Lecture 24: Process modeling & balance laws

- Balance laws
  - Differential balances
  - Material derivative

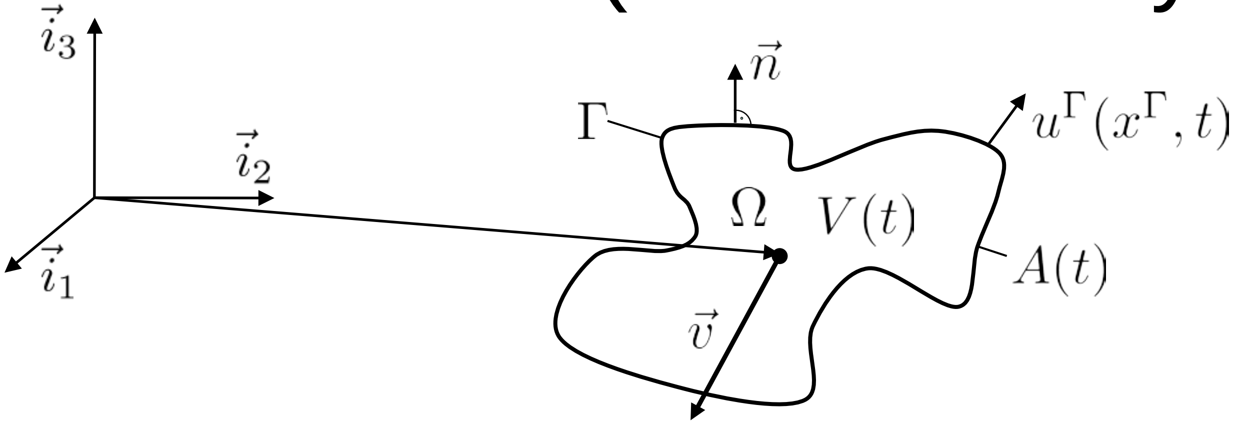
Book: 10.4, 11.1-11.4

Computational fluid dynamics

- CFD = solving momentum + mass balances (that is, Navier-Stokes + continuity equation) for different setups

http://physbam.stanford.edu/~fedkiw/

Control volume (infinitesimally small)



- How can the extensive property Ψ change in the domain Ω ?

• production rate : $\Sigma_\Psi \hat{=} \dfrac{\text{produced/consumed } \Psi \text{ in } \Omega}{\text{time}}$

• transport rate : $\Phi = \dfrac{\text{over } \Gamma \text{ in/out of the domain } \Omega}{\text{time}}$

→ Integral balance: $\dfrac{d}{dt}\Psi = \Phi_\Psi + \Sigma_\Psi$

storage → effort transport source

General integral balance

- Arbitrary size: In order to get a local character we have to introduce properties with local characteristics

$$\psi(x,t) = \lim_{V \to 0} \frac{\Psi}{V}\Big|_{x,t}$$ [intensive property]

$$\Psi(t) = \int_{\Omega} \psi(x,t)\, dV$$

$$\Sigma_\psi(t) = \int_{\Omega} \sigma_\psi(x,t)$$

← source density

remote effects

$$\sigma_\psi(x,t) = \sigma_\psi^{p}(x,t) + \sigma_\psi^{F}(x,t)$$

$$\phi_\psi(x,t) = \lim \frac{\Phi}{A}\Big|_{x^\Gamma,t}$$ ← physiochemical phenomena in Ω

$$\rightarrow \Phi_\psi(t) = -\int_{\Gamma} \langle \phi_\psi(x^\Gamma,t) \rangle\, dA$$

general integral balance

$$\frac{d}{dt}\int_{\Omega} \psi\, dV = -\int_{\Gamma} \phi_\psi \cdot \underline{n}\, dA + \int_{\Omega} \sigma_\psi\, dV$$

Derivation of differential balance I

- Goal: Find a derivative of the local density ψ instead of the total amount of extensive property Ψ

$$\frac{d}{dt}\int_\Omega \psi dV = -\int_\Gamma \phi_\psi \underline{n} dA + \int_\Omega \sigma_\psi dV$$

