Lecture 20: Process modeling & balance laws

- Process modeling, structure and methodology
- Balance laws
  - Mass balances
  - Mass balances for multi-component systems

Book: 10.4, 11.1-11.4

What are process modeling and balance laws used for?

Process modeling & balance laws:

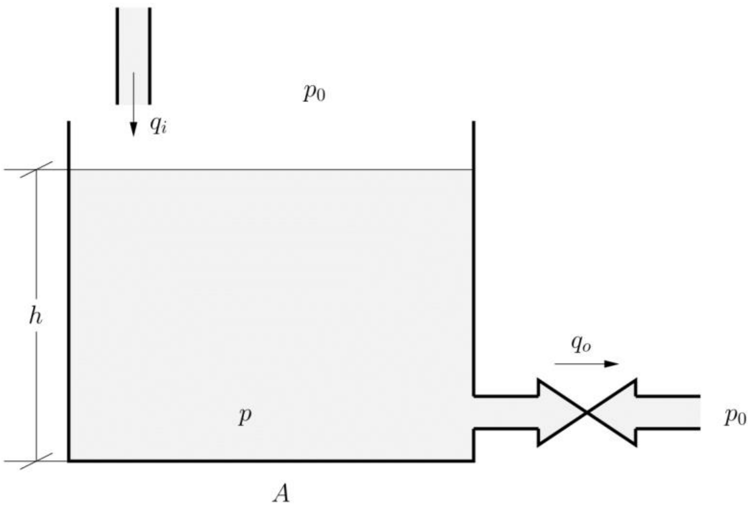
- Basically, modeling of anything that changes in the physical world.
- In this context, we will be concerned with fluids (liquids and gas) in (chemical) **process systems**

Autoignition of hydrogen in a turbulent hot air coflow

Process modeling: Structure and methodology

- Goal of process modeling: Construct mathematical models of the process under study.
- These mathematical models consists of process variables (variables and parameters) and the equations that link these

Process



Process variables

(variables and parameters)

- Level
  - Variability: Variable
  - Symbol: *h*
  - Value: 1.1
  - Unit: m
  - ...
- Area
  - Variability: Parameter
  - Symbol: *A*
  - Value: 2.2
  - Unit: m^2
  - ...
- ...

Process equations

$$\frac{\mathrm{d}h}{\mathrm{d}t} = \frac{1}{A}(q_i - q_o)$$

$$q_o = C\sqrt{p - p_0}$$

$$p = p_0 + \rho g h$$

Number of equations must match number of (unknown) variables.

Process equations

- Balance laws
  - Mass
  - Momentum
  - Energy
  - ...

- Constitutive equations
  - For (generalized) flows
  - Thermodynamic equations of state (e.g. ideal gas law)
  - Phenomenological relationships (e.g. between friction force and flow in a pipe)
  - ...

- Constraints
  - Geometric relationships
  - Equilibrium conditions
  - ...

Also called «closure relations» as they «close» the balance laws (such that #equations = #variables)

Example Tank:

$$\frac{\mathrm{d}h}{\mathrm{d}t} = \frac{1}{A}\left(q_i - q_o\right)$$

$$q_o = C\sqrt{p - p_0}$$
$$p = p_0 + \rho g h$$

$$V = Ah$$

Process variables

- Thermodynamic state variables
  - Mass, pressures, levels, ...
  - Velocities
  - Temperatures
  - ...

- (Generalized) flows
  - Transport (single phase)
  - Exchange (between phases)
  - Sources (reactions)
  - ...

- Phenomenological coefficients
  - Viscosity
  - Reaction rates
  - Valve constants
  - ...

- Geometric dimensions
  - Lengths, Areas, Volumes
  - ...

