Lecture 1

Tuesday, January 9, 2018 8:56 AM

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use syllabus problem-solving format on Hwk + Exams

MAP OF HEAT TRANSFER

$$\Delta U = Q + W$$

$$\frac{dU}{dt} = \sum_{in} \dot{m}_{in} h_{in} - \sum_{out} \dot{m}_{out} + \dot{Q} + \dot{W}$$

Thermodynamics Equilibrium

Course starts here

Chapter 1 Non-Equilibrium

Leads to temperature gradients and heat transfer

causes flow, 2nd law

Heat transfers through a solid ("diffusion")

Chapter 2 Heat Transfer Mechanisms

Heat transfers through the space

Chapter 3 - Conduction governing equations and boundary conditions

Heat transfers through a fluid

Chapter 8 - Radiation

Chapter 4 - Conduction Steady State – Temperature **does not change** with time

Chapter 5 - Conduction Non-Steady State Temperature **changes** with time

Chapter 6 - Convection Governing equations and Boundary conditions

Chapter 7 Freezing and Thawing

couples mass & heat transfer

Change/rate in system

branch of thermo → non-equilibrium thermo

energy conservation

Thermodynamics Equilibrium versus Transport Phenomena?

quiz example

- First Law states:
  energy conserved ----?
- Second Law states:
  entropy > 0 ----?
- These laws do not tell you:
  What --------? transport

go over slides before class

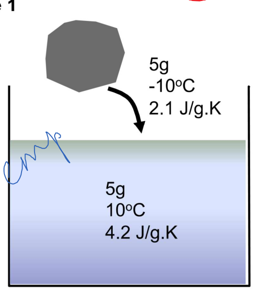
ENERGY CONSERVATION – First Law

Example 1

quiz example

before solving, educated guess

i.e. this temp should be > 0



do not know how fast, dist of Temp → need transport

$m_1 c_{p_1} \Delta T_1 = C_{p_2} \Delta T_2 m$

Assume no heat loss
What is the final temperature of the system?
System?
Open or closed system?

ENERGY CONSERVATION – First Law

Example 2

Quantities of water and ice are mixed, and we want to know how much ice melts

We have two situations

1. We wait a long time – what happens?

2. We wait a shorter time what happens? Could we calculate how much ice melts? What is the final temperature

- **Can we say how long it takes to reach the final temperature using equilibrium thermodynamics?**
- **Since we will be studying systems that are changing we will be studying non-equilibrium processes and we will be need additional laws to the thermodynamics laws**

Thermodynamics Equilibrium Review

more restrictive than steady state

- Two systems are said to be in thermal equilibrium when their temperatures are equal. **There are no heat flow in equilibrium**
- Non-equilibrium drives transport, which is the subject of this course
- In steady state, temperature does not change with time but **still there are heat flows**.

can change w/ time

can still have spatial differences

Thermodynamics Equilibrium versus Transport Phenomena?

What is the meaning of **transport phenomena**? interchange mass, heat, momentum

How many **transport phenomena** do we know to describe biological processes? fusion/fission of cells, oxygen uptake (lungs) digestion, intestine flow

What are the basic laws used to describe/model these **transport phenomena**?

1D transport in direction *x*

$$\boxed{Transport\,of\;Y\,(x) = -\,Property \cdot \frac{dY}{dx}}$$

Momentum	shear stress $\sigma = -\mu \dfrac{dv}{dx}$ a diff scalars	Newton Law - viscosity
Energy	energy $q(x) = -k\dfrac{dT}{dx}$	Fourier Law – Thermal conductivity
Mass	mass flux $j(x) = -D\dfrac{dC_A}{dx}$	First Fick Law – Diffusivity

extrapolate from 1D → 2D → 3D

What happens when the heat flow or the mass flow are not 1D, i.e. they transfer in all directions?

$$\underline{q}(x,y,z) = -k\ \nabla T(x,y,z)$$

$$\underline{j}_A(x,y,z) = -D\ \nabla C_A(x,y,z)$$

What is ∇ ? gradient operator.

∇ is the Vector Gradient

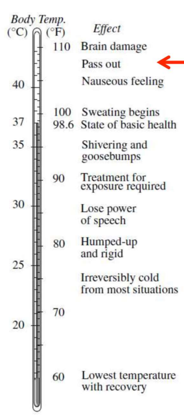
→ can analyze each direction individually

STOP 1/9

OBJECTIVES OF LECTURE 1

- Understand the physical processes and the laws describing modes **of heat transfer,** which are:
  - **Conduction**
  - **Convection** and
  - **Radiation**
- Understand the material properties that affect heat conduction in a material

Body, normal temperature



Locally, tissue is destroyed at 43-45°C

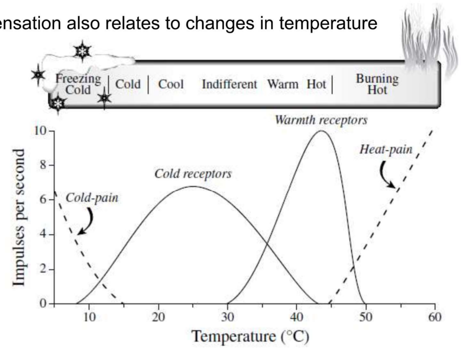
And below -45°C

Figure 1.4: Effect of various deep body temperatures on humans. Data from Egan (1975).