→ change differentiation and integration

- Use: Reynold's transport theorem:

$$\frac{d}{dt}\int_\Omega \psi dV = \int_\Omega \frac{\partial \psi}{\partial t} dV + \int_\Gamma \psi \underline{u}^\Gamma \underline{n} dA$$

change of moving surface

$$\rightarrow \int_\Omega \frac{\partial \psi}{\partial t} dV = -\int_\Gamma \psi \underline{u}^\Gamma \underline{n} dA - \int_\Gamma \phi_\psi \cdot \underline{n} dA + \int_\Omega \sigma_\psi dV$$

Derivation of differential balance II

$$\int_\Omega \frac{\partial \psi}{\partial t} dV = -\int_\Gamma \psi \underline{u}^\Gamma \underline{n} dA - \int_\Gamma \phi_\psi \underline{n} dA + \int_\Omega \sigma_\psi dV$$

- Finally we have to transfer the surface integrals into volume integrals to get the same integration domain
- Use: Divergence theorem

$$\int_\Gamma \phi_\psi n \, dA = \int_\Omega \nabla \cdot q_\psi \, dV$$

Nabla Operator: $\nabla = \left(\frac{\partial}{\partial x_1}, \ldots \frac{\partial}{\partial x_n} \right) = \sum_{i=1}^{n} \vec{e}_i \frac{\partial}{\partial x_i}$

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

Cylindric coordinates: $(\nabla \cdot v) = \frac{1}{r} \frac{\partial}{\partial r}(r \cdot v_r) + \frac{1}{r} \frac{\partial v_\theta}{\partial \theta} + \frac{\partial v_z}{\partial z}$

Derivation of differential balance III

$$\int_\Omega \frac{\partial \psi}{\partial t} dV = -\int_\Gamma \psi \underline{u}^\Gamma \underline{n} dA - \int_\Gamma \phi_\psi \underline{n} dA + \int_\Omega \sigma_\psi dV$$

- Apply divergence theorem:

velocity of volume

$$\int_\Omega \frac{\partial \psi}{\partial t} dV = -\int_\Omega \bar{\nabla} \cdot \psi \underline{\omega} dV - \int_\Omega \nabla \cdot \phi_\psi dV + \int_\Omega \sigma_\psi dV$$

$\rightarrow$ Ω is arbitrary since integration must be zero

$$\frac{\partial \psi}{\partial t} + \nabla \cdot \psi \underline{\omega} + \nabla \phi_\psi = \sigma_\psi$$

$\phi^t = \psi \underline{\omega} + \phi_\psi$

$\rightarrow$ general differential balance of density ψ

$$\frac{\partial \psi}{\partial t} + \nabla \phi_\psi^t = \sigma_\psi$$

Mass balance

velocity of center of mass: $\underline{\omega} = \frac{1}{\rho} \sum_{i=1}^{n_c} \rho_i V_i =: \underline{v}$

· diffusive flux: $\phi_{\rho_i} = \rho_i (v_i - v) =: j_i$

$$\rightarrow \quad \frac{\partial \rho_i}{\partial t} + \nabla \rho_i \underline{v} + \nabla \underline{j}_i = r_i^V$$

Equation of continuity of substance i

→ sum over all substances

local rate of mass accumulation

$$\frac{\partial \rho}{\partial t} + \nabla \rho \underline{v} = 0$$

[Equation of continuity]

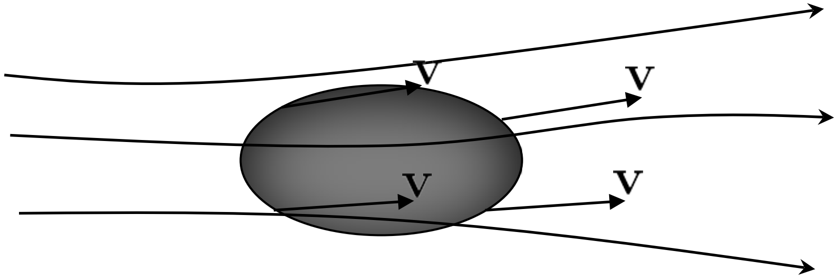
net rate of mass inflow

incompressible fluid

$\nabla \cdot v = 0$

$$\underbrace{\frac{\partial \rho}{\partial t} + v \cdot \nabla \rho}_{\frac{D\rho}{Dt}} + \rho \nabla \cdot v = 0$$