Example Tank:

h, ρ, p, p_0

q_i, q_o

C, g

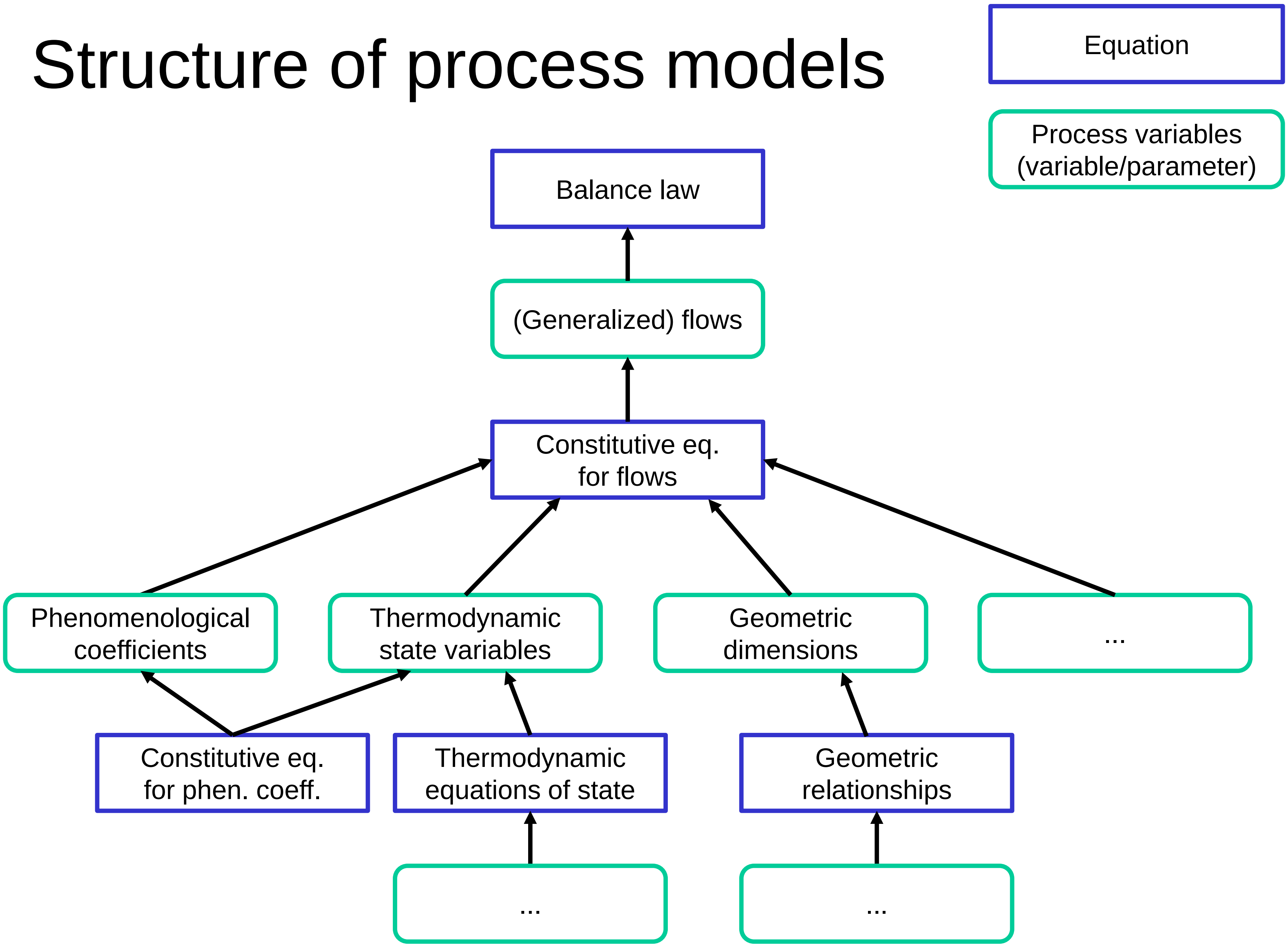
A

$$\frac{\mathrm{d}h}{\mathrm{d}t} = \frac{1}{A}(q_i - q_o)$$

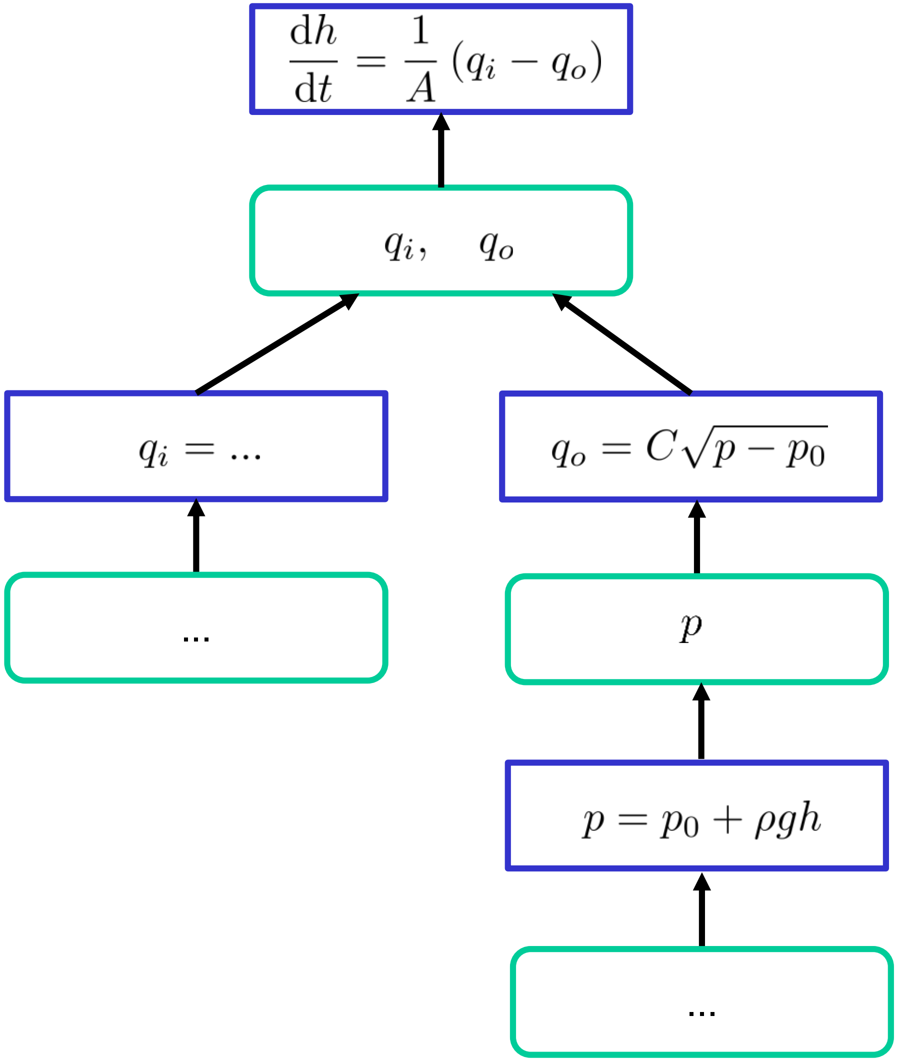
$$q_o = C\sqrt{p - p_0}$$

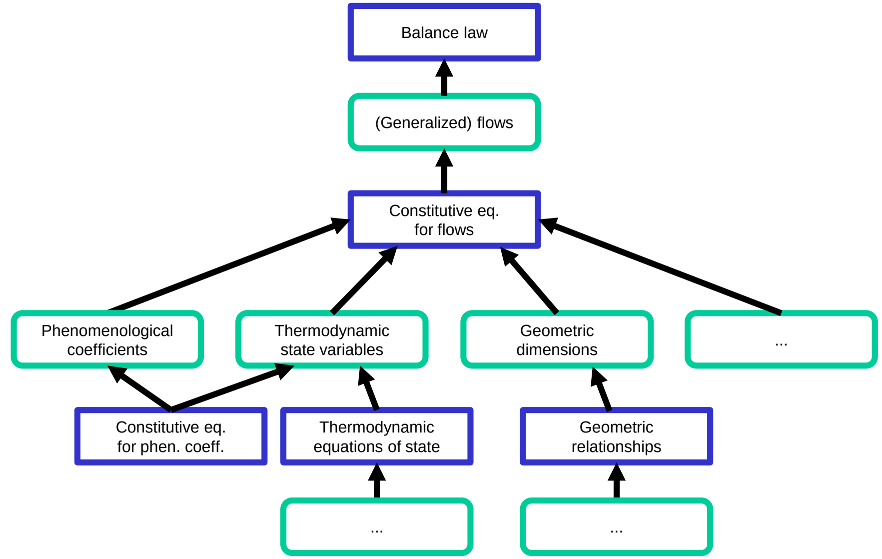
$$p = p_0 + \rho g h$$

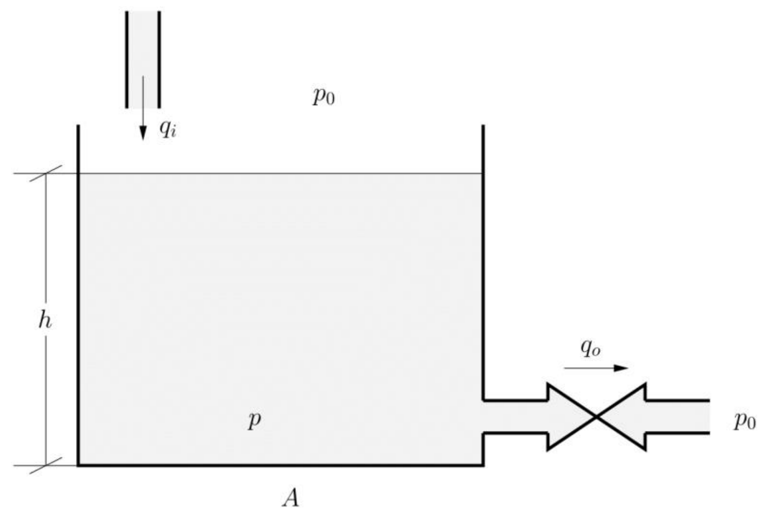
Structure of process models



Example: Tank







BALANCE LAWS

Physical balance principles are based on

Conservation laws

That a physical property is *conserved*, means that it will remain constant in a closed system

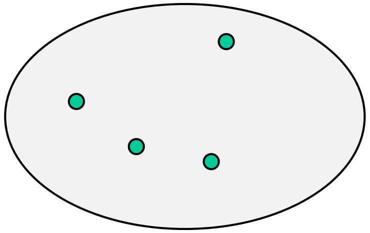
The following physical quantities are conserved:

- Mass
- Energy
- Momentum (norsk: impuls)
