Lecture 22: Balance equations – Momentum and energy balances

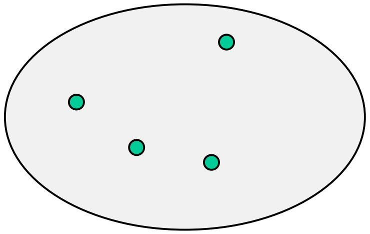
- Recap balance laws
- The momentum balance
- The energy balance
- Differential balance laws

Book: Ch. 11.2, 11.4

Process modeling and balance laws

- The balance laws are formulated for «conserved quantities»:
  - Mass (or other quantities that are «equivalent» to mass, such as moles, particles, etc.)
  - Momentum
  - Energy
- Process modeling is done by
  1. formulating the relevant balance laws, and
  2. finding the «closure relations» that is used to determine the flows in a balance law, as function of the state («inventory») of the balance law
- The state («inventory») of a balance law is what is used as a measure for the conserved quantity
  - Such as mass, moles, concentration, level, pressure, … for mass balance,
  - velocity or flows for momentum balance, and
  - temperature for energy balance

The basic physical principles



Consider a volume consisting of a fixed number of fluid particles, with total mass m, total momentum $\vec{p}$ and total energy E. From basic physics (conservation laws), we know the following principles hold:

- Conservation of mass (mass balance):

$$\frac{\mathrm{d}m}{\mathrm{d}t} = 0$$

- Newton's second law (momentum balance)

$$\frac{{}^{i}\mathrm{d}\vec{p}}{\mathrm{d}t} = \vec{F}$$

Also holds for angular momentum, $\vec{h} = \vec{r} \times \vec{p}$:

$$\frac{{}^{i}\mathrm{d}}{\mathrm{d}t}\vec{h} = \vec{r} \times \vec{F} = \vec{T}$$

- First law of thermodynamics (conservation of energy, energy balance):

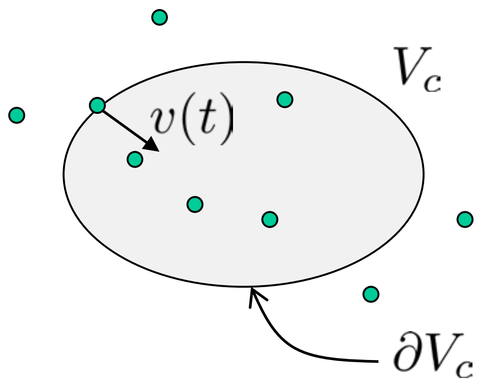
Rate of heat flowing into volume from surroundings

$$\frac{\mathrm{d}E}{\mathrm{d}t} = \dot{Q} - \dot{W}$$

Rate at which work is done by the body at surroundings

The balance laws

- Assume a fixed control volume (of arbitrary size and shape), where fluid flows across the control volume

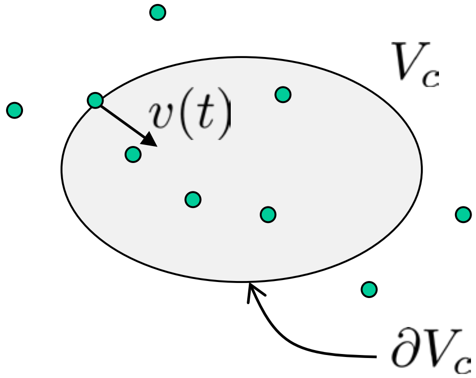


$$B = \iiint\limits_{V_c} \rho\beta(\mathbf{x}, t)\mathrm{d}V$$

- The general integral (macroscopic) balance law for *B* is

$$\frac{\mathrm{d}}{\mathrm{d}t}B = \left\{ \begin{array}{c} \text{transfer of } B \text{ through} \\ \text{surface } \partial V_c \text{ by} \\ \text{fluid flow (convection)} \end{array} \right\} + \left\{ \begin{array}{c} \text{other effects that} \\ \text{transfer } B \text{ into } V_c \\ \text{(indep. of fluid flow)} \end{array} \right\}$$

