Lecture 24: Process modeling & balance laws

- Balance laws
  - Differential balances
  - Material derivative

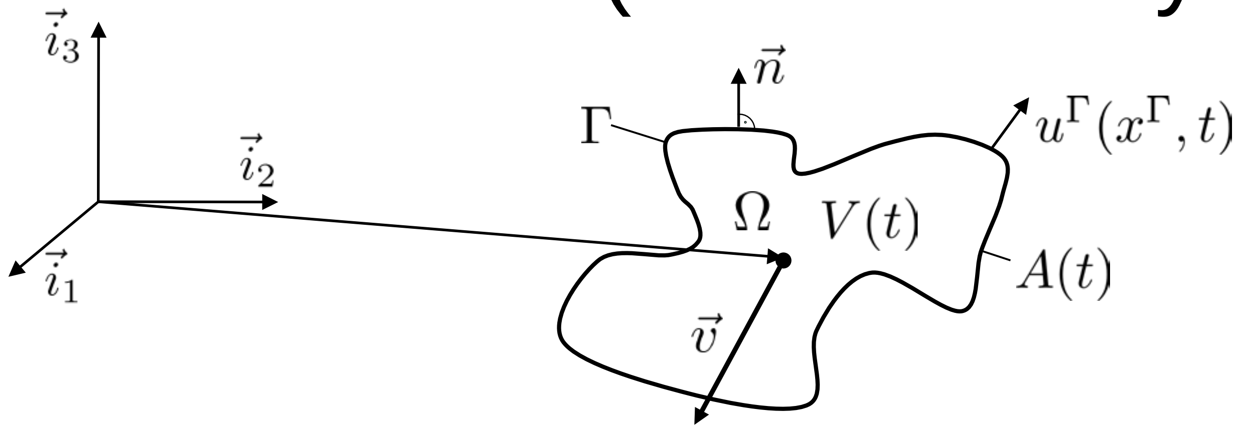
Book: 10.4, 11.1-11.4

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

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

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

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

→ Ω is arbitrary since integration must be zero

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

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

→ 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]

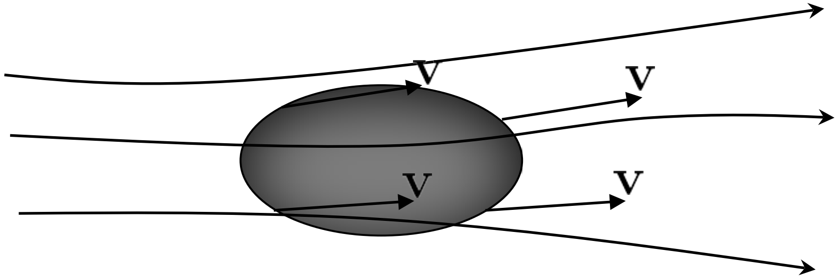
↖ net rate of mass inflow

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

incompressible fluid

$\nabla \cdot v = 0$

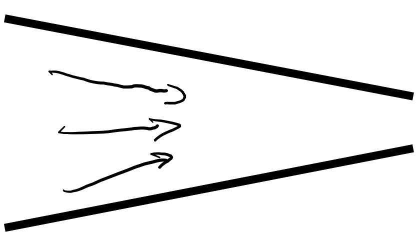
"Moving with the flow"



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

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

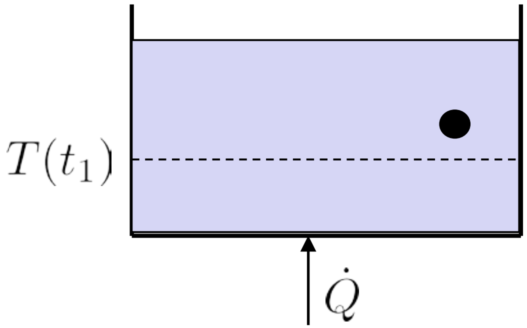
- Example:



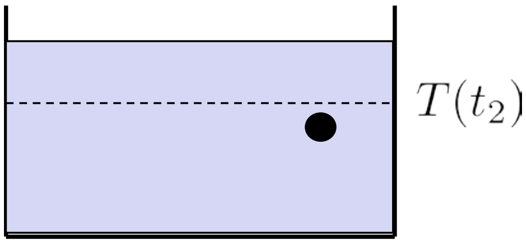
∘ velocity increases as pipe narrows [Bernoulli's law]

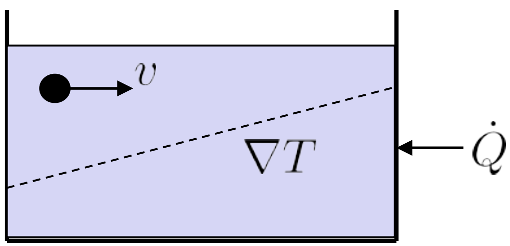
Example: Material derivative $\frac{D}{Dt} = \frac{\partial}{\partial t} + v \cdot \nabla$

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



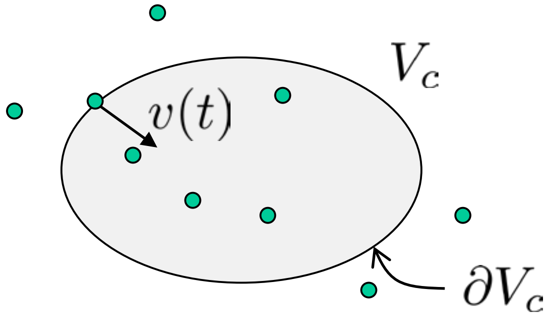
Temperature rise with time





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

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))

