Dynamic modelling and model analysis based on first engineering principles

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BME Modelling - 2015

All models are wrong ...
... some are useful !

George Box

Contents

The concept of a model

What is a model?

- "A model (**M**) for a system (**S**) and an experiment (**E**) is anything to which **E** can be applied in order to answer questions about **S**" (Minsky, 1965)

Engineering models

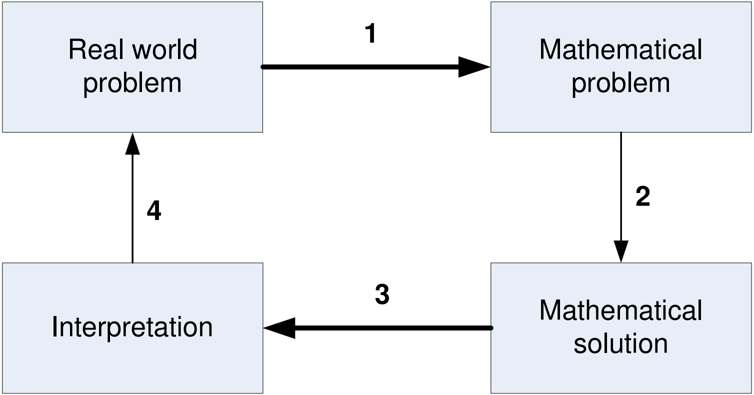
- "A mathematical representation (**M**) of a physical system (**S**) for a specific purpose (**P**) and experiment (**E**)"

Model application areas

1. system design
   - good accuracy
   - mostly static
2. control design
   - dynamic (time-dependent)
   - accurate description of the main dynamic processes
3. monitoring, troubleshooting and diagnosis
   - dynamic (time-dependent)
   - not very accurate but selective
4. simulation and operator training
   - great level of details
   - good accuracy
5. safety and risk analysis
   - mostly static
   - stochastic

The modelling process

A circular iterative process



Model classification

a **Mechanistic** vs. Empirical
- use first engineering principles
- conservation of mass, energy, etc.
- consider physical laws for the mechanisms

b Stochastic vs. **Deterministic**
- application area: control, monitoring, diagnosis

c **Lumped** vs. Distributed
- no state dependency (perfectly stirred volumes, concentrated parameter)

d **Dynamic** vs. Steady state
- application area: control, monitoring, diagnosis

e **Continuous** vs. Discrete (time and range space)

f **Linear** vs. **Nonlinear**

The general modelling problem

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

$$\frac{dh}{dt} = \frac{v_{be}}{A} sz_{be} - \frac{v_{ki}}{A} sz_{ki}$$

$$\frac{dT}{dt} = \frac{v_{be}}{Ah}(T_{be} - T) sz_{be} + \frac{Q_H}{c_p \rho A h} k$$

$$h(0) = h_0 \ , \ T(0) = T_0$$

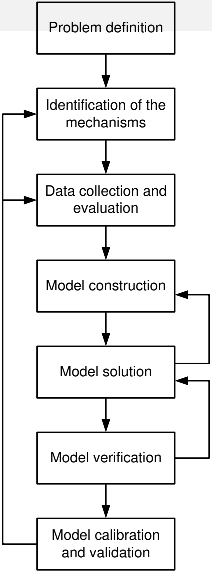
The modelling goal

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

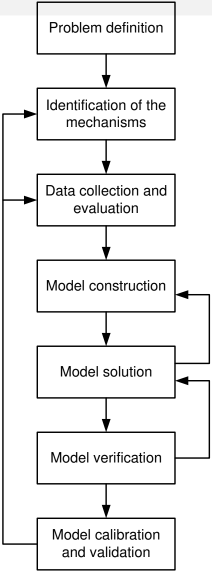
1. Problem definition
   formal description
   - system definition
   - modelling goal determination
   - flowsheet construction (equipments, variables)
2. Mechanisms identification
   - collection of phenomena
     (e.g. convection, transfer, reaction, evaporation)
3. Data collection and evaluation
   - 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