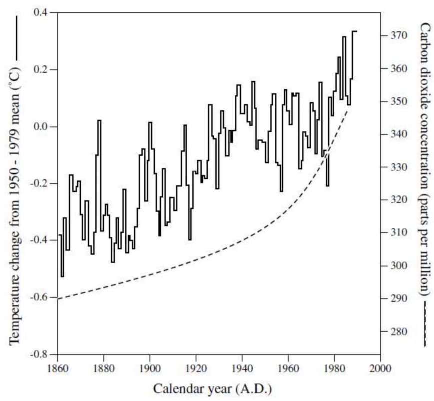
- Thermal Gradations discriminated by
  - Heat receptors
  - Cold receptors
  - Pain receptors

  Nerve ending under skin

- Thermal sensation also relates to changes in temperature



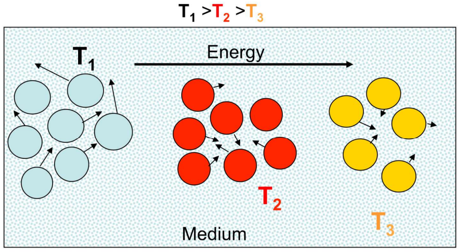
Global Warming – CO_2 concentration in recent times



- 0.5°C of real warming
- Few degree of warming can raise the sea level 0.2-1.5m

Conductive Heat Transfer (Heat Conduction)

$T_1 > T_2 > T_3$

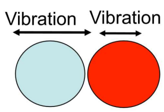


Conductive heat transfer is energy (heat) moving through a medium from its more energetic particles to the less energetic particles

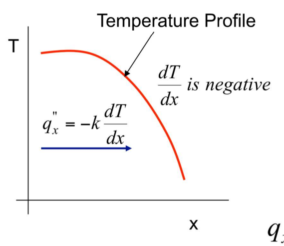
Structure of Materials

- Gas – molecules has freedom to move so energy is related to translation/rotation and vibration of the molecules
- Liquid – some between gases and solids, molecules move more randomly than in solids
- Solid – translation and rotation are restricted, so only vibration exists

Energy Transfer – Diffusion of Energy



Fourier Equation



$$\boxed{\frac{q_x}{A} = q''_x = -k\frac{dT}{dx}}$$

q_x : Rate of Heat Flow (Watts)

A : Area perpendicular to the flow (m^2)

k : Thermal conductivity ($W/m.K$)

$q''_x = \frac{q}{A}$: Heat Flux ($\frac{W}{m^2}$)

Fourier Equation

In three dimensions, heat flux is a vector that is oriented normal to surfaces of constant temperature known as *isotherms*

$$\vec{q}'' = q''_x \vec{i} + q''_y \vec{j} + q''_z \vec{k}$$

For isotropic materials (*k* is the same for each direction)

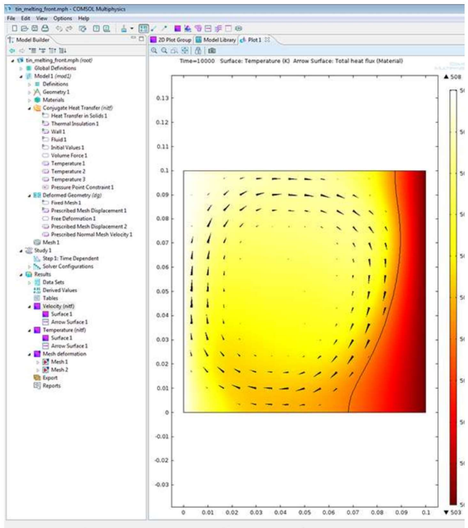
$$\vec{q}'' = -k\left[\frac{\partial T}{\partial x}\vec{i} + \frac{\partial T}{\partial y}\vec{j} + \frac{\partial T}{\partial z}\vec{k}\right]$$

Another short form to express the 3D Fourier Equation is:

$$\vec{q}'' = -k\nabla T \qquad \nabla: \text{Gradient Operator}$$

Read how this gradient can be expressed in different coordinate systems

Heat flux in 2D directions



Thermal Conductivity Units

$$q_x'' = -k\frac{dT}{dx}$$

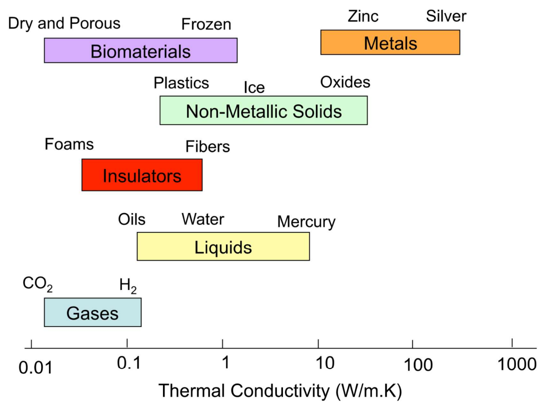
$$k = \frac{[q_x'']}{\left[\frac{dT}{dx}\right]} = \frac{[q_x]}{[A]\left[\frac{dT}{dx}\right]} = \frac{W(or\,\frac{J}{s})}{m^2\cdot\frac{K}{m}} = \frac{W}{m\cdot K} \qquad \text{(SI)}$$

$$k = \frac{[q_x'']}{\left[\frac{dT}{dx}\right]} = \frac{[q_x]}{[A]\left[\frac{dT}{dx}\right]} = \frac{\frac{BTU}{hr}}{ft^2\cdot\frac{F}{ft}} = \frac{BTU}{ft\cdot hr\cdot F} \qquad \text{(US)}$$