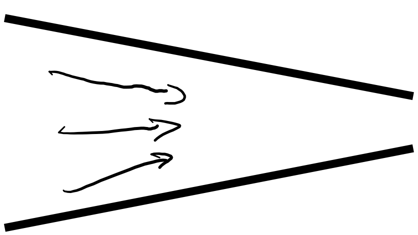
"Moving with the flow"



- The boundary of the element moves with the bulk velocity
- Property change:
  - Unsteady flow
  - Motion through a gradient of the property

$$\frac{\partial V}{\partial t} + V \cdot \nabla V$$

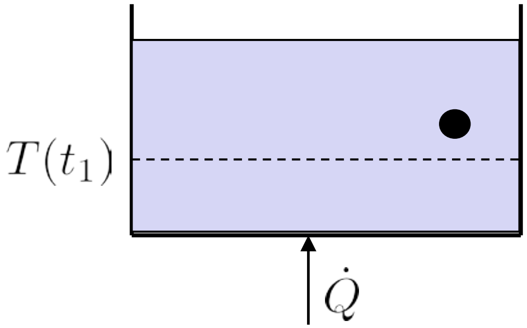
- Example:



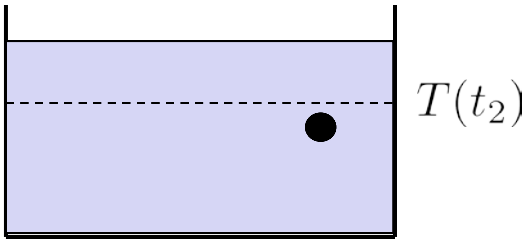
∘ velocity increases
as pipe narrows
[Bernoulli's law]

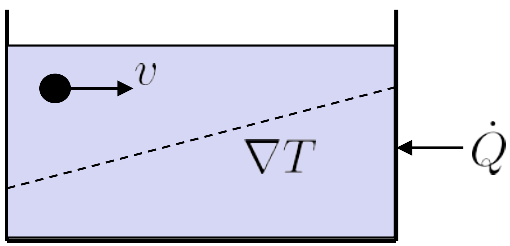
Example: Material derivative $\frac{D}{Dt} = \frac{\partial}{\partial t} + v \cdot \nabla$

$$\frac{DT}{Dt} = \underbrace{\frac{\partial T}{\partial t}}_{>0} + \underbrace{v \cdot \nabla T}_{0}$$



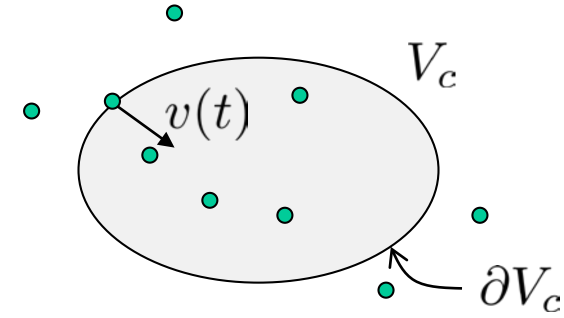
Temperature rise with time





$$\frac{DT}{Dt} = \underbrace{\frac{\partial T}{\partial t}}_{0} + \underbrace{v \cdot \nabla T}_{>0}$$

The momentum balance I



- In words

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{p} = \left\{ \begin{array}{c} \text{transfer of momentum into} \\ V_c \text{ by fluid flow} \\ \text{across surface } \partial V_c \end{array} \right\} + \left\{ \begin{array}{c} \text{generation of momentum} \\ \text{in } V_c \text{ due to forces} \\ \text{acting on } V_c \end{array} \right\}$$

- Mathematically

$$\frac{{}^i\mathrm{d}}{\mathrm{d}t}\vec{p} = \frac{{}^i\mathrm{d}}{\mathrm{d}t}\iiint\limits_{V_c} \rho\vec{v}\mathrm{d}V = -\iint\limits_{\partial V_c} \rho\vec{v}\vec{v}\cdot\vec{n}\mathrm{d}A + \vec{F}^{(r)}$$

where $\vec{F}^{(r)}$ is resultant force on fluid in control volume

(often: gravity (hydrostatic) and/or friction (hydrodynamic))

