

Modelling fundamentals



Vehicle dynamics



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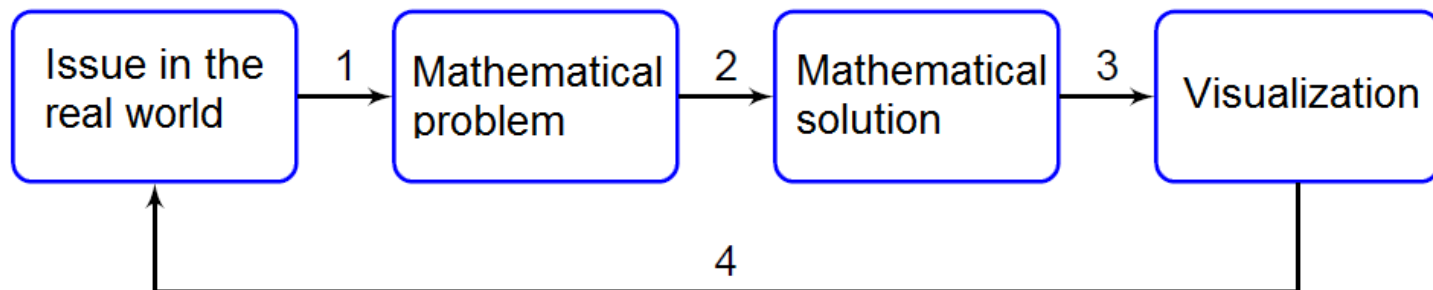
Steps of modelling

The **model** is a simplified part of the real world.

The **mathematical model** is a special representation of the model.

Modelling process:

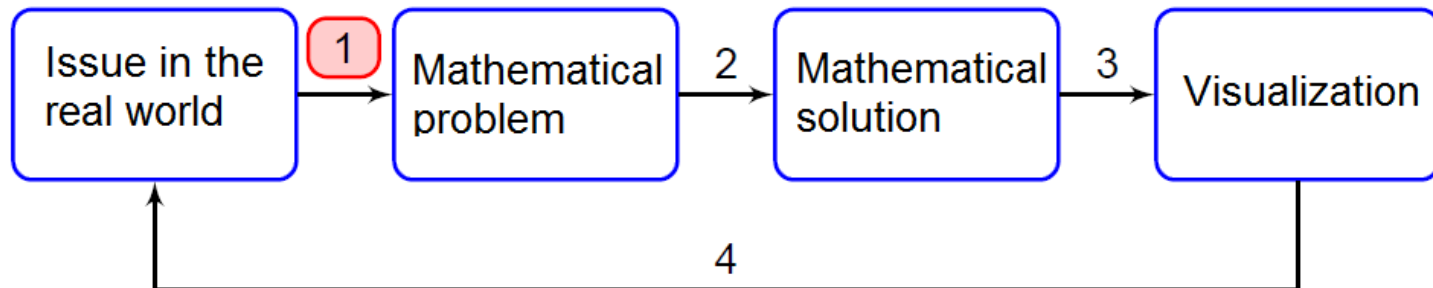
- Transforming the issue from the real world to mathematical problem
- Solving the mathematical problem
- Visualization of the results
- Using the results to solve the issue in the real world



1st step: mathematics from reality

Transforming the issue from the real world to mathematical problem:

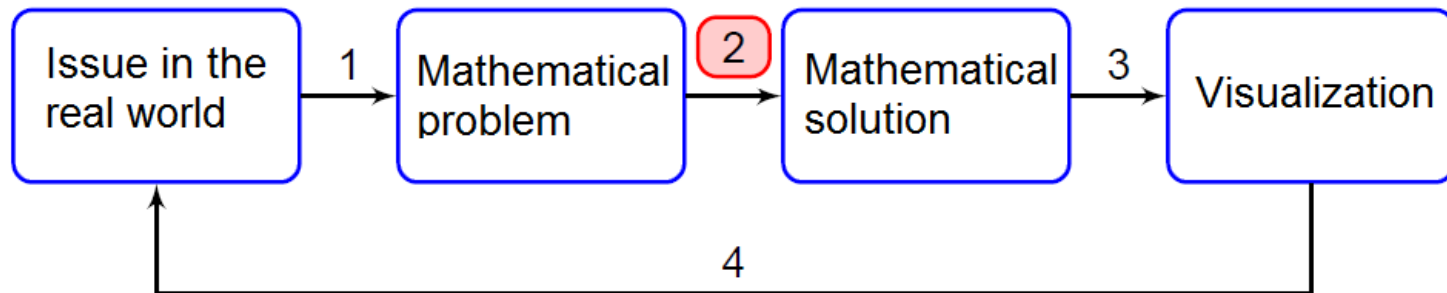
- Defining the boundaries of the issue/system
- Defining the inputs, the outputs, the states and the disturbances
- Defining the modelling aims
- Determining the mechanisms of the model
- Defining the class of the model
- Defining the accuracy of the model
- Collection and analyzation of the available system data



2nd step: solution of mathematical problem

Solving the equations of the built model:

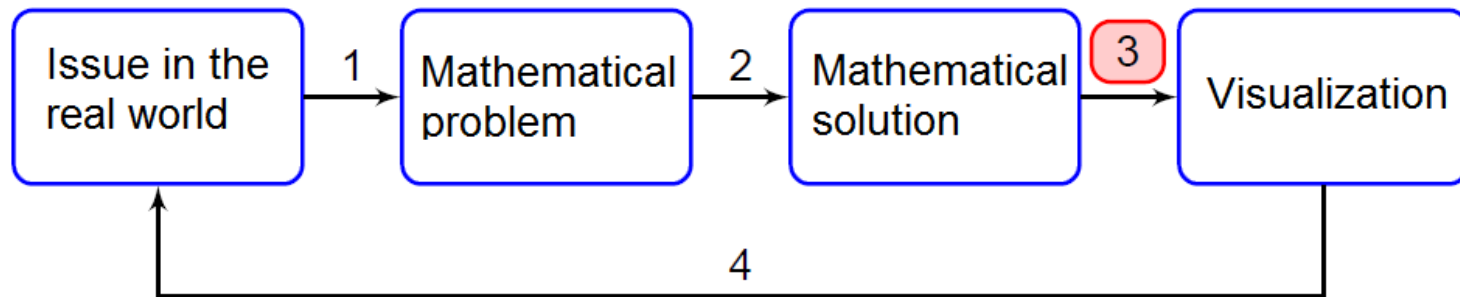
- Defining the variables based on the model's degree of freedom
- Analysing the solvability
- Selecting the way of the solution
- Analysing the divideability of the problem
- Sensitivity analysis of the solution by paying attention the accuracy of the inputs and the parameters
- Selecting the visualization modes of the solution



3rd step: plotting the outputs of the model

Verification, validation, estimation of the parameters and simplification:

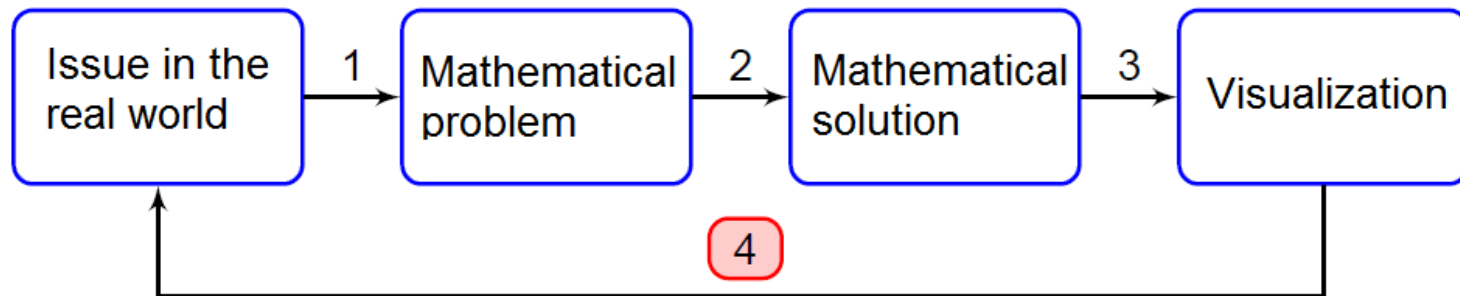
- Collecting the verification and validation possibilities
- Defining the verification and validation level
- Data analysis for the verification, for the validation and for the parameter estimation
- Determining the necessary modifications
- Collecting the simplification possibilities



4th step: using the solution to solve the issue

Utilization of the model:

- Checking the solving time (simulation speed)
- Noting the maintenance of the model
- Documenting the model



The application areas of a model

Process development:

- Practicability analysis
- Analysis of the parameter changes
- Optimization of the parameters or of the model structure

Process control:

- Analysis of the model dynamics
- Sensitivity analysis
- Control algorithm design
- Control algorithm tests

Troubleshooting:

- Determining the possible errors

Process safety:

- Analysis of the risky operations
- Planning of an emergency stop strategy

Environmental impact assessment:

- Determining the harmful emission
- Social and economical impact assessment

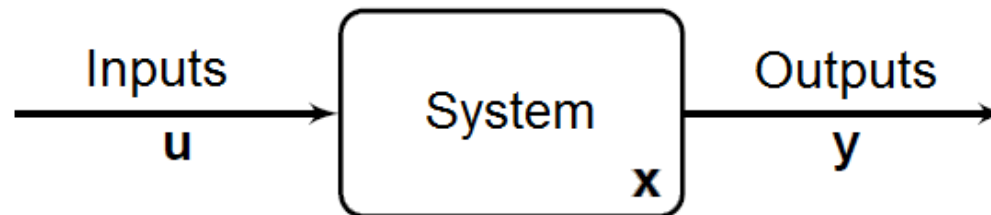
Model classes

Mechanistic	Based on mechanisms of physical laws
Empirical	Based on input-output data or on experiences
Stochastic	Contains probability variables
Deterministic	Based on cause effects
Concentrated p.	The variables are not function of the spatial location
Distributed p.	The variables are function of the spatial location
Linear	The superposition principle is applicable
Nonlinear	The superposition principle is not applicable
Continuous	The variables are defined in the space-time continuum
Discrete	The variables are defined as discrete space/time values
Hybrid	Contains both continuous and discrete variables

The system

Definition of the system:

- The system is a part of a real world with well-defined boundaries
- The system's behaviour is influenced by its inputs (\mathbf{u}) by the environment
- The system has an impact on the environment through its outputs (\mathbf{y})
- The states of the system can be assigned to the system's conservation quantities (mass, energy, momentum, etc.)
- Inputs, outputs and states can be considered as time dependent vector-valued functions

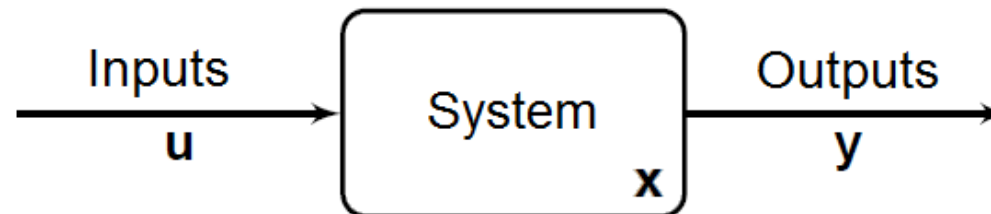


Modelling aims

Modelling aims:

- The modelling aims determine the utilization of the model (for example static/dynamic simulation, design, control process, etc.)
- They have a strong effect on the considered processes, on the mathematical form and on the accuracy
- Determine model's the validity range

Mathematical model: describes the system's behaviour for the given aim



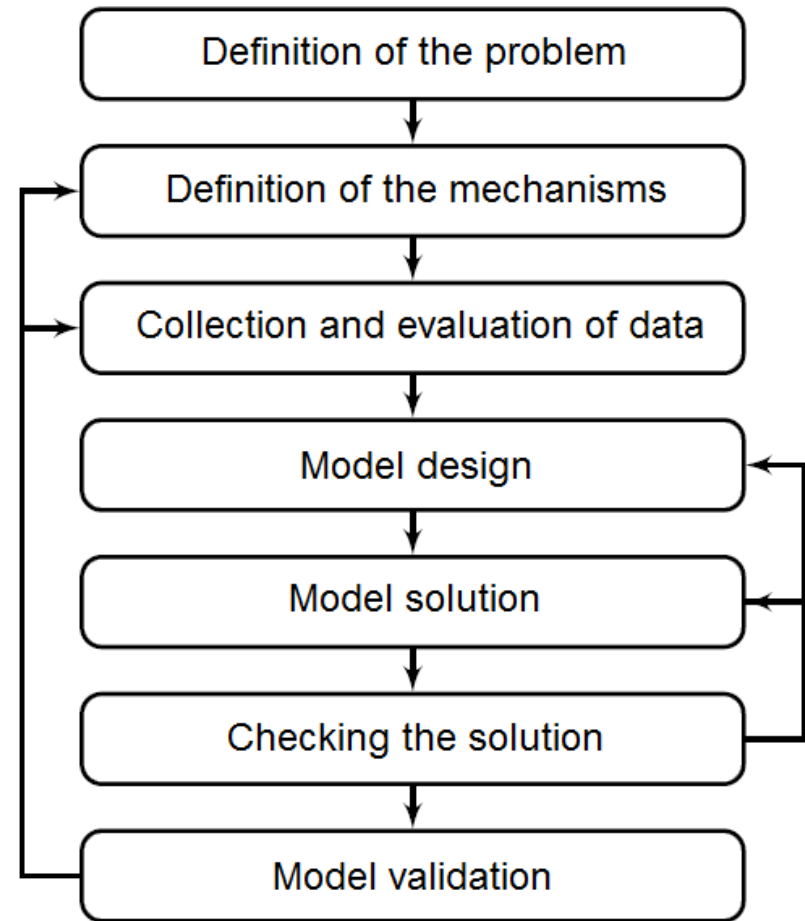
7 steps modelling process

Given:

- The system
- The modelling aims
- Validation criterion

To be determined:

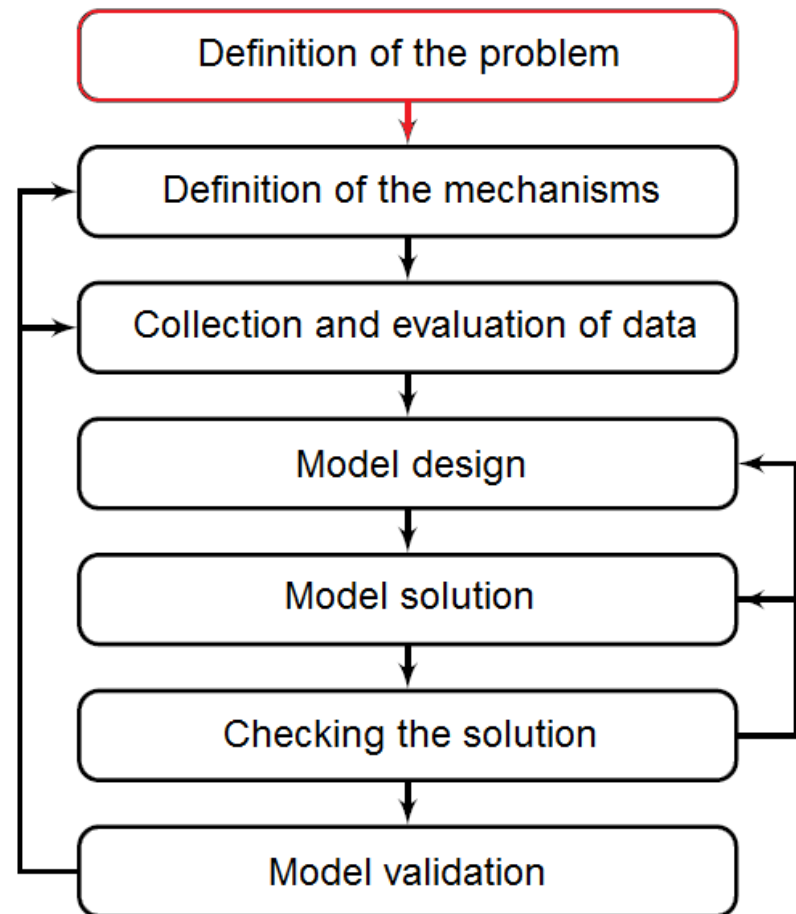
- Mathematical model that describes the system's behaviour for the given aim