Units of Thermal Conductivity

$$k = 0.69\frac{W}{m\,K} = 0.69W/m\cdot K = 0.69W/(mK)$$

Range of Thermal Conductivities



Thermal Conductivity and other transport properties

Thermal conductivities (and other transport properties) of most materials **must be measured**, only for gases (and some liquids) could be predicted from the molecular characteristics of the gas

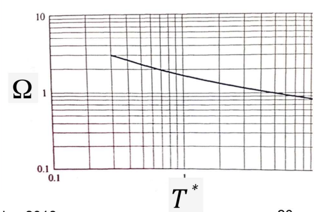
Thermal Conductivity

$$k = 83.3x10^{-3}\frac{\sqrt{\frac{T}{M}}}{\sigma^2\Omega} \quad (W/m.K)$$

T is given in degrees Kelvin

$$T^* = \frac{T}{\varepsilon/k_B} = \frac{k_B T}{\varepsilon}$$

Compound	σ (Å)	$\varepsilon/k_B\,(K)$	M
Hydrogen	2.83	59.7	2
Neon	2.82	32.8	20
Air	3.71	78.6	29
Oxygen	3.47	107	32
Argon	3.54	93.3	40
Benzene	5.35	412	58
Water	2.64	809	18



Prediction of Diffusivity D_{AB}

Diffusion of gas A in a medium B

$$D_{AB} = 1.86\times10^{-7}\frac{T^{3/2}}{\sqrt{M_{AB}}\,P\sigma_{AB}^2\Omega} \quad (\frac{m^2}{s})$$

$$M_{AB} = \frac{2M_A M_B}{M_A + M_B}$$

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

T is given in degrees Kelvin
P is given is atmosphere

Compound	σ (Å)	$\varepsilon/k_B\,(K)$	M
Hydrogen	2.83	59.7	2
Neon	2.82	32.8	20
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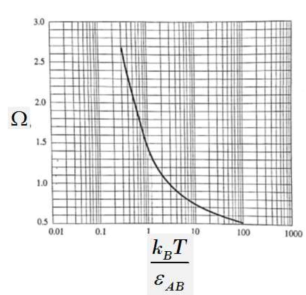

Prediction of viscosity μ

Viscosity $$\mu = 2.67x10^{-6} \frac{\sqrt{M\,T}}{\sigma^2 \Omega} \quad (Pa.s)$$

Compound	σ (Å)	$\varepsilon / k_B (K)$	*M*
Hydrogen	2.83	59.7	2
Neon	2.82	32.8	20
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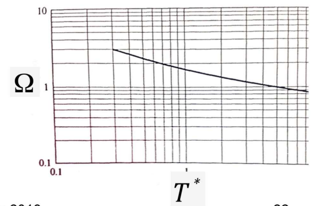
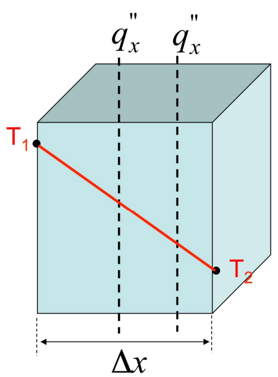


Simplified Heat Conduction Equations (Simple Systems)



$$q_x'' = -k\frac{dT}{dx}$$

- Steady State
- Constant *k*

$$q_x'' = -k\frac{\Delta T}{\Delta x}$$

$$q_x'' = -k\frac{T_2 - T_1}{\Delta x}$$

$$q_x'' = k\frac{T_1 - T_2}{\Delta x}$$

Thermal Diffusivity

$$q_x'' = -k\frac{dT}{dx}$$

$$q_x'' = -\frac{k}{\rho \cdot c}\frac{d(\rho \cdot c \cdot T)}{dx}$$

$$[\rho]\cdot[c]\cdot[T] = \frac{kg}{m^3}\cdot\frac{kJ}{kg\cdot K}\cdot K = \frac{kJ}{m^3}$$

$U = \rho \cdot c \cdot T$ [Energy per unit of Volume] ← "*concentration*" of energy"

$$q_x'' = -\frac{k}{\rho \cdot c}\frac{dU}{dx} = -\alpha\frac{dU}{dx}$$

Concept of Thermal Diffusivity

$$q_x'' = -\alpha \frac{dU}{dx}$$

U: "Concentration" of Energy

$\alpha : Thermal\text{"} Diffusivity\text{"}$

$$\boxed{Flux\ of\ Energy = -\alpha \cdot Gradient\ of\ Energy\ Concentration}$$

$$\alpha = \frac{k}{\rho \cdot c} \qquad \alpha = \frac{[k]}{[\rho]\cdot[c]} = \frac{\frac{W}{m \cdot K}}{\frac{kg}{m^3} \cdot \frac{J}{kg \cdot K}} = \frac{m^2}{s}$$

Thermal Diffusivity

$$q_x'' = -k \frac{dT}{dx}$$

Unsteady State Heat Transfer (temperature will change with time) and *k* independent of temperature – To be studied later – now accept the model equations

1D –Heat Transfer

$$\rho c \frac{\partial T}{\partial t} = k \frac{\partial^2 T}{\partial x^2} \longrightarrow \boxed{\frac{\partial T}{\partial t} = \frac{k}{\rho c} \frac{\partial^2 T}{\partial x^2} = \alpha \frac{\partial^2 T}{\partial x^2}}$$

