Modelling and Numerical Methods

Lecture 4

Conservation Equations and Rheology

Outline

- Conservation equations
- Energy equation
- Constitutive equations: Rheology
- Elasticity and Wave Equation
- Newtonian Viscosity and Navier Stokes

Learning Objectives

- Learn main conservation equations used in continuum mechanics modelling and understand what different terms in these equations represent
- Be able to solve conservation equations for basic analytical solutions given boundary/initial conditions.
- Understand basic properties of elastic and viscous rheology and understand how the choice of rheology leads to different forms of the momentum conservation equation
- Using tensor analysis to obtain relations between the main isotropic elastic parameters

Continuum Mechanics Equations

General:

1. Kinematics – describing deformation and velocity without considering forces
2. Dynamics – equations that describe force balance, conservation of linear and angular momentum
3. Thermodynamics – relations temperature, heatflux, stress, entropy

Material-specific

4. Constitutive equations – relations describing how material properties vary as a function of T,P, stress,…. Such material properties govern dynamics (e.g., ***density***), response to stress (***viscosity***, ***elastic parameters***), heat transport (***thermal conductivity***, ***heat capacity***)

Thermodynamics: Conservation of Energy

- First law of thermodynamics
- Preservation of energy, i.e any change in kinetic or internal energy is balanced by work done and heat used/produced

$$\frac{D(K+U)}{Dt} = W + Q$$

K- kinetic energy, U- internal energy,
W – power input, Q – heat input

- Let's start with the form that describes preservation of thermal energy, in 2-D

