027 | 0.805 |

- Note that the transition for cylindrical cross flow is $R_{x,c} \approx 2 \times 10^5$

- Technically, there is a more accurate equation for the average Nusselt number for cylindrical cross-flow given by the following expression,

$$\overline{Nu}_D = 0.3 + \frac{0.62 Re_D^{1/2} Pr^{1/3}}{\left[1 + \left(\frac{0.4}{Pr}\right)^{2/3}\right]^{1/4}} \left[1 + \left(\frac{Re_D}{282000}\right)^{5/8}\right]^{4/5}$$

that is valid for all $Re_D$ and $Pr > 0.2$

- For a sphere,

$$\boxed{\overline{Nu}_D = 2 + 0.6 Re_D^{1/2} Pr^{1/3}}$$

- Technically, there is a more accurate equation for the average Nusselt number for spherical cross-flow given by,

$$\overline{Nu}_D = 2 + \left(0.4 Re_D^{1/2} + 0.06 Re_D^{2/3}\right) Pr^{0.4} \left(\frac{\mu_\infty}{\mu_s}\right)^{1/4}$$

where all properties except $\mu_s$ are evaluated at $T_\infty$ and is applicable for $0.71 < Pr < 380$, $3.5 < Re_D < 7.6 \times 10^4$, and $1 < \frac{\mu}{\mu_s} < 3.2$

## 3.3 Potential Flow

- There really isn't much to say here. See my Transport Phenomena I review packet for a detailed description of potential flow

- The stream functions are defined as

$$u = -\frac{\partial \psi}{\partial y}$$

and

$$v = \frac{\partial \psi}{\partial x}$$

- As streamlines are more compact closer to the sphere or cylinder in potential flow, it means the velocity of the fluid is increasing

## 3.4 Sphere in a Water Bath

Problem: Consider a hot sphere in a cold bath such that it is quiescent (i.e. no flow - only conduction) and is at steady state

- Always start with boundary conditions. They are, for $T(r)$:

$$T(\infty) = T_\infty$$

$$T(R) = T_R$$

- There are two ways to approach this (both will yield the same answer). We can try a differential approach (as opposed to a microscopic energy balance) where

$$4\pi r^2 q_r \big|_{r=r} - 4\pi r^2 q_r \big|_{r=r+\Delta r} = 0$$

such that it reads "conduction in minus conduction out equals zero." Note that it is area times flux in minus area times flux out. The area here is $4\pi r^2$ for a sphere

- This expression can be rewritten by dividing through $4\pi$ and dividing by $dr$ such that

$$\frac{d}{dr}\left(r^2 q_r\right) = 0$$

- Using Fourier's Law,

$$\frac{d}{dr}\left(r^2 \frac{dT}{dr}\right) = 0$$

  once constants (i.e. $-k$) are factored out

  - Note that this equation could also have been obtained using the spherical equation of the microscopic energy balance such that

  $$\nabla^2 T = 0 \rightarrow \frac{1}{r^2}\frac{d}{dr}\left(r^2 \frac{dT}{dr}\right) = 0 \rightarrow \frac{d}{dr}\left(r^2 \frac{dT}{dr}\right) = 0$$

- Anyhow, we can integrate the above expression twice to yield

$$T = -\frac{C_1}{r} + C_2$$

  which turns to the following when boundary conditions are applied:

  $$T = \frac{R}{r}(T_R - T_\infty) + T_\infty \rightarrow \frac{T - T_\infty}{T_R - T_\infty} = \frac{R}{r}$$

- The radial flux from the sphere surface can be found by

$$q_r|_{r=R} = -k\frac{dT}{dr}\bigg|_{r=R} = \frac{k(T_R - T_\infty)}{R}$$

- We know that Newton's law of cooling applies at the solid-liquid interface, so

$$\frac{k(T_R - T_\infty)}{R} = h(T_R - T_\infty) \rightarrow h = \frac{k}{R} = \frac{2k}{D}$$

- Recall that the Nusselt number is defined as $Nu = \dfrac{hD}{k}$, so

$$Nu = 2$$

  for solely conduction in a sphere

# 4 Tube Flows

## 4.1 Area Average Quantities

- An area average quantity is defined as

$$\langle f \rangle = \frac{\iint f \, dA}{\iint dA}$$

- For the area average shear stress around a sphere,

$$\langle \tau \rangle = \frac{\iint \tau(r, z) \, r \, dr \, d\theta}{\int_0^{2\pi}\int_0^r r \, dr \, d\theta}$$

- The mixing cup temperature is defined as

$$T_{mc} = \frac{\langle v_z \cdot T \rangle}{\langle v_z \rangle}$$

- At a constant heat flux,

$$\frac{\partial T(r, z)}{\partial z} = \frac{dT_{mc}}{dz}$$

  where both quantities are for fully developed thermal regions and laminar flow in a tube. Therefore, the axial temperature gradient is independent of the radial location

## 4.2  Laminar Flow in Circular Tubes

### 4.2.1  Heat Flow

- The log-mean temperature difference is defined as

$$\Delta T_{lm} \equiv \frac{\Delta T_o - \Delta T_i}{\ln\left(\dfrac{\Delta T_o}{\Delta T_i}\right)}$$

  where the subscript $i$ represents the fluid flow through the tube, and the subscript $o$ represents fluid flow over the tube

- For internal flow in a circular cylinder,

$$Q = h\pi DL\Delta T_{lm}$$

- From Transport Phenomena I, we know that for laminar flow in a circular tube, $v_{z,max} = 2v_{z,mean}$ and

$$v_z = \frac{(\mathscr{P}_0 - \mathscr{P}_L)\,R^2}{4\mu L}\left[1 - \left(\frac{r}{R}\right)^2\right]$$

- It will simply be stated that

$$\boxed{Nu_D = \frac{hD}{k} = 4.36}$$

  for laminar flow in a circular tube with constant surface heat flux

- To see how the local Nusselt number changes with different conditions, consult Figure 14.2-1 in Bird, which shows a plot of $Nu_{loc}$ vs. $\dfrac{\alpha z}{\langle v_z\rangle D^2}$

# 5  Diffusivity and the Mechanisms of Mass Transport

## 5.1  Kinetic Theory and Lennard-Jones Potential

- The Kinetic Theory of Gases makes the assumption that all atoms are "hard spheres" that collide elastically and there are no intermoelcular forces. From this:

  - The mean free path is given as

$$\boxed{\lambda = \frac{1}{\sqrt{2}\pi d^2 n}}$$

    where $d$ is the diameter and $n$ is the number density

  - The mean molecular speed is

$$\boxed{\bar{u} = \sqrt{\frac{8k_B T}{\pi m}}}$$

    where $k_B$ is Boltzmann's constant (i.e. $1.38 \times 10^{-23}$ m$^2 \cdot$ kg $\cdot$ s$^{-2} \cdot$ K$^{-1}$, or, equivalently, $1.38 \times 10^{-23}$ J/K)

  - The collision frequency is

$$Z = \frac{1}{4}n\bar{u}$$

  - The dynamic viscosity is

$$\boxed{\mu = \frac{1}{3}nm\bar{u}\lambda = \frac{1}{3}\rho\bar{u}\lambda = \frac{2}{3\pi}\frac{\sqrt{\pi m k_B T}}{\pi d^2}}$$

– The thermal conductivity is given as

$$k = \frac{1}{2} n k_B \bar{u} \lambda = \frac{\sqrt{m k_B T / \pi}}{\pi d^2}$$

and has units of K/m

- The Lennard-Jones potential states that that

$$\phi(r) = 4\varepsilon \left[ \left( \frac{\sigma}{r} \right)^{12} - \left( \frac{\sigma}{r} \right)^{6} \right]$$

where $\phi(r)$ is the potential energy, $\sigma$ is the characteristic diameter of the molecules, and $\varepsilon$ is the maximum energy of attraction between a pair of molecules

– The values for $\sigma$ are tabulated in Table E.1 of BSL

- The viscosity of a pure monatomic gas may be written as

$$\mu = \frac{5}{16} \frac{\sqrt{\pi m k_B T}}{\pi \sigma^2 \Omega_\mu} = 2.6693 \times 10^{-5} \frac{\sqrt{MT}}{\sigma^2 \Omega_\mu}$$

where the second equation has $\sigma$ with units of angstrom, $T$ with units of Kelvins, $M$ is the molecular weight (unitless), and $\mu$ with units of g/cm$\cdot$s

– $\Omega_\mu$ is called the collision integral for viscosity and is tabulated in Table E.2 of BSL

- The thermal conductivity using Lennard-Jones parameters is

$$k = \frac{1.989 \times 10^{-4} \sqrt{\dfrac{T}{M}}}{\sigma^2 \Omega_\mu}$$

## 5.2   Fick's Law of Binary Diffusion (Molecular Mass Transport)

- If we define $w_i$ has the mass flow of substance $i$, $\omega_i$ as the mass fraction of substance $i$, $\mathscr{D}_{ij}$ as the diffusivity of $i$ in $j$,

$$\frac{w_i}{A} = \rho \mathscr{D}_{ij} \frac{\Delta \omega_i}{L}$$

where $\dfrac{w_i}{A}$ is the mass flux of substance $i$

– The units of $\mathscr{D}_{ij}$ are length-squared per unit time
– It is also important to recall that

$$\sum_i \omega_i = 1$$

- This can be rewritten as

$$\overrightarrow{j}_i = -\rho \mathscr{D}_{ij} \nabla \omega_i$$

where $j_i$ is the mass flux of substance $i$. This is Fick's Law.