1st: defining the solveable problem

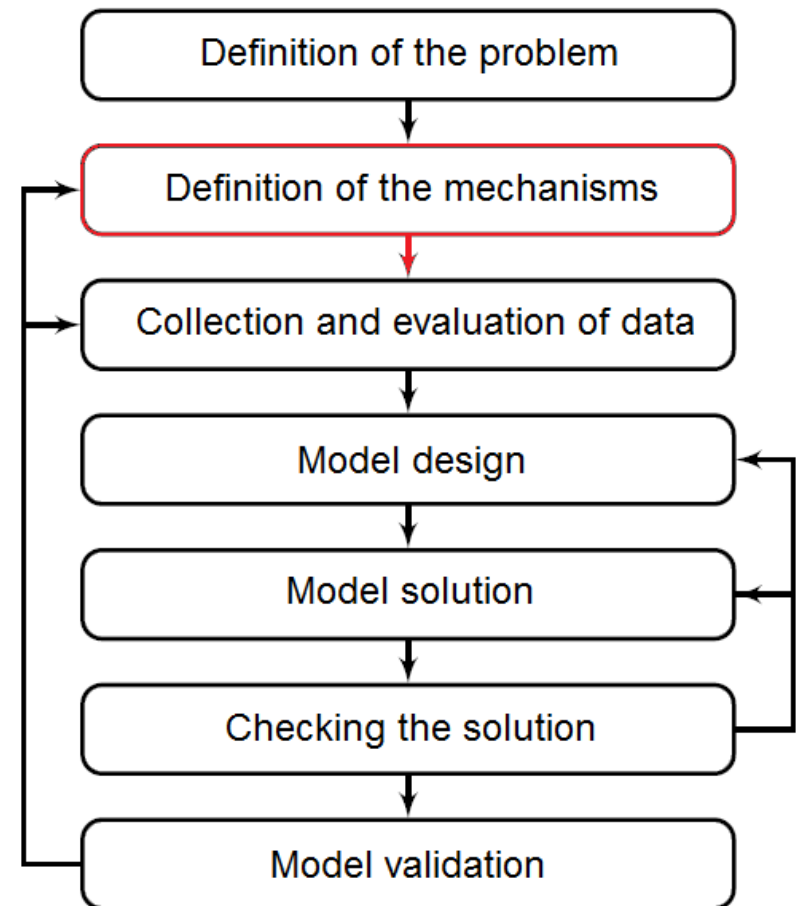
The system's formal description based on the modelling aim:

- Inputs, outputs, variables
- Model hierarchy (components and connections)
- Class of spatial distribution (concentrated, distributed)
- Operating range and accuracy
- Changes in time (static/dynamic)



2nd: determining the mechanisms

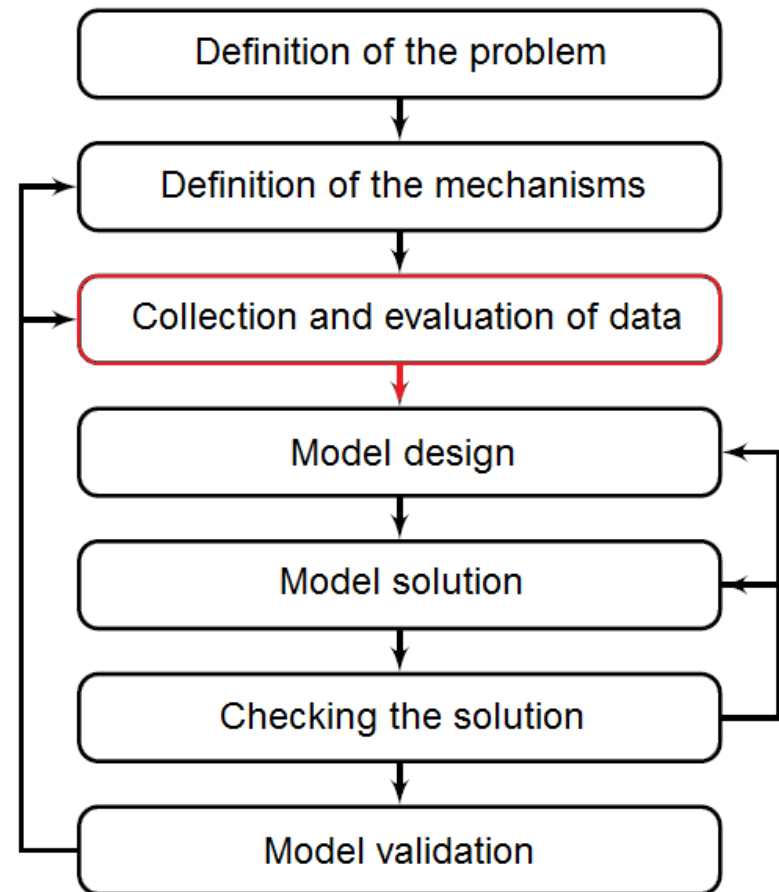
- Important processes from the aspects of the modelling aims
- Defining as few as possible process
- Modelling conditions



3rd: data collecting and evaluation

The modelling process always requires data:

- Measured and estimated data
- Basic data (source: manuals, tables)
- Data accuracy



