

Lecturer: Prof. Darryl Overby

Bioengineering Science 2

Heat and Mass Transport



Year 2 2020, Autumn Term

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Preface

These notes were partially built and compiled in Autumn 2020, during the outburst of COVID-19 in the UK and China. Although the teaching was conducted in a remote fashion and the class was barely able to meet each other in person, Prof. Darryl Overby managed to deliver this module, *Bioengineering Science 2*¹, without any compromise to the quality.

My procrastination impeded me from completing the writing and typesetting work until two years later, when I handed in my master's thesis and delivered my project presentation to the department. A long time from the hiatus, I guess a quick refresh to those classic thermo-fluids concepts would indeed be a good summer choice, given that my PhD work will be featuring bio-fluid mechanics.

The topics, convective heat transfer, boundary layers, and mass transport, were first built over the summer and appended to my previous work. Besides, figures in the notes were reproduced in the format of .eps hence the old, blocky ones could be replaced.

This module is now taught by Dr. S. Au and Dr. C. H. Yap, with slight revisions to the syllabus. These changes are mainly reflected in the last two chapters, where additional examples of external/internal flow are given, and derivations on the thermal/velocity boundary layers are removed. Yet, these changes have not been considered here. I will update them once those materials are accessible. Let us stay tuned.

Special thanks to G. Guo for his precious and continuous input in the notes, which motivated me to make corrections to the probed typos.

 \bigcirc The ET_EX files are now accessible on my GitHub repository. I hope this helps. Please report typos and inconsistencies to binghuan.li19@imperial.ac.uk.

To my undergraduate years.

September, 2023 & May, 2024 Rizhao, Shandong, China & London, UK

¹a.k.a. Heat and Mass Transport II

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1 Units and Energy

1.1 Dimensions and Units

Heat transport quantities are specified in terms of *dimensions*, and measured in terms of units.

Units Numbers are physical quantities with physical meanings and dimensions. All dimensional variables and parameters are assigned units. Variables and parameters without units are physically meaningless.

5 basic units used to describe all physical quantities						
Q	Quantity	Symbol	Unit	Quantity	Symbol	Unit
L	ength	L	m	Mass	М	kg
T C	Time Charge	T C	s C	Temperature	Т	K

1.2 Unit Conventions

Factor-Label Method

• Express conversion factors as unity fractions, representing the ratio of the same physical quantity expressed in two different units. For example:

$$\frac{760 \text{ mmHg}}{1 \text{ atm}} \quad \text{or} \quad \frac{101.3 \times 10^3 \text{ Pa}}{1 \text{ atm}}$$

- Unity fractions are multiplied together
- Similar units in the numerator and denominator cancel, to give desired units. For example:
- Exception: this does not work for temperature $T_{\text{Kelvin}} = T_{\text{Celsius}} + 273.15$

Always check units!

1.3 Laws of Thermodynamics

 0^{th} Law "If body A is in thermal equilibrium with body B, and B with C, then A is in thermal equilibrium with C."

1st Law "The energy of an isolated system is constant."

 2^{nd} Law "When two systems are brought into thermal contact, heat flows spontaneously from the one at higher temperature to the one at lower temperature, not the other way around."

1.4 First Law of Thermodynamics

Energy cannot be created nor destroyed, but only change forms.

$$du = \delta Q - \delta W$$
 [Joules, J]

- *u*: the total energy of a system (is a state variable, hence a true differential 'd')
- Q: heat flowing into the system (positive b.c U increases by heat inflow)
- W: work done by the system (negative b.c U decreases by doing work)

Express the 1st law in terms of rates of change:

$$\frac{\mathrm{d}U}{\mathrm{d}t} = \frac{\partial Q}{\partial t} - \frac{\partial W}{\partial t} = \dot{Q} - \dot{W} \text{ [Watts, W]}$$

- \dot{Q} : rate of heat flow into system
- \dot{W} : rate of work done by system

1.5 Two Types of Heat Transport Systems

1. Adiabatic: If the system is adiabatic, there is no heat transport ($\delta Q = 0$) and the system is thermally insulated from its surroundings.

$$dU = -\delta W$$

2. **Isometric:** If the system is isometric, there is no change in dimensions and therefore no work done ($\delta W = 0$). The system is mechanically insulated from its surroundings.

$$dU = \delta Q$$

1.6 Forms of energy

- Kinetic energy associated with a macroscopic mass in motion: $\frac{1}{2}mv^2$
- **Potential energy** associated with the position of an object in a gravitational or electromagnetic field: *mgz*
- Elastic strain energy energy stored within elastic deformation. e.g., spring of stiffness k and deformation x: $\frac{1}{2}kx^2$
- Thermal or "internal" energy energy associated with the motion of molecules (translation, rotation, vibration): mc_pT
- Many more forms of energy: chemical bond energy, nuclear energy, ...

2 Three Modes of Heat Transport



Figure 1: Conduction, convection, and radiation heat transfer modes

2.1 Conduction

• Heat Transport between molecules via random collisions.



Figure 2: Association of conduction heat transfer with diffusion of energy due to molecular activity.

Consider conduction within a gas under a temperature gradient where no bulk motion occurs. The energy is transferred from the high-energy molecules to the low-energy molecules by collision.

• In 1-D, heat conduction is governed by Fourier's Law:

$$\dot{Q} = -k \ A \ \frac{\mathrm{d}T}{\mathrm{d}x}$$

- k: thermal conductivity $[W/(m \cdot K)]$: an intrinsic property of material how good the material is to conduct heat?
- A: surface area $[m^2]$
- $\frac{dT}{dx}$: temperature gradient in x-direction [K/m]

2.2 Convection

• Heat transport due to bulk motion over a heated surface. It occurs at an interface between a fluid in motion and a bounding surface when the two are at different temperatures.



Figure 3: Boundary layer development in convection heat transfer.

• Convective heat flux is described by Newton's law of cooling:

$$\dot{Q} = h A \left(T_s - T_\infty \right)$$

- *h*: convective heat transport coefficient $[W/(m^2 \cdot K)]$
 - * highly sensitive to flow patterns, geometry, transport properties
 - * difficult to compute, but some analytical and tabulated values exist
- Two types of convective heat transport:
 - Forced convection: fluid motion is determined by the external source.
 - Free Convection: fluid motion is determined by temperature differences and buoyancy forces.