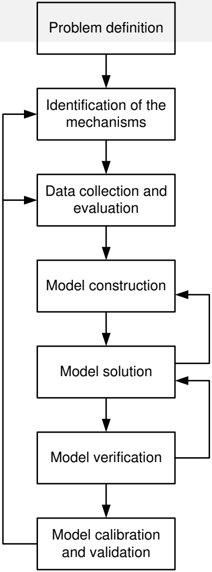
5 Model solution
- implementation or recasting of solution method
- model checking (plausibility and accuracy)



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

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

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
  - overall mass m - pressures p
  - energy U - temperature T
  - component mass m_X - concentration c_X (chemical potential)

Extensive - intensive relationships

- $U = c_P m T$ (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- ($c_{pB} v_B T_B$) and out-flows ($c_P v_K T$) 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:

$$\frac{dU}{dt} = c_{pB} v_B T_B - c_P v_K T - Q$$

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 assumptions

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/absence 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
  (e.g. T is between 30 and 40 ^oC)

Ingredients of a model

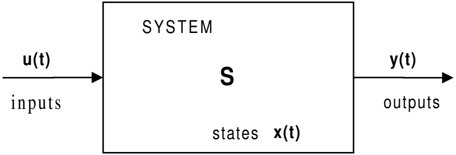
- System description (flowsheet, variables)
- Modelling goal
- Mechanisms
- Modelling assumptions
- Model data (data, unit, source, accuracy)
- Balance volumes (indicated on the flowsheet)
- Model equations (conservation balance equations, constitutive equations, initial and boundary conditions)
- Model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

Sate space model form

System (**S**): operates on signals

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

- inputs (u) and outputs (y); states (x)



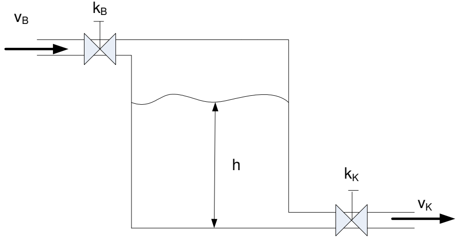
Signals of dynamic models based on first engineering principles

- state variables (x): conserved quantities (or their intensive pairs)
- input variables (u): on the right-hand sides of the conservation equations, manupulable (measurable)
- output variables (y): measurable, not directly manipulable (state variable or state dependent quantities)

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: gravitational tank

Mechanisms

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

Modelling assumptions

F1 perfectly stirred

F2 only water

F3 gravitational outflow

F4 constant cross section A

F5 constant density (ρ)

Example: gravitational tank

Conservation balances: overall mass balance

$$\frac{dm}{dt} = v_b - v_k \tag{1}$$

Constitutive equations

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

Example: gravitational tank

Model equation with measurable signals:

$$\frac{dh}{dt} = \frac{v_b^*}{A\rho}k_b - \frac{K}{A\rho}h \cdot k_K \tag{2}$$

State space model form

- state variable: h level
- input variables: binary valves k_B and k_K
- output variables: h level

Solution of dynamic models

Assume: concentrated parameter model

- **Given**:
  - the model equations: systems of ordinary differential and algebraic equations (DAEs)
  - initial values
  - parameter values
- **Contstruct**: the solution of the model (time dependent values of the variables) system

Numerical solution methods: finite difference approximations, e.g. Runge-Kutta methods

Properties

- numerical stability (explicit vs. implicit methods)
- accuracy (the order of the method)
- automatic selection of the integration steps, stiff models

Model verification

Aim: verifying qualitative properties of the solution **against engineering intuition**

Model and/or solution properties

- steady states
  - existence, multiplicity
- *structural* dynamic properties
  - controllability and observability
  - (stability)
- qualitative properties of the step response
  - sign of initial deviation
  - steady state deviation