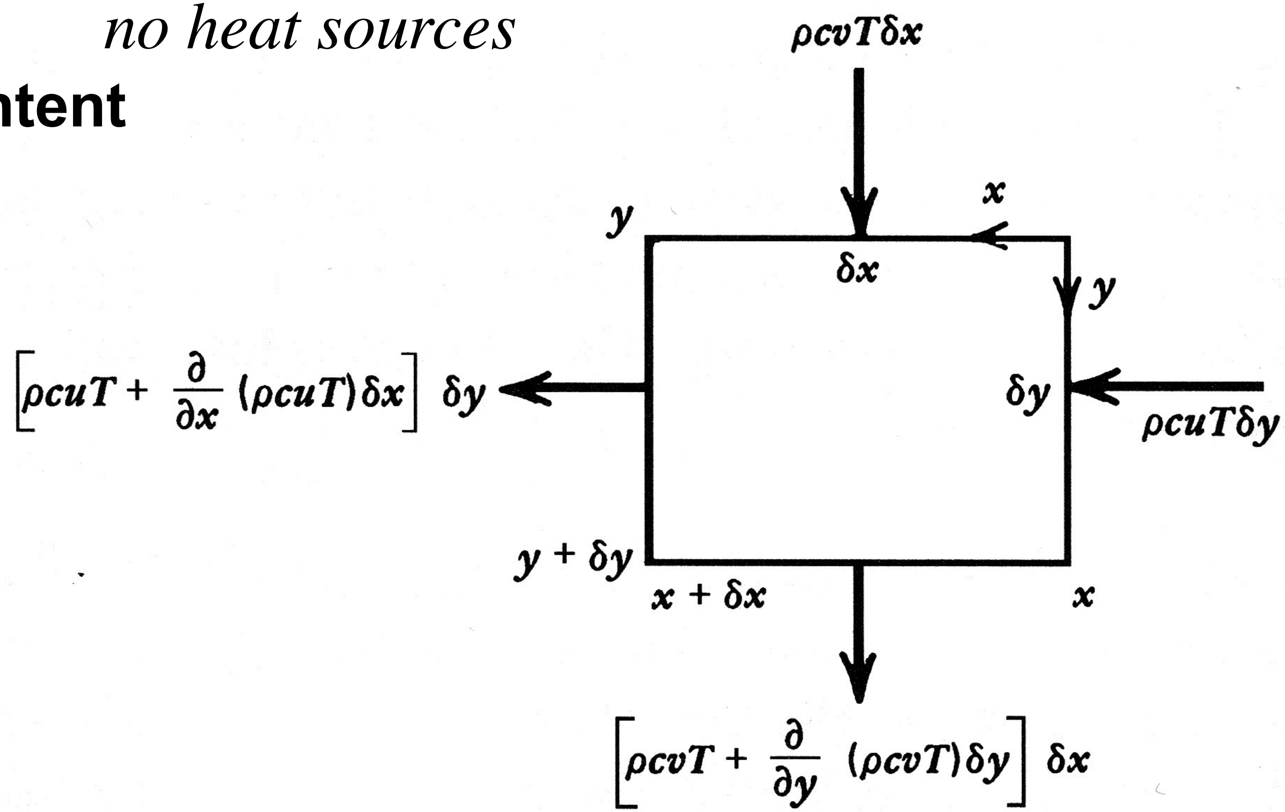
2-D energy equation

Spatial, constant ρ, C_P, k, incompressible
no heat sources

- **Change in heat content**

$$\frac{\partial\left(\rho C_P T\right)}{\partial t}\delta x\delta y$$

- **Advection**



- **Conduction**

C_P – heat capacity (J/kg/K)
u,v - velocity

2-D energy equation

Spatial, constant ρ, C_P, k, incompressible

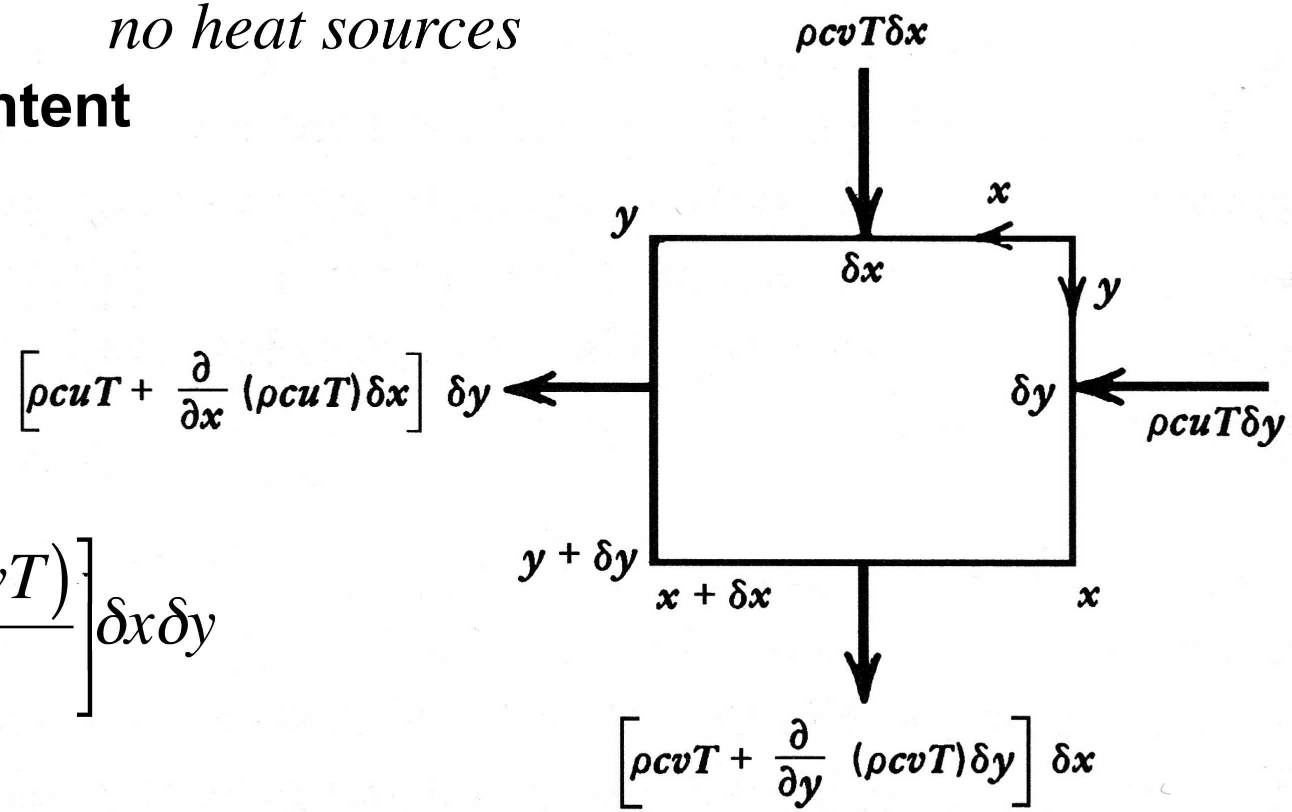
no heat sources

- **Change in heat content**

$$\frac{\partial\left(\rho C_P T\right)}{\partial t}\delta x\delta y$$

- **Advection**

$$\left[\frac{\partial\left(\rho C_P uT\right)}{\partial x}+\frac{\partial\left(\rho C_P vT\right)}{\partial y}\right]\delta x\delta y$$



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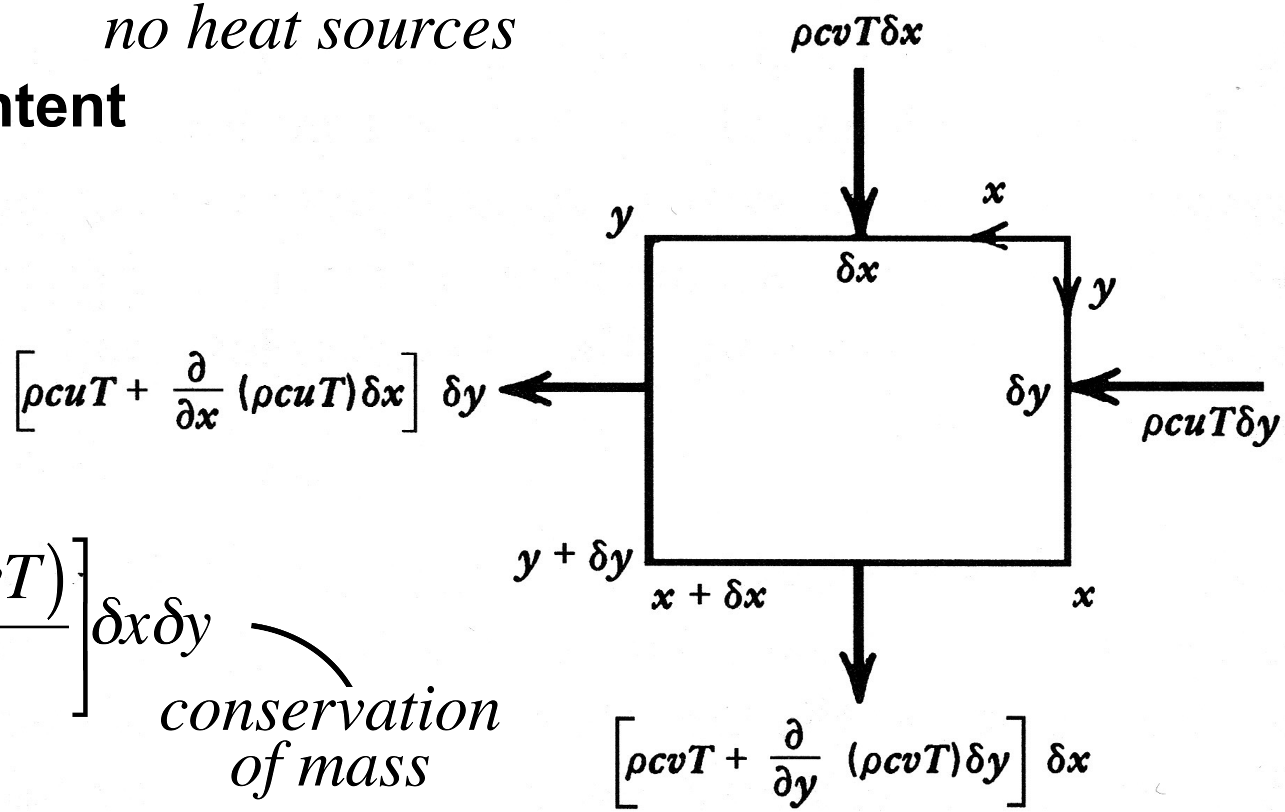