The integral balance laws



- Mass balance (without reactions/phase transfer)

$$\frac{\mathrm{d}}{\mathrm{d}t} m = \left\{ \begin{array}{c} \text{transfer of mass into} \\ V_c \text{ by fluid flow} \\ \text{across surface } \partial V_c \end{array} \right\}$$

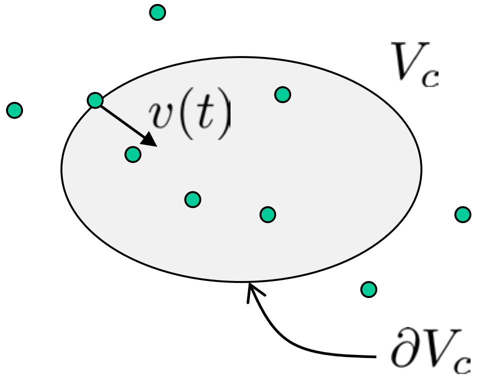
- Momentum (note: momentum is a vector)

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

- Energy

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

The mass balance



- In words

$$\frac{\mathrm{d}}{\mathrm{d}t}m = \left\{ \begin{array}{c} \text{transfer of mass into} \\ V_c \text{ by fluid flow} \\ \text{across surface } \partial V_c \end{array} \right\}$$

- Mathematically

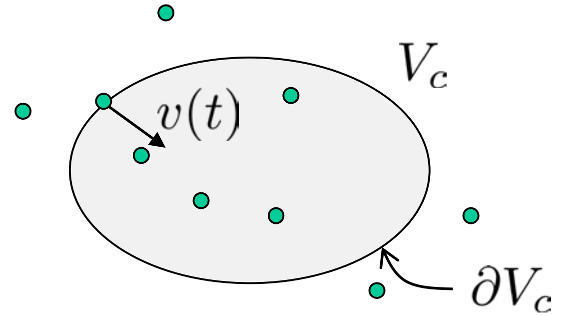
"Convection"

$$\frac{\mathrm{d}}{\mathrm{d}t}m = \frac{\mathrm{d}}{\mathrm{d}t}\iiint_{V_c} \rho \mathrm{d}V = -\iint_{\partial V_c} \rho \vec{v} \cdot \vec{n} \mathrm{d}A$$

- Often, we have one (or more) «point inflows» $w_{\mathrm{in},i}$, and outflows $w_{\mathrm{out},i}$. Then mass balance can be formulated as

$$\frac{\mathrm{d}}{\mathrm{d}t}m = \sum_i w_{\mathrm{in},i} - \sum_i w_{\mathrm{out},i}$$