4th: making the model

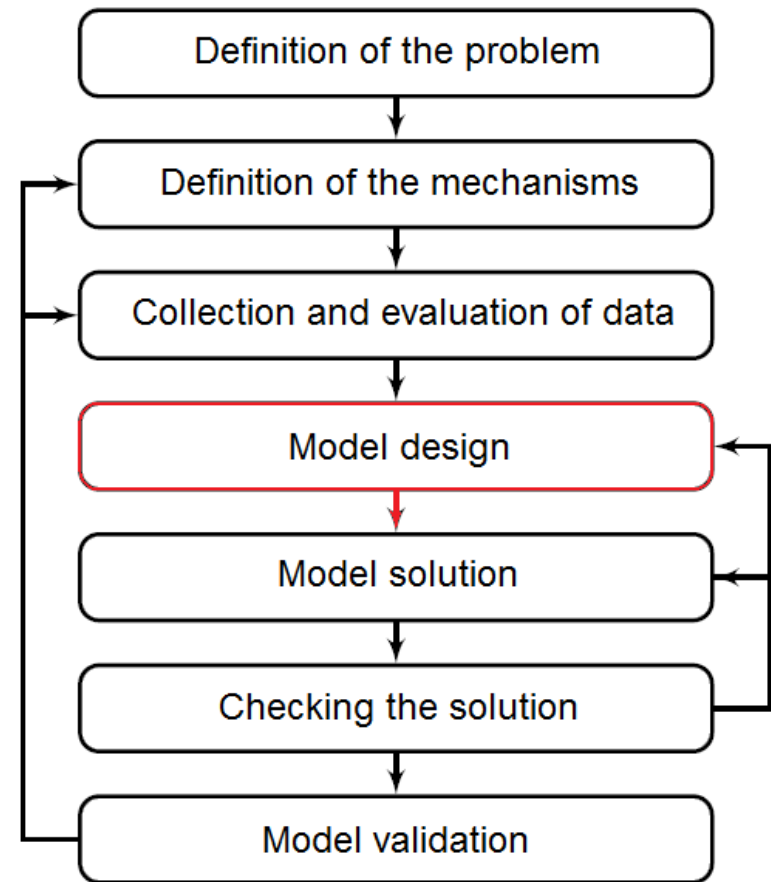
1st: definition of the balance volumes

2nd: definition of the conditions

3rd: making the model equations

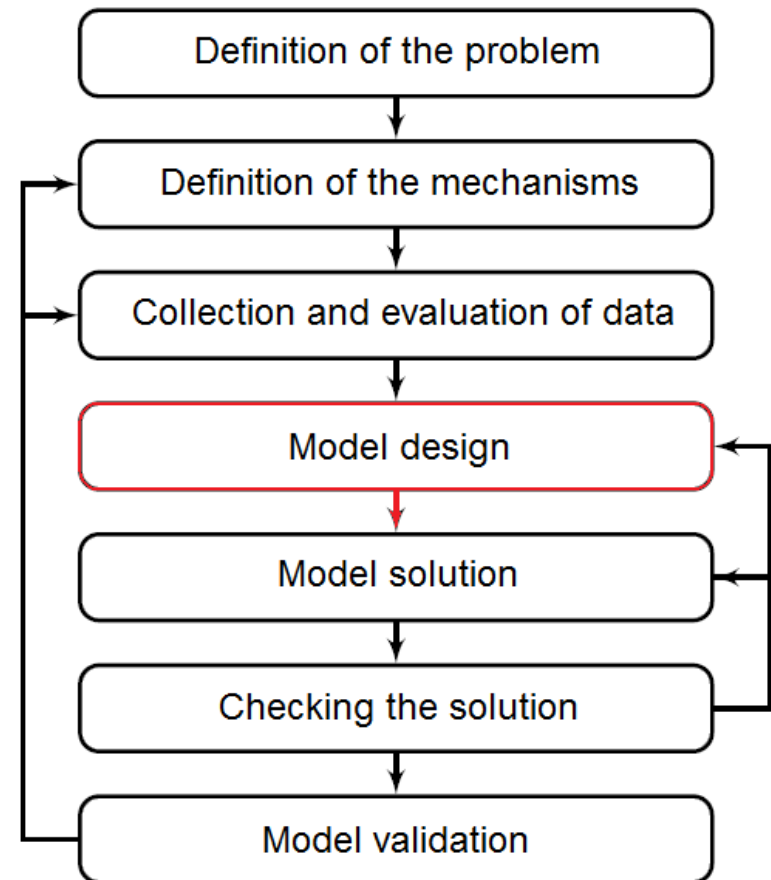
4th: setting the initial and the boundary conditions

5th: setting the variables and the parameters



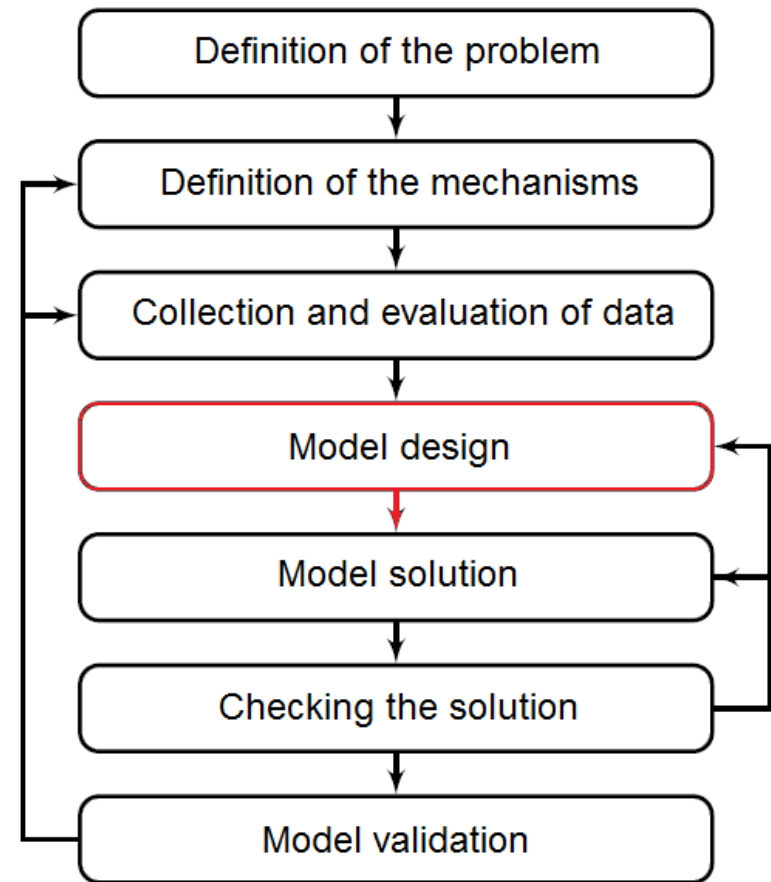
4.1: definition of the balance volumes

- Dividing the system to subsystems
- Balance volumes determine the conservation equations