3D –Heat Transfer

$$\rho c \frac{\partial T}{\partial t} = k \nabla^2 T \longrightarrow \boxed{\frac{\partial T}{\partial t} = \frac{k}{\rho c} \nabla^2 T = \alpha \nabla^2 T}$$

Because *T(x,t)* $\frac{dT}{dt} \Rightarrow \frac{\partial T}{\partial t}$ **and** $\frac{d^2 T}{dx^2} \Rightarrow \frac{\partial^2 T}{\partial x^2}$

Thermal Diffusivity

$$\alpha = \frac{k}{\underbrace{\rho \cdot c}}$$

Ability of a material to transfer heat

Thermal mass of the material (J/m^{3}K)

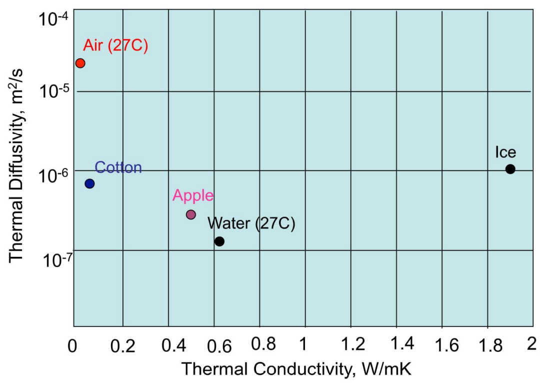
"Volumetric" Heat Capacity

$$\alpha = \frac{k}{\rho \cdot c}$$

Non porous Material – Density ?
Solid Density

Porous Material – Density ?
Bulk Density

Thermal Diffusivity

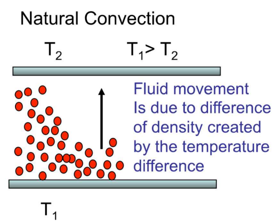


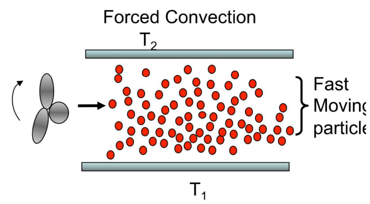
CONVECTIVE HEAT TRANSFER

Heat is transferred because the medium moves, it occurs in the presence of liquids or gases

$$q_{1-2} = hA(T_1 - T_2)$$

(**It is not a law**, *h,* the convection coefficient, depends on several factors, temperature, geometry, etc. in addition to the properties of the material





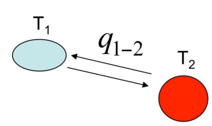
RADIACTIVE HEAT TRANSFER

Any matter at T > 0K will emit radiation. That radiation is attributed to changes in the electron configuration with temperature. Radiation is an electromagnetic wave. **No medium is necessary to transfer radiation**. Stefan- Boltzman Law

$$\frac{q}{A} = \sigma T^4$$

$$\sigma = 5.676x10^{-8} \frac{W}{m^2 K^4}$$

$$\sigma = 0.174x10^{-8} \frac{BTU}{hr \cdot ft^2 R^4}$$



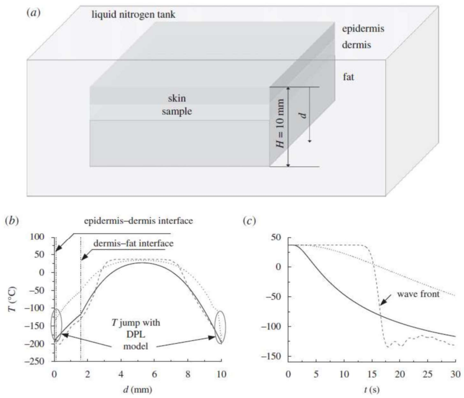
$$\frac{q_{1-2}}{A} = \sigma(T_1^4 - T_2^4)$$

$$\frac{q_{1-2}}{A} = h_r(T_1 - T_2)$$

$$h_r ?$$

Here K and C or F or R cannot be exchanged as when you have a temperature differences

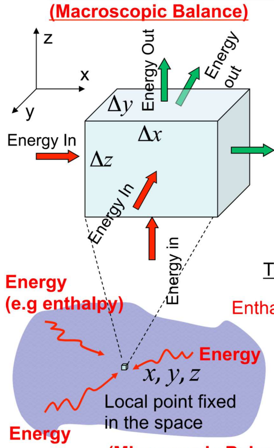
Energy Balance Equation
Microscopic versus Macroscopic



Energy Balance Equation
Objectives

- Identify the different terms (conduction, convection, heat generation, etc) in the equation of the energy balance.
- Define commonly used boundary conditions
- Applications of the energy equation

HEAT TRANSFER FROM AN ENERGY CONSERVATION STANDPOINT
(Macroscopic Balance)



(Microscopic Balance)

$$\boxed{\dot{E}_{in} - \dot{E}_{out} + \dot{E}_{gen} = \dot{E}_{st}}$$

$$Energy \equiv Heat$$

We need to consider heat transferred to any location ***macroscopically*** represented as a rectangular volume $V = \Delta x \cdot \Delta y \cdot \Delta z$