– The mass flux is defined as $j_i \equiv \rho \omega_i \Delta v_i$

– The mass flux is measured with respect to the motion of the center of mass, so

$$\sum_i j_i = 0$$

• In general, for a mixture,

$$v = \sum_i \omega_i v_i$$

which translates to "the velocity is equal to the sum of the mass fraction of each substance times its respective velocity"

• The Schmidt number is defined as

$$\text{Sc} = \frac{\nu}{\mathscr{D}_{ij}}$$

• The Lewis number is defined as

$$\text{Le} = \frac{\alpha}{\mathscr{D}_{ij}}$$

• Also, recall that the ideal gas law states

$$\rho = \frac{MP}{RT}$$

and

$$\boxed{c = \frac{P}{RT}}$$

where $c$ is a molar density defined as $c \equiv \dfrac{\rho}{M}$

• The mass fraction is most frequently written as

$$\boxed{\omega_i = \frac{\rho_i}{\rho}}$$

when volume is constant

– In addition,

$$c = \frac{\rho\omega}{M}$$

• The mole fraction is most frequently written as

$$x_i = \frac{c_i}{c}$$

when volume is constant

## 5.3  Temperature and Pressure Dependence of Diffusivities

• For a binary-gas mixture at low pressure,

$$\boxed{\frac{P\mathscr{D}_{AB}}{(P_{cA}P_{cB})^{1/3}\,(T_{cA}T_{cB})^{5/12}\left(\dfrac{1}{M_A} + \dfrac{1}{M_B}\right)^{1/2}} = a\left(\frac{T}{\sqrt{T_{cA}T_{cB}}}\right)^b}$$

where the subscript $c$ represents a critical property, which can be obtained from Table E1 in BSL. In this equation, $\mathscr{D}_{AB}$ has units of cm$^2$/s, $P$ has units of atm, and $T$ has units of K

– For a non-polar gas pair, $a = 2.745 \times 10^{-4}$ and $b = 1.823$ (excluding helium and hydrogen)

- For a non-polar gas and water, $a = 3.640 \times 10^{-4}$ and $b = 2.334$

- Interdiffusion is synonymous with self-diffusion and is denoted by $\mathscr{D}_{AA^*}$

  - Using reduced temperatures and pressures, one can find the reduced self-diffusivity from Figure 17.2-1 in BSL if $c\mathscr{D}_{AA^*}$ is given at a specific temperature and pressure. Recall that

    $$\text{Reduced quantity} = \frac{\text{Regular quantity}}{\text{Critical Quantity}}$$

    * To implement this method, realize that the $(c\mathscr{D}_{AA^*})_r$ is constant for a given system even if temperature and pressure changes. Therefore, if you are given $c\mathscr{D}_{AA^*}$ at one temperature and pressure and want it at another temperature and pressure, use Figure 17.2-1 to find the critical diffusivity, and then use this value at the new reduced pressure and temperature to find the new (not critical) diffusivity

  - Another way to find the self-diffusivity is to use the equation

    $$\boxed{(c\mathscr{D}_{AB})_c = 2.96 \times 10^{-6} \left( \frac{1}{M_A} + \frac{1}{M_B} \right)^{1/2} \frac{P_{cA}^{2/3}}{T_{cA}^{1/6}}}$$

    where $c$ is a concentration given in mol/cm$^3$

- For a binary-gas mixture at high density and low pressure, one can use Figure 17.2-1 by replacing the above formula with

  $$\boxed{(c\mathscr{D}_{AB})_c = 2.96 \times 10^{-6} \left( \frac{1}{M_A} + \frac{1}{M_B} \right)^{1/2} \frac{(P_{cA}P_{cB})^{1/3}}{(T_{cA}T_{cB})^{1/12}}}$$

## 5.4 Theory of Diffusion in Gases at Low Density

- The kinetic theory of gases states that, for rigid spheres,

  $$\boxed{\mathscr{D}_{AB} = \frac{2}{3} \sqrt{\frac{k_B T}{\pi}} \sqrt{\frac{1}{2} \left( \frac{1}{m_A} + \frac{1}{m_B} \right)} \frac{1}{\pi \left( \frac{(d_A + d_B)}{2} \right)^2 n}}$$

- With the use of Lennard-Jones constants, the above equation can be rearranged to

  $$\boxed{c\mathscr{D}_{AB} = 2.2646 \times 10^{-5} \sqrt{T \left( \frac{1}{M_A} + \frac{1}{M_B} \right)} \frac{1}{\sigma_{AB}^2 \Omega_{\mathscr{D},AB}}}$$

  - If the ideal gas law is assumed,

    $$\boxed{\mathscr{D}_{AB} = 0.0018583 \sqrt{T^3 \left( \frac{1}{M_A} + \frac{1}{M_B} \right)} \frac{1}{P\sigma_{AB}^2 \Omega_{\mathscr{D},AB}}}$$

    where the variables are in the conventional units previously described. The values for the collision integral for diffusivity can be found in Tables E1 and E2 of BSL

- If not given, the values for $\sigma_{AB}$ and $\varepsilon_{AB}$ can be given by (for nonpolar gas pairs)

  $$\boxed{\sigma_{AB} = \frac{\sigma_A + \sigma_B}{2}}$$

  and

  $$\boxed{\varepsilon_{AB} = \sqrt{\varepsilon_A \varepsilon_B}}$$

## 5.5 Mass Average and Molar Average Velocity

- When we state $v_i$, or the velocity of species $i$, this is not the velocity of an individual molecule of $i$. Instead, it is the mean of all the velocities of molecules of species $i$. In essence,

$$\overrightarrow{v} = \frac{\sum_{i=1}^{N} \rho_i \overrightarrow{v}_i}{\sum_{i=1}^{N} \rho_i} = \sum_{i=1}^{N} \omega_i \overrightarrow{v}_i$$

  is the mass average velocity

- The molar average velocity is given as

$$\overrightarrow{v^*} = \frac{\sum_{i=1}^{N} c_i \overrightarrow{v}_i}{\sum_{i=1}^{N} c_i} = \sum_{i=1}^{N} x_i \overrightarrow{v}_i$$

## 5.6 Summary of Mass and Molar Fluxes

- As stated earlier, Fick's Law states that the mass flux is

$$\overrightarrow{j}_A = -\rho \mathscr{D}_{AB} \nabla \omega_A$$

- This can be stated as

$$\overrightarrow{J_A^*} = -c \mathscr{D}_{AB} \nabla x_A$$

  where this is now the mole flux

- The combined mass flux for one species is

$$\overrightarrow{n_A} = \overrightarrow{j_A} + \rho_A \overrightarrow{v}$$

- The combined molar flux for one species is

$$\overrightarrow{N_A} = \overrightarrow{J_A^*} + c_A \overrightarrow{v^*}$$

- The mass flux for $N$ species is

$$\overrightarrow{j_A} = \overrightarrow{n_A} - \omega_A \sum_{i=1}^{N} \overrightarrow{n_i}$$

- The molar flux for $N$ species is

$$\overrightarrow{J_A^*} = \overrightarrow{N_A} - x_A \sum_{i=1}^{N} \overrightarrow{N_i}$$

- For a binary system with one-dimensional diffusion,

$$N_{A,z} = -c \mathscr{D}_{AB} \frac{\partial x_A}{\partial z} + x_A \left( N_{A,z} + N_{B,z} \right)$$

# 6 Concentration Distributions in Solids and in Laminar Flows

## 6.1 Shell Mass Balances and Boundary Conditions

- The molar flux can be related to the concentration gradient by

$$\boxed{N_A = -c \mathscr{D}_{AB} \nabla x_A + x_A \left( N_A + N_B \right)}$$

  − Note that $\nabla$ is acting as a gradient here since $x_A$ is a scalar

- For small $x_A$, the right-hand term drops out, and implementing

$$x_a = \frac{c_A}{c}$$

  yields

$$N_A = -\mathscr{D}_{AB}\nabla c_A$$

  when $x_A$ is small. This is frequently encountered at surfaces.

- In words, the shell mass balance states "rate of mass of $A$ in minus rate of mass of $A$ out plus rate of production of mass of $A$ by homogeneous reaction equals zero"

- The boundary conditions include:

  - The concentration at a surface can be specified (e.g. $x_A = x_{A0}$)
  - The mass flux at a surface can be specifies (e.g. $N_A = N_{A0}$)
  - If diffusion occurs in a solid, $N_{A0} = k_c\,(c_{A0} - c_{Ab})$ may apply, where $N_{A0}$ is the molar flux at the surface, $c_{A0}$ is the surface concentration, $c_{Ab}$ is the concentration in the bulk fluid stream, and $k_c$ is the mass transfer coefficient
  - The rate of chemical reaction at a surface can be specified. For an $n$-th order reaction, $N_{A0} = k_c c_{A0}^n$ may apply

## 6.2 Diffusion Through a Stagnant Gas Film

Problem: Consider the schematic shown below. Note that $B$ is immiscible with $A$, so while $B$ can be present in the system at steady state, there is no net flux of $B$ down or out, just across such that $N_{B.z} = 0$. For the full description of the problem, see Section 18.2 of BSL.
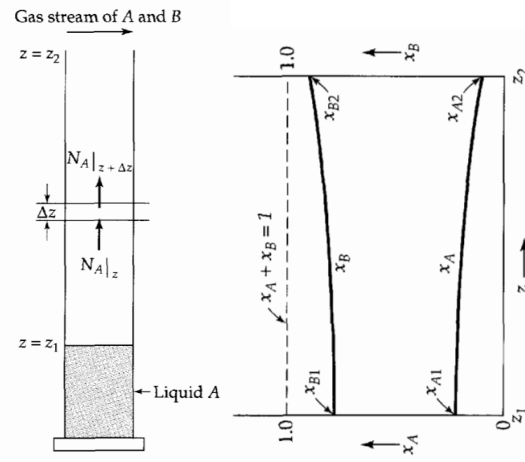