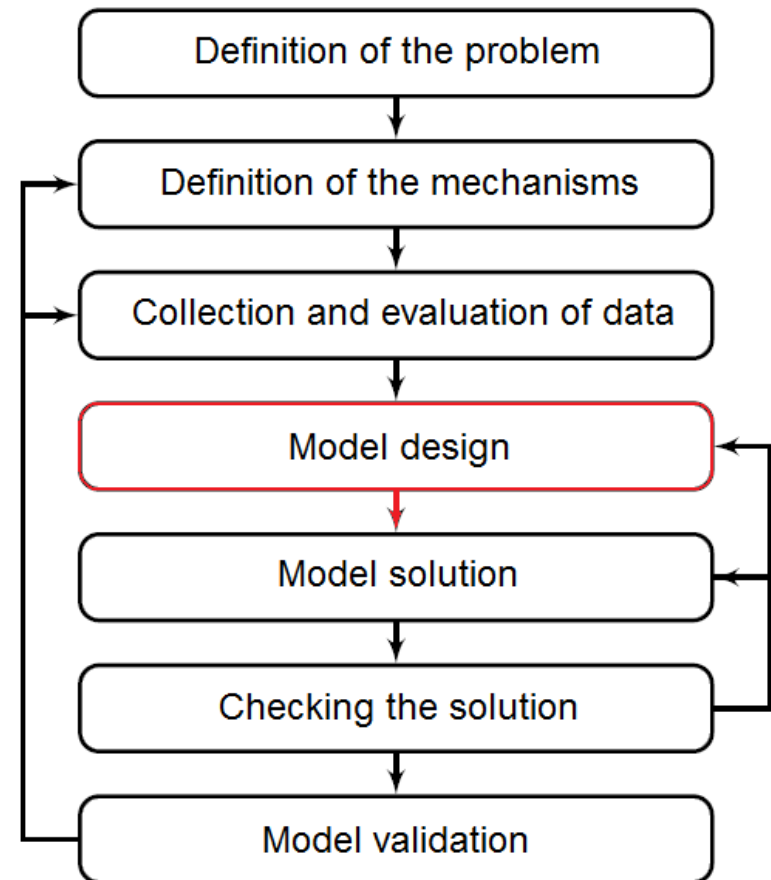
4.2: definition of the conditions

- The conditions determine the operation range of the model
- Typical modelling conditions:
 - Behaviour over time: *for example dynamic or stationary*
 - Balance volumes: *for example gaseous volumes or liquid volumes*
 - Spatial distribution: *concentrated or distributed*
 - Phenomenon: *for example evaporation, heat transfer*
 - Negligible processes: *for example specific heat is a constant*
 - Range of the states: *for example temperature interval*



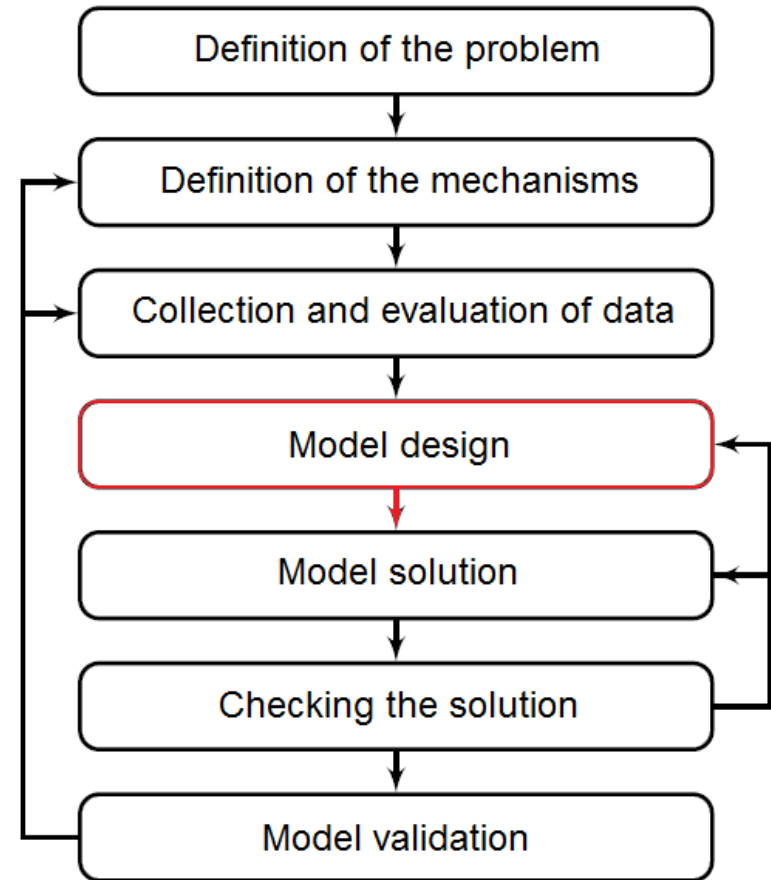
4.3: making the model equations

- Balance equations/conservation equations are usually differential equations:
 - Mass conservation
 - Energy conservation
 - Momentum conservation
- Complementary equations:
 - Usually algebraic equations
 - Equations for the whole mathematical description