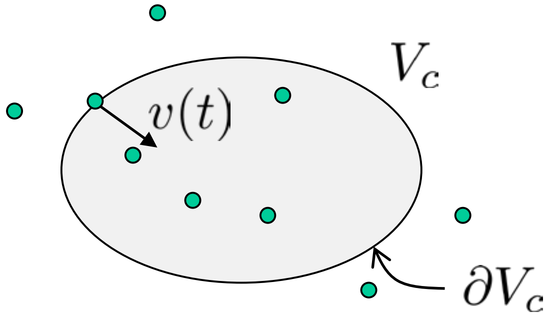
The momentum balance II

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

$$\vdots$$

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

The energy balance I



- In words

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

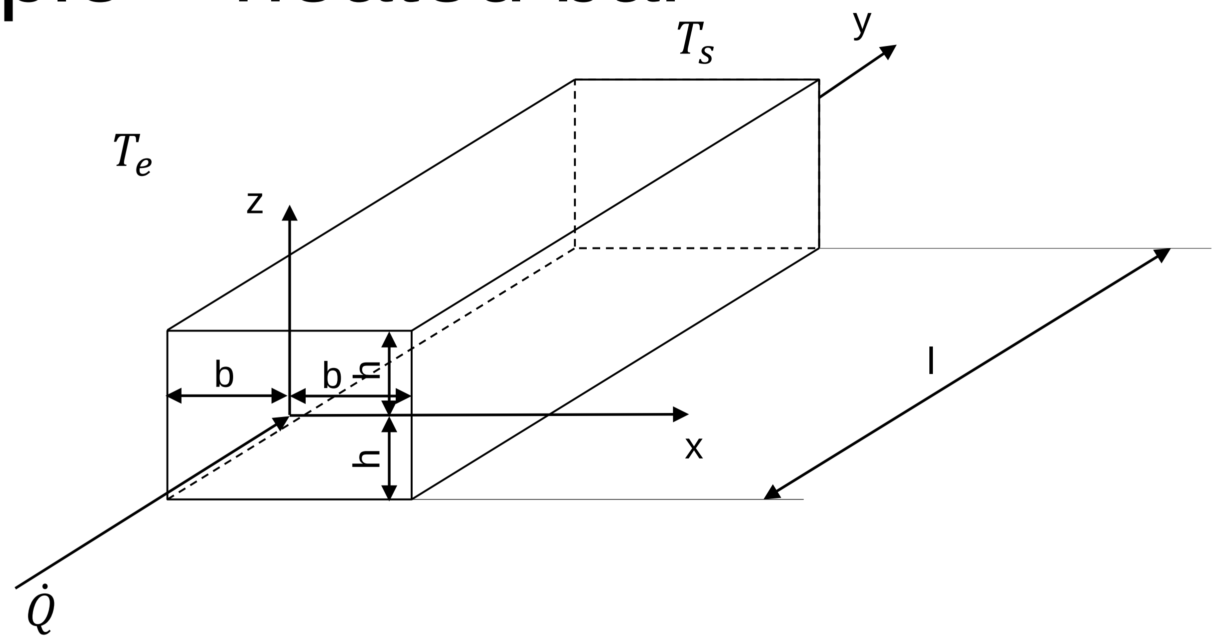
- Mathematically

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

The energy balance II

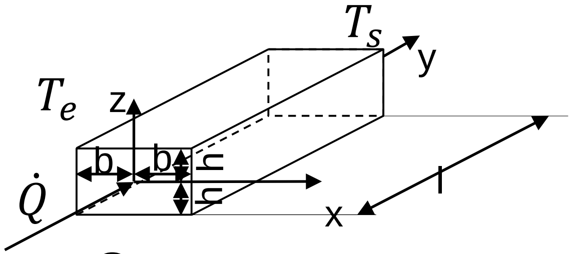
$$\frac{d}{dt}\int_{\Omega}\rho e dV = -\int_{\Gamma}\rho e \cdot \underline{v} \cdot \underline{n} dA + \frac{dQ}{dt} - \frac{dW}{dt}$$