1. We write the mass balance in the $z$ direction as

$$N_{A,z} = -c\mathscr{D}_{AB}\frac{dx_A}{dz} + x_A N_{A,z}$$

2. Solving for $N_{A,z}$ yields

$$N_{A,z} = \frac{-c\mathscr{D}_{AB}}{1 - x_A}\frac{dx_A}{dz}$$

3. A steady-state mass balance can be written as

$$SN_{A,z}|_z - SN_{A,z}|_{z+\Delta z} = 0$$

  where $S$ is a cross-sectional area

4. Dividing by $S\Delta z$ and letting $\Delta z \to 0$ yields

$$\frac{-dN_{Az}}{dz} = 0$$

5. This can therefore be written as

$$\frac{d}{dz}\left(\frac{c\mathscr{D}_{AB}}{1 - x_A}\frac{dx_A}{dz}\right) = 0$$

   (a) For an ideal gas mixture, $c$ is constant for a constant $T$ and $P$. Also, for gases, $\mathscr{D}_{AB}$ is usually independent of the composition such that

$$\frac{d}{dz}\left(\frac{1}{1 - x_A}\frac{dx_A}{dz}\right) = 0$$

   which can be integrated to yield[6]

$$-\ln\left(1 - x_A\right) = C_1 z + C_2$$

6. Although this is not obvious, we can let $C_1 = -\ln K_1$ and $C_2 = -\ln K_2$ such that[7]

$$1 - x_A = K_1^z K_2$$

7. The boundary conditions are: $x_A(z_1) = x_{A1}$ and $x_A(z_2) = x_{A2}$

8. Applying the boundary conditions yields $1 - x_{A1} = K_1^{z_1} K_2$ and $1 - x_{A2} = K_1^{z_2} K_2$, which can be combined to yield

$$\frac{1 - x_{A2}}{1 - x_{A1}} = K_1^{z_2 - z_1}$$

   (a) A little algebraic manipulation yields

$$K_1 = \left(\frac{1 - x_{A2}}{1 - x_{A1}}\right)^{1/(z_2 - z_1)}$$

   (b) We need an expression for $K_2$, so

$$1 - x_{A1} = \left(\frac{1 - x_{A2}}{1 - x_{A1}}\right)^{z_1/(z_2 - z_1)} K_2 \to K_2 = (1 - x_{A1})\left(\frac{1 - x_{A2}}{1 - x_{A1}}\right)^{-z_1/(z_2 - z_1)}$$

9. Plugging in the results for $K_1$ and $K_2$ yields

$$1 - x_A = \left(\frac{1 - x_{A2}}{1 - x_{A1}}\right)^{z/(z_2 - z_1)} (1 - x_{A1})\left(\frac{1 - x_{A2}}{1 - x_{A1}}\right)^{-z_1/(z_2 - z_1)}$$

   which can be rearranged to

$$\frac{1 - x_A}{1 - x_{A1}} = \left(\frac{1 - x_{A2}}{1 - x_{A1}}\right)^{(z - z_1)/(z_2 - z_1)}$$

10. To obtain the profile for $x_B$, recognize that $x_A + x_B \equiv 1$

---

[6]Note that a useful integral for these types of problems is $\int \dfrac{1}{ax + b}\, dx = \dfrac{1}{a}\ln|ax + b|$

[7]Generally speaking, for an equation of the form $a\ln\left(1 + bx_A\right) = C_1 z + C_2$, you want to make $C_1 = a\ln K_1$ and $C_2 = a\ln K_2$. From this, the final equation will be of the form $1 + bx_A = K_1^z K_2$.

11. Now, if the average concentration of $B$ is desired,

$$\overline{x}_B = \frac{\int_{z_1}^{z_2} x_B \, dz}{\int_{z_1}^{z_2} dz}$$

so

$$\frac{\overline{x}_B}{x_{B1}} = \frac{\int_{z_1}^{z_2} \left(\frac{x_B}{x_{B1}}\right) dz}{\int_{z_1}^{z_2} dz}$$

12. Define the non-dimensional height variable $\xi = \dfrac{z - z_1}{z_2 - z_1}$, such that $dz = (z_2 - z_1) \, d\xi$ and

$$\frac{\overline{x}_B}{x_{B1}} = \frac{\int_0^1 \left(\frac{x_B}{x_{B1}}\right)^{\xi} d\xi}{\int_0^1 d\xi}$$

13. The integral table states that $\int a^x \, dx = \dfrac{a^x}{\ln x}$, so

$$\frac{\overline{x}_B}{x_{B1}} = \frac{\left(\frac{x_{B2}}{x_{B1}}\right)^{\xi}}{\ln \left(\frac{x_{B2}}{x_{B1}}\right)} \Bigg|_0^1$$

which yields

$$\overline{x}_B = \frac{x_{B2} - x_{B1}}{\ln \left(\dfrac{x_{B2}}{x_{B1}}\right)} \equiv (x_B)_{\ln}$$

14. The rate of evaporation is the rate of mass transfer at the liquid-gas interface and can be found by calculating $N_{A,z}$ at $z = z_1$. Therefore,

$$N_{A,z}\big|_{z_1} = -\frac{c \mathscr{D}_{AB}}{1 - x_{A1}} \frac{dx_A}{dz}\bigg|_{z_1} = \frac{c \mathscr{D}_{AB}}{x_{B1}} \frac{dx_B}{dz}\bigg|_{z_1}$$

    (a) Implementing the dimensionless length,

$$\frac{c \mathscr{D}_{AB}}{x_{B1}} \frac{dx_B}{d\xi}\bigg|_{\xi=0} \frac{d\xi}{dz} = \frac{c \mathscr{D}_{AB}}{z_2 - z_1} \frac{d \left(x_B/x_{B1}\right)^{\xi}}{d\xi}\bigg|_{\xi=0}$$

15. The final expression is

$$N_{A,z}\big|_{z_1} = \frac{c \mathscr{D}_{AB}}{z_2 - z_1} \ln \left(\frac{x_{B2}}{x_{B1}}\right) = \frac{c \mathscr{D}_{AB}}{(z_2 - z_1)(x_B)_{\ln}} (x_{A1} - x_{A2})$$

    (a) This expression can be used to find the diffusivity constant of an evaporating substance

16. For diffusion with a moving interface, see Example 18.2-1 in BSL

## 6.3    Diffusion through a Spherical Film

Problem: Consider diffusion through a spherical shell with radii $r_1$ and $r_2$ where $r_1 < r < r_2$. For the full problem statement, see Example 18.2-3.

1. The shell balance states that in the $r$ direction states that

$$N_A 4\pi r^2\big|_r - N_A 4\pi r^2\big|_{r+\Delta r} = 0$$

which can be rewritten as

$$\frac{d}{dr}\left(r^2 N_A\right) = 0$$

2. We can state that $N_{B,r} = 0$ since $B$ is insoluble in $A$. Therefore,

$$N_{A,r} = -c\mathscr{D}_{AB}\frac{dx_A}{dr} + x_A N_{A,r}$$

which can be solved for $N_{A,r}$ as

$$N_{A,r} = -\frac{c\mathscr{D}_{AB}}{1-x_A}\frac{dx_A}{dr}$$

3. Therefore,

$$\frac{d}{dr}\left(r^2 \frac{c\mathscr{D}_{AB}}{1-x_A}\frac{dx_A}{dr}\right) = 0$$

4. Integrating this yields

$$-\ln\left(1 - x_A\right) = \frac{C_1}{r} + C_2$$

5. Let $C_1 = -\ln K_1$ and $C_2 = -\ln K_2$ such that

$$1 - x_A = K_1^{1/r} K_2$$

6. As in the previous subsection, this comes out to

$$\frac{1 - x_A}{1 - x_{A1}} = \left(\frac{1 - x_{A2}}{1 - x_{A1}}\right)^{(1/r_1 - 1/r)/(1/r_1 - 1/r_2)}$$

when the boundary conditions are applied

7. The molar flow can be found as

$$W_A = 4\pi r_1^2 N_{A,r}\big|_{r_1} = \frac{4\pi c\mathscr{D}_{AB}}{\frac{1}{r_1} - \frac{1}{r_2}}\ln\left(\frac{1 - x_{A2}}{1 - x_{A1}}\right)$$

which is applicable for any spherical surface of radius $r$ between $r_1$ and $r_2$

## 6.4 Diffusion with a Heterogeneous Chemical Reaction (e.g. Gas Reacting on Solid Catalyst)

### 6.4.1 Diffusion with an Instantaneous Heterogeneous Reaction

Problem: Consider the heterogeneous chemical reaction of $2A \to B$ shown in the diagram below. For the full problem statement, see Section 18.3 in BSL.
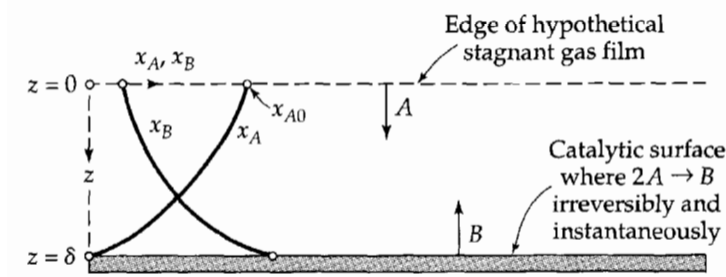