The momentum balance II

$$\frac{d}{dt}\int_\Omega \rho \underline{v} dV = -\int_\Gamma \rho \underline{v}\cdot\underline{v}\cdot\underline{n} dA + \int_\Omega B dV + \int_\Gamma \underline{n}\cdot\underline{\sigma} dA$$

$$\vdots$$

$$\frac{\partial \rho \underline{v}}{\partial t} + \nabla\cdot\underline{v}\rho\underline{v} - \nabla\underline{\sigma} \quad = B$$

product rule:

$$\rho\frac{\partial v}{\partial t} + \underbrace{\underline{v}\frac{\partial\rho}{\partial t} + \underline{v}\nabla\rho\underline{v}}_{=0 \text{ [Eq. of Cont.]}} + \rho\underline{v}\cdot\nabla\underline{v} - \nabla\sigma = B$$

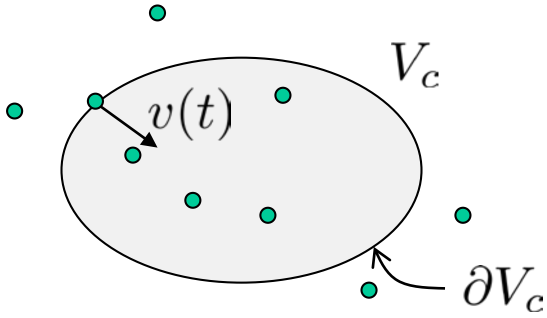
$$\rho\left(\frac{\partial v}{\partial t} + \underline{v}\nabla\underline{v}\right) = B + \nabla\underline{\sigma}$$

local rate of change of vel. over time

convective term

$$\rightarrow \rho\frac{Dv}{Dt} = B + \nabla\underline{\sigma}$$

The energy balance I



- In words

$$\frac{\mathrm{d}}{\mathrm{d}t}E = \left\{ \begin{array}{c} \text{transfer of energy into} \\ V_c \text{ by fluid flow} \\ \text{across surface } \partial V_c \end{array} \right\} + \left\{ \begin{array}{c} \text{transfer of energy into} \\ V_c \text{ by heat transfer} \\ \text{and by work} \end{array} \right\}$$

- Mathematically

$$\frac{\mathrm{d}}{\mathrm{d}t}E = \frac{\mathrm{d}}{\mathrm{d}t}\iiint_{V_c} \rho e \mathrm{d}V = \underbrace{-\iint_{\partial V_c} \rho e \vec{v}\cdot\vec{n}\mathrm{d}A}_{\text{Energy flow by convection}} + \dot{Q} - \dot{W}$$

The energy balance II

$$\frac{d}{dt}\int_\Omega \rho e dV = -\int_\Gamma \rho e \cdot \underline{v} \cdot \underline{n} dA + \frac{dQ}{dt} - \frac{dW}{dt}$$

$$\frac{dQ}{dt} = -\int_\Gamma \underline{n}\, \underset{\sim}{q}\, dA - \int_\Omega q''' dV$$

heat flux vector

heat rate generation

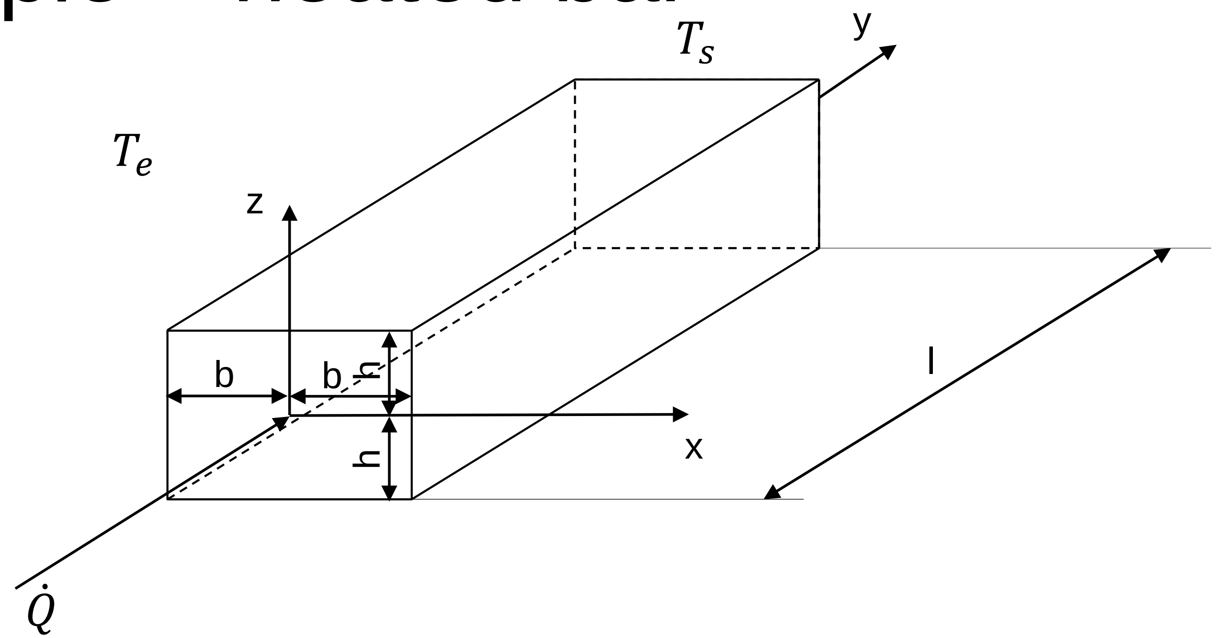
$$\frac{dW}{dt} = -\int_\Gamma \underline{n} (\sigma \underline{v}) dA$$