The structure of state space models

Linearized state space models around a *steady state point*

$$
\begin{array}{lcll}
\frac{dx}{dt} & = & Ax + Bu & \text{(state eq.)} \\
y & = & Cx + Du & \text{(output eq.)}
\end{array}
$$

for a nonlinear input-affin state space model

$$
\begin{array}{lcll}
\frac{dx}{dt} & = & f(x) + g(x)u & \text{(state eq.)} \\
y & = & h(x) & \text{(output eq.)}
\end{array}
$$

Signed strukture matrices: $[A]$

$$
[A]_{ij} = \begin{cases} + & \text{if} \quad a_{ij} > 0 \\ 0 & \text{if} \quad a_{ij} = 0 \\ - & \text{if} \quad a_{ij} < 0 \end{cases}
$$

Structure graph

Signed directed graph $S = (V, \mathcal{E}; w)$

- **vertex set** corresponds to state, input and output variables

$$V = X \cup U \cup Y$$
$$X \cap U = X \cap Y = U \cap Y = \emptyset$$

- **edges** correspond to *direct* effects between variables
- edge **weights** describe the *sign* of the effect

The occurrence matrix of a structure graph

An o_{ij} entry in the occurrence graph O

$$o_{ij} = \begin{cases} w_{ij} & ha \qquad\qquad (v_i, v_j) \in E \\ 0 & egyebkent \end{cases}$$

For a linear(ized) LTI state space model with (A, B, C, D) (order (u, x, y))

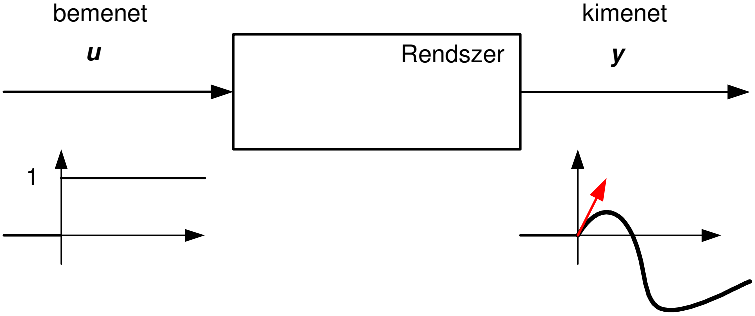
$$O = \begin{pmatrix} 0 & 0 & 0 \\ [B] & [A] & 0 \\ [D] & [C] & 0 \end{pmatrix}$$

For an input-affine SISO state space model

$$\begin{aligned} [A]_{ij} &= \left[\frac{\partial f_i}{\partial x_j} + \frac{\partial g_i}{\partial x_j} u_0\right] \quad , \quad [B]_{i1} = [g_i] \\ [C]_{1j} &= \left[\frac{\partial h}{\partial x_j}\right] \quad , \quad [D] = 0 \end{aligned}$$

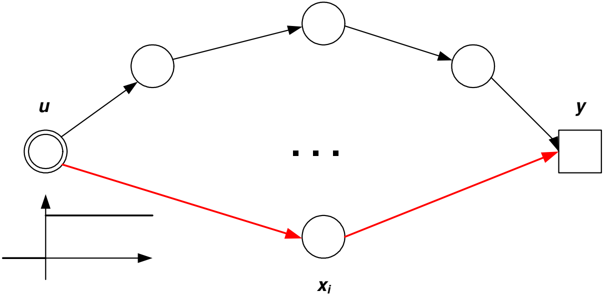
Initial deviation – 1

Unit step response



Initial deviation – 2

Sign-value of the shortest path(s!)