1. From the stoichiometry, we know that[8]

$$N_{B,z} = -\frac{1}{2}N_{A,z}$$

2. We also know that

$$N_{A,z} = -c\mathscr{D}_{AB} + x_A\left(N_{A,z} - \frac{1}{2}N_{A,z}\right)$$

   which simplifies to

$$N_{A,z} = -\frac{c\mathscr{D}_{AB}}{1 - \frac{1}{2}x_A}\frac{dx_A}{dz}$$

3. The shell mass balance states that

$$SN_{A,z}\big|_z - SN_{A,z}\big|_{z+\Delta z} = 0$$

   which leads to

$$\frac{dN_{A,z}}{dz} = 0$$

4. This yields

$$\frac{d}{dz}\left(\frac{c\mathscr{D}_{AB}}{1 - \frac{1}{2}x_A}\frac{dx_A}{dz}\right) = 0$$

5. Integrating this yields

$$-2\ln\left(1 - \frac{1}{2}x_A\right) = C_1 z + C_2$$

   for constant $c\mathscr{D}_{AB}$

6. Substituting $C_1 = -2\ln K_1$ and $C_2 = -2\ln K_2$ yields

$$1 - \frac{x_A}{2} = K_1^z K_2$$

7. The boundary conditions are $x_A(0) = x_{A0}$ and $x_A(\delta) = 0$

---

[8]For a reaction $aA \to bB$, $N_{B,z} = -\dfrac{b}{a}N_{A,z}$

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8. Applying the boundary conditions yields

$$1 - \frac{1}{2}x_A = \left(1 - \frac{1}{2}x_{A0}\right)^{1-z/\delta}$$

9. To get the molar flux, we need $\dfrac{dx_A}{dz}$. Since we want the molar flux at the film, and the film is at $z = 0$, we technically want $\dfrac{dx_A}{dz}\bigg|_{z=0}$. The final result yields[9] so'

$$N_{A,z} = \frac{2c\mathscr{D}_{AB}}{\delta} \ln \left(\frac{1}{1 - \frac{1}{2}x_{A0}}\right)$$

### 6.4.2 Diffusion with a Slow Heterogeneous Reaction

Problem: Attempt the previous problem with a slow reaction (i.e. not instantaneous). Assume that the rate $A$ disappears at the catalyst surface is given as $N_{A,z} = k_1'' c_A = k_1'' c x_A$, in which $k_1''$ is a rate constant for the pseudo-first-order surface reaction. For the full problem statement, see Example 18.3-1 in BSL.

1. The set-up is identical up until the boundary conditions at which point $x_A(\delta) = \dfrac{N_{A,z}}{k_1'' c}$ instead of $x_A(\delta) = 0$

2. Applying the boundary conditions yields

$$\left(1 - \frac{1}{2}x_A\right) = \left(1 - \frac{1}{2}\frac{N_{A,z}}{k_1'' c}\right)^{z/\delta} \left(1 - \frac{1}{2}x_{A0}\right)^{1-z/\delta}$$

3. Evaluating $\dfrac{dx_A}{dz}\bigg|_{z=0}$ and solving for $N_{A,z}$ yields,

$$N_{A,z} = \frac{2c\mathscr{D}_{AB}}{\delta} \ln \left(\frac{1 - \frac{1}{2}\left(\frac{N_{A,z}}{k_1'' c}\right)}{1 - \frac{1}{2}x_{A0}}\right)$$

4. If $k_1''$ is large (note that this means the reaction is fast, but not so fast that it is instantaneous) then

$$N_{A,z} = \frac{2c\mathscr{D}_{AB}/\delta}{1 + \frac{\mathscr{D}_{AB}}{k_1'' \delta}} \ln \left(\frac{1}{1 - \frac{1}{2}x_{A0}}\right)$$

   which can be obtained by a Taylor expansion on the logarithm term and keeping just the first term such that $\ln(1 + p) \approx p$ for small $p$

5. The Damkohler Number of the second order can be defined as

$$\mathrm{Da}^{\mathrm{II}} = \frac{k_1'' \delta}{\mathscr{D}_{AB}}$$

   (a) In the limit of $\mathrm{Da}^{\mathrm{II}} \to \infty$, we obtain the expression for the instantaneous reaction
   (b) In words, the Damkohler number is the ratio of the chemical reaction rate compared to the diffusion rate (i.e. mass transfer)
   (c) A very fast reaction is governed by mass transfer, but a very slow reaction is governed by kinetics

---

[9]The following is a helpful identity: $\dfrac{d}{dx}\left(a^{bx}\right) = ba^{bx}\ln(a)$

## 6.5 Diffusion with a Homogeneous Chemical Reaction (e.g. Gas Dissolving in Liquid)

Problem: Consider a gas $A$ diffusing into a liquid $B$. As it diffuses, the reaction $A + B \rightarrow AB$ occurs. You can ignore the small amount of $AB$ that is present (this is the pseudobinary assumption).
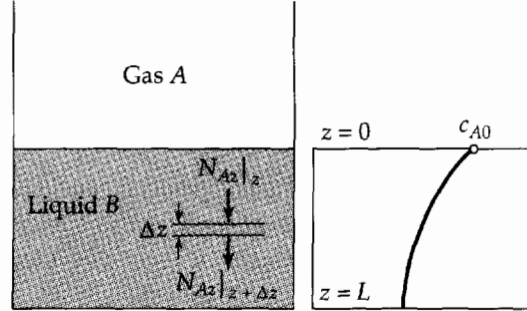


1. Note that the reaction rate can be given as $k_1''' c_A$ if we assume pseudo-first order. This makes the shell mass balance

$$SN_{A,z}|_z - SN_{A,z}|_{z+\Delta z} - k_1''' c_A S \Delta z = 0$$

2. This can be rewritten as

$$\frac{dN_{A,z}}{dz} + k_1''' c_A = 0$$

3. If the concentration of $A$ is small (i.e. dilute), then we can state that $x_A$ goes to zero in

$$N_{A,z} = -c \mathscr{D}_{AB} \frac{dx_A}{dz} + x_A (N_{A,z} + N_{B,z})$$

such that

$$N_{A,z} = -\mathscr{D}_{AB} \frac{dc_A}{dz}$$

4. Combining this with the equation in step 2 yields

$$\mathscr{D}_{AB} \frac{d^2 c_A}{dz^2} - k_1''' c_A = 0$$

5. The boundary conditions are $c_A(0) = c_{A0}$ and $N_{A,z}(L) = \left.\frac{dc_A}{dz}\right|_L = 0$. The first boundary condition states that the concentration of $A$ at the surface is fixed. The second boundary condition states that no $A$ diffuses through the bottom of the container.

6. Multiply the equation in Step 4 by $\dfrac{L^2}{c_{A0} \mathscr{D}_{AB}}$ for later simplicity. This yields

$$\frac{L^2}{c_{A0}} \frac{d^2 c_A}{dz^2} - \frac{k_1''' c_A L^2}{c_{A0} \mathscr{D}_{AB}} = 0$$

7. Let's define the dimensionless variable known as the Thiele modulus:

$$\phi \equiv \sqrt{k_1''' L^2 / \mathscr{D}_{AB}}$$

8. Let's also define the dimensionless length

$$\xi \equiv \frac{z}{L}$$

such that

$$dz = L d\xi$$

9. The concentration ratio ca be defined as
$$\Gamma \equiv \frac{c_A}{c_{A0}}$$

10. Using these variables,
$$\frac{d^2\Gamma}{d\xi^2} - \phi^2\Gamma = 0$$

11. The general solution is given as
$$\Gamma = C_1 \cosh\left(\phi\xi\right) + C_2 \sinh\left(\phi\xi\right)$$

since
$$\cosh\left(p\right) \equiv \frac{e^p + e^{-p}}{2}$$

and
$$\sinh\left(p\right) \equiv \frac{e^p - e^{-p}}{2}$$

12. The boundary conditions are at $\xi = 0$, $c_A = c_{A0}$, so $\Gamma = 1$ and $\xi = 1$, $\frac{d\Gamma}{d\xi} = 0$. Applying boundary condition,
$$1 = C_1 \cosh\left(0\right) + C_2 \sinh\left(0\right) \rightarrow C_1 = 1$$

and
$$\frac{d\Gamma}{d\xi} = \phi \sinh\left(\phi\xi\right) + C_2\phi \cosh\left(\phi\xi\right)$$

and invoking the second boundary condition yields
$$0 = \phi \sinh\phi + C_2\phi \cosh\phi \rightarrow C_2 = -\tanh\phi$$

13. This yields
$$\Gamma = \cosh\left(\phi\xi\right) - \tanh\left(\phi\right)\sinh\left(\phi\xi\right)$$

which can be rearranged to[10]
$$\Gamma = \frac{\cosh\left(\phi\right)\cosh\left(\phi\xi\right) - \sinh\left(\phi\right)\sinh\left(\phi\xi\right)}{\cosh\left(\phi\right)} = \frac{\cosh\left[\phi\left(1-\xi\right)\right]}{\cosh\phi}$$