Figure 4: (a) Forced convection, (b) Free convection

- Mixed convection: convection influenced by both the external source and buoyancy

2.3 Radiation

- In radiation, heat transport is due to the propagation of electromagnetic waves (photons). It occurs at any finite temperature for solid, liquid or gas, and does not require physical contact or material medium (efficient in vacuum).
- Black body radiation, E_b , is described by Stefan-Boltzmann law:

$$E_b = \sigma T^4$$

where σ is the Stefan-Boltzmann constant with its value $5.67 \times 10^{-8} [W/(m^2K^4)]$

• However, real materials are not ideal black bodies:

$$E = \epsilon \sigma T^4$$

where ϵ is the emissivity with its value $0 \le \epsilon \le 1$

• Radiation also incident on the surface from surroundings (irradiation or *G*). But only a portion of *G* is absorbed, the rest is reflected or transmitted. This can be described by

$$G_{abs} = \alpha G$$

where α is absorptivity with its value $0 \le \alpha \le 1$

3 Reynolds Transport Theorem

3.1 Conservation Laws

dU =	δQ -	$-\delta W$ -	+ d <i>S</i>
$\overline{}$	\smile	\smile	\smile
1	2	3	4

Increase in energy
 Amount of inflow
 Amount of outflow
 Amount of generation

Written in terms of rate of change:

$$\frac{\mathrm{d}U}{\mathrm{d}t} = \frac{\partial Q}{\partial t} - \frac{\partial W}{\partial t} + \frac{\partial S}{\partial t} = \dot{Q} - \dot{W} + \dot{S}$$

3.2 Control Volume

Control Volume (CV) is a defined region of space where a conservation law is applied.

- can be any shape and size chosen based on convenience;
- must be used consistently throughout the problem;

3.3 Kinematics Description and Material Derivative

Kinematics Description of motion of mass in time and space, noting about forces driving that motion.

Two general approaches used in kinematics are Lagrangian and Eulerian.



Figure 5: Eulerian and Lagrangian descriptions of the kinematics.

Lagrangian	Eulerian
 keeps track of individual particles as they move through space 	• describes particle velocity as a function of space
 often called the "material-following" approach 	• Convenient in mathematical approach, but leads to some paradoxes
• Difficult in practice	

Material Derivative The material derivative (or, total derivative) links the Eulerian and Lagrangian reference frames. For a certain quantity g, the material derivative of g is

$$\frac{Dg}{Dt} = \frac{\partial g}{\partial t} + (\vec{\mathbf{v}} \cdot \nabla)g$$

Derivation

Let $g(\vec{x}, t) = g(x, y, z, t)$ be an arbitrary property of a mass particle defined in an Eulerian field. As the particle moves through the field, the property assumes the local value of $g(\vec{x}, t)$. What is the rate of change of $g(\vec{x}, t)$?

$$\frac{Dg}{Dt} = \frac{d}{dt}g(\overbrace{X(t), Y(t), Z(t)}^{\overline{x}(t)}, t)$$

$$= \frac{\partial g}{\partial x} \frac{dX}{dt} + \frac{\partial g}{\partial y} \frac{dY}{dt} + \frac{\partial g}{\partial z} \frac{dZ}{dt} + \frac{\partial g}{\partial t}$$

$$= v_x \frac{\partial g}{\partial x} + v_y \frac{\partial g}{\partial y} + v_z \frac{\partial g}{\partial z} + \frac{\partial g}{\partial t}$$

$$= \underbrace{\frac{\partial g}{\partial t}}_{\text{unsteady}} + \underbrace{(\overrightarrow{v} \cdot \nabla)g}_{\text{advection}}$$

where the vector $\vec{v} \in [v_x, v_y, v_z]$.

3.4 Flow and Flux

3.4.1 Flow

Flow Flow quantifies how much of a substance or property is being transported across a surface per unit of time. **Flow is an** *extensive* **property.**

Typical Units of Flows

- flux of solute: M/s
- flux of heat: J/s = W
- flux of solvent: m³/s

Extensive Property is a physical property that depends on the size or the amount of material contained in system. It cannot be defined at a point.

• Examples: mass, energy, momentum

3.4.2 Flux

Flux Flux quantifies how much of a substance or property is being transported across a surface per unit of time and per unit area. **Flux is an** *intensive* **property.**

Typical Units of Fluxes

- flux of solute: $M/(m^2s)$
- flux of heat: $J/(m^2s) = W/(m^2)$
- flux of solvent: $m^3/(m^2s) = m/s$

Intensive Property is independent of size or the amount of material contained in the system. It cannot be defined at each point (per unit volume, unit area, unit mass);

• Examples: density, concentration.

Integrating an intensive property over space containing mass translates an intensive property into an extensive property.

3.4.3 Flux Orientation and Volume Flow Rate

Flow across a surface depends on the relative orientation between flux and surface.



Mathematically, the intensive volume flow rate is

$$\mathrm{d}V = (\vec{\mathbf{v}} \cdot \hat{\mathbf{n}}) \mathrm{d}A \mathrm{d}t$$
 or $\frac{\mathrm{d}V}{\mathrm{d}t} = (\vec{\mathbf{v}} \cdot \hat{\mathbf{n}}) \mathrm{d}A$

where

- \hat{n} represents the outward facing normal or a control surface: $\hat{n} = n_x \hat{e}_x + n_y \hat{e}_y + n_z \hat{e}_z$.
- \vec{v} represents the velocity of flux crossing the surface: $\vec{v} = v_x \hat{e}_x + v_y \hat{e}_y + v_z \hat{e}_z$.

Extensive flow rate:

$$Q = \int_A (\vec{\boldsymbol{v}} \cdot \hat{\boldsymbol{n}}) \, \mathrm{d}A$$

Generalize to any arbitrary extensive property *B*, where $\beta = \frac{dB}{dm}$ (see examples after the derivation in subsection 3.5), total rate of transport of *B* across surface area *A* due to fluid flow is:

$$Q = \int_A \rho \beta(\vec{\boldsymbol{v}} \cdot \hat{\boldsymbol{n}}) \, \mathrm{d}A$$

3.5 Reynolds Transport Theorem (RTT)

For a conserved physical quantity B, RTT is mathematically expressed as

$$\frac{\mathrm{d}B_{\mathrm{system}}}{\mathrm{d}t} = \frac{\partial}{\partial t} \int_{CV} \rho\beta \mathrm{d}V + \oint_{CS} \rho\beta(\vec{\mathbf{v}}\cdot\hat{\mathbf{n}}) \mathrm{d}A.$$
(3.5.1)

In other words,



Term B: rate of change of *B* within CV (Eulerian) $\lim_{\Delta t \to 0} \frac{B_{CV}|_{t+\Delta t} - B_{CV}|_{t}}{\Delta t} = \frac{\partial B_{CV}}{\partial t} = \frac{\partial}{\partial t} \int_{CV} \rho \beta dV$ **Term C**: rate of change of *B* within CV as it is lost by fluid flow (Eulerian) $\lim_{\Delta t \to 0} \frac{\text{Net amount of } B \text{ leaving CV due to flow}}{\Delta t}$ = rate of *B* leaving CV due to flow $= \sigma f \rho \beta(\vec{v} \cdot \hat{n}) dA$ To equate these three terms, **Term A = Term B + Term C** $\Rightarrow \frac{dB_{\text{system}}}{dt} = \frac{\partial}{\partial t} \int_{CV} \rho \beta dV + \oint_{CS} \rho \beta(\vec{v} \cdot n) dA$ which states the RTT expressed in Equation 3.5.1.