Example – heated bar

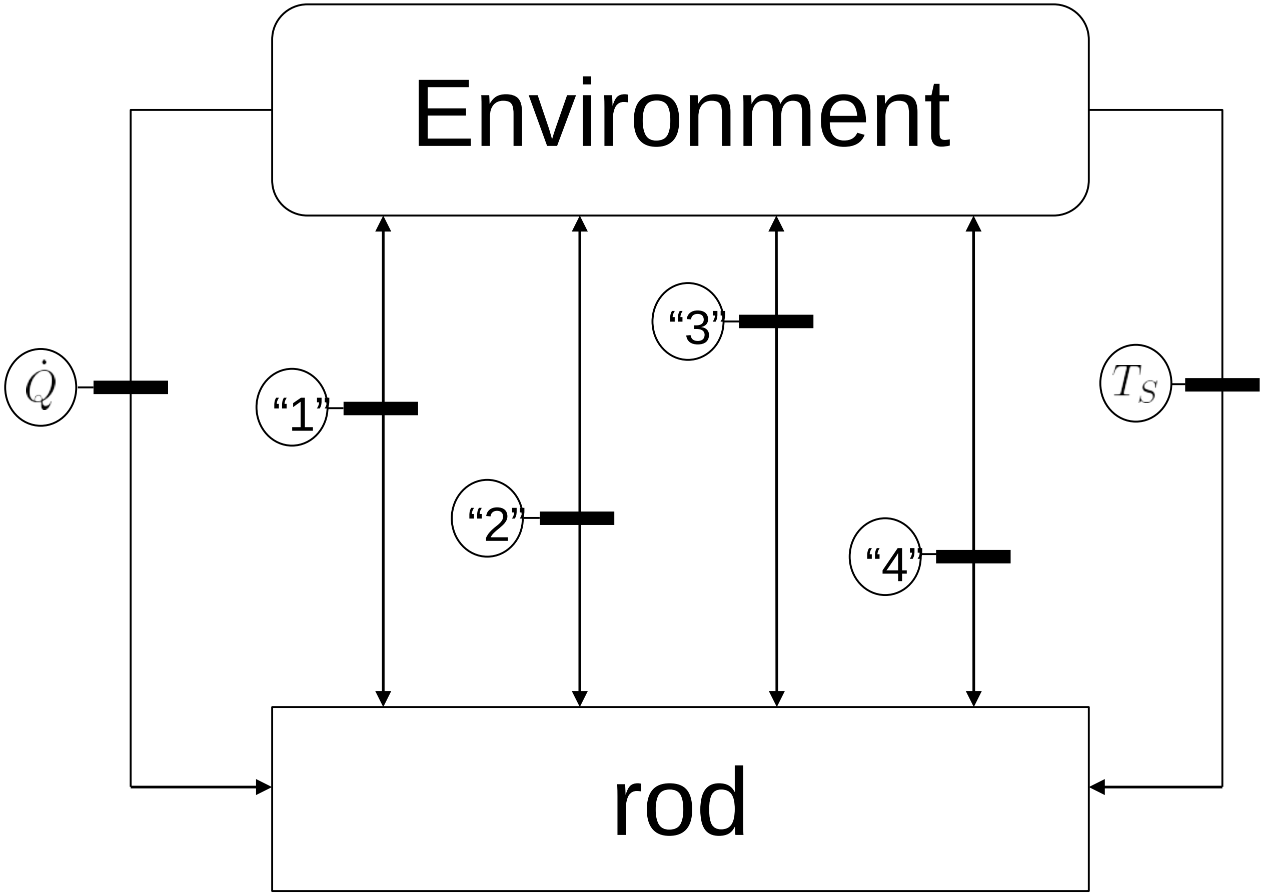


- At all sidewalls there is heat exchange with the environment (T_e, heat exchange coefficient α)
- At the front side there is a heat flux $\dot{Q}$
- At the back side there is a constant temperature T_s

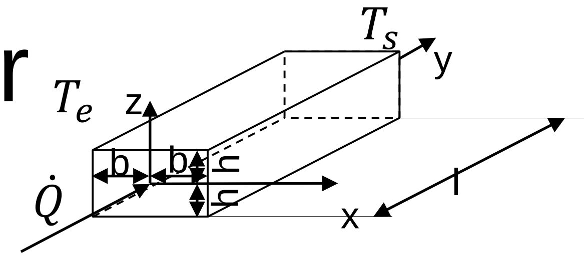
Abstraction of process



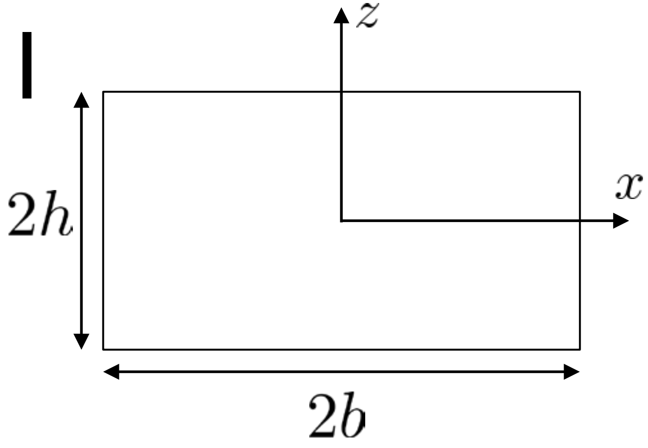
- How many interaction with the environment?



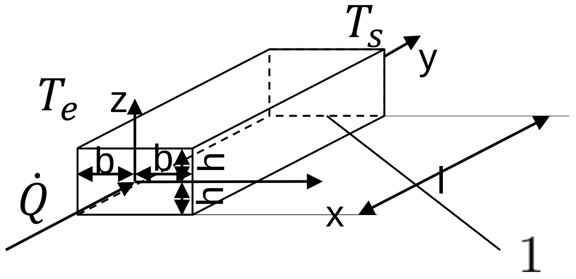
Energy balance – heated bar



Solve differential balance I



Boundary conditions



Solve differential balance II (pde)