14. Reverting to the original notation yields,
$$\frac{c_A}{c_{A0}} = \frac{\cosh\left[\sqrt{k_1''' L^2/\mathscr{D}_{AB}}\left(1-\frac{z}{L}\right)\right]}{\cosh\left(\sqrt{k_1''' L^2/\mathscr{D}_{AB}}\right)}$$

15. The average concentration in the liquid phase can be given by
$$\frac{\bar{c}_A}{c_{A0}} = \frac{\int_0^L \frac{c_A}{c_{A0}}\, dz}{\int_0^L dz} = \frac{\tanh\phi}{\phi}$$

16. The molar flux at the surface is
$$N_{A,z}\big|_{z=0} = -\mathscr{D}_{AB}\frac{dc_A}{dz}\bigg|_{z=0} = \left(\frac{c_{A0}\mathscr{D}_{AB}}{L}\right)\phi\tanh\left(\phi\right)$$

---

[10]Note that $\cosh\left(x \pm y\right) = \cosh x \cosh y \pm \sinh x \sinh y$ and $\sinh\left(x \pm y\right) = \sinh x \cosh y \pm \cosh x \sinh y$

## 6.6 Gas Absorption with Chemical Reaction in Agitated Tank

Problem: Consider the diagram shown below. Assume that each gas bubble is surround by a stagnant liquid film of thickness $\delta$, which is small compared to the bubble diameter. Assume a quasi-steady concentration profile is quickly established in the liquid film after the bubble is formed. The gas $A$ is only sparingly soluble in the liquid, so we can neglect the convection term. The liquid outside the stagnant film is at concentration $c_{A\delta}$ and is constant. Even though this is a spherical bubble, it is a thin shell, so you can treat it as a slab. For the full problem statement, see Example 18.4-1 in BSL.
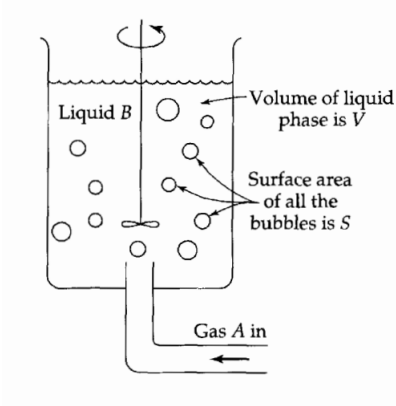


1. The setup is the same as before, but the boundary conditions are at $z = 0$, $\xi = 0$, $c_A = c_{A0}$, $\Gamma = 1$, and at $z = \delta$, $\xi = 1$, $c_A = c_{A\delta}$, $\Gamma = B$ if we state that $B = \dfrac{C_{A\delta}}{C_{A0}}$. Note that the dimensionless length should be redefined accordingly as $\xi = \dfrac{z}{\delta}$ and the Thiele modulus is redefined as $\phi = \sqrt{k_1''' \delta^2 / \mathscr{D}_{AB}}$

2. From the previous problem,
$$\Gamma = C_1 \cosh\left(\phi\xi\right) + C_2 \sinh\left(\phi\xi\right)$$

3. Applying boundary condition 1 yields
$$C_1 = 1$$

4. Applying boundary conditions 2 yields
$$C_2 = \frac{B - \cosh\phi}{\sinh\phi}$$

5. This means
$$\Gamma = \cosh\left(\phi\xi\right) + \frac{B - \cosh\phi}{\sinh\phi}\sinh\left(\phi\xi\right) = \frac{\sinh\phi\cosh\left(\phi\xi\right) + (B - \cosh\phi)\sinh\left(\phi\xi\right)}{\sinh\phi}$$

6. Now equate $A$ entering the liquid at $z = \delta$ to amount consumed in bulk:
$$-S\mathscr{D}_{AB}\frac{dc_A}{dz}\bigg|_{z=\delta} = Vk_1''' c_{A\delta}$$

7. We need the $\dfrac{dc_A}{dz}\bigg|_{z=\delta}$ term. This can be rewritten as
$$\frac{dc_A}{dz} = \frac{dc_A}{d\xi}\frac{d\xi}{dz} = \frac{dc_A}{d\xi}\frac{1}{\delta}$$

8. Therefore,

$$\frac{dc_A}{dz}\bigg|_{z=\delta} = \frac{c_{A0}}{\delta}\left(\frac{\phi\sinh^2\phi - \phi\cosh^2\phi + B\phi\cosh\phi}{\sinh\phi}\right)$$

using the identity $\cosh x^2 - \sinh x^2 = 1$ yields

$$\frac{dc_A}{dz}\bigg|_{z=\delta} = \frac{c_{A0}}{\delta}\left(\frac{B\phi\cosh\phi - \phi}{\sinh\phi}\right)$$

9. So,

$$-S\mathscr{D}_{AB}\frac{c_{A0}}{\delta}\left(\frac{B\phi\cosh\phi - \phi}{\sinh\phi}\right) = Vk_1'''c_{A\delta}$$

10. This can be solved for $B$ as

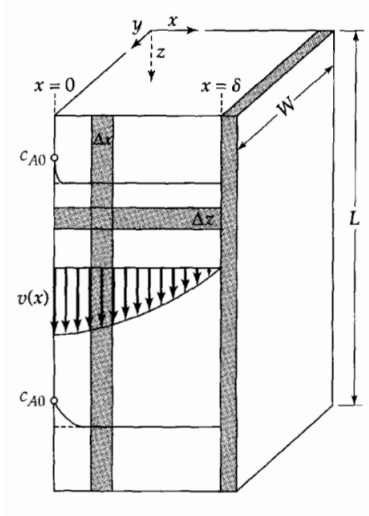$$B = \frac{1}{\cosh\phi + \dfrac{V}{S\delta}\phi\sinh\phi}$$

11. The total rate of absorption is

$$\check{N} \equiv \frac{N_{A,z}|_{z=0}\,\delta}{c_{A0}\mathscr{D}_{AB}} = \frac{\phi}{\sinh\phi}\left(\cosh\phi - \frac{1}{\cosh\phi + \frac{V}{S\delta}\phi\sinh\phi}\right)$$

which is plotted in Figure 18.4-4 of BSL

## 6.7 Diffusion into a Falling Liquid Film (Gas Absorption)

Problem: Consider the absorption of $A$ into a falling film of liquid $B$. For the full problem, see Section 18.5 in BSL.



1. The velocity profile is found from Transport I as

$$v_z(x) = v_{max}\left[1 - \left(\frac{x}{\delta}\right)^2\right]$$

2. The concentration will change in the $x$ and $z$ direction, so

$$N_{A,z}|_z\,W\Delta x - N_{A,z}|_{z+\Delta z}\,W\Delta x + N_{A,x}|_x\,W\Delta z - N_{A,x}|_{x+\Delta x}\,W\Delta z = 0$$

at steady state

3. This then yields
$$\frac{\partial N_{A,z}}{\partial z} + \frac{\partial N_{A,x}}{\partial x} = 0$$

4. We now want expressions for the molar mass flux:
$$N_{A,z} = -\mathscr{D}_{AB}\frac{\partial c_A}{\partial z} + x_A\left(N_{A,z} + N_{B,z}\right)$$

which reduces to the following because the transport of $A$ in the $z$ direction will be primarily by convection (not diffusion)
$$N_{A,z} = x_A\left(N_{A,z} + N_{B,z}\right) \approx c_A v_z\left(x\right)$$

and in the $x$ direction we have
$$N_{A,x} = -\mathscr{D}_{AB}\frac{\partial c_A}{\partial z}$$

since there is mostly diffusion in the $x$ direction (not convection)

5. Therefore,
$$v_z\frac{\partial c_A}{\partial z} = \mathscr{D}_{AB}\frac{\partial^2 c_A}{\partial x^2}$$

6. Inserting the velocity component yields
$$v_{z,max}\left[1 - \left(\frac{x}{\delta}\right)^2\right]\frac{\partial c_A}{\partial z} = \mathscr{D}_{AB}\frac{\partial^2 c_A}{\partial x^2}$$

7. The boundary conditions are: at $z = 0$, $c_A = 0$ and $x = 0, c_A = c_{A0}$ and $x = \delta$, $\dfrac{\partial c_A}{\partial x} = 0$ since there is pure $B$ at the top, the liquid-gas interface is determined by the solubility of $A$ in $B$, and $A$ can't diffuse through the wall

8. We shall use the limiting case of the Penetration Model, which states that there is only penetration in the outer layers of the film such that $v_z \approx v_{z,max}$. This means,
$$v_{z,max}\frac{\partial c_A}{\partial z} = \mathscr{D}_{AB}\frac{\partial^2 c_A}{\partial x^2}$$

and the third boundary condition is changed to at $x = \infty$, $c_A = 0$

9. This looks like a semi-infinite solid problem, so
$$\frac{c_A}{c_{A0}} = 1 - \mathrm{erf}\left(\frac{x}{\sqrt{4\mathscr{D}_{AB}z/v_{z,max}}}\right)$$

10. The local mass flux at the gas-liquid interface may be found by
$$N_{A,x}\big|_{x=0} = -\mathscr{D}_{AB}\frac{\partial c_A}{\partial x}\bigg|_{x=0} = c_{A0}\sqrt{\frac{\mathscr{D}_{AB}v_{max}}{\pi z}}$$

11. The total molar flow across the surface at $x = 0$ is
$$W_A = \int_0^W \int_0^L N_{A,x}\big|_{x=0}\, dz\, dy = WLc_{A0}\sqrt{\frac{4\mathscr{D}_{AB}v_{max}}{\pi L}}$$

## 6.8 Gas Absorption from Rising Bubbles

Problem: Estimate the rate at which gas bubbles of $A$ are absorbed by liquid $B$ as the gas bubbles rise at their terminal velocity, $v_t$, through a clean quiescent liquid. See Example 18.5-1 in BSL for more information.