What is the quantity β in RTT? β denotes the amount of *B* per unit mass, *i.e.*, $\beta = dB/dm$. Examples to follow:

• If *B* denotes mass *m*:
$$\beta = \frac{\mathrm{d}m}{\mathrm{d}m} = 1;$$

• If *B* denotes volume *V*:
$$\beta = \frac{\mathrm{d}V}{\mathrm{d}m} = 1/\rho;$$

- If *B* denotes linear momentum $\vec{P} = m\vec{v}$: $\beta = \frac{\mathrm{d}\vec{P}}{\mathrm{d}m} = \vec{v}$;
- If *B* denotes angular momentum $\vec{L} = \vec{r} \times \vec{P} = m\vec{r} \times \vec{v}$: $\beta = \frac{\mathrm{d}\vec{L}}{\mathrm{d}m} = \vec{r} \times \vec{v}$.

4 Heat Equation

4.1 Integral Form of Heat Equation

When $B \to U$, $\beta \to U_M$, RTT can be expressed as

$$\frac{\mathrm{d}U_{\mathrm{system}}}{\mathrm{d}t} = \frac{\partial}{\partial t} \int_{CV} \rho U_M \,\mathrm{d}V + \oint_{CS} \rho U_M(\vec{v} \cdot \hat{n}) \,\mathrm{d}A$$

The rate of change of the system, $\frac{dU_{\text{system}}}{dt}$ can be further expand with the expression $\dot{Q} - \dot{W} + \dot{S}$,

$$\dot{Q} - \dot{W} + \dot{S} = \frac{\partial}{\partial t} \int_{CV} \rho U_M \, \mathrm{d}V + \oint_{CS} \rho U_M (\vec{v} \cdot \hat{n}) \, \mathrm{d}A$$

By applying the following constraints and rearranging the expressions,

1. Only the thermal energy is considered: $\rho U_M = \rho c_p T$, where c_p is specific heat at constant pressure [J/kg K],

$$\dot{Q} - \dot{W} + \dot{S} = \frac{\partial}{\partial t} \int_{CV} \rho c_p T \, \mathrm{d}V + \oint_{CS} \rho c_p T (\vec{v} \cdot \hat{n}) \, \mathrm{d}A$$

- 2. \dot{Q} is the rate of heat transport into CV through CS: $\dot{Q} = -\oint_{CS} (\vec{q} \cdot \hat{n}) dA$, where \vec{q} is the heat flux vector;
 - neglect contributions of work terms: $\dot{W} = 0$;

- heat generation per unit volume: $\dot{S}_{v} : \dot{S} = \int_{CV} \dot{S}_{v} dV.$ $- \oint_{CV} (\vec{q} \cdot \hat{n}) dA + \dot{S}_{v} = \frac{\partial}{\partial t} \int_{CV} \rho c_{p} T dV + \oint_{CV} \rho c_{p} T (\vec{v} \cdot \vec{q}) dA$

Re-arrange the above expression, this gives us the final expression of conservation of mass.

$$\underbrace{\frac{\partial}{\partial t} \int_{CV} \rho c_p dV}_{\text{rate of change}} = \int_{CV} \dot{S}_v dV - \oint_{CS} (\vec{q} \cdot \hat{n}) dA - \oint_{CS} \rho c_p T(\vec{v} \cdot \hat{n}) dA}_{\text{rate of heat generation}} + \underbrace{\int_{CS} c_S}_{\text{rate of heat loss}} \underbrace{\int_{CV} \rho c_p T(\vec{v} \cdot \hat{n}) dA}_{\text{by fluid flow across CS}}$$
(4.1.1)

4.2 An Example



- \vec{f} can be any arbitrary vector
- $\nabla \cdot$ is the divergence operator, where $\nabla \cdot \vec{f} = \frac{\partial f_x}{\partial x} + \frac{\partial f_y}{\partial y} + \frac{\partial f_z}{\partial z}$

4.3.2 Differential Form of Heat Equation

$$\rho c_p \left(\underbrace{\frac{\partial T}{\partial t}}_{\odot} + \underbrace{(\vec{v} \cdot \nabla)T}_{@} \right) = \underbrace{\dot{S_v}}_{@} + \underbrace{k \nabla^2 T}_{@}$$

unsteady term
 convective term
 source term
 diffusive term

Derivation

Apply the divergence theorem to the heat equation:

$$\oint_{CS} (\vec{q} \cdot \hat{n}) dA = \int_{CV} (\nabla \cdot \vec{q}) dV$$
$$\oint_{CS} \rho c_p T(\vec{v} \cdot \hat{n}) dA = \int_{CV} (\nabla \cdot (\rho c_p T \vec{v})) dV$$

Therefore,

$$\frac{\partial}{\partial t} \int_{CV} \rho c_p T dV = \int_{CV} \dot{S}_v dV - \oint_{CS} (\vec{q} \cdot \hat{n}) dA - \oint_{CS} \rho c_p T(\vec{v} \cdot \hat{n}) dA$$
$$= \int_{CV} \dot{S}_v dV - \int_{CV} (\nabla \cdot \vec{q}) dV - \int_{CV} (\nabla \cdot (\rho c_p T \vec{v})) dV$$

Rearrange:

$$\int \underbrace{\left[\frac{\partial}{\partial t}\rho c_{p}T - \dot{S}_{v} + (\nabla \cdot \vec{q}) + (\nabla \cdot (\rho c_{p}T\vec{v}))\right]}_{0} dV = 0$$

Since:

•
$$\frac{\partial}{\partial t}(\rho c_p T) = \rho \frac{\partial (c_p T)}{\partial t} + c_p T \frac{\partial \rho}{\partial t}$$

• $\nabla \cdot (\rho c_p T \vec{v}) = c_p T (\nabla \cdot \rho \vec{v}) + \rho (\vec{v} \nabla \cdot c_p T)$

Thus,

$$\rho \frac{\partial (c_p T)}{\partial t} + c_p T \frac{\partial \rho}{\partial t} = \dot{S}_v - (\nabla \cdot \vec{q}) - c_p T (\nabla \cdot \rho \vec{v}) - \rho (\vec{v} \nabla \cdot c_p T)$$

Rearrange: assume c_p is constant and uniform

$$\underbrace{c_p T\left(\frac{\partial \rho}{\partial t} + \nabla \cdot \rho \vec{v}\right)^{+} \rho c_p \left(\frac{\partial T}{\partial t} + (\vec{v} \cdot \nabla)T\right) = \dot{S}_v - (\nabla \cdot \vec{q})$$

Since $\nabla \cdot \vec{q} = -k\nabla^2 T$.