Transport of Energy by the movement of the fluid

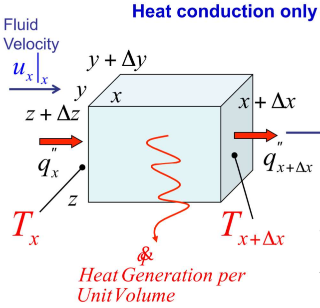
Enthalpy $\rightarrow$ $\dot{m}c(T - T_{ref})$ $\quad T_{ref} = 0$

$$\dot{m} = uA\rho = \left[\frac{m}{s}\right]\cdot\left[m^2\right]\cdot\left[\frac{kg}{m^3}\right] = \left[\frac{kg}{s}\right]$$

$$\dot{m}c(T - T_{ref}) = \left[\frac{kg}{s}\right]\left[\frac{kJ}{kg \cdot K}\right]\left[K\right] = \left[\frac{kJ}{s}\right] = \left[kW\right]$$

HEAT TRANSFER FROM AN ENERGY CONSERVATION STANDPOINT

Heat conduction only in one direction (direction *x*)



$u_x|_{x+\Delta x}$ Fluid Velocity

Macroscopic Energy Balance

$$\boxed{\dot{E}_{in} - \dot{E}_{out} + \dot{E}_{gen} = \dot{E}_{st}}$$

$$\dot{E}_{in} = q_x'' A_x + A_x u_x \rho c T_x$$

$$\dot{E}_{out} = q_{x+\Delta x}'' A_{x+\Delta x} + A_{x+\Delta x} u_{x+\Delta x} \rho c T_{x+\Delta x}$$

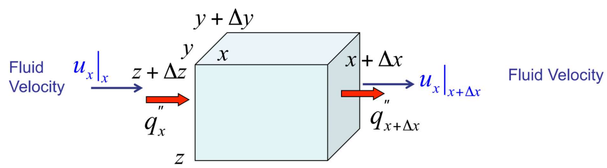
$$\dot{E}_{gen} = \dot{q}\Delta x \Delta y \Delta z$$

$$\dot{E}_{st} = \Delta x \Delta y \Delta z \rho c \frac{\Delta T}{\Delta t}$$

In an interval of time Δt

$$\left[\left(q_x'' + \rho c (uT)_x\right) - \left(q_{x+\Delta x}'' + \rho c (uT)_{x+\Delta x}\right)\right]\Delta y \Delta z \Delta t + \dot{q}\Delta x \Delta y \Delta z \Delta t = \Delta x \Delta y \Delta z \rho c \Delta$$

HEAT TRANSFER FROM AN ENERGY CONSERVATION STANDPOINT



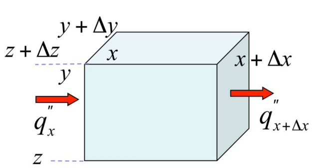
$$\left[\left(q_x'' + \rho c (uT)_x\right) - \left(q_{x+\Delta x}'' + \rho c (uT)_{x+\Delta x}\right)\right]\Delta y \Delta z \Delta t + \dot{q}\Delta x \Delta y \Delta z \Delta t = \Delta x \Delta y \Delta z \rho c \Delta T$$

$$\left(\underbrace{q_x'' - q_{x+\Delta x}''} + \rho c \left((uT)_x - (uT)_{x+\Delta x}\right)\right)\Delta y \Delta z \Delta t + \dot{q}\Delta x \Delta y \Delta z \Delta t = \Delta x \Delta y \Delta z \rho c \Delta T$$

Fourier Law $\longrightarrow$ $q_x'' - q_{x+\Delta x}'' = -k\left.\frac{\partial T}{\partial x}\right|_x - \left(-k\left.\frac{\partial T}{\partial x}\right|_{x+\Delta x}\right) = -\left(k\left.\frac{\partial T}{\partial x}\right|_x - k\left.\frac{\partial T}{\partial x}\right|_{x+\Delta x}\right)$

$$\left(-\left(k\left.\frac{\partial T}{\partial x}\right|_x - k\left.\frac{\partial T}{\partial x}\right|_{x+\Delta x}\right) + \rho c\left((uT)_x - (uT)_{x+\Delta x}\right)\right)\Delta y \Delta z \Delta t + \dot{q}\Delta x \Delta y \Delta z \Delta t = \Delta x \Delta y \Delta z \rho c \Delta$$

HEAT TRANSFER FROM AN ENERGY CONSERVATION STANDPOINT



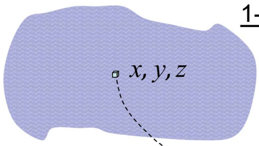
$$\underbrace{\frac{-\left(k\left.\frac{\partial T}{\partial x}\right|_x - k\left.\frac{\partial T}{\partial x}\right|_{x+\Delta x}\right)}{\Delta x}}_{\text{Conduction}} + \underbrace{\rho c \frac{\left((uT)_x - (uT)_{x+\Delta x}\right)}{\Delta x}}_{\text{Convection}} + \underbrace{\dot{q}}_{\text{Generation}} = \underbrace{\frac{\rho c \Delta T}{\Delta t}}_{\text{Storage/ Accumulation}}$$

If we consider $\Delta x \to 0$ *and* $\Delta t \to 0$

$$\underbrace{\frac{\partial}{\partial x}\left(k\frac{\partial T}{\partial x}\right)}_{\text{Conduction}} - \underbrace{\rho c \frac{\partial}{\partial x}(uT)}_{\text{Convection}} + \underbrace{\dot{q}}_{\text{Generation}} = \underbrace{\rho c \frac{\partial T}{\partial t}}_{\text{Storage/ Accumulation of energy}}$$