- **Change in heat content**

$$\frac{\partial(\rho C_P T)}{\partial t}\delta x \delta y$$

- **Advection**

$$\left[\frac{\partial(\rho C_P u T)}{\partial x} + \frac{\partial(\rho C_P v T)}{\partial y}\right]\delta x \delta y$$

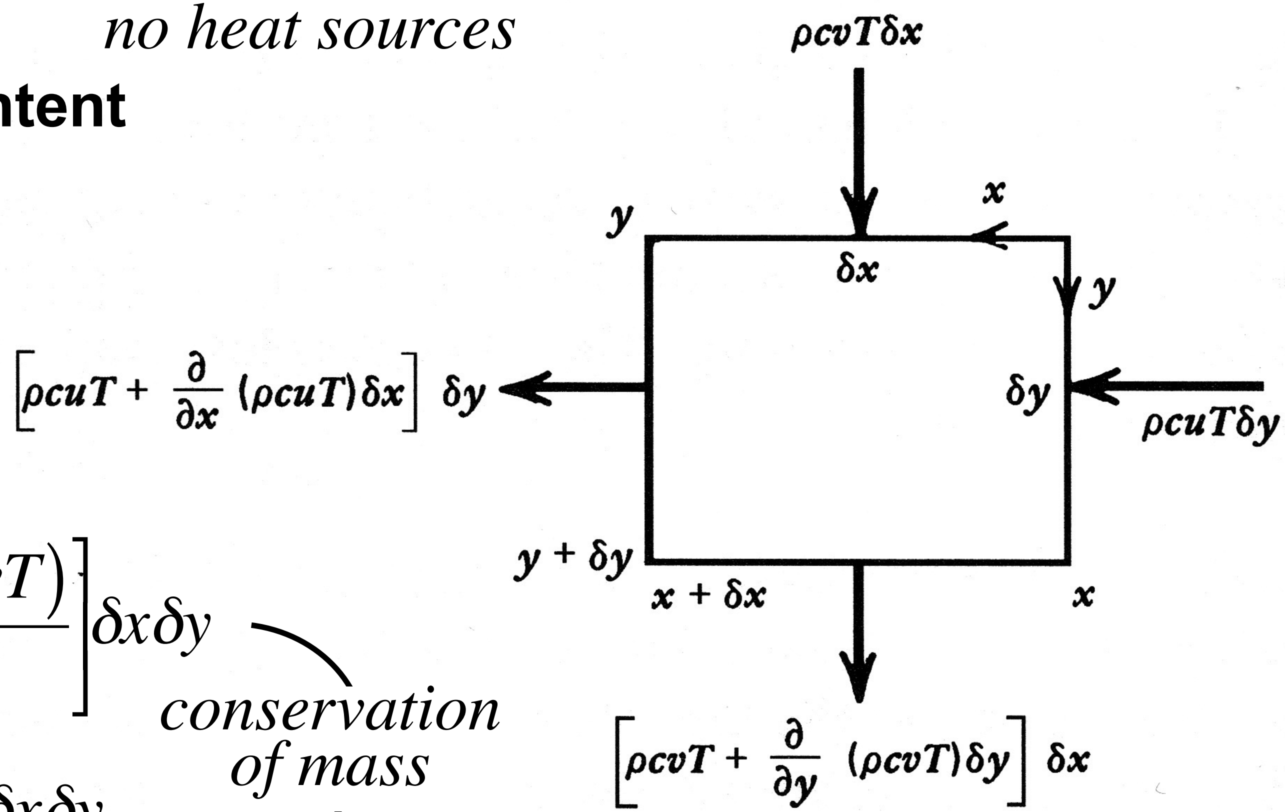
conservation of mass

How does this simplify?