Result

$$\rho c_p \left(\frac{\partial T}{\partial t} + (\vec{\mathbf{v}} \cdot \nabla) T \right) = \dot{S_v} + k \nabla^2 T$$

Alternatively

$$\underbrace{\rho c_p \frac{DT}{Dt}}_{\odot} = \underbrace{\dot{S_v}}_{\odot} + \underbrace{k \nabla^2 T}_{\odot}$$

- ① Rate of change of heat in fluid particle
- ② Rate of heat generation
- ③ Rate of heat accumulation by conduction

4.3.3 Special Cases of the Differential Form of Heat Equation

No heat generation ($\dot{S}_v = 0$)

$$\frac{\partial T}{\partial t} + (\vec{\mathbf{v}} \cdot \nabla)T = \alpha \nabla^2 T$$

where $k \to \alpha = \frac{k}{\rho c_p}$ is the **thermal diffusivity**, with the unit m²/s.

No advection ($\vec{v} = 0$)

$$\frac{\partial T}{\partial t} = \alpha \nabla^2 T + \frac{\dot{S}_v}{\rho c_p}$$

Steady-state ($\frac{\partial T}{\partial t} = 0$)

$$(\vec{\mathbf{v}}\cdot\nabla)T = \alpha\nabla^2 T + \frac{\dot{S}_v}{\rho c_p}$$

4.4 Similarity

Transport of	Governing Equation	"Diffusivity"	Source Term
Heat	$\frac{\partial T}{\partial t} + (\vec{\mathbf{v}} \cdot \nabla)T = \alpha \nabla^2 T + \dot{S}_T$	$\alpha = k/\rho c_p$	$\dot{S}_T = \dot{S}_v / \rho c_p$
Mass	$\frac{\partial C}{\partial t} + (\vec{\mathbf{v}} \cdot \nabla)C = \mathcal{D}\nabla^2 C + S_C$	${\cal D}$	S_C
Momentum (N-S)	$\frac{\partial \vec{\mathbf{v}}}{\partial t} + (\vec{\mathbf{v}} \cdot \nabla) \vec{\mathbf{v}} = v \nabla^2 \vec{\mathbf{v}} + \dot{S}_v$	$v = \mu/\rho$	$\dot{S}_v = (-\nabla p + \rho \mathbf{g})/\rho$

5 Steady-State Heat Conduction

5.1 Boundary Conditions

The 1-D heat equation is second-order in spatial coordinates (x) and first-order in time (t), so two *boundary conditions* and one *initial condition* are needed.



Table 1: Three types of boundary conditions: Dirichlet, Neumann, Newton's Law of Cooling

5.2 Example 1: 1-D Steady-State Conduction in a Wall





5.2.1 Thermal Resistance

The linear temperature profile from the above example allows us to use the concept of **resistance** to construct an equivalent "**thermal circuit**".

Thermal Resistance Analogous to the electrical resistance,

current flow <i>I</i> [A]	heat flux $\dot{\mathcal{Q}}[\mathrm{W}]$
$I = \frac{1}{R} \Delta V$	$\dot{Q} = \frac{kA}{L}\Delta T$
$V_1 \qquad \begin{array}{c} R \qquad V_2 \\ \bullet \qquad \\ \Delta V \end{array}$	$\begin{array}{c} T_1 & \underbrace{L}_{kA} & T_2 \\ \bullet & & & \\ \bullet & & & \\ & & & \\ \Delta T & & \\ \end{array}$

the **thermal resistance** of heat conduction, $R_{T,cond} = \frac{L}{kA} \begin{bmatrix} K \\ W \end{bmatrix}$, impedes the process of conduction.

• For other modes of heat transport in a *plane wall*, the thermal resistances are

Conduction , $R_{T,cond}$	Convection , $R_{T,conv}$	Radiation , $R_{T,rad}$
L	L	L
\overline{kA}	\overline{hA}	$\overline{h_r A}$

• For different geometries, the thermal resistances for conduction are

Geometry	Thermal Resistance, R _{T,cond}
plane wall	$\frac{L}{kA}$
cylindrical wall	$\frac{\ln(r_2/r_1)}{2\pi LA}$
spherical wall	$\frac{1}{4\pi k}(\frac{1}{r_1} - \frac{1}{r_2})$

Contact Resistance Conduction across the true contact area. Convection/radiation across gaps.

5.3 Example 2: Steady-State Conduction in a Cylinder

Example: Conduction Through a CylinderAssumptions1-D steady-state conduction $\Rightarrow \partial/\partial t = 0;$ $T = T_{s,2}$ \cdot no external heat generation $\Rightarrow \dot{S}_v = 0;$ r_1 r_2 \cdot no convection is considered $\Rightarrow (\vec{v} \cdot \nabla)T = 0;$ r_1 \cdot constant k.L

Solution Procedure Start from the heat equation:

$$oc_p \left(\frac{\partial T}{\partial t} + (\vec{\nu} \cdot \nabla) T \right)^0 = \dot{S}_v^0 + k \nabla^2 T$$

In cylindrical coordinates:

$$\nabla^2 T = \frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial T}{\partial r} \right) + \frac{1}{r^2} \frac{\partial^2 \mathcal{T}}{\partial \theta^2} + \frac{\partial^2 \mathcal{T}}{\partial z^2} + \frac{\partial^2 \mathcal{T}}{\partial z^2}$$

Therefore:

$$\nabla^2 T = 0 \implies T = C_1 \ln(r) + C_2$$

Impose the Dirichlet boundary conditions for constants C_1 and C_2 :

•
$$r = r_1, T = T_{s,1} \implies C_1 = \frac{T_{s,1} - T_{s,2}}{\ln(r_1/r_2)}$$

• $r = r_2, T = T_{s,2} \implies C_2 = T_{s,2} - \frac{T_{s,1} - T_{s,2}}{\ln(r_1/r_2)} \ln(r_2)$

Therefore,

$$T(r) = \frac{T_{s,1} - T_{s,2}}{\ln(r_1/r_2)} \ln\left(\frac{r}{r_2}\right) + T_{s,2}$$



5.4 Example 3: Wall Exposed to Convection

Example: Wall Exposed to Convection

Assumptions

- 1-D steady-state conduction $\Rightarrow \partial/\partial t = 0$;
- no external heat generation $\Rightarrow \dot{S}_v = 0$;
- exposed to fluid convection T_{∞} at x = L;
- constant k.
- Aim Solve for T(x) in wall.