"Microscopic" Equation to describe Heat Transfer in a local point

1-D Equation



$$\frac{\partial}{\partial x}\left(k\frac{\partial T}{\partial x}\right) - \rho c\frac{\partial}{\partial x}(uT) + \dot{q} = \rho c\frac{\partial T}{\partial t}$$

$$\boxed{\underbrace{\rho c\frac{\partial T}{\partial t}}_{\text{Heat Storage}} + \underbrace{\rho c\frac{\partial}{\partial x}(uT)}_{\text{Convection}} = \underbrace{\frac{\partial}{\partial x}\left(k\frac{\partial T}{\partial x}\right)}_{\text{Conduction}} + \underbrace{\dot{q}}_{\text{Heat Generation}}}$$

A more convenient form

$$\boxed{\frac{\partial T}{\partial t} + \frac{\partial}{\partial x}(uT) = \frac{1}{\rho c}\frac{\partial}{\partial x}\left(k\frac{\partial T}{\partial x}\right) + \frac{\dot{q}}{\rho c}}$$

Heat Transfer Equation (Microscopic Energy Balance)

$$\boxed{\rho c\frac{\partial T}{\partial t} + \rho c\frac{\partial}{\partial x}(uT) = \frac{\partial}{\partial x}\left(k\frac{\partial T}{\partial x}\right) + \dot{q}}$$

Units

$$\rho c\frac{\partial T}{\partial t} = \left[\frac{kg}{m^3}\right]\cdot\left[\frac{kJ}{kg\,K}\right]\left[\frac{K}{s}\right] = \left[\frac{kJ}{s}\right] = \left[\frac{kW}{m^3}\right] \ or \ \left[\frac{W}{m^3}\right]$$

$$\rho c\frac{\partial (uT)}{\partial x} = \left[\frac{kg}{m^3}\right]\cdot\left[\frac{kJ}{kg\,K}\right]\left[\frac{\frac{m}{s}\cdot K}{m}\right] = \left[\frac{kJ}{s}\right] = \left[\frac{kW}{m^3}\right] \ or \ \left[\frac{W}{m^3}\right]$$

$$\frac{\partial}{\partial x}\left(k\frac{\partial T}{\partial x}\right) = \left[\frac{1}{m}\right]\cdot\left[\frac{W}{m\cdot K}\cdot\frac{K}{m}\right] = \left[\frac{W}{m^3}\right] \ or \ \left[\frac{kW}{m^3}\right]$$

$$\dot{q} = Heat\,Generation\ per\,Unit\,Volume = \frac{kW}{m^3}$$

Phil. Trans. R. Soc. A (2010) **368**, 561–583
doi:10.1098/rsta.2009.0248

REVIEW

Multi-scale heat and mass transfer modelling of cell and tissue cryopreservation

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Cells and tissues undergo complex physical processes during cryopreservation. Understanding the underlying physical phenomena is critical to improve current cryopreservation methods and to develop new techniques. Here, we describe multi- scale approaches for modelling cell and tissue cryopreservation including heat transfer at macroscale level, crystallization, cell volume change and mass transport across cell membranes at microscale level. These multi-scale approaches allow us to study cell and tissue cryopreservation.

Keywords: multi-scale modelling; heat and mass transfer; cryopreservation

1. Introduction

Cryopreservation aims to preserve cells/tissues without significantly impacting their function (e.g. viability, mechanical properties; Whittingham *et al.* 1972; Ludwig *et al.* 1999; Agca 2000; Stachecki & Cohen 2004). Biological activity is first slowed down or even stopped through cooling down to subzero temperatures. This activity is retrieved after warming back to physiological temperature. Cryopreservation has been used for many important applications such as *in vitro* fertilization (i.e. oocyte (Porcu *et al*. 1997; Isachenko *et al*. 2005; Antinori *et al*. 2007) and sperm (Guthrie & Welch 2005; van den Berg *et al*. 2007) preservation); stem cell research (Bakken 2006; Demirci & Montesano 2007*a*; Hunt & Timmons 2007; Kashuba Benson *et al*. 2008); preservation of organs for transplantation surgery (Ishine *et al*. 2000); and storage and transportation of tissue engineered products (Nerem 2000). Recent advances in nano- and micro-technologies have

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One contribution of 9 to a Theme Issue 'Multi-scale biothermal and biomechanical behaviours of biological materials'.

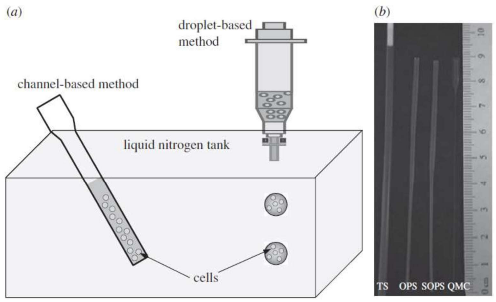


Figure 1. Channel-based and droplet-based methods for cryopreservation. (*a*) In channel-based methods, cells are mixed with media, e.g. CPAs, inside a channel. The whole channel is then immersed in liquid nitrogen for freezing. In droplet-based methods, cell-laden droplets are ejected into nitrogen for freezing (Demirci & Montesano 2007*a*). (*b*) A comparison of the devices used in channel-based methods (Arav *et al.* 2002; He *et al.* 2008): the traditional straw (TS), the open-pulled straw (OPS), the superfine open-pulled straw (SOPS) and the quartz micro-capillary (QMC). Adapted from He *et al.* (2008).