- The molar absorption rate is

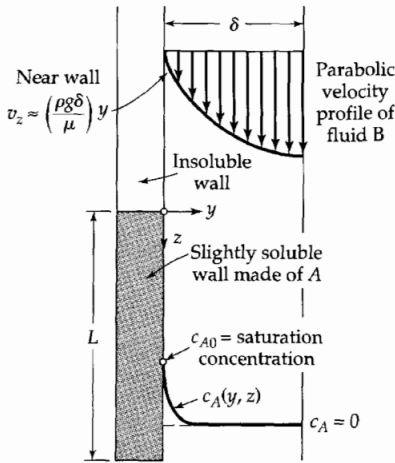$$(N_A)_{avg} = c_{A0}\sqrt{\frac{4\mathscr{D}_{AB}v_t}{\pi D}}$$

and is applicable for potential flow and for gas bubbles between 0.3 cm and 0.5 cm

- For creeping flow around the bubble,

$$(N_A)_{avg} = c_{A0}\sqrt{\frac{4\mathscr{D}_{AB}v_t}{3\pi D}}$$

## 6.9 Diffusion into a Falling Liquid Film (Solid Dissolution)

Problem: See Section 18.6 in BSL for the full problem statement.



1. The velocity profile can be obtained from Transport I as

$$v_z = \frac{\rho g \delta^2}{2\mu}\left[1 - \left(1 - \frac{y}{\delta}\right)^2\right] = \frac{\rho g \delta^2}{2\mu}\left[2\left(\frac{y}{\delta}\right)^2 - \left(\frac{y}{\delta}\right)^2\right]$$

for the case where $\cos\beta = 1$ and $x = \delta - y$

2. To make the equation simpler, we can state that $\left(\frac{y}{\delta}\right)^2 \ll \frac{y}{\delta}$,

$$v_z = \frac{\rho g \delta y}{\mu} = ay$$

since

$$a \equiv \frac{\rho g \delta}{\mu}$$

3. The boundary conditions are at $z = 0$, $c_A = 0$ and $y = 0$, $c_A = c_{A0}$ and $y = \infty$, $c_A = 0$

4. Define the combination variable of

$$f(\eta) = \frac{c_A}{c_{A0}}$$

where

$$\eta \equiv y\left(\frac{a}{9\mathscr{D}_{AB}z}\right)^{1/3}$$

5. The partial differential equation is

$$\frac{d^2 f}{d\eta^2} + 3\eta^2 \frac{df}{d\eta} = 0$$

6. This solution is tabulated as

$$f = C_1 \int_0^\eta \exp\left(-\bar{\eta}^3\right) d\bar{\eta} + C_2$$

7. It turns out that

$$\frac{c_A}{c_{A0}} = \frac{\int_\eta^\infty \exp\left(-\bar{\eta}^3\right) d\bar{\eta}}{\int_0^\infty \exp\left(-\bar{\eta}^3\right)^3 d\bar{\eta}} = \frac{\int_\eta^\infty \exp\left(-\bar{\eta}^3\right)}{\Gamma\left(\frac{4}{3}\right)}$$

8. The local mass flux at the wall can be obtained as follows

$$N_{A,y}\big|_{y=0} = -\mathscr{D}_{AB} \frac{\partial c_A}{\partial y}\bigg|_{y=0} = -\mathscr{D}_{AB} c_{A0} \left[\frac{d}{d\eta}\left(\frac{c_A}{c_{A0}}\right) \frac{\partial \eta}{\partial y}\right]\bigg|_{y=0}$$

$$= -\mathscr{D}_{AB} c_{A0} \left[-\frac{\exp\left(-\eta^3\right)}{\Gamma\left(\frac{4}{3}\right)}\left(\frac{a}{9\mathscr{D}_{AB}z}\right)^{1/3}\right]\Bigg|_{y=0} = \frac{\mathscr{D}_{AB} c_{A0}}{\Gamma\left(\frac{4}{3}\right)}\left(\frac{a}{9\mathscr{D}_{AB}z}\right)^{1/3}$$

9. Therefore the molar flow of $A$ across the surface is

$$W_A = \int_0^W \int_0^L N_{A,y}\bigg|_{y=0} dz\, dz = \frac{2\mathscr{D}_{AB} c_{A0} WL}{\Gamma\left(\frac{7}{3}\right)}\left(\frac{a}{9\mathscr{D}_{AB}L}\right)^{1/3}$$

## 6.10 Diffusion and Chemical Reaction Inside a Porous Catalyst

Problem: We shall describe diffusion within a porous catalyst pellet. We shall describe an effective diffusivity, which is an averaged quantity. Consider a pellet of radius $R$ that is submerged in gaseous reactant $A$ and gaseous product $B$. Species $A$ diffuses inside the catalyst and is converted to $B$ on the surface. For the full problem statement, see Section 18.7 of BSL.

1. The mass balance states that

$$N_{A,r} 4\pi r^2\big|_r - N_{A,r} 4\pi r^2\big|_{r+\Delta r} + R_A 4\pi r^2 \Delta r = 0$$

where the rightmost term is the molar rate of production of $A$ by chemical reaction in the shell of thickness $\Delta r$

2. This translates to

$$\frac{d}{dr}\left(r^2 N_{A,r}\right) = r^2 R_A$$

3. The effective diffusivity is

$$N_{A,r} = -\mathscr{D}_{eff} \frac{dc_A}{dr}$$

4. Therefore,

$$\mathscr{D}_{eff} \frac{1}{r^2} \frac{d}{dr}\left(r^2 \frac{dc_A}{dr}\right) = -R_A$$

for constant $\mathscr{D}_{eff}$

5. The boundary conditions are $c_A = c_{AR}$ at $r = R$ and $c_A =$ finite at $r = 0$

6. A change of variables can be implemented to yield

$$\frac{d^2 f}{dr^2} = \left(\frac{k_1'' a}{\mathscr{D}_{eff}}\right) f$$

7. This has the solution of

$$\frac{c_A}{c_{AR}} = \frac{C_1}{r} \cosh\left(r\sqrt{\frac{k_1'' a}{\mathscr{D}_{eff}}}\right) + \frac{C_2}{r} \sinh\left(r\sqrt{\frac{k_1'' a}{\mathscr{D}_{eff}}}\right)$$

8. Using the boundary conditions yields

$$\frac{c_A}{c_{AR}} = \left(\frac{R}{r}\right) \frac{\sinh\left(r\sqrt{\frac{k_1'' a}{\mathscr{D}_{eff}}}\right)}{\sinh\left(R\sqrt{\frac{k_1'' a}{\mathscr{D}_{eff}}}\right)}$$

9. The molar flow at the surface $r = R$ is

$$W_{AR} = 4\pi R^2 N_{AR} = -4\pi R^2 \mathscr{D}_{eff} \frac{dc_A}{dr}\bigg|_{r=R}$$

10. Evaluating the derivative and plugging it in yields

$$W_{AR} = 4\pi R \mathscr{D}_{eff} c_{AR} \left(1 - R\sqrt{\frac{k_1'' a}{\mathscr{D}_{eff}}}\right) \coth\left(R\sqrt{\frac{k_1'' a}{\mathscr{D}_{eff}}}\right)$$

11. The best possible scenario is if every element's surface is exposed such that $c_A = c_{AR}$ and then

$$W_{AR,0} = -\frac{4}{3}\pi R^3 a k_1'' c_{AR}$$

12. The efficiency factor is defined as

$$\eta_A \equiv \frac{W_{AR}}{W_{AR,0}} = \frac{3}{\phi^2}\left(\phi \coth\left(\phi\right) - 1\right)$$

where $\phi$ is once the Thiele modulus of $\phi = R\sqrt{\frac{k_1'' a}{\mathscr{D}_{eff}}}$. Note that this Thiele modulus has a different functional form.

(a) For $\phi = 10$, $\coth \approx 1$, so for large $\phi$, $\eta_A \approx \frac{3}{\phi}$

13. For a nonspherical particle,

$$R_{\text{nonsphere}} = 3\left(\frac{V_P}{S_P}\right)$$

where $V_P$ is the volume and $S_P$ is the external surface

14. The conversion rate is then

$$|W_{AR}| \approx V_P a k_1'' c_{AR} \eta_A$$

for nonspherical particles where

$$\eta_A = \frac{1}{3\Lambda^2}\left(3\Lambda \coth\left(3\Lambda\right) - 1\right)$$

and the generalized modulus is defined as

$$\Lambda \equiv \frac{\phi}{R}\frac{V_P}{S_P} = \frac{V_P}{S_P}\sqrt{\frac{k_1'' a}{\mathscr{D}_{eff}}}$$

# 7 Equations of Change for Multicomponent Systems

## 7.1 The Equations of Continuity for a Multicomponent Mixture

- The microscopic mass balance states that

$$\frac{\partial \rho_\alpha}{\partial t} = -\left(\nabla \cdot \rho_\alpha \vec{v}\right) - \left(\nabla \cdot \vec{j}_\alpha\right) + r_\alpha$$

- The continuity equation for the mixture is

$$\frac{\partial \rho}{\partial t} = -\left(\nabla \cdot \rho \vec{v}\right)$$

and at steady-state conditions with constant density,

$$\nabla \cdot \vec{v} = 0$$

- The molar equation of continuity states that

$$\frac{\partial c_\alpha}{\partial t} = -\left(\nabla \cdot \vec{N}_\alpha\right) + R_\alpha$$

## 7.2 Summary of the Multicomponent Equations of Change

- For a binary system with constant $\rho \mathscr{D}_{AB}$,

$$\boxed{\rho\left(\frac{\partial \omega_A}{\partial t} + (\vec{v} \cdot \nabla \omega_A)\right) = \rho \mathscr{D}_{AB} \nabla^2 \omega_A + r_A}$$

   - For a system also at steady-state, you can divide by the molar mass, $M_A$, to get

$$\boxed{\vec{v} \cdot \nabla c_A = \mathscr{D}_{AB} \nabla^2 c_A + r_A}$$

- For a binary system with constant $c\mathscr{D}_{AB}$,

$$c\left(\frac{\partial x_A}{\partial t} + (\vec{v}^* \cdot \nabla x_A)\right) = c\mathscr{D}_{AB} \nabla^2 x_A + (x_B R_A - x_A R_B)$$

- For binary systems with zero velocity and no chemical reaction, Fick's Law states that

$$\frac{\partial c_A}{\partial t} = \mathscr{D}_{AB} \nabla^2 c_A$$

## 7.3 Simultaneous Diffusion, Convection, and Reaction with a Porous Plug

Problem: See Example 19.1-1 in BSL.

