ETH zürich

Course Introduction

2016 Lecture #1

Systems Analysis and Mathematical Modeling
in Urban Water Management (SAMM)

http://www.ifu.ethz.ch/SWW/education/lectures/Systems_Analysis
6 credits   4 hours of lectures/exercises

(1) Prof. Eberhard Morgenroth, eberhard.morgenroth@ifu.baug.ethz.ch
(2) Prof. Max Maurer, max.maurer@ifu.baug.ethz.ch

Your Professors

Prof. Morgenroth

- Process Engineering in Urban Water Management
- ETH/Eawag
- Focus
  - Biological treatment of water and wastewater
  - Nutrient removal and recovery
  - Gravity driven membrane filtration
  - Processes for decentralized treatment

Prof. Maurer

- Urban Water Systems
- ETH/Eawag
- Focus
  - Water infrastructure management
  - Evaluation of water systems
  - Concepts for decentralized treatment

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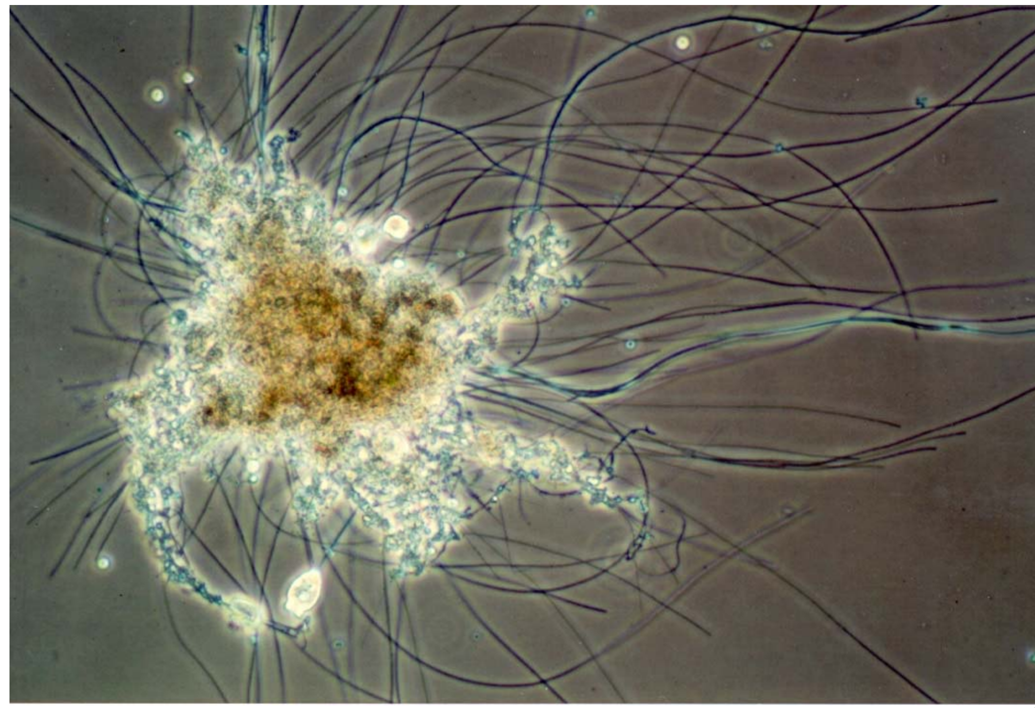
Both courses cover a range of scales

Systems Analysis and Mathematical Modeling in Urban Water Management



Process Engineering I (Biological Processes)