$$\frac{\partial \rho e}{\partial t} + \nabla \rho e \underline{v} + \nabla q - q''' - \nabla(\underline{\sigma} \cdot \underline{v}) = 0$$

product rule + Eq. of cont.

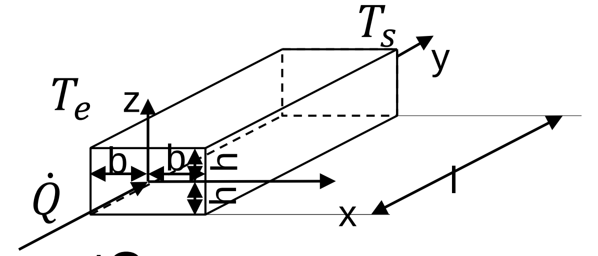
$$\rho \frac{De}{Dt} = -\nabla \underline{q} + q''' + \nabla(\sigma \cdot v)$$

Example – heated bar

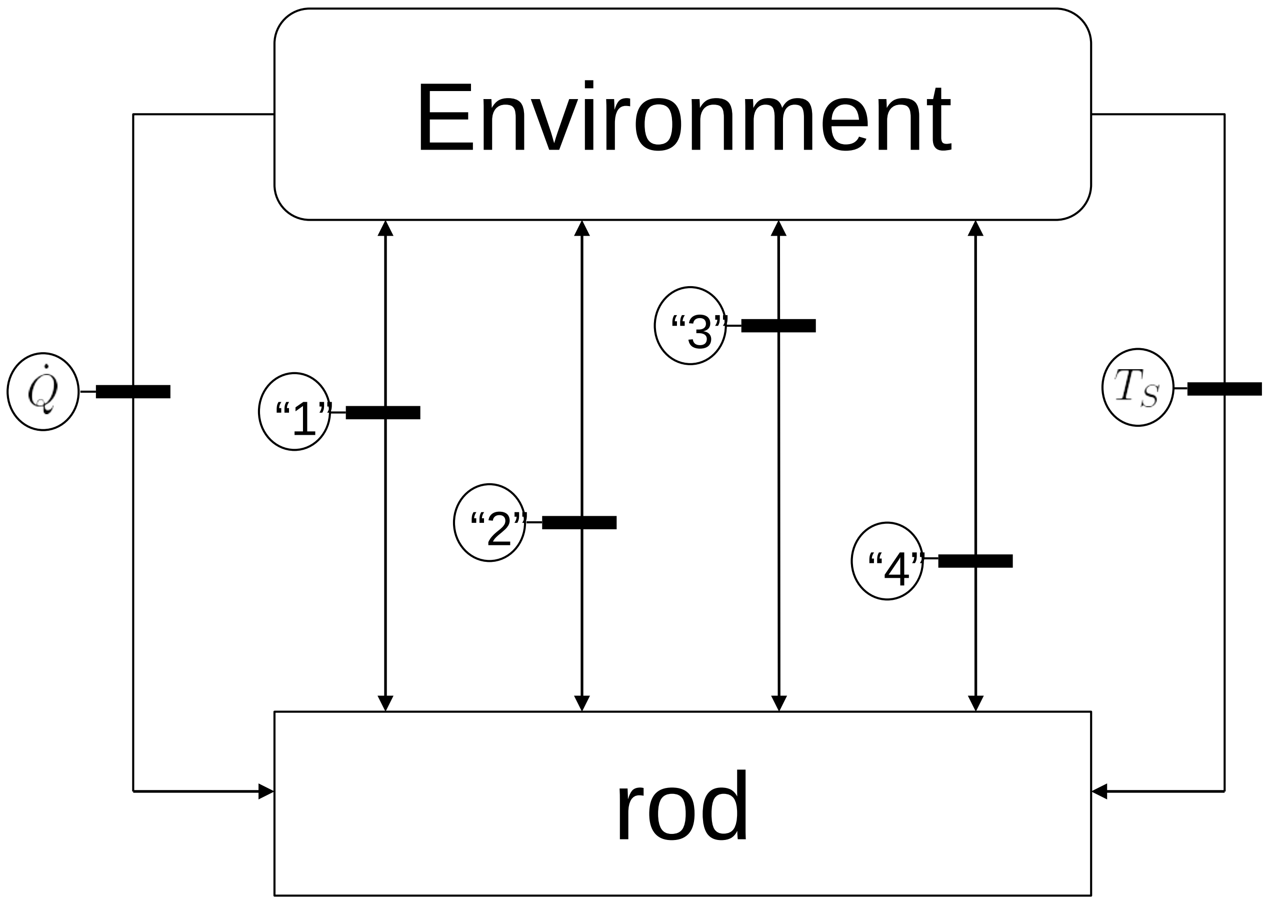


- At all sidewalls there is heat exchange with the environment (T_e, heat exchange coefficient α)
- At the front side there is a heat flux $\dot{Q}$
- At the back side there is a constant temperature T_s

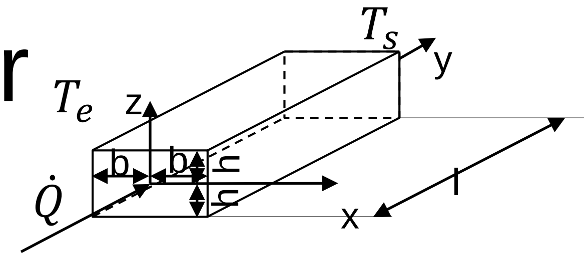
Abstraction of process



- How many interaction with the environment?