1. We can use the equation for binary systems with constant $\rho \mathscr{D}_{AB}$,

$$\rho\left(\frac{\partial \omega_\alpha}{\partial t} + (\vec{v} \cdot \nabla \omega_\alpha)\right) = \rho \mathscr{D}_{AB} \nabla^2 \omega_A + r_A$$

2. We can set the time-derivative term equal to zero since it is at steady-state. We can also divide by $M_A$ (the molecular mass) to get

$$v_0 \frac{dc_A}{dz} = \mathscr{D}_{AB} \frac{d^2 c_A}{dz^2} - k_1''' c_A$$

3. Dividing by $\mathscr{D}_{AB}$ yields

$$\frac{d^2 c_A}{dz^2} - \frac{v_0}{\mathscr{D}_{AB}} \frac{dc_A}{dz} - \frac{k_1'''}{\mathscr{D}_{AB}} c_A$$

4. Set the boundary conditions as $c_A = c_{A0}$ at $z = 0$ since nothing has reacted the inlet and $c_A = 0$ at $z = \infty$ when it has all reacted

5. The final solution is tabulated as

$$\boxed{\frac{c_A}{c_{A0}} = \exp\left(\frac{v_0 z}{2\mathscr{D}_{AB}}\left(1 - \sqrt{1 + \frac{4k_1''' \mathscr{D}_{AB}}{v_0^2}}\right)\right)}$$

## 7.4   Concentration Profile in Tubular Reactors

Problem: See Example 19.4-2 in BSL.

1. We can use the equation for binary systems with constant $\rho\mathscr{D}_{AB}$,

$$\rho\left(\frac{\partial \omega_\alpha}{\partial t} + (\vec{v}\cdot\nabla\omega_\alpha)\right) = \rho\mathscr{D}_{AB}\nabla^2\omega_A + r_A$$

2. The system is at steady-state, so the time-derivative term goes to zero. We can also ignore $r_A$ for reasons I do not completely understand. Therefore,

$$v_z \frac{\partial c_A}{\partial z} = \mathscr{D}_{AB}\left[\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial c_A}{\partial r}\right) + \frac{\partial^2 c_A}{\partial z^2}\right]$$

3. We can ignore the axial diffusion compared to the axial convection,

$$v_z \frac{\partial c_A}{\partial z} = \mathscr{D}_{AB}\left[\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial c_A}{\partial r}\right)\right]$$

4. The velocity profile is given as

$$v_z = v_{z,max}\left(1 - \left(\frac{r}{R}\right)^2\right)$$

5. Plugging this expression for $v_z$ into our differential equation yields

$$v_{z,max}\left(1 - \left(\frac{r}{R}\right)^2\right)\frac{\partial c_A}{\partial z} = \mathscr{D}_{AB}\left[\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial c_A}{\partial r}\right)\right]$$

6. The boundary conditions are $c_A = c_{A0}$ at $z = 0$, $c_A = 0$ at $r = R$, and $c_A = $ finite at $r = 0$

7. We can define $y = R - r$ such that the second boundary condition becomes $c_A = 0$ at $y = 0$ and the third boundary condition becomes $c_A = $ finite and at $y = \infty$

8. This allows us to rewrite our expression as

$$2v_{z,max}\frac{y}{R}\frac{\partial c_A}{\partial z} = \mathscr{D}_{AB}\frac{\partial^2 c_A}{\partial y^2}$$

9. One can find that the solution to this expression

$$\boxed{\frac{c_A}{c_{A0}} = \frac{\int_0^\eta \exp\left(-\bar{\eta}^3\right) d\bar{\eta}}{\Gamma\left(\frac{4}{3}\right)}}$$

where

$$\boxed{\eta \equiv \frac{y}{R}\left(\frac{2v_{z,max}R^2}{9\mathscr{D}_{AS}z}\right)^{1/3}}$$

# 8  Concentration Distributiuons with More than One Independent Variable

## 8.1  Time-Dependent Diffusion

### 8.1.1  Gas Adsorption with Rapid Reaction

Problem: See Example 20.1-2 in BSL.

1. The concentration profiles can be described as

$$\frac{\partial c_A}{\partial t} = \mathscr{D}_{AS} \frac{\partial^2 c_A}{\partial z^2}$$

for $0 \leq z \leq z_R(t)$ and

$$\frac{\partial c_B}{\partial t} = \mathscr{D}_{BS} \frac{\partial^2 c_B}{dz^2}$$

for $z_R(t) \leq z \leq \infty$

2. The initial conditions state that at $t = 0$, $c_B = c_{B\infty}$ and $c_A = 0$ for all $z > 0$. The boundary conditions are at $z = 0$, $c_A = c_{A0}$. At $z = z_R(t)$, $c_A = c_B = 0$. At $z = z_R(t)$, $-\frac{1}{a}\mathscr{D}_{AS}\frac{\partial c_A}{\partial z} = \frac{1}{b}\mathscr{D}_{BS}\frac{\partial c_B}{\partial z}$. At $z = \infty$, $c_B = c_{B\infty}$

3. If we define $\eta \equiv \dfrac{z}{\sqrt{4\mathscr{D}t}}$ and $\phi \equiv \dfrac{c_A}{c_{A0}}$ so that

$$\frac{d^2\phi}{d\eta^2} + 2\eta\frac{d\phi}{d\eta} = 0$$

4. Let $\psi \equiv \dfrac{d\phi}{d\eta}$ so that

$$\frac{d\psi}{d\eta} + 2\eta\psi = 0 \rightarrow \frac{d\psi}{\psi} = -2\eta d\eta \rightarrow \psi = C' \exp\left(\eta^2\right)$$

5. From this, we can state that

$$\phi = C'' + C' \int_0^\eta \exp\left(-\bar\eta^2\right)\, d\bar\eta$$

6. Try

$$\frac{c_A}{c_{A0}} = C_1 + C_2\text{erf}\left(\frac{z}{\sqrt{4\mathscr{D}_{AS}t}}\right)$$

and

$$\frac{c_B}{c_{B\infty}} = C_3 + C_4\text{erf}\left(\frac{z}{\sqrt{4\mathscr{D}_{BS}t}}\right)$$

7. Applying the boundary conditions yields

$$\boxed{\frac{c_A}{c_{A0}} = 1 - \frac{\text{erf}\left(\dfrac{z}{\sqrt{4\mathscr{D}_{AS}t}}\right)}{\text{erf}\left(\dfrac{z_R}{\sqrt{4\mathscr{D}_{AS}t}}\right)}}$$

$$\boxed{\frac{c_B}{c_{B\infty}} = 1 - \frac{\text{erf}\left(\dfrac{z}{\sqrt{4\mathscr{D}_{BS}t}}\right)}{\text{erf}\left(\dfrac{z_R}{\sqrt{4\mathscr{D}_{BS}t}}\right)}}$$

8. The mass transfer at the interface is then

$$N_{Az0} = -\mathscr{D}_{AS} \left.\frac{\partial c_A}{\partial z}\right|_{z=0} = \frac{c_{A0}}{\mathrm{erf}\left(\sqrt{\dfrac{\gamma}{\mathscr{D}_{AS}}}\right)}\sqrt{\frac{\mathscr{D}_{AS}}{\pi t}}$$

9. The average rate of absorption up to time $t$ is then

$$N_{Az0,avg} = \frac{1}{t}\int_0^t N_{Az0}dt = \frac{2c_{A0}}{\mathrm{erf}\left(\sqrt{\dfrac{\gamma}{\mathscr{D}_{AS}}}\right)}\sqrt{\frac{\mathscr{D}_{AS}}{\pi t}} = 2N_{Az0}$$

### 8.1.2   Mass Transfer at an Interface with a Semi-Infinite Body

Problem: See Example 20.1-4 in BSL.