http://www.saskatoon.ca, Jürg Kappeler

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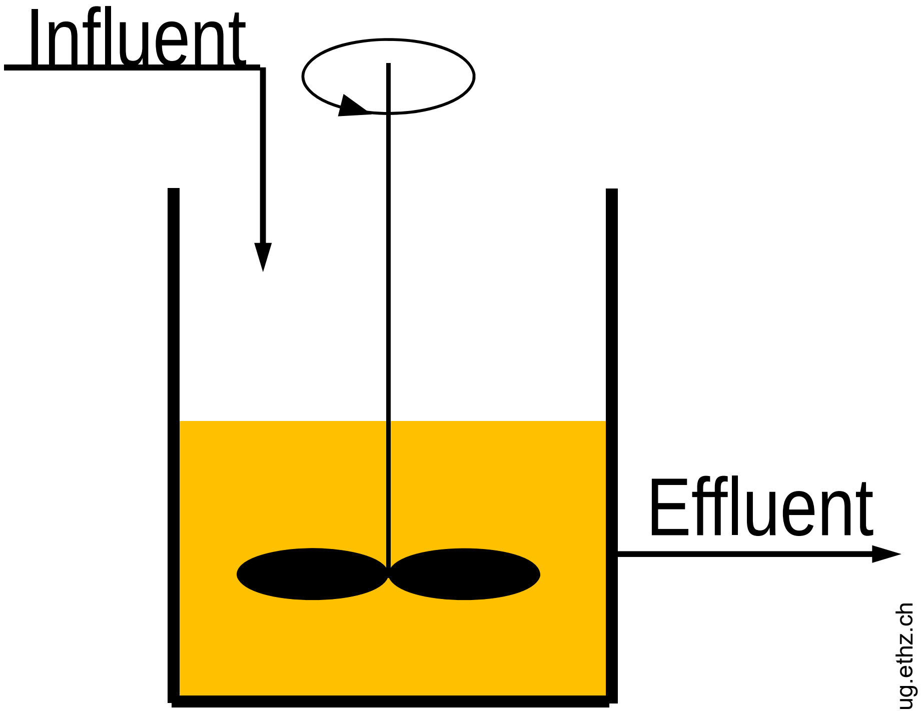
Both courses develop idealized models

Systems Analysis and Mathematical Modeling
in Urban Water Management



Process Engineering I (Biological Processes)

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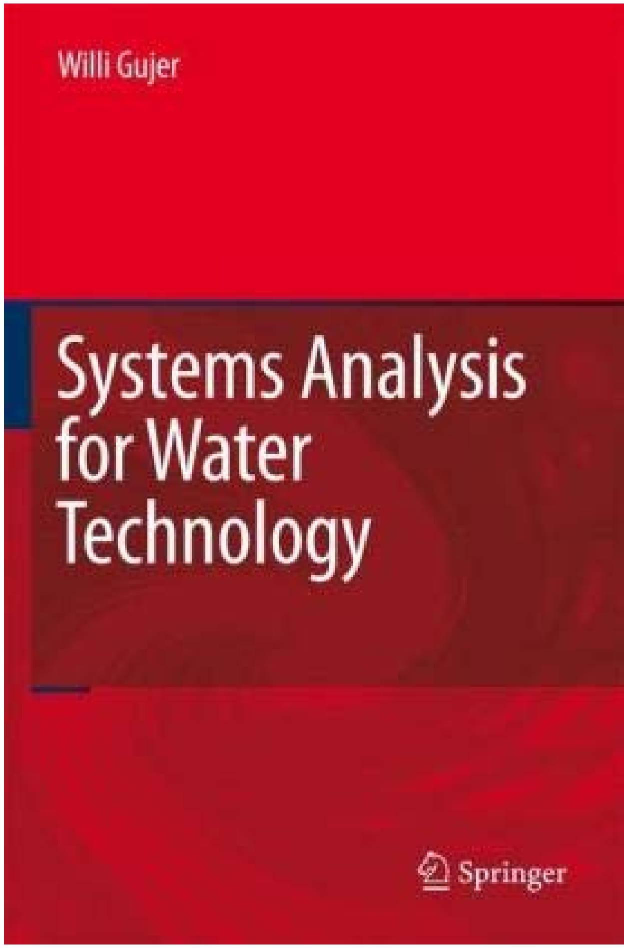
Similar topics in Process Engineering Ia and Systems Analysis and Mathematical Modeling – at different levels

Topic	Your previous BSc courses	PE Ia (PE Ib)	SAMM
Material balances	CSTR, PFR, batch	CSTR, PFR, batch	CSTR, PFR, batch, non-ideal mixing, dispersion, implicit/explicit
Residence time distribution (RTD)	Only averages (HRT, SRT)	Only averages (HRT, SRT)	HRT, SRT, RTD, dispersion coefficient
Matrix notation to describe parallel processes	-	Be able to read and write	Systematic evaluation based on conservation principles
Numerical modeling	Some	Use SUMO simulator to evaluate treatment systems	You do your own programing in Berkeley Madonna (also in exams)