  - Linear and angular

No one has ever observed that conservation laws have been violated

- Conservation laws are exact laws

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

State variables for process systems

- What variables are relevant as state variable(s) for balance laws based on conservation of mass (that is, mass balances)?
  - Mass
  - Density
  - Moles, and mole concentration
  - Derived quantities: Pressure, level, …
  - (number of particles, etc.)
- For energy balances:
  - Internal energy
  - Temperature
- For momentum balances
  - Linear or angular momentum
  - Velocities

Extensive and intensive properties

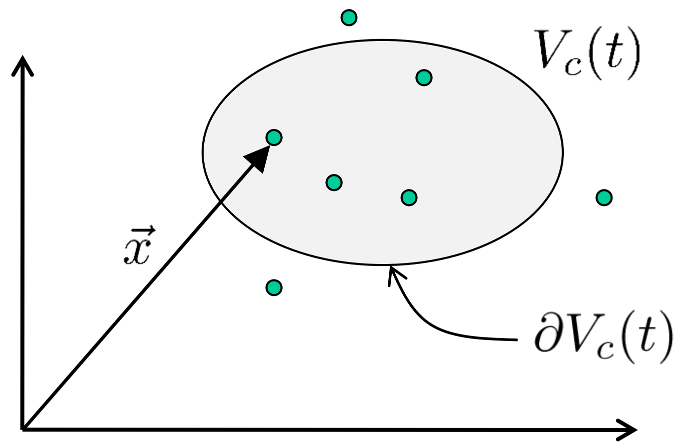
- We must choose properties (thermodynamic variables) to describe our process, and these are either *intensive* or *extensive*
- Intensive properties are scale invariant (does not change if we divide a volume in two), while extensive variables are proportional to amount of material
- In this course, we use mostly *mass-intensive* properties/variables (that is, we measure amount of material with mass):

Extensive properties	Symbol	Unit	Intensive properties	Symbol	Unit
mass	m	kg	1	-	-
volume	V	m^3	specific volume	v	m^3/kg
internal energy	U	J	specific internal energy	u	J/kg
enthalpy	H	J	specific enthalpy	h	J/kg
entropy	S	J/K	Specific entropy	s	J/K/kg