Some of the Calculations

(a) Heat transfer during cryopreservation

The lumped model, in which temperature variation across CPAs is negligible has often been widely used for slow freezing methods. However, this model is not applicable for fast freezing methods like vitrification owing to the non-uniform temperature distribution around CPAs (Han *et al.* 2008). The frequently used heat equation is given as

$$\rho c \frac{\partial T}{\partial t} = \nabla \cdot \lambda \nabla T + \dot{q}_{\mathrm{met}} + \dot{q}_{\mathrm{ext}}, \qquad (2.1)$$

Other Equations Used

$$\rho c \frac{\partial T}{\partial t} = \frac{1}{r}\frac{\partial}{\partial r}\left(\lambda r \frac{\partial T}{\partial r}\right) + \frac{\partial}{\partial z}\left(\lambda \frac{\partial T}{\partial z}\right) + \dot{q}_{\mathrm{met}}$$

Heat Transfer Equation (Microscopic Energy Balance)

$$\rho c \frac{\partial T}{\partial t} + \rho c \frac{\partial}{\partial x}(uT) = \frac{\partial}{\partial x}\left(k \frac{\partial T}{\partial x}\right) + \dot{q}$$

$$\Downarrow$$

$$\frac{\partial T}{\partial t} + \frac{\partial}{\partial x}(uT) = \frac{1}{\rho c}\frac{\partial}{\partial x}\left(k \frac{\partial T}{\partial x}\right) + \frac{\dot{q}}{\rho c}$$

Simplifications of the General Equation

k = constant (it does not vary with position)

$$\frac{\partial T}{\partial t} + \frac{\partial}{\partial x}(uT) = \frac{k}{\rho c}\frac{\partial^2 T}{\partial x^2} + \frac{\dot{q}}{\rho c}$$

Heat Transfer Equation (Microscopic Energy Balance)

Simplifications of the General Equation

$$\frac{\partial T}{\partial t} + \frac{\partial}{\partial x}(uT) = \alpha \frac{\partial^2 T}{\partial x^2} + \frac{\dot{q}}{\rho c}$$

$$\boxed{\alpha = \frac{k}{\rho c}}$$

- No Heat Generation and constant fluid velocity

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

- No Heat Generation and no fluid movement ("*no convection*")

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

Examples of Heat Generation

$$\frac{\partial T}{\partial t} + \frac{\partial}{\partial x}(uT) = \alpha \frac{\partial^2 T}{\partial x^2} + \frac{\dot{q}}{\rho c}$$

Table C.3

Organ	($\dot{q}V$) Metabolic Rate (W)
Heart Muscle	10-31
Skeletal Muscle	17-350
Skin	4-30
Liver	18
Kidney	6
Brain	17

Utility of the Heat ("Energy") Equation

- Only applies if the **Continuum Theory** applies (Nanoscale ?)
- It is useful for **any material**
- It is useful for any size or shape (rectangular, cylindrical, spherical, or any shape)
- If used, start with the more general equation and start to simplify based on suitable ("realistic") assumptions. It is safer – as you drop terms, that you be aware of the reasons

Can it be done more general?

1. Include compressible fluids – maybe less application to biomaterials
2. Properties vary with temperature ("location") – Solutions are not longer analytical solutions (numerical approaches are used, e.g. Finite Element, FE)
3. To include fluid mechanics (fluid velocity) or mass transfer, e.g. water evaporation during the heating process [Multiphysics Equations]

Multiphysics Problems

- Momentum Equation (Navier-Stokes)
- Energy Equation
- Mass Transfer Equation

Typical “Multiphysics” Problem

Navier Stokes Equation (Fluid Mechanics)

$$\rho\left(\frac{\partial \underline{u}}{\partial t} + \underline{u}\cdot\nabla\underline{u}\right) = \rho g - \nabla p + \nabla.\mu\nabla\underline{u}$$

$$\mu = f(Temperature)$$

Energy Equation (this class) – 1D equation

$$\frac{\partial T}{\partial t} + \frac{\partial}{\partial x}\left(uT\right) = \alpha\frac{\partial^2 T}{\partial x^2} + \frac{\overbrace{\mu\nabla\underline{u}\cdot\nabla\underline{u}}^{\text{Viscous Friction}}}{\rho c}$$

Heat (“Energy”) Equation – 1D problem

$$\frac{\partial T}{\partial t} + \frac{\partial}{\partial x}\left(uT\right) = \alpha\frac{\partial^2 T}{\partial x^2} + \frac{\dot{q}}{\rho c}$$

Some Applications and Simplifications

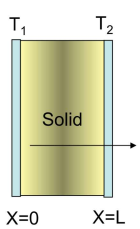
- No fluid velocity
- No heat generation
- Steady state
- constant properties
- 1D Heat Flux

$$0 = \alpha\frac{\partial^2 T}{\partial x^2} \Longrightarrow \frac{d^2 T}{dx^2} = 0$$

$$\frac{d^2 T}{dx^2} = 0 \xrightarrow{\text{Solution}} \boxed{T = C_1 x + C_2}$$

To get the solution to the problem we need to determine the constants
BOUNDARY CONDITIONS ARE NEEDED

Heat (“Energy”) Equation – (simple solution)



Heat Conduction

$$\frac{d^2 T}{dx^2} = 0 \Longrightarrow T = C_1 x + C_2$$

$$C_2 = T_1$$

$$C_1 = \frac{T_2 - T_1}{L}$$

Solution

$$\boxed{T = \frac{T_2 - T_1}{L}x + T_1}$$

Boundary Conditions

$$\begin{cases} T = T_1 \quad at \quad x = 0 \\ T = T_2 \quad at \quad x = L \end{cases}$$

