Dynamic system modeling for control and diagnosis Modelling fundamentals

Katalin Hangos

UniPannonia Dept. of Electrical Engng and Information Systems

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The general modelling problem

- **Given**: the system to be modelled, modelling goal
- **Contstruct**: a mathematical model that describes the behaviour of the system



$$\begin{aligned} \frac{dh}{dt} &= \frac{v_{be}}{A} s z_{be} - \frac{v_{ki}}{A} s z_{ki} \\ \frac{dT}{dt} &= \frac{v_{be}}{Ah} (T_{be} - T) s z_{be} + \frac{Q_H}{c_p \rho Ah} k \\ h(0) &= h_0 \quad , \quad T(0) = T_0 \end{aligned}$$

The modelling goal

Problem description: a pair of the system and the **modelling goal** Modelling goal

- possibilities and categories
 - dynamic and static (steady-state) simulation
 - system design
 - process control (prediction, regulation, identification, diagnosis)
- determines the (vailidity) domain of the model
- influences the following model properties
 - which mechanisms should be taken into account
 - the mathematical form (algebraic equations, differential equations, graphs etc)
 - the accuracy (of the characteristic variables)

The 7 steps modelling procedure - 1

- 1 Problem definition formal description
 - system definition
 - modelling goal determination
 - flowsheet construction (equipments, variables)
- 2 Mechanisms identification
 - collection of phenomena
 (e.g. convection, transfer, reaction, evaporation)
- 3 Data collection and evaluation
 - constants from data tables (accuracy!)
 - properties of equipments and operation
 - measured data (preliminary)



The 7 steps modelling procedure - 2

- 4 Model construction
 - determination of balance volumes
 - formulation of modelling assumptions
 - construction of model equations (conservation balances, constitutive equations)
 - determination of initial and boundary conditions
- **5** Model solution
 - implementation or recasting of solution method
 - model checking (plausibility and accuracy)



The 7 steps modelling procedure - 3

- 6 Model verification
 - verifying qualitative model
 behaviour against engineering intuition
 - checking dynamic properties (e.g. stability) on the model
- 7 Model calibration and validation
 - model calibration estimating unknown/uncertain model parameters using measured data
 - model validation

comparing the model and the real system (measured data) using statistical methods



Mechanisms - phenomena



These depend on the type of the physical systems:

- mechanical systems
- thermodynamical (process, energy) systems
- electrical systems
- chemical, biological, etc. systems

Most important mechanisms in thermodynamical systems

- flows: convective, diffusive
- heating, cooling
- mass and energy transfer
- phase transitions (evaporation, boiling melting, ...)

Conservation balances - 1



Balance volumes: for constructing conservation balances

- most often with *constant volume*
- *perfectly stirred* (concentrated parameter, the balance is in the form of ordinary differential equations)

Conserved (extensive) quantities:

- ovarall mass
- energy (entalpy, internal energy)
- component mass, (momentum)

Dynamic conservation balance in general form: for a conserved quantity

$$\left\{\begin{array}{c} rate \ of \\ change \end{array}\right\} = \left\{\begin{array}{c} in-\\ flow \end{array}\right\} - \left\{\begin{array}{c} out-\\ flow \end{array}\right\} + \left\{\begin{array}{c} source \\ sink \end{array}\right\}$$

Intensive quantities



Intensive quantities equilibrate when joining sub-systems

- potential (driving force) type quantities
- drive flows and transfer (usually linear approximation without any cross-effects)
- measurable quantities
- extensive intensive pairs
 - $^{\circ}$ overall mass m pressures p
 - $^{\circ}$ energy U temperature T
 - $^{\circ}$ component mass m_X concentration c_X (chemical potential)

Extensive - intensive relationships

- $U = c_P mT$ (c_P specific heat)
- $m_X = \frac{m}{\rho} c_X$ (ρ density)