Energy balance – heated bar



1) Derive 3D energy balance

$$\frac{\partial \rho h}{\partial t} = -\nabla \underline{q}$$

Solve Nabla operator:

$$\frac{\partial \rho h}{\partial t} = -\frac{\partial}{\partial x}(q_x) - \frac{\partial}{\partial y}(q_y) - \frac{\partial}{\partial z}(q_z)$$

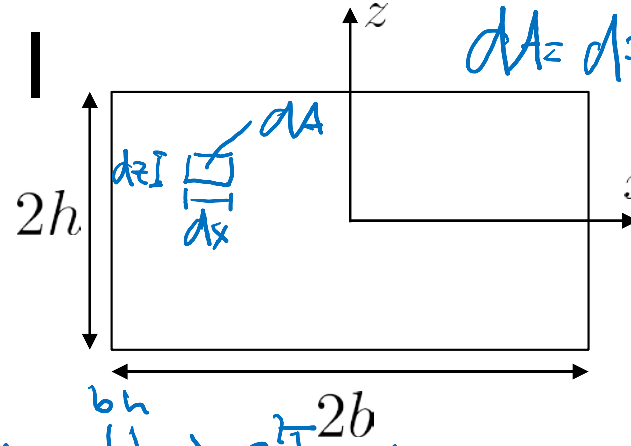
Fourier's law: $q = -\lambda \frac{\partial T}{\partial x}$

heat capacities: $\frac{\partial h}{\partial t} = c_p \frac{\partial T}{\partial t}$

$$\rho \frac{\partial h}{\partial t} = \rho c_p \frac{\partial T}{\partial t} = \lambda \frac{\partial^2 T}{\partial x^2} + \lambda \frac{\partial^2 T}{\partial y^2} + \lambda \frac{\partial^2 T}{\partial z^2}$$