Deviation of the input (from its steady state value): $[\Delta u]_S = +$
Sign of the derivative: $[\frac{dx_i}{dt}]_S = \delta x_i = s_{u,x_i} \otimes_S [\Delta u]_S = s_{u,x_i}$
Sign of the **initial deviation** of the output:

$$[\frac{dy}{dt}]_S = \delta y = S^*_{u,y} \otimes_S [\Delta u]_S = s_{u,x_i} \otimes_S s_{x_i,y}$$

Grey-box Models

Dynamic models

- developed from first engineering principles – **white box part**
- part of their parameters and/or structure unknown – **black box part**

are called grey-box models

Model calibration – 1

Model Calibration – Conceptual Problem Statement

Given

- a grey-box model
- calibration data (measured data)
- measure of fit (loss function)

Compute

- an estimate of the parameter values and/or structural elements

Identification: dynamic model structure and parameter estimation

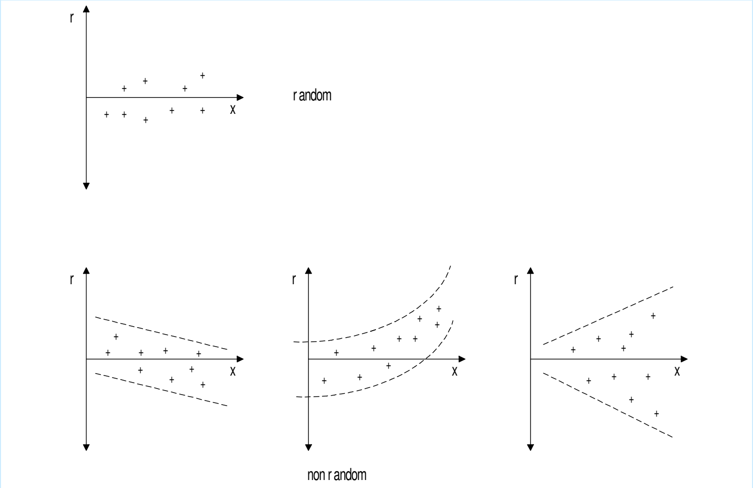
Model calibration – 2

Conceptual steps of solution

- Analysis of model specification
- Sampling of continuous time dynamic models
- Data analysis and preprocessing
- Model parameter and structure estimation
- Evaluation of the quality of the estimate

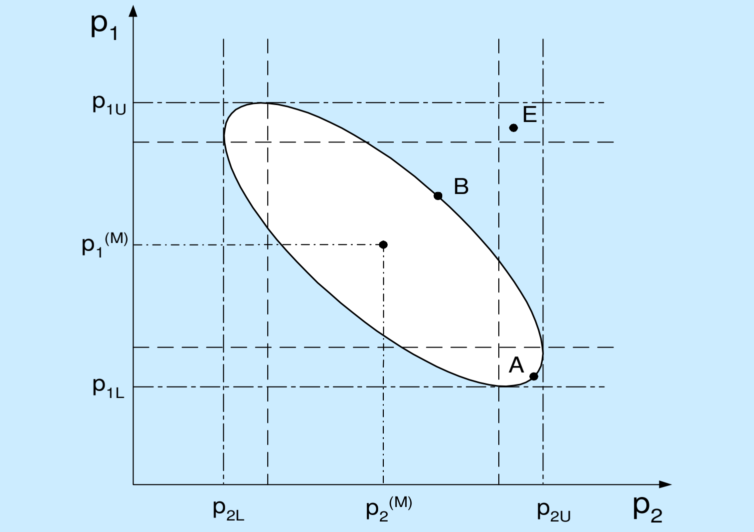
Evaluation of the quality of the estimates – 1

In the space of model outputs: ***residuals*** *should form white noise processes*



Evaluation of the quality of the estimates – 2

In the space of parameters: ***independent estimates*** *with low variance*



Statistical model validation

Conceptual problem statement

Given:

- a **calibrated** model
- validation data (measured data): independently measured from the calibration data (!!)
- measure of fit (loss function): in the space of output variables driven by the modelling goal

Decide (Question):

- Is the calibrated model "good enough" for the purpose (see modelling goal)?
  (Does it reproduce the data well?)