Heat ("Energy") Equation

More on Boundary Conditions

$$\frac{\partial T}{\partial t} + \frac{\partial}{\partial x}(uT) = \alpha \frac{\partial^2 T}{\partial x^2} + \frac{\dot{q}}{\rho c}$$

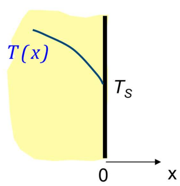
Solution

$$T = T(x,t)$$

- For the location (*x*) we need **two boundary conditions**
- For the time (*t*) we need another boundary condition.
  In general the Temperature is known at the start of the process *t=0*
  so the time boundary condition is more known as ***Initial Condition***

Heat/Energy Equation – General Boundary Conditions

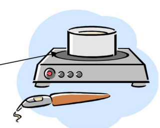
1. Surface Temperature is Specified



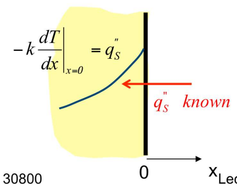
$$T\big|_{x=0} = T_s$$

constant or a function of time for example

The temperature of the surface could change with time



2. Surface Heat flow is specified



$$-k\frac{dT}{dx}\Big|_{x=0} = q''_S$$

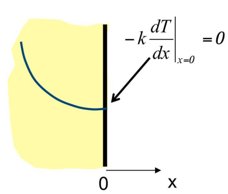
It could be constant or a function of time

Heat/Energy Equation – General Boundary Conditions

2. Surface heat flow is specified – Special Cases

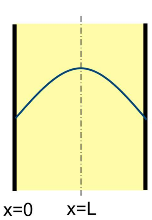
2a. Insulated Condition

$$-k\frac{dT}{dx}\Big|_{x=0} = 0$$

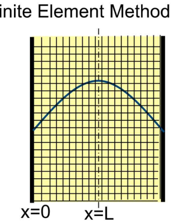


2b. Symmetry Condition

$$-k\frac{dT}{dx}\Big|_{x=L} = 0$$

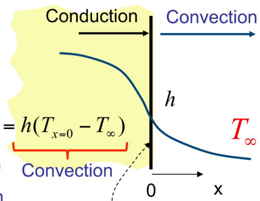


Grid for Numerical Solutions Finite Element Method (FEM)



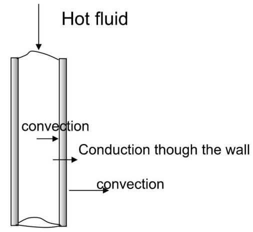
Heat/Energy Equation – General Boundary Conditions

3. Convection at the surface



$$-k\left.\frac{dT}{dx}\right|_{x=0} = h(T_{x=0} - T_\infty)$$

Conduction — Convection



$T_{x=0}$ *is unknown*

Many times (e.g. when the fluid is a liquid moving with a high velocity we can assume that $h \to \infty$ and $T_{x=0} \to T_\infty$

Heat/Energy Equation – Only conduction in different coordinate systems

Cartesian

$$\frac{\partial T}{\partial t} = \frac{k}{\rho c}\left[\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} + \frac{\partial^2 T}{\partial z^2}\right] + \frac{\dot{q}}{\rho c} \longrightarrow \boxed{T = T(x, y, z, t)}$$

Cylindrical

$$\frac{\partial T}{\partial t} = \frac{k}{\rho c}\left[\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial T}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2 T}{\partial \varphi^2} + \frac{\partial^2 T}{\partial z^2}\right] + \frac{\dot{q}}{\rho c} \longrightarrow \boxed{T = T(r, \phi, z, t)}$$

Spherical

$$\frac{\partial T}{\partial t} = \frac{k}{\rho c}\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial T}{\partial r}\right) + \frac{1}{r^2 \sin^2\theta}\frac{\partial^2 T}{\partial \varphi^2} + \frac{1}{r^2 \sin^2\theta}\frac{\partial}{\partial \theta}(\sin\theta\frac{\partial T}{\partial \theta})\right] + \frac{\dot{q}}{\rho c}$$

$$\longrightarrow \boxed{T = T(r, \phi, \theta, t)}$$

Heat/Energy Equation – General Case

Only Conduction

$$\frac{\partial T}{\partial t} = \frac{k}{\rho c}\nabla^2 T + \frac{\dot{q}}{\rho c}$$

Conduction + Convection

$$\frac{\partial T}{\partial t} + \underbrace{\underline{u}\cdot\nabla T}_{\text{Convection}} = \underbrace{\frac{k}{\rho c}\nabla^2 T}_{\text{Conduction}} + \frac{\dot{q}}{\rho c}$$

Heat/Energy Equation – General Case

Application – Sterilization Process

Sterilization: A process under which a sample is heated at a certain temperature for a given time in order to reduce the number of microorganisms and thus avoid contamination. Standard process applied to foods (e.g. cans)

Temperature will not be uniform in the can so sterilization will be based on the slowest heating point

What is the difference between the two cans besides the dimensions?

Content is a liquid

$$\frac{\partial T}{\partial t} + \underline{u} \cdot \nabla T = \frac{k}{\rho c} \nabla^2 T + \overset{=0}{\cancel{\frac{\dot{q}}{\rho c}}}$$

Content is a solid

$$\frac{\partial T}{\partial t} = \frac{k}{\rho c} \nabla^2 T + \overset{=0}{\cancel{\frac{\dot{q}}{\rho c}}}$$

Which one will heat faster?
What equations should we use?

In this case the slowest heating point is the geometrical center