2-D energy equation

Spatial, constant ρ, C_P, k, incompressible

no heat sources



- **Change in heat content**

$$\frac{\partial(\rho C_P T)}{\partial t}\delta x\delta y$$

- **Advection**

$$\left[\frac{\partial(\rho C_P uT)}{\partial x} + \frac{\partial(\rho C_P vT)}{\partial y}\right]\delta x\delta y$$

conservation of mass

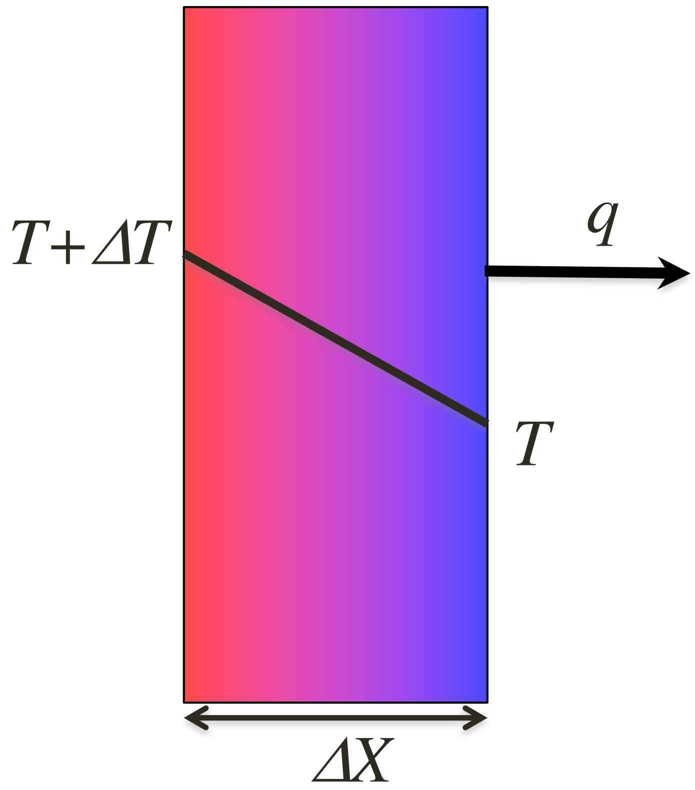
$$\rho C_P\left[u\frac{\partial T}{\partial x} + v\frac{\partial T}{\partial y}\right]\delta x\delta y$$

- **Conduction**

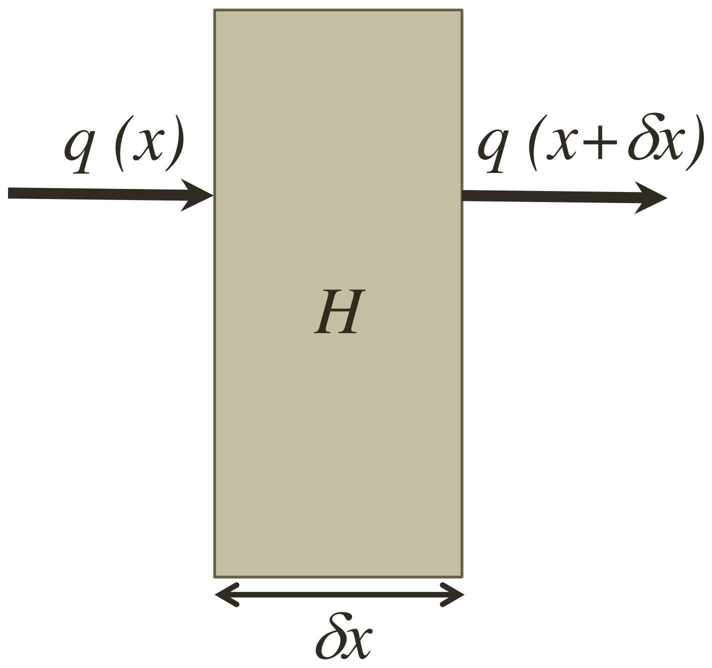
Fourier's Law for conduction

$$q = -k\frac{dT}{dx}$$

- ***Heat flux***, q, = heat/area = energy/time/area, unit: J/s/m^2 = W/m^2
- Heat flux proportional to ***temperature gradient***
- Minus sign because heat flows from hot to cold
- Constant of proportionality: ***thermal conductivity***, k, unit: W/m/K



1-D Steady State Conduction



- **net heat flow/unit area/unit time =**

$q(x+\delta x)$-$q(x)$

$$q(x+\delta x) = q(x) + \delta x \frac{dq}{dx} + \ldots.$$

$$q(x+\delta x) - q(x) \approx \delta x \frac{dq}{dx}$$

$$\delta x \frac{dq}{dx} = \delta x \left[\frac{d}{dx}\left(-k \frac{dT}{dx} \right) \right]$$

$$\delta x \frac{dq}{dx} = \delta x \left[-k \frac{d^2T}{dx^2} \right]$$ *for constant k*