Solution Procedure Start from the heat equation:

$$\rho c_p \left(\frac{\partial T}{\partial t} + (\vec{v} \cdot \nabla) T \right)^0 = \dot{S}_v^0 + k \nabla^2 T$$

Rearrange,

$$\frac{\mathrm{d}^2 T}{\mathrm{d} x^2} = 0 \implies T = C_1 x + C_2$$

Impose the boundary conditions for constants C_1 and C_2 :

- Dirichlet condition: $x = 0, T = T_0 \implies C_2 = 0$
- Newton's Law of Cooling: x = L, $-k \frac{\mathrm{d}T}{\mathrm{d}x} = h(T_0 T_\infty) \implies C_1 = -\frac{h(T_0 T_\infty)}{k + hL}$

Therefore,

$$T(x) = -\frac{h(T_0 - T_\infty)}{k + hL}x + T_0$$

How does the temperature profile within the wall look like? The gradient of T(x) is $-\frac{h(T_0 - T_{\infty})}{k + hL}$. Since $T_0 - T_{\infty}$ is constant, what determines the temperature distribution within the wall is the term $\frac{h}{k + hL}$ (ignore the minus symbol) \Rightarrow need to discuss the following cases

- *h* >> *k*, *i.e.*, convection is greater than conduction;
- $h \approx k$, *i.e.*, convection is about the same as conduction;
- *h* << *k*, *i.e.*, conduction is grater than convection.

We thus introduce the Biot number, Bi, that represents the ratio of convection to conduction.



5.4.1 The Biot Number

The Biot number, *Bi*, is a dimensionless number, that represents the relative magnitude of *surface convection* to *conduction within a solid*.

Bi =
$$\frac{\frac{L}{kA}}{\frac{1}{hA}} = \frac{hL}{k} = \frac{\text{temperature drop in wall}}{\text{temperature drop across surface}} \begin{bmatrix} \frac{W/(m^2 - K) \cdot m}{W/(m \cdot K)} \end{bmatrix}$$

- if $Bi \ll 1$: convection is more dominant \Rightarrow assume *uniform* temperature within solid;
- if $Bi \gg 1$: cannot assume uniform temperature within solid.

Therefore, the temperature profile within the solid from the above example



5.5 Example 4: Internal Heat Generation



Start from the heat equation:

$$\rho c_p \left(\frac{\partial T}{\partial t} + (\vec{v} \cdot \nabla) T \right)^0 = \dot{S}_v + k \nabla^2 T$$

Rearrange,

$$k \frac{\mathrm{d}^2 T}{\mathrm{d}x^2} + \dot{S}_v = 0 \quad \Rightarrow \quad T = -\frac{\dot{S}_v}{2k}x^2 + C_1 x + C_2$$

Impose the boundary conditions for constants C_1 and C_2 :

• Neumann condition: $x = 0, \frac{\mathrm{d}T}{\mathrm{d}x} = 0 \implies C_1 = 0$

• Newton's Law of Cooling: x = L, $-k \frac{\mathrm{d}T}{\mathrm{d}x} = h(T - T_{\infty}) \implies C_2 = \frac{\dot{S_v}L}{h} + \frac{\dot{S_v}L^2}{2k} + T_{\infty}$

Therefore,

$$T(x) = \frac{\dot{S}_{v}L^{2}}{2k} \left(1 - \frac{x^{2}}{L^{2}}\right) + \frac{\dot{S}_{v}L}{h} + T_{\infty}$$

Symmetry of the solution along the centreline As we only solved the solution from x = 0 to x = L (right half of the geometry), the full temperature profile can be obtained by mapping the solution along the centreline.

6 Transient Heat Conduction

6.1 Lumped Capacitance Method

Problem Formulation Consider a planar wall at an initial uniform temperature T_i -

- At t = 0, the wall is exposed to fluid at temperature T_{∞} ;
- Time-dependent changes in wall temperature from T_i to T_{∞} (figure).

No convection and heat generation were considered. Given the initial and boundary conditions (x, t):

- [IC] At $t = 0^-$ (*immediately* before the initial convection exposure), $T = T_i$, for all $x \ge 0$
- [BC] At x = 0, $T = T_s$, for all $t \ge 0^+$ (after the convection exposure)
- [BC] At $x \to \infty$, $T \to T_i$, for all $t \ge 0^+$

Aim Determine the temperature profile T(x, t).

Solution Procedure If $Bi \ll 1$: temperature is nearly *uniform* within the solid at each point in time,

- Conduction is very fast within the solid;
- Convection is very slow from the contact surface.

Therefore, we could simplify the problem $T(x, t) \rightarrow T(t)$.

Start from the differential form of the heat equation,

$$\frac{\partial}{\partial t} \int_{CV} \rho c_p T dV = \int_{CV} \dot{S}_v dV - \oint_{CS} (\vec{q} \cdot \hat{n}) dA - \oint_{CS} \rho c_p T (\vec{v} \cdot n) dA = 0, \text{ no advection}$$

As ρ , c_p and T are uniform within CV, only T changes with time ($\partial \rightarrow d$):

$$\rho c_p V \frac{\mathrm{d}T}{\mathrm{d}t} = -q_h A \quad \Rightarrow \quad \rho c_p V \frac{\mathrm{d}T}{\mathrm{d}t} = -\underbrace{h(T - T_\infty)}_{q_h} A$$

The above equation states the balance of the *rate of change of the thermal energy* and *the convective heat transfer from surface*.