Required reading for Systems Analysis and Mathematical Modeling

- Book:
  W. Gujer (2008) Systems Analysis for Water Technology, Springer, 129 CHF
- We provide you with copies of overheads, etc.
- Software and further information available at www.berkeleymadonna.com for Windows and Mac



Credit requirements

- Solve all 10 problem sets. Make sure you understand the solution in detail.
- ~~Hand in at least 7 problem sets, that you worked out yourself.~~
  [Note: No more "Testate" at ETH]
- <u>TWO MIDTERMS AND ONE FINAL EXAM</u> which will be evaluated and graded. Your final grade is a weighted average of these three evaluations (25/25/50%).
- In case of non passing grade:
  Repetition only possible after re-enrolling in the course next year

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Your preparation for lectures

- Lectures: You profit most from the lectures if you read the text before the lectures.

- Problem sessions: You should read and understand the problem set before the class.

If you do not work during the semester and you do not solve the problems yourself, you will not profit from this course!

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Modeling software: Berkeley Madonna

- www.berkeleymadonna.com
- The demo version is sufficient for this course, however you would require a full license if ever you want to do professional work (Costs: 49 – 299 US$)
- In the demo-version:
  - You cannot save any complete models.
  - But - you can save the equations under:
    <File> <Save Equations as … >
  - Clipboard is not active.
  - Graphic output can be printed but is marked.
  - We will not use flowcharts – do not load the Java Tool
- You will be programming Berkeley Madonna in exercises and in 2nd midterm and final exam

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Content of this course

- Systems analysis:
  - System definition, mass balances, transport processes,
  - Kinetics, stoichiometry
  - Ideal reactors
  - Residence time distribution, modeling of real reactors — Morgenroth
  - Heterogeneous processes and systems
  - Dynamic behavior of reactors

  - Model identification: Model structure and parameters
  - Local sensitivity, error propagation (MC simulation)
- Basics of process control
- Introduction in time series analysis — Maurer
- Design under uncertainty

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Program: Lecture and Exercises HS 2016

Schedule (2016)

#	Date	Lecture (8^{00}-10^{00})	Lecturer	Exercise (10^{00}-12^{00})	Room (Exercise)	Chapter
1	Fr. 23.09	Course Introduction / Material Balances	E. Morgenroth	Exercise 1: Ideal Reactors I	HIL E15.2	1/2/3
2	Fr. 30.09	Transformation Processes	E. Morgenroth	Exercise 2: Stoichiometric Matrix	HIL E15.2	5
3	Fr. 07.10	Ideal Reactors	E. Morgenroth	Exercise 3: Mass Balances	HIL D10.2	6
4	Fr. 14.10	Ideal Reactors / Residence Time Distribution (RTD)	E. Morgenroth	Exercise 4: Ideal Reactors II	TBC [2]	7
5	Fr. 21.10	Residence Time Distribution (RTD)	E. Morgenroth	Exercise 5: Residence Time Distribution [1]	HIL C29	8
6	Fr. 28.10	Heterogeneous Systems	E. Morgenroth	**First Midterm Exam**	TBC [2]	9
7	Fr. 04.11	Dynamic Behavior of Reactors	E. Morgenroth	Exercise 6: Dynamic Behavior of Reactors	HIL C29	10
8	Fr. 11.11	Sensitivity and Parameter Identification	M. Maurer	**Mock Exam:** Exercise 7: Sensitivity and Parameter Identification	HIL E15.2	11/12
9	Fr. 18.11	Sensitivity and Parameter identification	M. Maurer	Exercise 8: River-Model (Sensitivity) [1]	HIL C29	12
10	Fr. 25.11	Error Propagation	M. Maurer	**Second Midterm Exam**	HIL E15.2	12

Learning objectives for lecture/exercise
SAMMbook Chapter 1/2

- You have a clear picture of <u>content and organization of this course</u>
- You know some important <u>terms from systems analysis</u>
  (e.g., such as system, model, simulation, intensive/extensive properties, variables, transformation processes, transport processes, dynamic/equilibrium processes, calibration, validation, verification, uncertainty, variation)
- You know what the <u>goals of systems analysis</u> are
- You have started to develop an approach that allows you to <u>link the different topics of the course</u>
- You are able to use <u>Berkeley Madonna</u> to implement your own mathematical models (→ Exercise on first day of class)

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System – Model – Simulation

- What do the following terms mean to you:
  - System
  - Model
  - Simulation

- How do we use these terms in our daily life?