- **heat produced** = $\rho H \delta x = A \delta x$

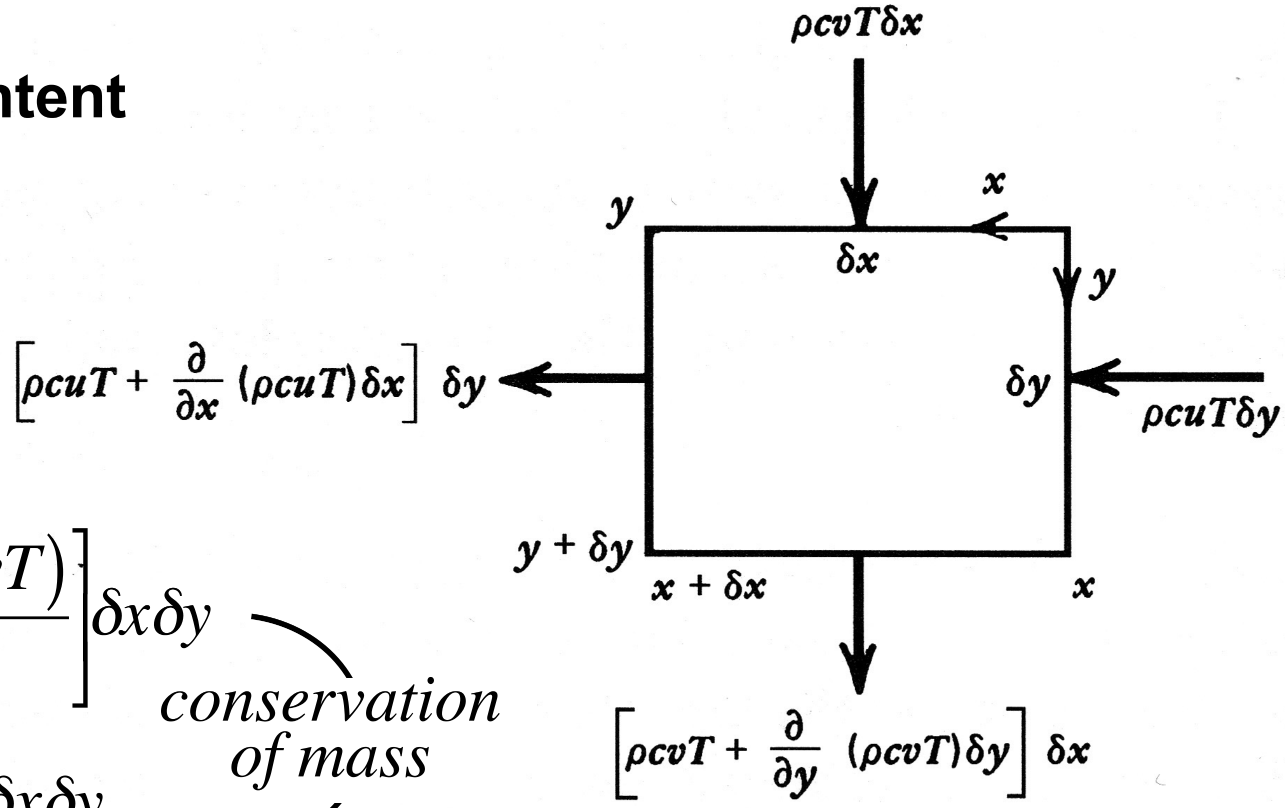
H - heat production rate/unit mass (W/kg)

A – heat production/unit volume (W/m^3)

$$\boxed{-k \frac{d^2T}{dx^2} = \rho H = A}$$

2-D energy equation

Spatial, constant ρ, C_P, k, , incompressible, no heat production



- **Change in heat content**

$$\frac{\partial(\rho C_P T)}{\partial t}\delta x\delta y$$

- **Advection**

$$\left[\frac{\partial(\rho C_P uT)}{\partial x} + \frac{\partial(\rho C_P vT)}{\partial y}\right]\delta x\delta y$$

conservation of mass

$$\rho C_P\left[u\frac{\partial T}{\partial x} + v\frac{\partial T}{\partial y}\right]\delta x\delta y$$

- **Conduction**

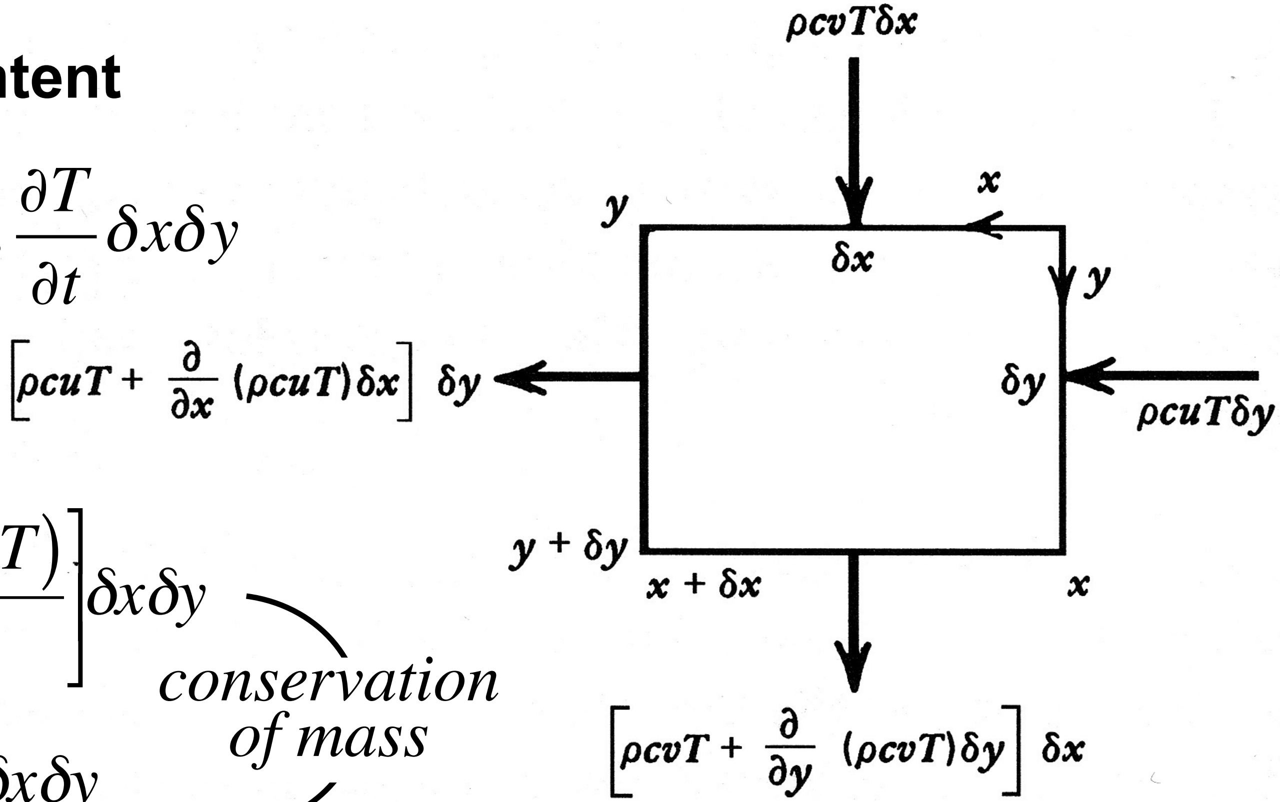
$$-k\left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2}\right)\delta x\delta y$$