It can be further re-arranged to a first-order ODE:

$$\frac{\mathrm{d}T}{\mathrm{d}t} = -\frac{hA}{\rho c_p V} (T - T_\infty)$$

Define two parameters $\Theta = T - T_{\infty}, \tau = \frac{\rho c_p V}{hA}$,

$$\frac{\mathrm{d}\Theta}{\mathrm{d}t} = -\frac{1}{\tau}\Theta \quad \xrightarrow{\text{solve the ODE}} \quad \Theta = C_1 e^{-t/\tau}$$

where the constant C_1 is subjected to the initial condition $\Rightarrow C_1 = T_i - T_{\infty}$. The general solution is

$$\Theta = (T_i - T_{\infty})e^{-t/\tau} \quad \xrightarrow{\text{expand}} \quad T = (T_i - T_{\infty})e^{-t/\tau} + T_{\infty}$$

where $\tau = \frac{\rho c_p V}{hA} = \underbrace{\frac{1}{hA}}_{R_t} \underbrace{\rho c_p V}_{C_t}$ can be interpreted as the product of thermal resistance (R_t) and the

heat capacity of the wall (C_t) .

6.2 Transient Conduction through Semi-Infinite Solid

Start from the differential form of the heat equation,

$$\rho c_p \left(\frac{\partial T}{\partial t} + (\vec{v} - \nabla) T \right)^0 = \dot{S}_v^0 + k \nabla^2 T \quad \Rightarrow \quad \frac{\partial T}{\partial t} = \alpha \frac{\partial^2 T}{\partial x^2}$$

Define dimensionless variables:

- $T^* = \frac{T}{\hat{r}}$, where \hat{T} is the characteristic temperature scale;
- $t^* = \frac{t}{\hat{t}}$, where \hat{t} is the characteristic time scale;
- $x^* = \frac{x}{\hat{x}}$, where \hat{x} is the characteristic length scale.

Using chain rule:

$$\frac{\partial T}{\partial t} = \alpha \frac{\partial^2 T}{\partial x^2} \quad \Rightarrow \quad \frac{\hat{T}}{\hat{t}} \frac{\partial T^*}{\partial t^*} = \frac{\alpha \hat{T}}{\hat{x}^2} \frac{\partial^2 T^*}{\partial x^{*2}} \quad \xrightarrow{\text{divide by } \hat{T}} \quad \frac{1}{\hat{t}} \frac{\partial T^*}{\partial t^*} = \frac{\alpha}{\hat{x}^2} \frac{\partial^2 T^*}{\partial x^{*2}}$$

Since $\frac{\partial T^*}{\partial t^*} \sim O(1)$ and $\frac{\partial^2 T^*}{\partial x^{*2}} \sim O(1)$, *i.e.*, dimensionless derivatives have an order of magnitude of 1 since both the denominator and numerator quantities are of the same dimension; the remaining terms must also have similarities in order for the equation holds true:

$$\frac{1}{t^*} \sim \frac{\alpha}{x^{*2}} \quad \Rightarrow \quad x^* \sim \sqrt{\alpha t^*}$$

Given the temperature profile at time t_1 , what does the temperature profile look like at some later time t_2 ? Motivated by the concept of "self-similarity", define a similarity variable, η

$$\eta = \frac{x}{2\sqrt{\alpha t}}$$

This would allow us to perform change of variable,

$$\frac{\partial T}{\partial t} = \alpha \frac{\partial^2 T}{\partial x^2} \quad \Leftrightarrow \quad \left[-2\eta \frac{\mathrm{d}T}{\mathrm{d}\eta} = \frac{\mathrm{d}^2 T}{\mathrm{d}\eta^2} \right]$$

Derivation

The partial differentials of η with respect to t and x are

$$\frac{\partial \eta}{\partial t} = -\frac{x\alpha}{4(\alpha t)^{\frac{3}{2}}} = -\frac{1}{4}\frac{x}{\sqrt{\alpha t}}\frac{\alpha}{\alpha t} = -\frac{\eta}{2t} \text{ and } \frac{\partial \eta}{\partial x} = \frac{1}{2\sqrt{\alpha t}}$$

By chain rule, the first term in heat equation can be expressed as

$$\frac{\partial T}{\partial t} = \frac{\mathrm{d}T}{\mathrm{d}\eta} \frac{\partial \eta}{\partial t} = \underbrace{-\frac{\eta}{2t} \frac{\mathrm{d}T}{\mathrm{d}\eta}}_{\text{new LHS}}$$

the second term in heat equation can be expressed as

$$\frac{\partial^2 T}{\partial x^2} = \frac{\mathrm{d}^2 T}{\mathrm{d}\eta^2} \left(\frac{\partial\eta}{\partial x}\right)^2 = \underbrace{\frac{1}{4\alpha t} \frac{\mathrm{d}^2 T}{\mathrm{d}\eta^2}}_{\text{new R.H.S.}}$$

Equate the new L.H.S. to the new R.H.S., and rearrange, the new ODE is

$$-2\eta \frac{\mathrm{d}T}{\mathrm{d}\eta} = \frac{\mathrm{d}^2 T}{\mathrm{d}\eta^2}$$

$$-2\eta \frac{\mathrm{d}T}{\mathrm{d}\eta} = \frac{\mathrm{d}^2 T}{\mathrm{d}\eta^2} \implies -2\eta\xi = \frac{\mathrm{d}\xi}{\mathrm{d}\eta} \implies -\int 2\eta \mathrm{d}\eta = \int \frac{1}{\xi} \mathrm{d}\xi$$

This gives us

$$-\eta^2 = \ln \xi + C_1 \quad \Rightarrow \quad \xi = C_2 e^{-\eta^2}$$

Therefore, by definition $\xi = dT/d\eta$:

$$T = C_2 \int_0^{\eta} e^{-s^2} \mathrm{d}s + C_3$$

where *s* here within the integral is a dummy variable.

Impose the boundary conditions:

• at $\eta = 0, T = T_s, \Rightarrow C_3 = T_s$

• as
$$\eta \to \infty, T \to T_i, \Rightarrow C_2 = \frac{2(T_i - T_s)}{\sqrt{\pi}}$$

Therefore,

$$T = \frac{2(T_i - T_s)}{\sqrt{\pi}} \int_0^{\eta} e^{-s^2} \mathrm{d}s + T_s$$

Define the error function erf as

$$\operatorname{erf}(z) = \frac{2}{\sqrt{\pi}} \int_0^z e^{-s^2} \mathrm{d}s$$

and substitute

$$T = (T_i - T_s) \operatorname{erf}(\eta) + T_s$$

Alternatively, define the co-error function, ${\rm erfc}$ as

$$\operatorname{erfc}(z) = 1 - \operatorname{erf}(z)$$

The solution becomes

$$T = (T_s - T_i) \operatorname{erfc}(\eta) + T_i \implies T = (T_s - T_i) \operatorname{erfc}\left(\frac{x}{2\sqrt{\alpha t}}\right) + T_i$$