- What alternatives are there to mass-intensive?
- Is temperature an intensive or extensive property? Pressure? (yes and no…)

The concept of control volume

- We use a control volume for separating what we are interested in from the rest of the world (surroundings)
- Generally, material flow into (or out of) the control volume, across the surface



Extensive Property B of one particle

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

Summed over all particles in $V_c(t)$

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

- We are interested in
  - knowing how the extensive property B varies inside the control volume
  - ***or*** (equivalently?) how the intensive property $\beta(\mathbf{x},t)$ varies inside the volume
- Control volumes can move or change shape, but we will assume they are fixed (more on this in fluid mechanics)

Lumped vs distributed modeling

- If we do *lumped modeling*, we assume that intensive properties are constant (or averaged) over the control volume

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

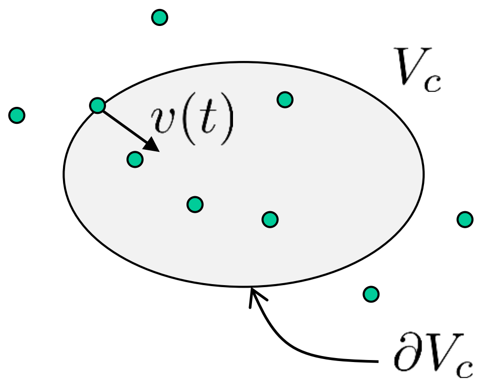
- The balance laws used for lumped modeling are the *integral* (or *macroscopic*) balance laws
  - Formulated for extensive (e.g. mass), or averaged intensive (e.g. average temperature), variables

- The alternative to lumped modeling is *distributed* modeling, where we are interested in how $\beta(\mathbf{x}, t)$ varies as a function of position ***x***
- The balance laws for distributed modeling are the differential balance laws

(This course: Mainly lumped modeling and integral balance laws)

The balance laws I

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

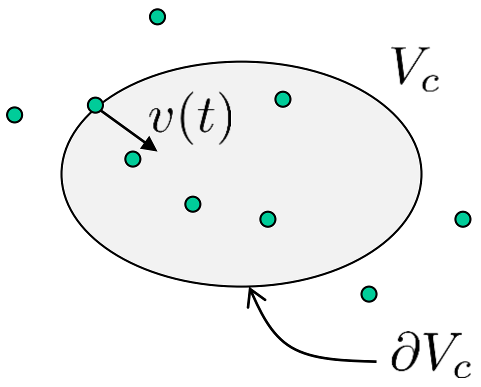


$$B = \iiint_{V_c} \rho\beta(\mathbf{x}, t)\mathrm{d}V$$

- 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 balance laws II



- 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

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

Mathematical formulation of convection

$$\frac{\mathrm{d}}{\mathrm{d}t}B = \underbrace{\left\{ \begin{array}{c} \text{transfer of } B \text{ through} \\ \text{surface } \partial V_c \text{ by} \\ \text{fluid flow (convection)} \end{array} \right\}}_{-\iint\limits_{\partial V_c} \rho\beta\vec{v}\cdot\vec{n}\mathrm{d}A} + \left\{ \begin{array}{c} \text{other effects that} \\ \text{transfer } B \text{ into } V_c \\ \text{(indep. of fluid flow)} \end{array} \right\}$$