The momentum balance



- In words

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

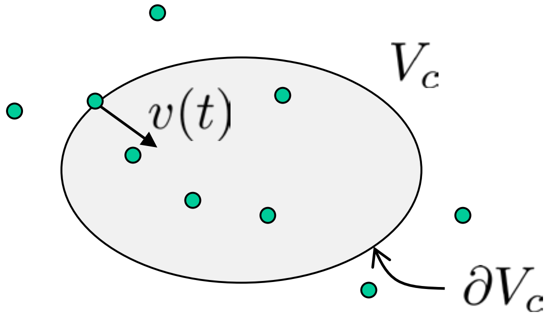
- Mathematically

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

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

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

The energy balance



- In words

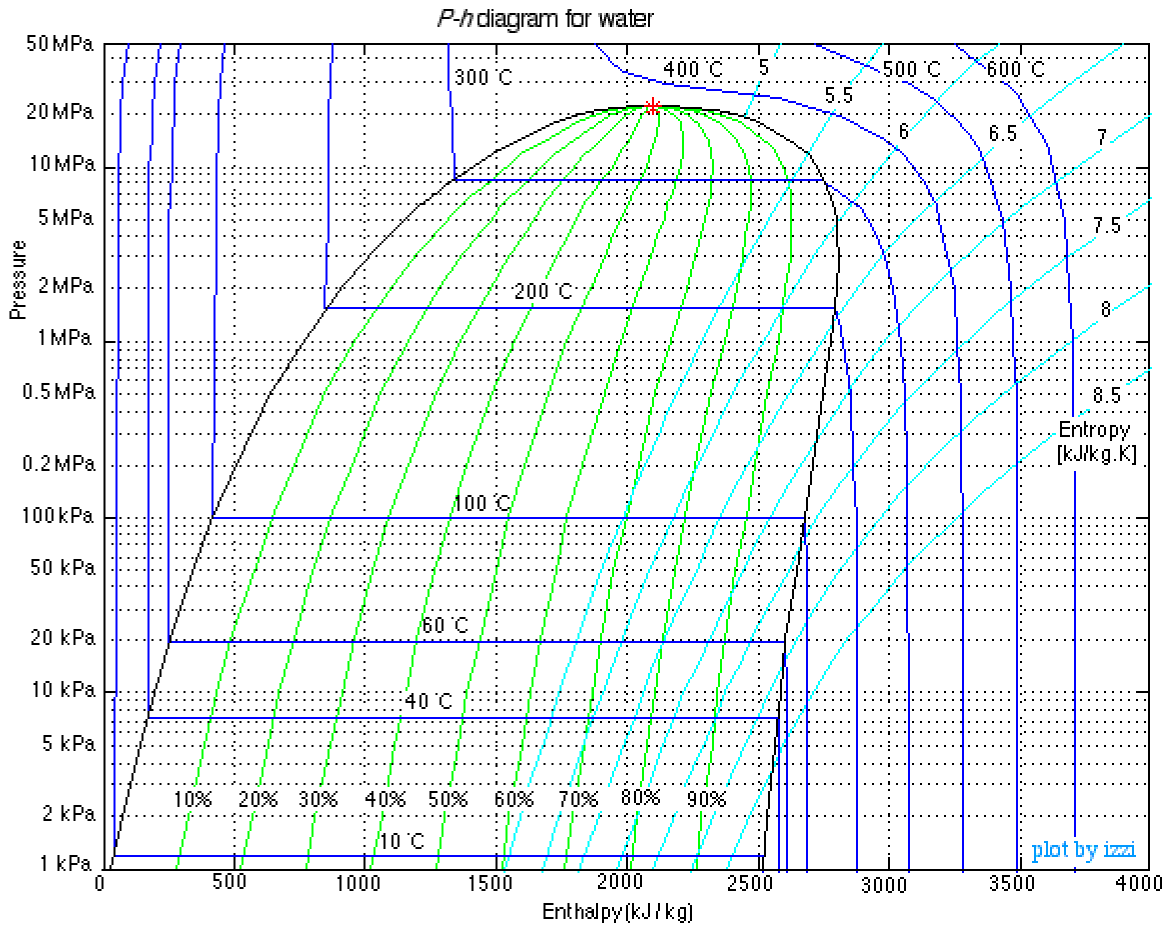
$$\frac{\mathrm{d}}{\mathrm{d}t}E = \left\{ \begin{array}{c} \text{transfer of energy into} \\ V_c \text{ by fluid flow} \\ \text{across surface } \partial V_c \end{array} \right\} + \left\{ \begin{array}{c} \text{transfer of energy into} \\ V_c \text{ by heat transfer} \\ \text{and by work} \end{array}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

- Mathematically

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

- What is the energy of a fluid?

P-h-diagram for water



Energy

$$\frac{\mathrm{d}}{\mathrm{d}t}E = \frac{\mathrm{d}}{\mathrm{d}t}\iiint_{V_c} \rho e \mathrm{d}V = -\iint_{\partial V_c} \rho e \vec{v} \cdot \vec{n} \mathrm{d}A + \dot{Q} - \dot{W}$$