Z	$\operatorname{erf}(z)$		$\operatorname{erf}(z)$	Z	$\operatorname{erf}(z)$
0.000	0.00000	0.360	0.38933	1.040	0.85865
0.020	0.02256	0.380	0.40901	1.080	0.87333
0.040	0.04511	0.400	0.42839	1.120	0.88679
0.060	0.06762	0.440	0.46623	1.160	0.89910
0.080	0.09008	0.480	0.50275	1.200	0.91031
0.100	0.11246	0.520	0.53790	1.300	0.93401
0.120	0.13476	0.560	0.57162	1.400	0.95229
0.140	0.15695	0.600	0.60386	1.500	0.96611
0.160	0.17901	0.640	0.63459	1.600	0.97635
0.180	0.20094	0.680	0.66378	1.700	0.98379
0.200	0.22270	0.720	0.69143	1.800	0.98909
0.220	0.24430	0.760	0.71754	1.900	0.99279
0.240	0.26570	0.800	0.74210	2.000	0.99532
0.260	0.28690	0.840	0.76514	2.200	0.99814
0.280	0.30788	0.880	0.78669	2.400	0.99931
0.300	0.32863	0.920	0.80677	2.600	0.99976
0.320	0.34913	0.960	0.82542	2.800	0.99992
0.340	0.36936	1.000	0.84270	3.000	0.99998

Table 2: Values of z and erf(z)

7 Convective Heat Transfer

Convection The energy transfer between a surface and a fluid moving over the surface.

To find the *total convective heat flow*, \dot{Q}_h ,

$$\dot{Q}_h = \int\limits_{A_s} q_h \mathrm{d}A = (T_s - T_\infty) \int\limits_{A_s} h \mathrm{d}A$$

Define the *average* convection coefficient, \bar{h} , has the following expression:

$$\bar{h} = \frac{1}{A_s} \int_{A_s} h \mathrm{d}A_s$$

Therefore,

$$\dot{Q}_h = \bar{h}A_s(T_s - T_\infty)$$

This expression is useful in describing convective heat transfer for a whole body.

7.1 Boundary Layers and Heat Convective Coefficient

Convection occurs at a surface, but how does fluid interact with the surface? This requires knowledge of boundary layers.

7.1.1 Velocity Boundary Layer

Consider a uniform free-stream flow contacting a flat surface, the velocity u increases from 0 at the surface (non-slip condition) to approximately u_{∞} at some distance from the surface, δ_V .

Figure 6: A uniform "free-stream" flow contacting a flat surface

where

- u_{∞} : free stream velocity;
- u(x, y): boundary layer velocity profile;
- δ_V : velocity boundary layer thickness.

Velocity boundary layer thickness $\delta_v \sim \sqrt{vt}$, where v is defined as effective diffusivity with the expression $v = \mu/\rho$.

7.1.2 Thermal Boundary Layer

Consider a uniform free-stream flow contacting an isothermal flat surface: at y = 0, there is a thermal equilibrium between the flow and the surface; Thermal "diffusion" transfers heat through fluid.

Figure 7: A uniform "free-stream" flow contacting a flat surface

where

- T_{∞} : free stream temperature;
- T(x, y): boundary layer temperature profile;
- δ_T : temperature boundary layer thickness.

Thermal boundary layer thickness $\delta_T \sim \sqrt{\alpha t}$, where α is defined as **effective diffusivity** with the expression $\alpha = k/\rho c_p$.

Thermal and velocity boundary layers occur simultaneously!

7.1.3 Heat Convective Coefficient

Given a thermal boundary layer, how do we calculate *h*? At y = 0, both convection and conduction occur, this states two fluxes must be balanced, $q_h = q_k$,

$$\underbrace{h(T_s - T_m)}_{q_h} = \underbrace{-k \frac{\mathrm{d}T}{\mathrm{d}y}}_{q_k} \implies h = -\frac{k}{(T_s - T_\infty)} \frac{\mathrm{d}T}{\mathrm{d}y}\Big|_{y=0}$$

Define the dimensionless temperature, Θ , and the dimensionless y-length scale, y^* ,

$$\Theta = \frac{T - T_{\infty}}{T_s - T_{\infty}}, \qquad y^* = \frac{y}{\delta_T}$$

Hence,

$$h = -\frac{k}{(T_s - T_{\infty})} \frac{\mathrm{d}T}{\mathrm{d}y} \bigg|_{y=0}$$
$$= -\frac{k}{(T_s - T_{\infty})} \frac{(T_s - T_{\infty})}{\delta_T} \frac{\mathrm{d}\Theta}{\mathrm{d}y^*} \bigg|_{y=0}$$
$$= -\frac{k\sqrt{u_{\infty}}}{\sqrt{\alpha x}} \frac{\mathrm{d}\Theta}{\mathrm{d}y^*} \bigg|_{y=0}$$

This states

$$h \sim \frac{k\sqrt{u_{\infty}}}{\sqrt{\alpha x}} \frac{\mathrm{d}\Theta}{\mathrm{d}y^*}$$

where *h* decreases like $1/\sqrt{x}$.

7.2 Turbulence

Motivation The first step in a convection problem is to determine whether the boundary layer is laminar or turbulent.

What is turbulence?

- Laminar flow: fluid flows in parallel layers without mixing.
- Turbulent flow: irregular, non-laminar or chaotic flow pathways with mixing.

Figure 8: Velocity boundary layer development on a flat plate.

Figure 9: Turbulence in a pipe.

• Boundary layer transition to turbulence after a critical length, x_c . Reynolds number, Re, depicts the turbulent transition:

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

7.3 Boundary Layer Thickness

Dimensionless Number	Expression	Description
Reynolds Number	$\operatorname{Re}_x = \frac{u_{\infty}x}{v}$	ratio of internal to viscous forces
Prandtl Number	$\Pr = \frac{\nu}{\alpha}$	ratio of momentum to thermal diffusivity
Biot Number	$\mathrm{Bi} = \frac{hL}{k}$	ratio of conductive resistance to convective resis- tance (in solid)
Nusselt Number	$\mathrm{Nu} = \frac{hL}{k}$	dimensionless temperature gradient at surface (in fluid)

Table 3: Summary of dimensionless numbers

7.3.1 The Prandtl Number, Pr

The Prandtl number, Pr, represents the ratio of *momentum diffusivity* $\left(v = \frac{\mu}{\rho} \left[\frac{m^2}{s}\right]\right)$ to *thermal diffusivity* $\left(\alpha = \frac{k}{\rho c_p} \left[\frac{m^2}{s}\right]\right)$. It is an intrinsic property of the fluid at a set temperature.