Conservation balances - 2



Dynamic conservation balance for **overall mass**

- no source/sink
- the overall mass *m* is measurable (e.g. level measurement)
- for perfectly stirred balance volumes the in- (v_B) and out-flows (v_K) are mass flows [kg/s]

Example:

$$\frac{dm}{dt} = v_B - v_K$$

Conservation balances - 3



Dynamic conservation balance for energy

- source/sink: external (e.g. electrical) heating/cooling or heat transfer Q([J/s])
- for perfectly stirred balance volumes the in- $(c_{pB}v_BT_B)$ and out-flows (c_Pv_KT) are energy flows [J/s]
- The energy *U* is directly **not** measurable, we use the temperature instead in the equation => transformation into intensive form

Example:

$$\frac{dU}{dt} = c_{pB}v_BT_B - c_Pv_KT - Q$$



Constitutive equations

Further equations necessary to complete the model

- usually algebraic equations
- most common types:
 - ° extensive-intensive relationships
 - transfer rate equations
 - termodinamical reltionships
 - balance volume relations
 - equipment and control relations

Modelling assuptions



The list should be *collected incrementally* during the modelling procedure

Most common modelling assumption types:

- assumptions on the time-dependent behaviour of the (sub)system/mechanisms (e.g. dynamic, steady-state)
- assumptions on the balance volumes (e.g. only fluid phase, vapour and liquid phase)
- assumption on the spatial distributions (e.g. perfectly stirred/concentrated parameter)
- assumptions on the presence/absense or properties of mechanisms
 (e.g. no evaporation, linear heat transfer)
- assumptions on the negligible effects (e.g. density depends only on T, specific heat c_P is constant)
- assumptions on the required domain of state variables, and on the required accuracy

Ingredients of a modell



- System description (flowsheet, variables)
- Modelling goal
- Mechanisms
- Modelling assumptions
- Model data (data, unit, source, accuracy)
- Balance volumes (indicated on the flowsheet)
- Model equations (conservation balance equations, constitutive equations, initial and boundary conditions)
- Model variables and parameters

State-space model form

System (S): operates on signals (time-dependent, variables)

 $y = \mathbf{S}[u]$

• inputs (*u*) and outputs (*y*); states (*x*)



Signals in a state-space model originates from first engineering principles

- state variables (x): conserved extensive quantities (or their intensive pairs)
- input variables (*u*): appear on the right-hand sides of the differential equations, manipulable (measurable)
- output variables (y): measurable, not directly manipulable (state variable or depends therefrom)



Example: tank with gravitational outflow



Problem description

Given a tank with constant cross section that is used for storing water. The water flows into the tank through a binary input valve, the outflow rate is driven by gravitation, i.e. depends on the water level in the tank, but it is controlled by a binary output valve.



Construct the model of the tank for diagnostic purposes if we can measure the water level and the status of the valves.

Example: tank with gravitational outflow - 2 \rightarrow

Mechanisms

- in- and out-flow
- gravitational outflow (driven by the hydrostatic pressure)

Modelling assumptions

- F1 one balance volume (the tank) perfectly stirred
- F2 only water is present (only overall mass balance is considered)
- F3 gravitational outflow
- F4 constant cross-section A
- F5 density (ρ) is constant



Example: tank with gravitational outflow - 3

Conservation balance equation: for overall mass

$$\frac{dm}{dt} = v_b - v_k$$



Constitutive equations

- $m = A \cdot h \cdot \rho$ (water level h is measurable)
- $v_B = v_B^* k_B$ (valve status k_B is measurable)
- $v_K = K \cdot h \cdot k_K$ (gravitational outflow, valve status k_K is measurable)

Example: tank with gravitational outflow - 4

Model equation with measurable variables:

$$\frac{dh}{dt} = \frac{v_b^*}{A\rho} k_b - \frac{K}{A\rho} h \cdot k_F$$



State-space model form

- state variable: water level h
- input variables: status of the values k_B and k_K
- output variable: water level *h*