Mathematical formulation of mass balance

- For mass, the intensive variable is $\beta(\mathbf{x}, t) = 1$

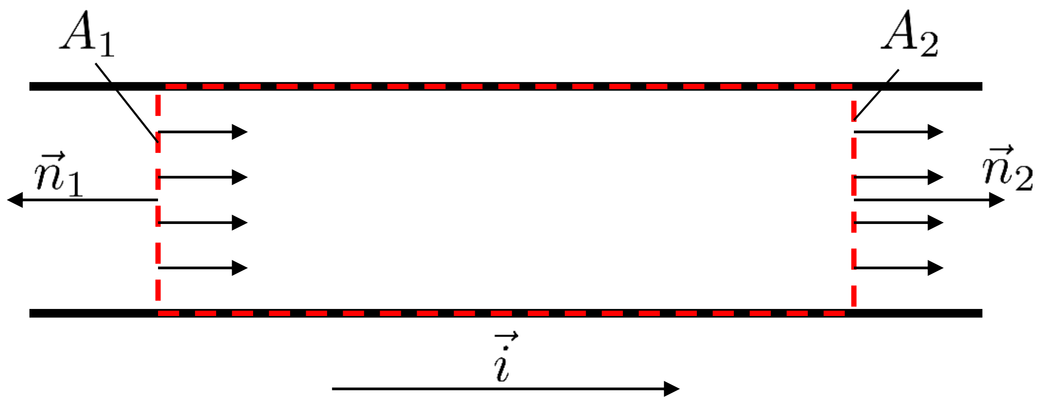
$$\frac{\mathrm{d}}{\mathrm{d}t} m = \underbrace{\left\{ \begin{array}{c} \text{transfer of mass into} \\ V_c \text{ by fluid flow} \\ \text{across surface } \partial V_c \end{array} \right\}}_{-\iint\limits_{\partial V_c} \rho \beta \vec{v} \cdot \vec{n} \mathrm{d}A}$$

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

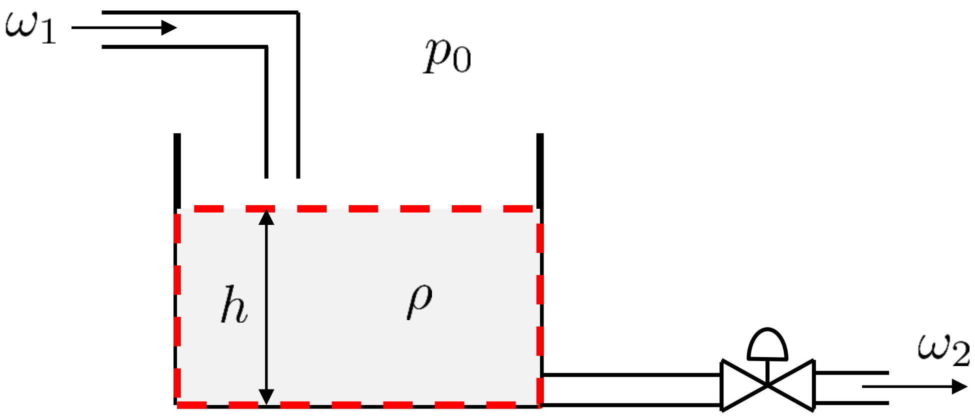
- Often, we have one (or more) «point inflows» $\omega_{in,i}$, and outflows $\omega_{out,i}$. Then mass balance can be formulated as

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

Example: Flow in a pipe



Example: Tank



Mass-type balance laws with generation

- Assume B is an extensive variable «equivalent to» mass
  - that is, mass of a component in a volume, or number of molecules of a component, number of particles, etc.
- These types of mass balance laws can have *internal generation*:

$$\frac{\mathrm{d}}{\mathrm{d}t}B = \sum_i W_{\mathrm{in},i} - \sum_i W_{\mathrm{out},i} + W_{\mathrm{generated}}$$

- More generally, if the local rate of generation of *B* is r_B:

$$\frac{\mathrm{d}}{\mathrm{d}t}B = \frac{\mathrm{d}}{\mathrm{d}t}\iiint_{V_c} \rho\beta \mathrm{dV} = -\iint_{\partial V_c} \rho\beta\vec{v}\cdot\vec{n}\mathrm{d}A + \iiint_{V_c} r_B \mathrm{dV}$$

