Model building using engineering principles
Modelling of energy systems

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Lecture overview

1. Thermal energy systems
   - Characterization of thermal energy systems
2. The basic principles of thermodynamics
   - Thermodynamical variables
   - The laws of thermodynamics
3. Balance equations in energy systems
   - Mass balances
   - Energy balances
4. Constitutive equations in energy systems
   - Extensive-intensive relationships
   - Transfer rates
5. State space model form of dynamic energy models
   - Energy balance equations in intensive variable form

Characterization of thermal energy systems

Characterization: through modelling objects and mechanisms

- Modelling objects: spatially homogeneous (perfectly stirred) balancing volumes with constant chemical composition as the simplest case
- Mechanisms
  - (diffusive and) convective transport
  - energy transfer through phase boundary or wall
  - phase change processes , such as evaporation, melting, boiling, freezing etc.

Basic principles of thermodynamics

1. Thermal energy systems

2. The basic principles of thermodynamics
    - Thermodynamical variables
    - The laws of thermodynamics

3. Balance equations in energy systems

4. Constitutive equations in energy systems

5. State space model form of dynamic energy models

Extensive and intensive quantities

There are two types of termodynamical quantities:

1. extensive quantities , that are additive when joining two subsystems of the same phase: such as mass, energy etc.
2. intensive quantities , that equilibrate when joining two subsystems of the same phase: such as pressure, temperature etc.

Canonical set of variables : necessary and sufficient set to describe the thermodynamical state of a single phase system, each such set consists of one extensive and some intensive variables.

$$\{m, p, T, c_i, i = 1, ..., K\}$$

m	overall mass of the system,
p	pressure,
T	temperature,
$c_i, i = 1, ..., K-1$	concentrations

The laws of thermodynamics

Thermodynamics is the discipline for studying energy, the conversion of energy between various forms and the ability of energy to do work.

The laws ($\approx$ axioms)

1. The first law states that energy or matter can neither be created nor destroyed.
   energy conservation
2. The second law postulates the evolution towards and the conditions of thermal equilibrium.
   entropy - an extensive property of a thermodynamical system - of any isolated system *never decreases*

Non-equilibrium processes

Non-equilibrium thermodynamics is concerned with transport processes (convection, transfer, diffusion, etc.) and with the rates of chemical reactions.

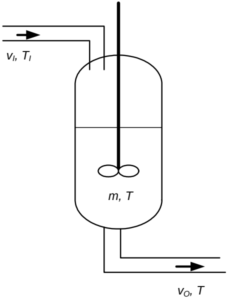
The conserved extensive - potential intensive pairs are as follows:

- overall mass $m \leftrightsquigarrow$ pressures p
- energy $U \leftrightsquigarrow$ temperature T
- component mass $m_X \leftrightsquigarrow$ concentration c_X (or more generally chemical potential μ)

In classical irreversible thermodynamics a linear relationship is assumed between the flow vector of conserved extensive variables and the difference of their potentials.
The cross-effects are also neglected.

Balance volumes and conserved extensive quantities

Balance volumes: perfectly stirred



Conserved extensive quantities:

- overall mass m
- energy U

Mass balances

For **perfectly stirred balance volumes**

- no source or sink term if the balance volume is connected to the environment only. Otherwise, the phase changes (evaporation, boiling, melting, etc.) may generate a mass source or sink through the interphase boundary.
- convective terms are the in- and out-flows entering or leaving the balance volume, that are mass flows $[kg/s]$.

$$\frac{dm}{dt} = v_I - v_O$$

Associated measurable quantity: level (e.g. with constant cross section)

Energy balances

For **perfectly stirred balance volumes**

- convective induced energy flows are induced by the convective mass flows of a balance volume, such that each v_I inflow induces an energy inflow $c_{pI} v_I T_I$ measured in $[J/s]$, where c_{pI} is the specific heat and T_I is the temperature of the flow.
- source or sink terms can be external (e.g. electrical) heating/cooling or heat transfer Q (again in unit $[J/s]$).

$$\frac{dU}{dt} = c_{pI} v_I T_I - c_p v_O T + Q$$

Associated measurable quantity: temperature

Constitutive equations – Extensive-intensive relationships

For **perfectly stirred balance volume with constant pressure**

$$U = c_p \cdot m \cdot T$$

where m is the overall mass, c_P is the specific heat measured in unit $[J/kg/K]$ that may depend on temperature, pressure and component concentrations.

$$m = V \cdot \rho$$

where V is the volume, m is the overall mass and ρ is the density of the balance volume.

Constitutive equations – II.

1. **property relations**
   - density relation: $\rho(p, T)$,
   - specific heat relation: $c_p(p, T)$,
   - dependence of equilibrium saturated pressure on the temperature $p^*(T)$
2. **thermodynamical state equations**: algebraic relationship between the canonical state variables (mass m, pressure p, temperature T and volume V) of a (gas phase) balance volume, e.g. ideal gas law

$$p \cdot V = \frac{m}{M} \cdot R \cdot T$$

Constitutive equations – III.

3. **energy transfer** term between two balance volumes with different temperatures T_1 and T_2

   $$Q_{transfer} = K_T \cdot A \cdot (T_1 - T_2)$$

   where A is the heat transfer area in $[m^2]$, K_T is the heat transfer coefficient measured in $[J/m^2/K/s]$, and the energy transfer rate $Q_{transfer}$ is measured in units $[J/s] = [W]$

4. **energy source terms caused by phase changes**, e.g. boiling, melting, evaporation, etc.

   $$Q_{Eevap} = E_{evap} \cdot Q^{(m)}_{mevap}$$

   where the unit of Q_{Eevap} is $[J/s]$

Transformation to state space model form

From the **extensive form of the dynamic energy balance equation**

1. The conservation balance equations should be transformed to have measurable (mostly intensive) quantities in them.
2. The constitutive algebraic equations should be substituted into the differential ones (if possible).

Energy balance equations in intensive form – 1

Assumptions for the transformation steps

- F1 A single perfectly stirred balance volume is considered with overall mass m and internal energy U.
- F2 One in- (v_I) and one out-flow (v_O) is assumed, that are mass flows $[kg/s]$.
- F3 Constant thermodynamical properties (specific heat c_p) are assumed.

Original equations

Mass balance

$$\frac{dm}{dt} = v_I - v_O$$

Energy balance

$$\frac{dU}{dt} = c_{pI} v_I T_I - c_p v_O T + Q$$

Energy balance equations in intensive form – 2

Original equations

Mass balance

$$\frac{dm}{dt} = v_I - v_O$$

Energy balance

$$\frac{dU}{dt} = c_{pI} v_I T_I - c_p v_O T + Q$$

with

$$c_P m \frac{dT}{dt} + c_P T \frac{dm}{dt} = c_{pI} v_I T_I - c_p v_O T + Q$$

State equation originating from the energy balance

$$\frac{dT}{dt} = \frac{v_I}{c_p m}(c_{pI} T_I - c_p T) + \frac{Q}{c_p m}$$

State space model in energy systems

- **State equations**: overall mass balances, energy balances in intensive form
- **State variables**: for each balance volume i

$$x = [\ m_i, T_i \mid i = 1, ..., N]^T$$

- **Output variables**: non-input variables that we can directly measure