1. It will simply be stated that

$$\frac{c_A}{c_{A0}} = 1 - \mathrm{erf}\left(\frac{z}{\sqrt{4\mathscr{D}_{AB}t}}\right)$$

2. At the interface,

$$N_{Az0} = c_{A0}\sqrt{\frac{\mathscr{D}_{AB}}{\pi t}}$$

   (a) Note that $\dfrac{d}{dz}\mathrm{erf}\left(u\right) = \dfrac{2}{\sqrt{\pi}}\exp\left(-u^2\right)\dfrac{du}{dz}$

## 8.2   Diffusion and Chemical Reaction in Isothermal Laminar Flow Along a Soluble Flat Plate

Problem: See Example 20.2-1 in BSL.

- The velocity boundary layer thickness can be described by

$$\delta = \sqrt{12\frac{\nu x}{v_\infty}}$$

- The Schmidt number can be expressed as

$$\frac{1}{\mathrm{Sc}} = \frac{4}{3}x\frac{d}{dx}\Delta^3 + \Delta^3 + 12\left[\frac{k_n^{'''}c_{A0}^{n-1}x}{(n+1)v_\infty}\right]\Delta^2$$

   where

$$\Delta \equiv \frac{\delta_c}{\delta}$$

- For no reaction,

$$\mathrm{Sc}^{-1/3} = \Delta$$

   for $\Delta \leq 1$

- For a slow reaction,

$$\Delta \approx \mathrm{Sc}^{1/3} - \frac{1}{7}$$

## 8.3 Taylor Dispersions

Problem: See Section 20.5 in BSL.

1. It will simply be stated that the axial dispersion coefficient is defined as

$$K \equiv \frac{R^2 \langle v_z \rangle^2}{48 \mathscr{D}_{AB}} = \frac{1}{48} \mathscr{D}_{AB} \mathrm{Pe}_{AB}^2$$

   where

$$\mathrm{Pe} \equiv \mathrm{ReSc}$$

2. The modified expression that holds for more values of $\mathscr{D}_{AB} t / R^2$ is

$$K \equiv \mathscr{D}_{AB} + \frac{R^2 \langle v_z \rangle^2}{48 \mathscr{D}_{AB}} = \mathscr{D}_{AB} \left( 1 + \frac{1}{48} \mathrm{Pe}_{AB}^2 \right)$$

## 8.4 Unsteady-State Interphase Diffusion

Problem: See Problem 20.D.2 in BSL.

1. It will simply be stated that the concentration profiles can be given by

$$\boxed{\frac{c_1 - c_1^\circ}{c_2^\circ - m c_1^\circ} = \frac{1 + \mathrm{erf}\left( \dfrac{z}{\sqrt{4 \mathscr{D}_1 t}} \right)}{m + \sqrt{\mathscr{D}_1 / \mathscr{D}_2}}}$$

   and

$$\boxed{\frac{c_2 - c_2^\circ}{c_1^\circ - c_2^\circ / m} = \frac{1 - \mathrm{erf}\left( \dfrac{z}{\sqrt{4 \mathscr{D}_2 t}} \right)}{1/m + \sqrt{\mathscr{D}_2 / \mathscr{D}_1}}}$$

   where $m$ is Henry's law constant (i.e. the "distribution coefficient")

2. The flux at the interface is

$$\boxed{N_{Az}|_{z=0} = - \left( \frac{c_2^\circ - m c_1^\circ}{m + \sqrt{\mathscr{D}_1 / \mathscr{D}_2}} \right) \sqrt{\frac{\mathscr{D}_1}{\pi t}}}$$

# 9 Interphase Transport in Nonisothermal Mixtures

## 9.1 Rotating Disks

- The molar flux at the surface can be given by

$$\boxed{N_{A0} = 0.620 c_A \left( \frac{\mathscr{D}_{AB}^{2/3} \Omega^{1/2}}{\nu^{1/6}} \right) = k_{c,m}^\circ \Delta c_A}$$

   where $\Omega$ is in rad/s

- The mean Sherwood number can be given by

$$\boxed{\overline{\mathrm{Sh}} = \frac{k_{c,m}^\circ D}{\mathscr{D}_{AB}} = 0.620 \mathrm{Re}^{1/2} \mathrm{Sc}^{1/3}}$$

- The Reynolds number is expressed in this case as

$$\text{Re} = \frac{vL}{\nu} = \frac{D^2\Omega}{\nu}$$

- To relate the mole fraction to concentration,

$$c_i = \frac{x_i\rho}{\sum x_i M_i}$$

where $\rho$ is the density of the mixture

## 9.2 Correlation of Binary Transfer Coefficients in One Phase

- For forced convection around a sphere,

$$\overline{\text{Sh}} = 2 + 0.60\text{Re}^{1/2}\text{Sc}^{1/3}$$

- Many of the heat transfer expressions we found earlier can be used for mass transfer analogues by replacing the Nusselt number with the Sherwood number and replacing the Prandtl number with the Schmidt number

## 9.3 Interaction of Phase Resistances (i.e. Leeching)

Problem: See Example 22.4-2 in BSL.

- It will simply be stated that

$$\frac{M_A(t)}{\frac{4}{3}\pi R^3 c_0} = 6\sum_{n=1}^{\infty} B_n \exp\left(-\lambda_n^2 \mathscr{D}_{AB}t/R^2\right)$$

- For infinite $k_c$ or $N$,

$$\lambda_n = n\pi$$

and

$$B_n = \left(\frac{1}{\pi n}\right)^2$$

- For finite $k_c$ or $N$,

$$\lambda_n \cot\left(\lambda_n\right) - (1 - N) = 0$$

and

$$B_n = \frac{N^2}{\lambda_n^3} \frac{\sin^2\left(\lambda_n\right)}{\lambda_n - \sin\left(\lambda_n\right)\cos\left(\lambda_n\right)}$$

# 10  Appendix

## 10.1  Gradient

$$\nabla f = \frac{\partial f}{\partial x}\hat{x} + \frac{\partial f}{\partial y}\hat{y} + \frac{\partial f}{\partial z}\hat{z}\ \text{(Cartesian)}$$

$$\nabla f = \frac{\partial f}{\partial r}\hat{r} + \frac{1}{r}\frac{\partial f}{\partial \theta}\hat{\theta} + \frac{\partial f}{\partial z}\hat{z}\ \text{(Cylindrical)}$$

$$\nabla f = \frac{\partial f}{\partial r}\hat{r} + \frac{1}{r}\frac{\partial f}{\partial \theta}\hat{\theta} + \frac{1}{r\sin\theta}\frac{\partial f}{\partial \phi}\hat{\phi}\ \text{(Spherical)}$$

## 10.2  Divergence

$$\nabla \cdot \vec{v} = \frac{\partial v_x}{\partial x} + \frac{\partial v_y}{\partial y} + \frac{\partial v_z}{\partial z}\ \text{(Cartesian)}$$

$$\nabla \cdot \vec{v} = \frac{1}{r}\frac{\partial}{\partial r}\left(rv_r\right) + \frac{1}{r}\frac{\partial v_\theta}{\partial \theta} + \frac{\partial v_z}{\partial z}\ \text{(Cylindrical)}$$

$$\nabla \cdot \vec{v} = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 v_r\right) + \frac{1}{r\sin\theta}\frac{\partial}{\partial \theta}\left(v_\theta \sin\theta\right) + \frac{1}{r\sin\theta}\frac{\partial v_\phi}{\partial \phi}\ \text{(Spherical)}$$

## 10.3  Curl

$$\nabla \times \vec{v} = \left(\frac{\partial v_z}{\partial y} - \frac{\partial v_y}{\partial z}\right)\hat{x} + \left(\frac{\partial v_x}{\partial z} - \frac{\partial v_z}{\partial x}\right)\hat{y} + \left(\frac{\partial v_y}{\partial x} - \frac{\partial v_x}{\partial y}\right)\hat{z}\ \text{(Cartesian)}$$

$$\nabla \times \vec{v} = \left(\frac{1}{r}\frac{\partial v_z}{\partial \theta} - \frac{\partial v_\theta}{\partial z}\right)\hat{r} + \left(\frac{\partial v_r}{\partial z} - \frac{\partial v_z}{\partial r}\right)\hat{\theta} + \frac{1}{r}\left(\frac{\partial (rv_\theta)}{\partial r} - \frac{\partial v_r}{\partial \theta}\right)\hat{z}\ \text{(Cylindrical)}$$

$$\nabla \times \vec{v} = \frac{1}{r\sin\theta}\left(\frac{\partial (v_\phi \sin\theta)}{\partial \theta} - \frac{\partial v_\theta}{\partial \phi}\right)\hat{r} + \left(\frac{1}{r\sin\theta}\frac{\partial v_r}{\partial \phi} - \frac{1}{r}\frac{\partial (rv_\theta)}{\partial r}\right)\hat{\theta} + \frac{1}{r}\left(\frac{\partial (rv_\theta)}{\partial r} - \frac{\partial v_r}{\partial \theta}\right)\hat{\phi}\ \text{(Spherical)}$$

## 10.4  Laplacian

$$\nabla^2 f = \frac{\partial^2 f}{\partial x^2} + \frac{\partial^2 f}{\partial y^2} + \frac{\partial^2 f}{\partial z^2}\ \text{(Cartesian)}$$

$$\nabla^2 f = \frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial f}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2 f}{\partial \theta^2} + \frac{\partial^2 f}{\partial z^2}\ \text{(Cylindrical)}$$

$$\nabla^2 f = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial f}{\partial r}\right) + \frac{1}{r^2 \sin\theta}\frac{\partial}{\partial \theta}\left(\sin\theta\frac{\partial f}{\partial \theta}\right) + \frac{1}{r^2 \sin^2\theta}\frac{\partial^2 f}{\partial \phi^2}\ \text{(Spherical)}$$