- Be aware that these terms have defined meaning in the context of this course

puts things together/shows us something important/pretends to be

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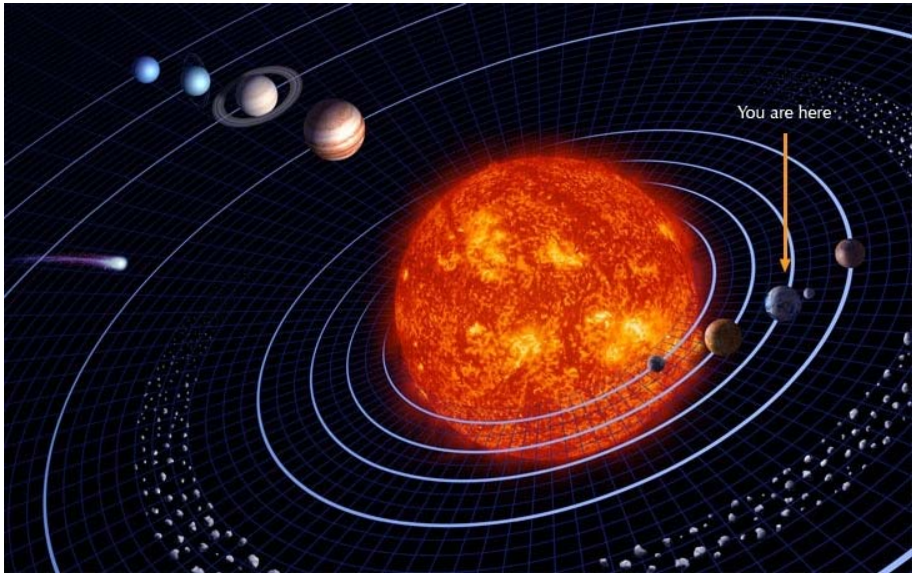
What is a system?



A system is a set of related and interacting elements which together serve a common purpose.
Here we consider systems that exist in time and space.

Therefore a system is composed of

- Interacting elements
- Relationships between these elements
- Exists over some time
- Has a boundary that separates clearly between the system and its environment

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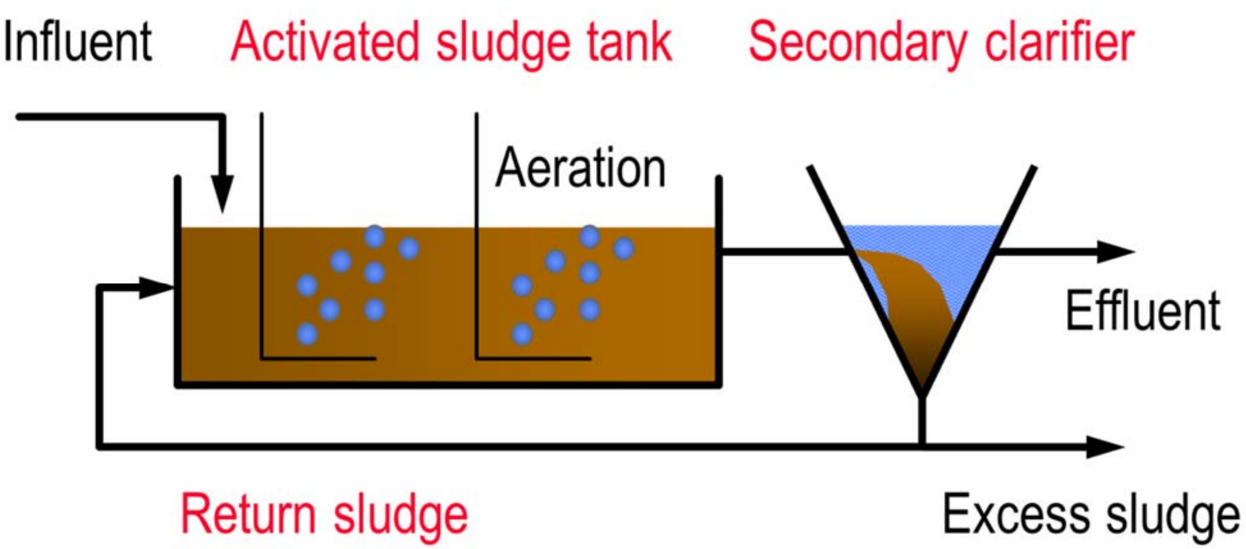
Important Properties of a System

- The environment may affect (disturb) the system!
- The system may affect its environment (output)!
- IMPORTANT: The effect of the system upon the environment may not affect the system again!
  - The output may not disturb the system!
  - Feed back exists only within the system! Or else we must understand it and include it in the system to be analyzed.