2-D energy equation

Spatial, constant ρ, C_P, k, , incompressible, no heat production

- **Change in heat content**

$$\frac{\partial\left(\rho C_P T\right)}{\partial t}\delta x\delta y = \rho C_P \frac{\partial T}{\partial t}\delta x\delta y$$



- **Advection**

$$\left[\frac{\partial\left(\rho C_P uT\right)}{\partial x} + \frac{\partial\left(\rho C_P vT\right)}{\partial y}\right]\delta x\delta y$$

conservation of mass

$$\rho C_P\left[u\frac{\partial T}{\partial x} + v\frac{\partial T}{\partial y}\right]\delta x\delta y$$

- **Conduction**

$$-k\left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2}\right)\delta x\delta y$$

$$\boxed{\rho C_P\left[\frac{\partial T}{\partial t} + u\frac{\partial T}{\partial x} + v\frac{\partial T}{\partial y}\right] = k\left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2}\right)}$$

$$\rho C_P\left[\frac{\partial T}{\partial t} + \mathbf{u}\cdot\nabla T\right] = k\nabla^2 T$$

Energy equation

$$\frac{D(K+U)}{Dt} = W + Q$$

- **Material derivative internal heat**

$$\rho C_P\left[\frac{\partial T}{\partial t} + u \cdot \nabla T\right] = \rho C_P \frac{DT}{Dt} \Rightarrow \frac{D\left(\rho C_P T\right)}{Dt}$$

Allowing for spatial variations of material parameters

- **Heat input**

$$k\nabla^2 T \Rightarrow \nabla \cdot k\nabla T \qquad\qquad +A$$

Conduction *Internal heat production*

- **Work done**

$\Rightarrow$ Changes in *motion* (kinetic energy) and *internal deformation*

Net effect of $W - \frac{DK}{Dt}$ becomes $\boldsymbol{\sigma} : \mathbf{D}$

$\mathbf{D}$ – strain rate

Energy equation

conservation of heat

I	II	III	IV	V	VI
$D(\rho C_p T)/Dt =$	$\nabla \cdot k \nabla T$	$+ A$	$+ \boldsymbol{\sigma} \mathbf{:D}$	$(+ \alpha T \mathbf{v} \cdot \nabla P$	$\ldots)$

I - change in temperature with time
II - heat transfer by conduction (and radiation)
III - heat production (including latent heat)
IV - heat generated by internal deformation

V - heat generated by adiabatic compression
VI - other heat sources, e.g. latent heat

Conservation equations

- Conservation of mass
  - Kinematics

$$\frac{D\rho}{Dt} + \rho \nabla \cdot \mathbf{v} = 0$$

- Conservation of momentum
  - Dynamics
  - Newton's second law
  - Angular momentum

$$\rho \frac{D\mathbf{v}}{Dt} = \nabla \cdot \underline{\underline{\sigma}} + \mathbf{f}$$

$$\boldsymbol{\sigma} = \boldsymbol{\sigma}^{\mathrm{T}}$$

- Conservation of energy
  - First law of thermodynamics

$$\frac{D\left(\rho C_P T\right)}{Dt} = \nabla \cdot k \nabla T + A + \boldsymbol{\sigma} : \mathbf{D}$$

- Entropy inequality

  Which law is this?

Rate of entropy increase of a particle always ≥ entropy supply

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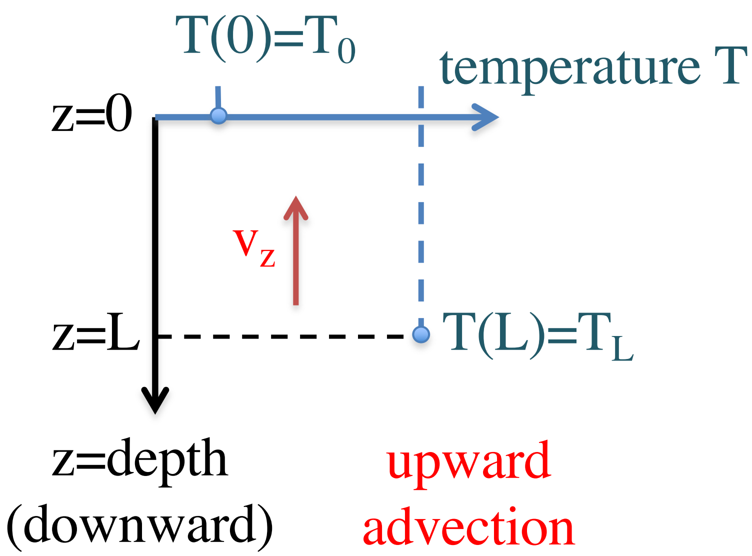
1-D advection-diffusion solution

$$\boxed{-v_z \frac{\partial T}{\partial z} = \kappa \frac{\partial^2 T}{\partial z^2}} \qquad \kappa = \frac{k}{\rho C_P}$$