Chemical reactions I

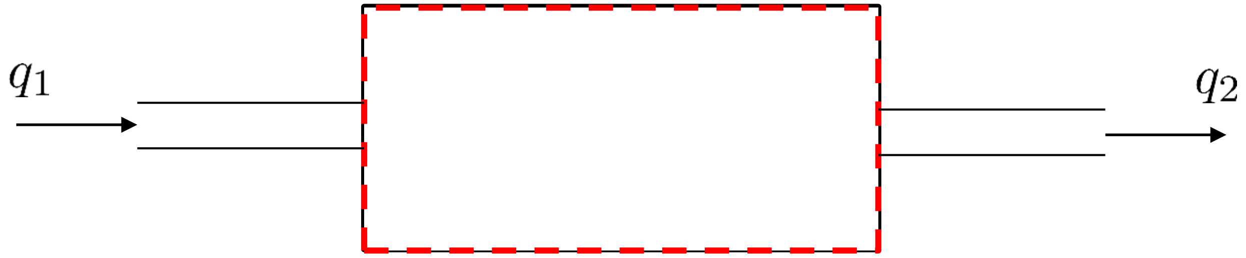
- Sometimes easier with amount of molecules than with masses
- Amount of molecules is measured in mol and the symbol n_k

→ Moleculebalance instead of massbalance

Molebalance

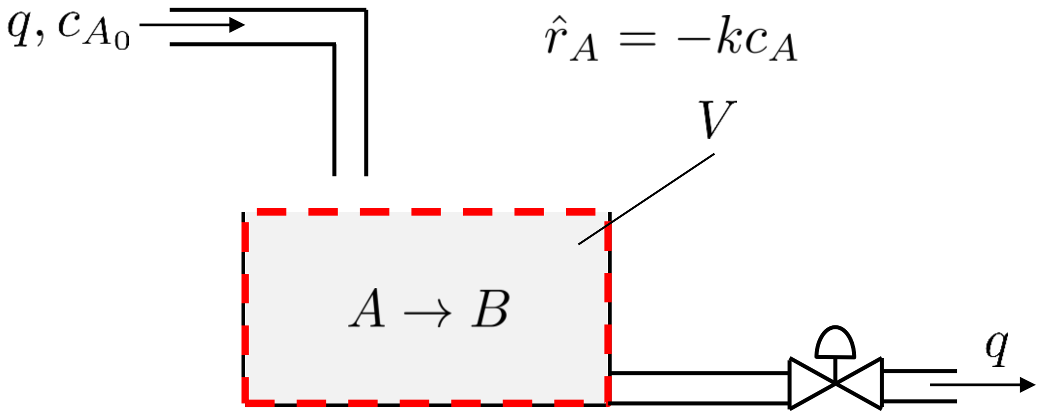
$$\frac{\mathrm{d}}{\mathrm{d}t}\iiint\limits_{V_c} c_k \mathrm{d}V = -\iint\limits_{\partial V_c} c_k \vec{v}\cdot\vec{n}\mathrm{d}A + \iiint\limits_{V_c} \hat{r}_k \mathrm{d}V$$

- Example:



Chemical reactions II

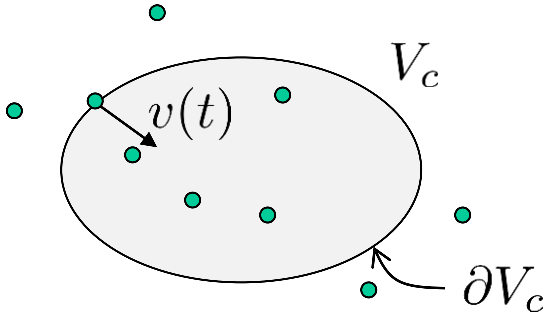
Example: Reaction in tank



Chemical reactions III

- Closed tank: $$\frac{\mathrm{d}}{\mathrm{d}t}\iiint\limits_{V_c} c_k \mathrm{d}V = -\iint\limits_{\partial V_c} c_k \vec{v}\cdot\vec{n}\mathrm{d}A + \iiint\limits_{V_c} \hat{r}_k \mathrm{d}V$$