Consider external flow over a flat plate,

$$\frac{\delta_V}{\delta_T} \sim \frac{\sqrt{\nu}}{\sqrt{\alpha}} = Pr^{\frac{1}{2}}$$

thus, Pr gives a physical indication of the relative thickness of the viscous boundary layer δ_V to the thermal boundary layer δ_T .

7.3.2 Velocity Boundary Layer Thickness, δ_V

$$\delta_V \sim x \ R e_x^{-\frac{1}{2}}$$

What is the scale of δ_V ?

Neglect any thermal effects \Rightarrow no change in ν and ρ .

Momentum diffuses from a flat plate into semi-infinite fluid \Rightarrow viscous penetration depth:

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

Re-arrange:

$$\delta_V \sim \left(\frac{\nu x}{u_{\infty}}\right)^{\frac{1}{2}} = \underbrace{\left(\frac{\nu}{u_{\infty} x}\right)^{\frac{1}{2}}}_{Re^{-\frac{1}{2}}} x = \boxed{x Re^{-\frac{1}{2}}}$$

7.3.3 Thermal Boundary Layer Thickness, δ_T

For $Pr \ll 1$ $\delta_V \ll \delta_T$,

$$h \sim \frac{k}{\delta_T} \sim k \; \frac{u_{\infty}^{\frac{1}{2}}}{\alpha^{\frac{1}{2}} \; x^{\frac{1}{2}}} \; \Rightarrow \; \delta_T \sim x \left(\alpha \frac{x}{u_{\infty}} \right)^{\frac{1}{2}}$$

Also,

$$\underbrace{\frac{h x}{k}}_{Nu_{x}} \sim \underbrace{\frac{u_{\infty}^{\frac{1}{2}} x^{\frac{1}{2}}}{v^{\frac{1}{2}}}}_{Re_{x}^{\frac{1}{2}}} \underbrace{\frac{v^{\frac{1}{2}}}{\alpha^{\frac{1}{2}}}}_{Pr^{\frac{1}{2}}} \Rightarrow Nu_{x} \sim Re_{x}^{\frac{1}{2}} Pr^{\frac{1}{2}}$$

1

For Pr >> 1

$$\delta_T \sim \left(\frac{\alpha x}{u}\right)^{\frac{1}{2}} \sim \left(\frac{\alpha x \,\delta_V}{u_\infty \,\delta_T}\right)^{\frac{1}{2}}$$

Thus,

$$\frac{\delta_T^3}{\delta_V^3} \sim \frac{\alpha x}{u_\infty \delta_V^2} \sim \frac{\alpha Re_x}{u_\infty x} = \frac{\nu Re_x}{u_\infty x} \frac{1}{\nu} \sim \frac{1}{Pr} \implies \frac{\delta_V}{\delta_T} \sim Pr^{\frac{1}{3}}$$

Since

$$\delta_V \sim x \ Re_x^{-\frac{1}{2}}$$
$$\delta_T \sim x \ Re^{-\frac{1}{2}} Pr^{-\frac{1}{3}}$$

7.4 Internal Flow

Velocity entrance length Hydrodynamic entrance length

 $x_{e,v} \approx 0.005 DRe_D$

Thermal entrance length

 $x_{e,T} = 0.005 DRe_D Pr$

• when $x > x_{e,T}$, there is no fixed free stream temperature T_{∞} - a mean temperature, T_m , replaced T_{∞} as the reference temperature.

$$T_m = \frac{2\pi}{Q} \int_0^R T u r \mathrm{d}r$$

• when the boundary layer is thermally fully developed: adding heat must increase the temperature - *T* changed in space, not time, general shape of the thermal profile is preserved.

Assume a constant profile,

$$\Theta' = a \left(1 - \frac{r^2}{R^2} \right) \quad \Rightarrow \quad T = a (T_m - T_s) \left(1 - \frac{r^2}{R^2} \right) + T_s$$
$$\Rightarrow \quad \frac{\partial T}{\partial r} = a (T_m - T_s) \left(- \frac{2r}{R^2} \right)$$

Therefore,

$$q_r = h(T_m - T_s) = -k \frac{\partial T}{\partial r} \Big|_{r=R}$$

$$\Rightarrow \quad h(T_m - T_s) = \frac{2ka}{R} (T_m - T_s)$$

$$\Rightarrow \quad h = \frac{4ka}{D}$$

Therefore, the Nusselt Number

$$Nu_D = \frac{hD}{k} = 4a \approx 4 \implies \begin{cases} 4.36, & \text{uniform surface heat flux} \\ 3.66, & \text{uniform surface temperature} \end{cases}$$

8 Mass Transport

8.1 Advection and Diffusion

• The total flux, \vec{j} ,

$$\vec{j} = \vec{j}_a + \vec{j}_d$$

• Advection of Solute, \vec{j}_a : If the solvent undergoes bulk motion, then there will be an additional solute flux as the solute is carried along with the flow.

$$\vec{j}_a = \vec{v}C$$

where C is the solute concentration.

• Diffusive Flux, \vec{j}_d : the diffusive flux of solute is driven by a concentration gradient.

$$\vec{j}_a = -\mathcal{D}_{AB}\nabla C$$

- The diffusivity, \mathcal{D}_{AB} , is determined by the Stokes-Einstein Relationship

$$\mathcal{D}_{AB} = \frac{k_B T}{6\pi\mu a}$$

where $k_B \approx 1.38 \times 10^{-2}$ J/K is the Boltzmann's constant; and $a = \left(\frac{3M_w}{4\pi\rho N_A}\right)^{\frac{1}{3}}$ with M_w being the molecular weight, N_A is Avogadro's number.

Pèclet number, Pe

$$\mathrm{Pe} = \frac{UL}{\mathcal{D}_{AB}}$$

which states the ratio of advection to diffusion.

8.2 The Integral and Differential Form of the Conservation of Mass

The Integral form

$$\frac{\partial}{\partial t} \int_{CV} C dV = \int_{CV} \dot{S}_{v} dV - \oint_{CS} (\vec{j}_{d} \cdot \hat{n}) dA - \oint_{CS} C(\vec{v} \cdot \hat{n}) dA$$

The differential form

$$\frac{\partial C}{\partial t} + (\vec{\mathbf{v}} \cdot \nabla)C = \mathcal{D}\nabla^2 C + \dot{S}_v$$

A special case: Fick's Second Law - no advection (u = 0) nor solute production ($\dot{S}_v = 0$)

$$\frac{\partial C}{\partial t} = \mathcal{D}\nabla^2 C$$

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