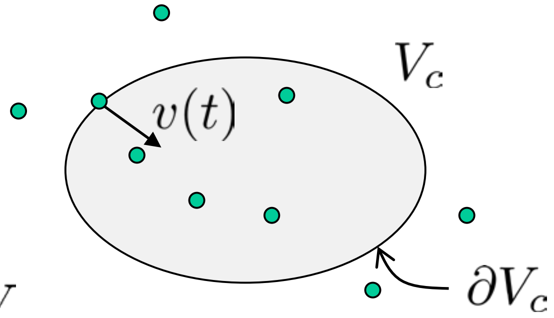
- The energy of a fluid of mass *m*, moving with a velocity *v* at a height *z* in a gravitational field:

$$E = \underbrace{U}_{\substack{\text{internal}\\ \text{energy}}} + \underbrace{\frac{1}{2}mv^2}_{\substack{\text{kinetic}\\ \text{energy}}} + \underbrace{mgz}_{\substack{\text{potential}\\ \text{energy}}}$$

- Specific energy:

$$e = u + \frac{1}{2}v^2 + gz$$

Heat and work flow



$$\frac{\mathrm{d}}{\mathrm{d}t}E = \frac{\mathrm{d}}{\mathrm{d}t}\iiint_{V_c} \rho e \mathrm{d}V = -\iint_{\partial V_c} \rho e \vec{v}\cdot\vec{n}\mathrm{d}A + \dot{Q} - \dot{W}$$

- Heat flow

$$\dot{Q} = \iint_{\partial V_c} \vec{j}_Q \cdot \vec{n}\mathrm{d}A$$

- Work flow

$$\dot{W} = \underbrace{\iint_{\partial V_c} p\vec{v}\cdot\vec{n}\mathrm{d}A}_{\text{flow work}} + \underbrace{\dot{W}_s}_{\text{shaft work}}$$

Enthalpy

- The energy balance can be written

$$\frac{\mathrm{d}}{\mathrm{d}t}\iiint\limits_{V_c} \rho e \mathrm{d}V = -\iint\limits_{\partial V_c} \rho \left(e + \frac{p}{\rho}\right) \vec{v}\cdot\vec{n}\mathrm{d}A - \dot{W}_s + \dot{Q}$$

where the first term on the RHS is convection and flow work

- Define **enthalpy** as

$$h = u + \frac{p}{\rho}$$

- Then

$$\frac{\mathrm{d}}{\mathrm{d}t}\iiint\limits_{V_c} \rho \left(u + \frac{1}{2}v^2 + gz\right)\mathrm{d}V = -\iint\limits_{\partial V_c} \rho \left(h + \frac{1}{2}v^2 + gz\right) \vec{v}\cdot\vec{n}\mathrm{d}A - \dot{W}_s + \dot{Q}$$

Internal energy and enthalpy

- Specific heat capacities:

$$c_v := \left.\frac{\partial u}{\partial T}\right|_{\text{constant volume}} \qquad c_p := \left.\frac{\partial h}{\partial T}\right|_{\text{constant pressure}}$$

(found in tables for different fluids, often assumed constant)

- If assumed constant, implies that energy and enthalpy is (linear) function of temperature only:

$$\frac{\mathrm{d}u}{\mathrm{d}t} = c_v \frac{\mathrm{d}T}{\mathrm{d}t} \qquad u(T_2) - u(T_1) = c_v\,(T_2 - T_1)$$

$$\frac{\mathrm{d}h}{\mathrm{d}t} = c_p \frac{\mathrm{d}T}{\mathrm{d}t} \qquad h(T_2) - h(T_1) = c_p\,(T_2 - T_1)$$

- For ideal gases:

$$c_v = c_p + R$$

- For incompressible fluids (often assumed for liquids):

$$c_v = c_p$$

Examples energy balances...