The momentum balance



- In words

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

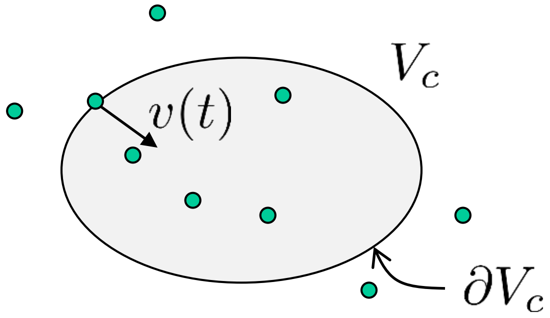
- Mathematically

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

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

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

The energy balance



- In words

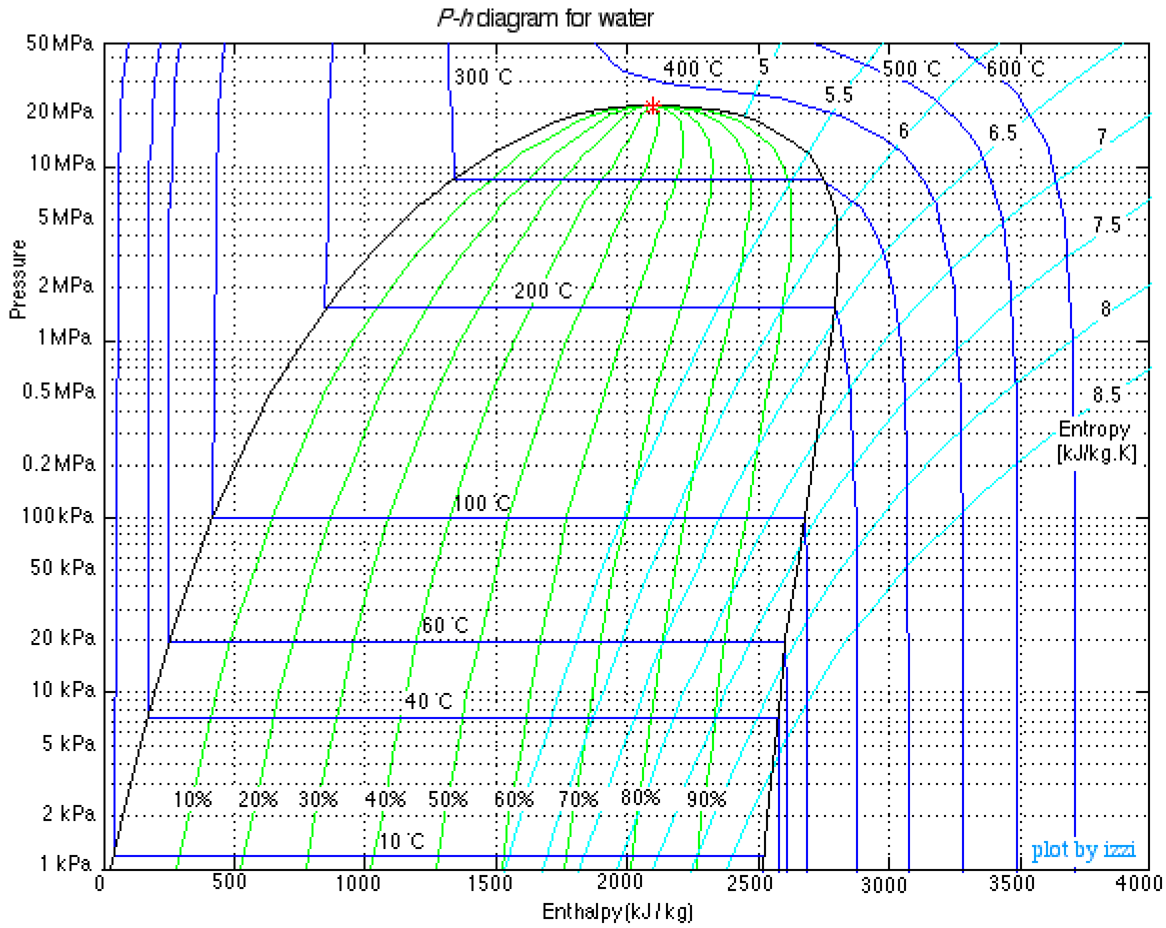
$$\frac{\mathrm{d}}{\mathrm{d}t}E = \left\{ \begin{array}{c} \text{transfer of energy into} \\ V_c \text{ by fluid flow} \\ \text{across surface } \partial V_c \end{array} \right\} + \left\{ \begin{array}{c} \text{transfer of energy into} \\ V_c \text{ by heat transfer} \\ \text{and by work} \end{array}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

- 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



Homework

- Read 11.1-11.2
- Formulate a momentum balance for a pipeflow with friction