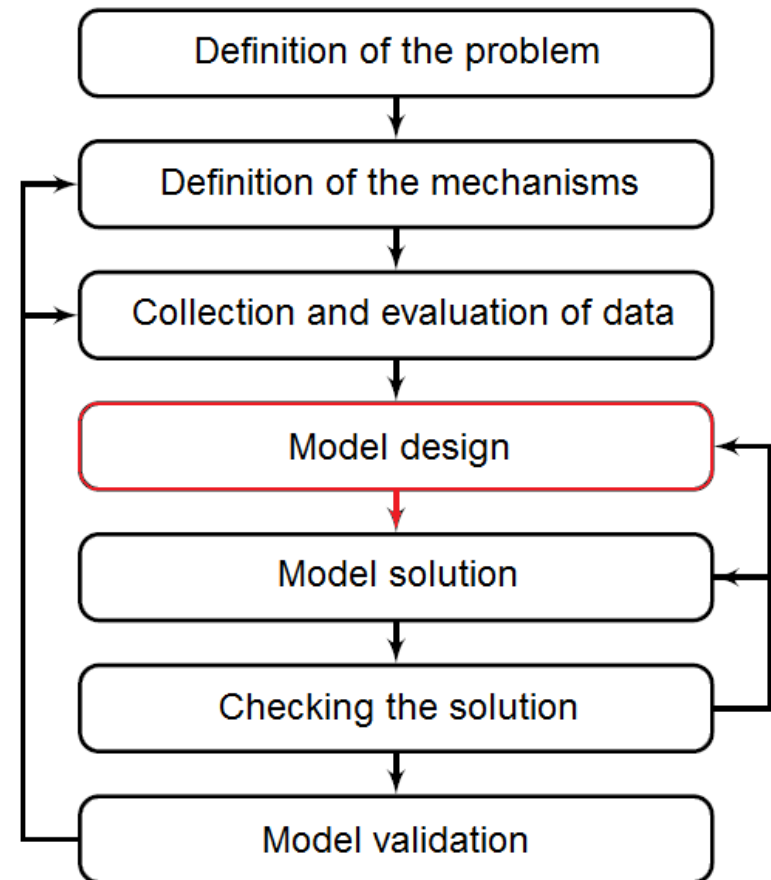
4.4: setting the initial and the boundary conditions

- Initial conditions for ordinary differential equations
- Boundary conditions for partial differential equations (distributed parameters)



4.5: setting the variables and the parameters

- Notation, meaning, unit
- For parameters: known/estimated, accuracy



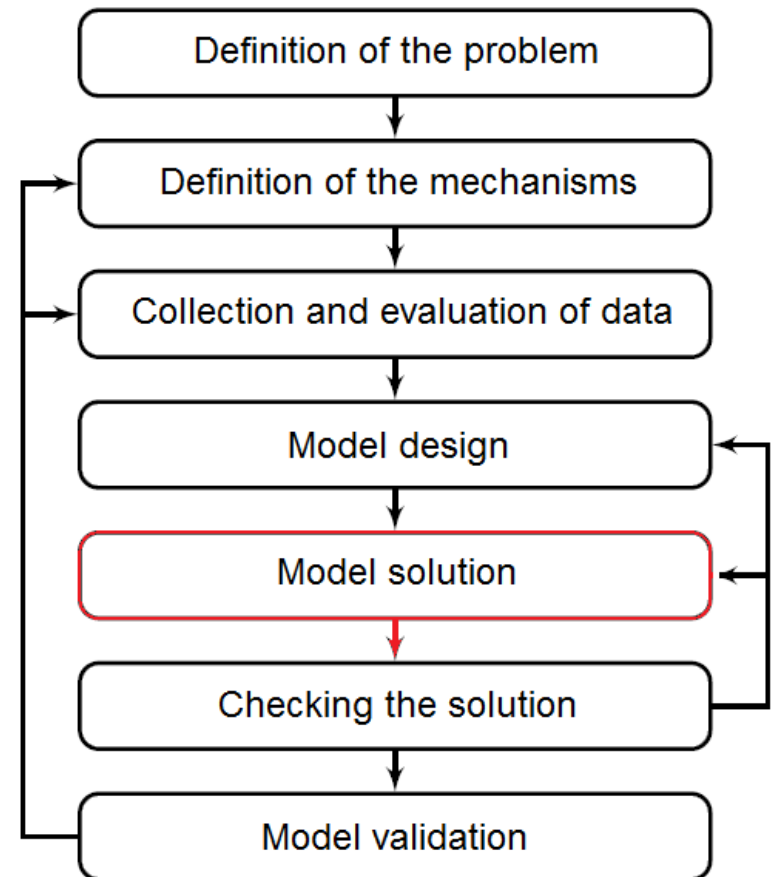
5th: solving the model

The mathematical model can be:

- Algebraic equations (AE)
- Ordinary differential equations (ODE)
- Differential algebraic equations (DAE)
- Partial differential equations (PDE)
- Integro-differential equations (IDE)

Solving the model:

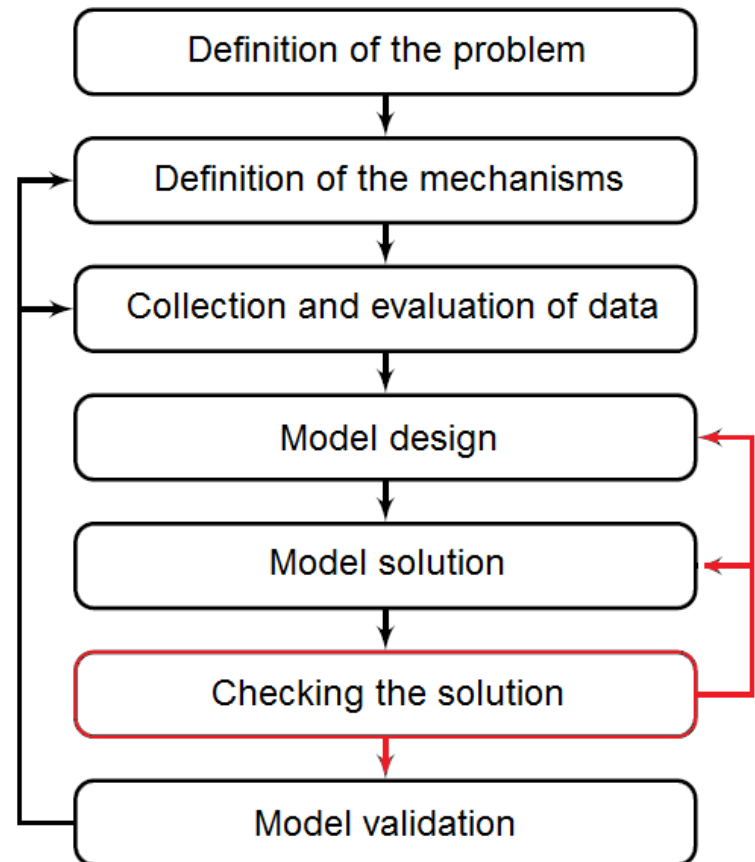
- Solvability analysis
- Selection of the solving method (for example analytical or numerical)



6th: checking the solution

Verification:

- Impacts of data changes on the solution
- Is the model behaviour compliance the expected behaviour from engineer aspects?
- Logical checking



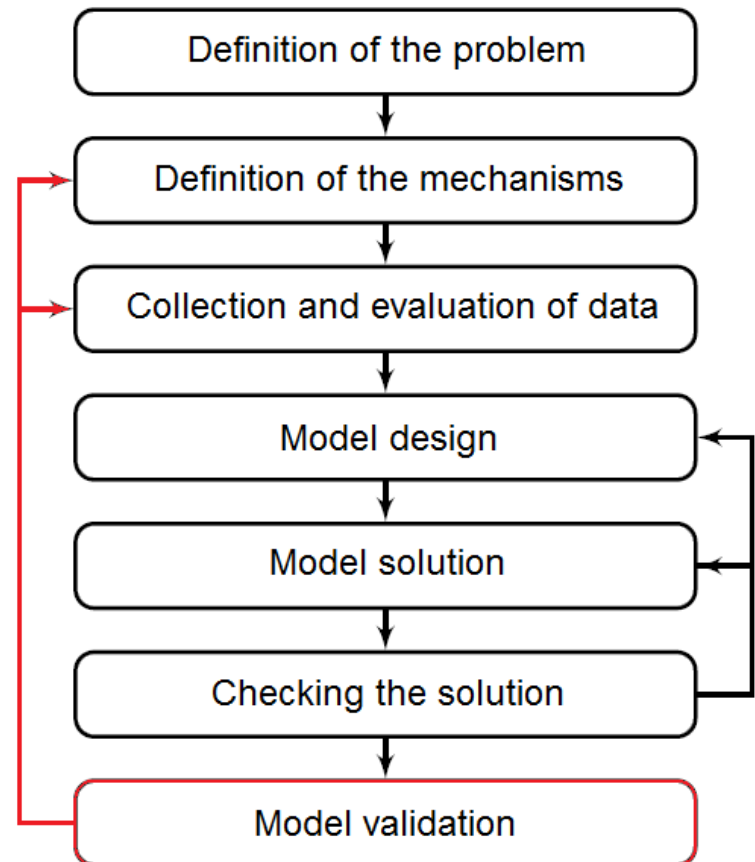
7th: model validation

Model calibration:

- Estimation of unknown or uncertain parameters

Model validation:

- Statistical comparison between the results of the mathematical model and between the measurements of the real system



Components of the model

A systematically built model has the following components:

- System description (text, illustrations)
- Modelling aims
- Mechanisms
- Modelling conditions
- Data (value, unit, source, accuracy)
- Balance volumes (with illustrations)
- Model equations
 - Conservation equations
 - Complementary equations
 - Initial and boundary conditions
- Variables, parameters

The general principle of conservation

The balance volume is a part of the space where the conservation laws/equations can be applied:

- A trivial balance can be made
- It can be open and it can have variable volume
- It can be homogeneous or inhomogeneous
- From the spatial distribution aspect: static or dynamic

Definition of the balance volumes:

- It is not trivial
- It is influenced by the modelling aims or by the required accuracy (or by the modeller's knowledge)

The general principle of conservation

$$\begin{aligned} \{ \text{change of the inner quantity} \} &= \{ \text{intake quantity} \} - \{ \text{output quantity} \} + \\ \text{(in time)} &+ \{ \text{sources} \} - \{ \text{sinks} \} \end{aligned}$$

The differential form of the balance equation:

$$\frac{\partial \hat{\Phi}}{\partial t} = -\nabla \cdot J + \hat{q}$$

$$\nabla \cdot J = \text{div}(J) = \frac{\partial J_x}{\partial x} + \frac{\partial J_y}{\partial y} + \frac{\partial J_z}{\partial z}$$

The same equation with concentrated parameters:

$$\frac{d\Phi}{dt} = J + q$$

Examples for balance equations

Mass conservation:

$$\frac{dm}{dt} = \sum_{j=1}^p \sigma_j - \sum_{k=1}^q \sigma_k$$

Energy conservation:

$$\frac{dE}{dt} = \sum_{j=1}^p \sigma_j (h + e_k + e_p) - \sum_{k=1}^q \sigma_k (h + e_k + e_p) + Q + W$$

Momentum conservation:

$$\frac{dM}{dt} = M^{in} - M^{out} + \sum_{k=1}^p F_k$$

Literature used

K. M. Hantos and I T. Cameron
*PROCESS MODELLING AND MODEL
ANALYSIS*
Academic Press, 2001.

Thank you for your attention!

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