Take $f(z) = \dfrac{\partial T}{\partial z}$ and $c = \dfrac{v_z}{\kappa}$

Then $\dfrac{\partial f}{\partial z} = -cf(z)$

$\Rightarrow$ This yields $f(z) = f(0)\mathrm{e}^{-cz}$, i.e. $\dfrac{\partial T}{\partial z}(z) = A\,\mathrm{e}^{-v_z z/\kappa}$

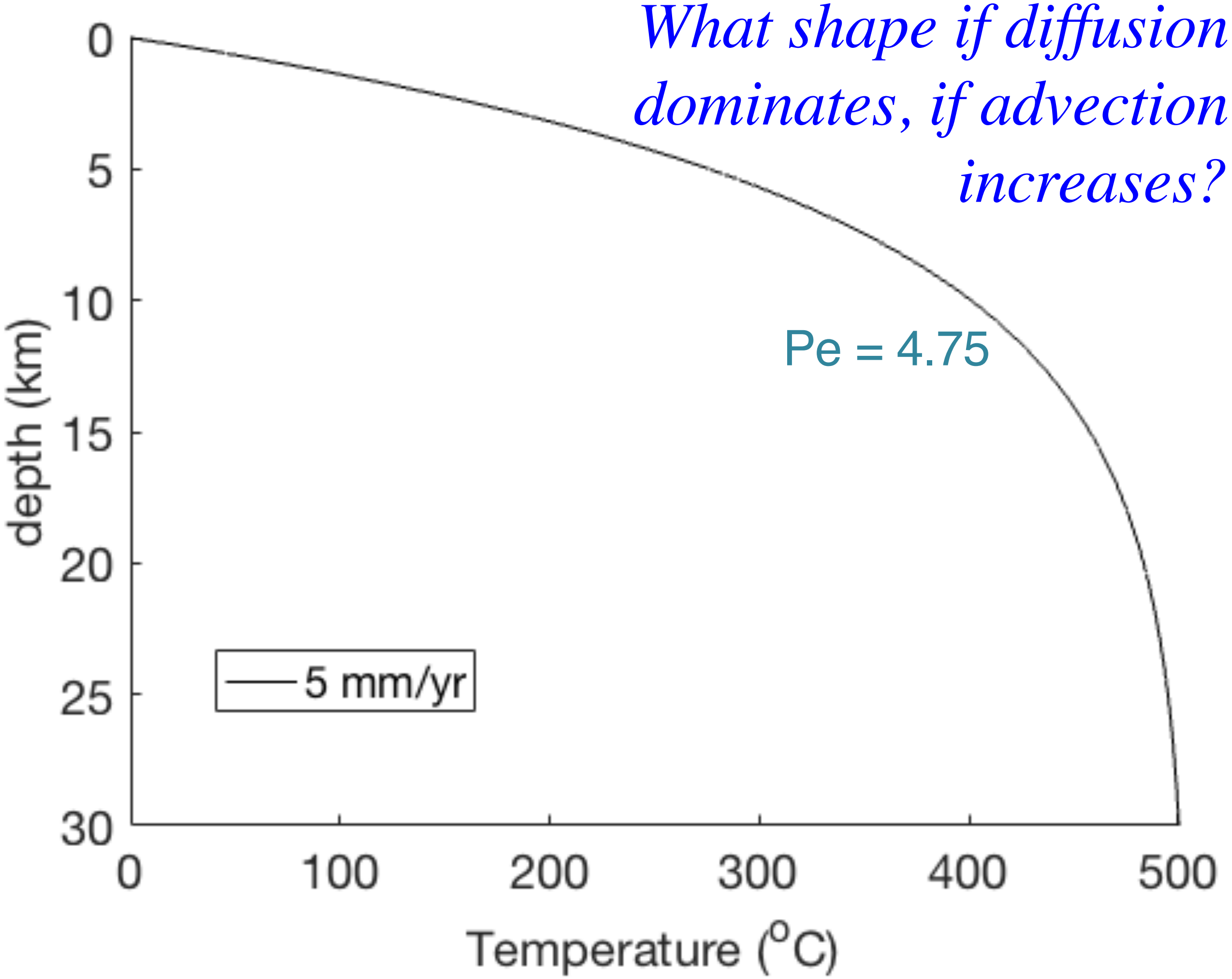
$$T(z) = B - \frac{A}{v_z/\kappa}\mathrm{e}^{-v_z z/\kappa}$$

where A, B are integration constants

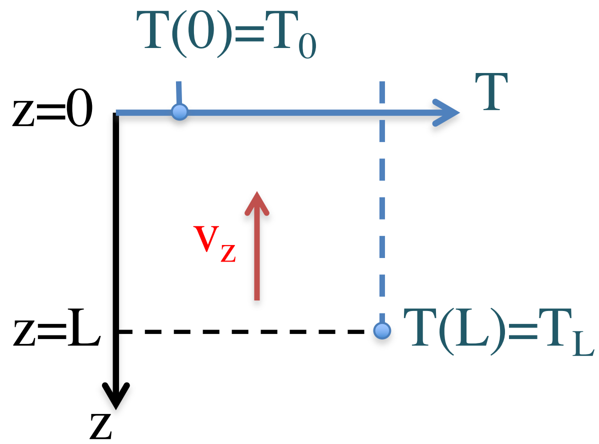
For constant temperature boundary conditions $T(z{=}0){=}0$ and $T(z{=}\mathrm{L}){=}\mathrm{T_L}$

$\Rightarrow$ Integration gives: $T(z) = T_L\left[\dfrac{1-\mathrm{e}^{-v_z z/\kappa}}{1-\mathrm{e}^{-v_z L/\kappa}}\right]$