Solve differential balance I

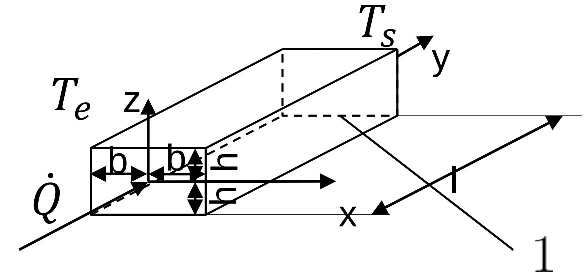
$dA = dz\,dx$



$$\int_{-b}^{b}\int_{-h}^{h} \rho c_p \frac{\partial T}{\partial t}\, dz\, dx = \int_{-b}^{b}\int_{-h}^{h} \lambda \frac{\partial^2 T}{\partial x^2}\, dz\, dx + \int_{-b}^{b}\int_{-h}^{h} \lambda \frac{\partial^2 T}{\partial y^2}\, dz\, dx + \int_{-b}^{b}\int_{-h}^{h} \lambda \frac{\partial^2 T}{\partial z^2}\, dz\, dx$$

$$4hb\,\rho c_p \frac{\partial \bar{\bar{T}}}{\partial t} = \int_{-h}^{h} \left(\left[\lambda \frac{\partial T}{\partial x}\right]_{x=b} - \left[\lambda \frac{\partial T}{\partial x}\right]_{x=-b} \right) dz + 4hb\,\lambda \frac{\partial^2 \bar{\bar{T}}}{\partial y^2} + \int_{-b}^{b} \left(\left[\lambda \frac{\partial T}{\partial z}\right]_{z=h} - \left[\lambda \frac{\partial T}{\partial z}\right]_{z=-h} \right) dx$$

Boundary conditions



energy balance boundary:

$$0 = q^- + q^+$$

$$q^+ = \alpha (T - T_e)$$ ← heat convection

$$q^- = \left[\lambda \frac{\partial T}{\partial x}\right]_{x=b}$$ ← heat conduction

All surfaces:

1: $\lambda \left[\frac{\partial T}{\partial x}\right]_{x=b} = -\alpha (T - T_e)$

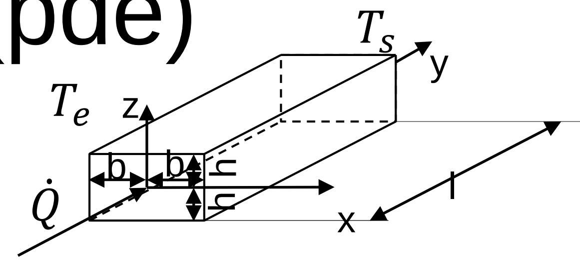
2: $\lambda \left[\frac{\partial T}{\partial z}\right]_{z=h} = -\alpha (T - T_e)$

3: $\lambda \left[\frac{\partial T}{\partial x}\right]_{x=-b} = \alpha (T - T_e)$

4: $\lambda \left[\frac{\partial T}{\partial z}\right]_{z=-h} = \alpha (T - T_e)$

$$\rightarrow \quad 4hb\rho c_p \frac{\partial \bar{\bar{T}}}{\partial t} = 4hb\lambda \frac{\partial^2 \bar{\bar{T}}}{\partial y^2} - 4(b+h)\alpha (T - T_e)$$

Solve differential balance II (pde)



- $\vartheta = T - T_e$
- steady-state

$$0 = \frac{\partial^2 \vartheta}{\partial y^2} - \underbrace{\frac{(b+h)\alpha}{hb\lambda}}_{\eta^2} \vartheta(y)$$

→ solution of 2nd order diff. eq.

$$\vartheta(y) = C_1 \sinh(\eta y) + C_2 \cosh(\eta y)$$

→ boundary conditions!

$$y = 0 : \quad \dot{Q} = -\lambda 4bh \left[\frac{\partial T}{\partial y}\right]_{y=0} = -4\lambda b h \eta \left[C_1 \cosh(0) + C_2 \sinh(0)\right]$$

$$y = l : \quad T_s - T_e = T(y=l) - T_e = C_1 \sinh(\eta l) + C_2 \cosh(\eta l)$$

Homework

- Read Section 4.5 (Hydraulic transmission lines)
- Read Chapter 10