Differential mass balance

- Recall the integral mass balance:

$$\underbrace{\frac{\mathrm{d}}{\mathrm{d}t}\iiint_{V_c} \rho \mathrm{d}V}_{} = -\underbrace{\iint_{\partial V_c} \rho \vec{v} \cdot \vec{n} \mathrm{d}A}_{}$$

Mathematics (obvious?)

$$\frac{\mathrm{d}}{\mathrm{d}t}\iiint_{V_c} \rho \mathrm{d}V = \iiint_{V_c} \frac{\partial \rho}{\partial t} \mathrm{d}V$$

Divergence theorem

$$\iint_{\partial V_c} \rho \vec{v} \cdot \vec{n} \mathrm{d}A = \iiint_{V_c} \vec{\nabla} \cdot (\rho \vec{v}) \mathrm{d}V$$

- That is:

$$\iiint_{V_c} \frac{\partial \rho}{\partial t} + \vec{\nabla} \cdot (\rho \vec{v}) \mathrm{d}V = 0$$

- This must hold for arbitrary control volumes, which implies

$$\boxed{\frac{\partial \rho}{\partial t} + \vec{\nabla} \cdot (\rho \vec{v}) = 0}$$

Differential mass balance, also called *continuity equation* or *advection equation*

Alternative formulations

- The differential mass balance

$$\frac{\partial \rho}{\partial t} + \vec{\nabla} \cdot (\rho \vec{v}) = 0$$

- From definition of nabla operator, this is the same as

$$\frac{\partial \rho}{\partial t} + \sum_{i=1}^{3} \frac{\partial}{\partial x_i} (\rho v_i) = 0, \quad \mathbf{v} = (v_1, v_2, v_3)^{\mathsf{T}}$$

- If we introduce the *material derivative*,

$$\frac{\mathrm{D}\phi}{\mathrm{D}t} := \frac{\partial \phi}{\partial t} + \mathbf{v}^{\mathsf{T}} \nabla \phi = \frac{\partial \phi}{\partial t} + \sum_{i=1}^{3} \frac{\partial \phi}{\partial x_i} v_i$$

The material derivative is the derivative following a particle (as opposed to the derivative at a fixed point in space)

and use product rule, we can write

$$\frac{\mathrm{D}\rho}{\mathrm{D}t} + \rho \nabla \cdot \vec{v} = 0$$

Differential momentum and energy balances

- Differential momentum balance for inviscid fluid (*Euler's equation*)

$$\rho \frac{\mathrm{D}\vec{v}}{\mathrm{D}t} = -\vec{\nabla} p + \rho \vec{f}, \quad \text{where } \rho\vec{f} \text{ is the mass force (e.g. gravity)}$$

- For viscous (Newtonian) fluids, the differential momentum balance is the famous *Navier-Stokes* equation:

$$\rho \frac{\mathrm{D}\vec{v}}{\mathrm{D}t} = -\vec{\nabla} p + \mu \vec{\nabla}^2 \vec{v} + \rho \vec{f}$$

- Differential energy balance (for example)

$$\rho \frac{\mathrm{D}}{\mathrm{D}t} \left(\frac{1}{2} \vec{v}^2 + u \right) = -\vec{\nabla} \cdot (p\vec{v}) - \vec{\nabla} \cdot \vec{j}_Q + \rho \vec{v} \cdot \vec{f}$$

Computational fluid dynamics

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

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

Example of differential energy balances: The heat equation of a solid

- The energy balance:

$$\rho \frac{\mathrm{D}}{\mathrm{D}t}\left(\frac{1}{2}\vec{v}^2 + u\right) = -\vec{\nabla}\cdot(p\vec{v}) - \vec{\nabla}\cdot\vec{j}_Q + \rho\vec{v}\cdot\vec{f}$$

- Solid: Disregard kinetic and potential energy, no velocity:

$$\rho\frac{\partial u}{\partial t} = -\vec{\nabla}\cdot\vec{j}_Q$$

- We need a «closure relation». Here in the form of *Fourier's law*:

$$\vec{j}_Q = -\alpha\vec{\nabla}(\rho c_p T)$$

- Combined with

$$\frac{\partial u}{\partial t} = c_p\frac{\partial T}{\partial t}$$

we get

$$\frac{\partial T}{\partial t} - \alpha\vec{\nabla}\cdot\vec{\nabla}T = 0$$

In one dimension:

$$\frac{\partial T(x,t)}{\partial t} - \alpha\frac{\partial^2 T(x,t)}{\partial x^2} = 0$$