1-D advection-diffusion solution



What shape if diffusion dominates, if advection increases?



$$T(z) = T_L\left[\frac{1-\mathrm{e}^{-v_z z/\kappa}}{1-\mathrm{e}^{-v_z L/\kappa}}\right]$$

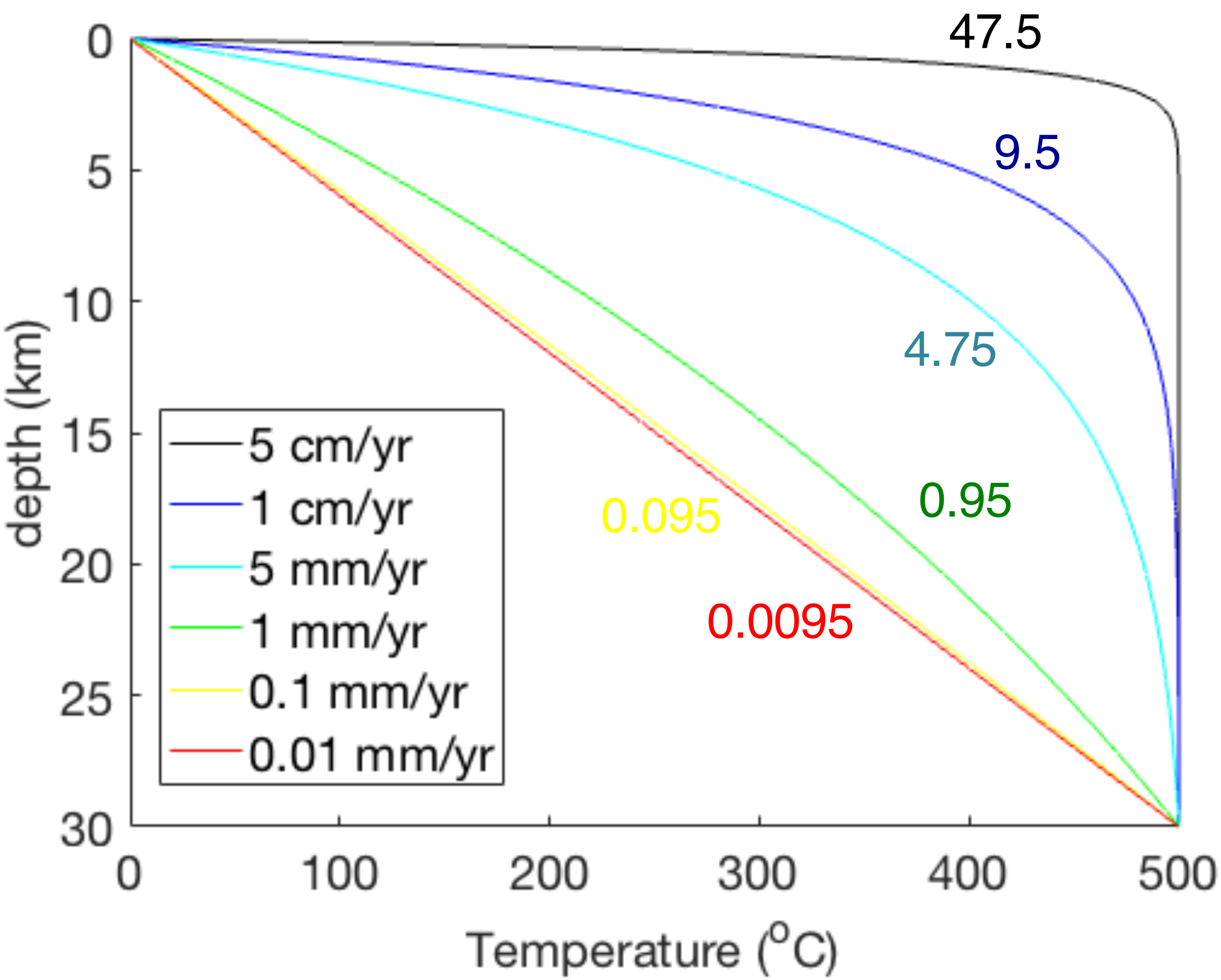
Peclet number, measure of relative importance advection/diffusion

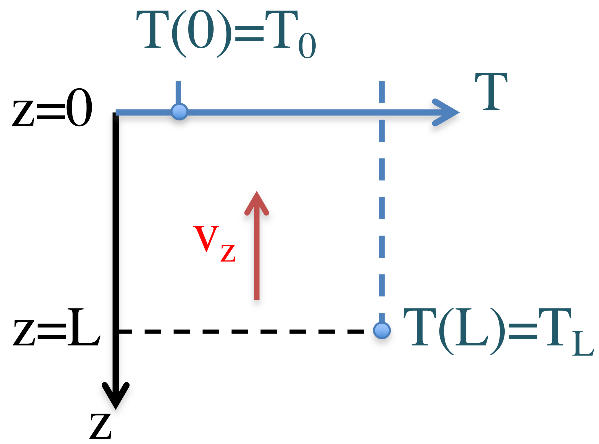
$$Pe = \frac{v_z L}{\kappa} = \frac{[(m/s)m]}{[m^2/s]}$$

Take a break

- Use ***Exercise 3*** in *chapter4.ipynb* to look at the shape of the solutions
- ***Exercise 4*** for afternoon workshop

1-D advection-diffusion solution





$$T(z) = T_L \left[\frac{1 - e^{-v_z z/\kappa}}{1 - e^{-v_z L/\kappa}} \right]$$

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