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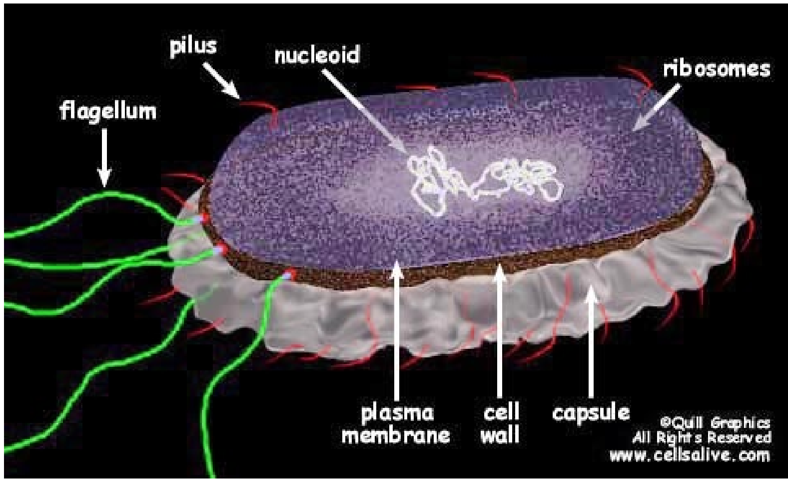
What is a model?



- A model is an abstract description of reality, which is developed in order to understand better some defined aspects of the system to be analyzed or designed.
- It is a semantically closed abstraction of a system.

- Models help us to improve our understanding of the behavior of reality.
- The analysis of the model is more effective than direct observation of reality.

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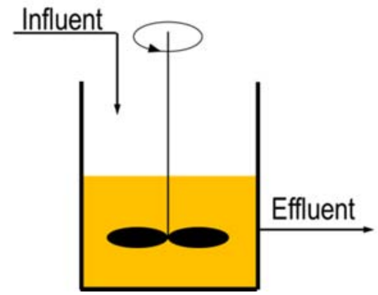
What is a model?

Reality

Conceptual model



Mathematical model

$$\frac{dS}{dt} = \frac{1}{\theta_H}(S_{in} - S) + r_S$$

$$\frac{dX}{dt} = \frac{1}{\theta_H}X_{in} - \frac{1}{\theta_X}X + r_X$$

Experimental model

Models in teaching and communication

- Models allow us to communicate in a structured way what we know about a system or a process.
- Models define a common base in communication between experts.
- Models allow us to follow the historic development of our understanding.

$$\frac{dS}{dt} = \frac{1}{\theta_H}\left(S_{in} - S\right) + r_S$$

$$\frac{dX}{dt} = \frac{1}{\theta_H} X_{in} - \frac{1}{\theta_X} X + r_X$$

Table 5. Model #3a: Based on Model #2 but taking into account switching functions for oxygen (S_O) and nutrients (S_{NH}, S_{PO4}).

	S_O	S	X_I	X	S_{NH}	S_{PO4}	Kinetics
Units	g O_2	g COD	g COD	g COD			ρ
Growth	$1-\frac{1}{Y_H}$	$-\frac{1}{Y_H}$		1	$-i_{NX}$	$-i_{PX}$	$\mu_{max}\frac{S}{K_S+S}\cdot\frac{S_O}{K_O+S_O}\cdot\frac{S_{NH}}{K_{NH}+S_{NH}}\cdot\frac{S_{PO4}}{K_{PO4}+S_{PO4}}X$
Decay	$-(1-f_I)$		f_I	-1	$(1-f_I)i_{NX}$	$(1-f_I)i_{PX}$	$b\cdot X$

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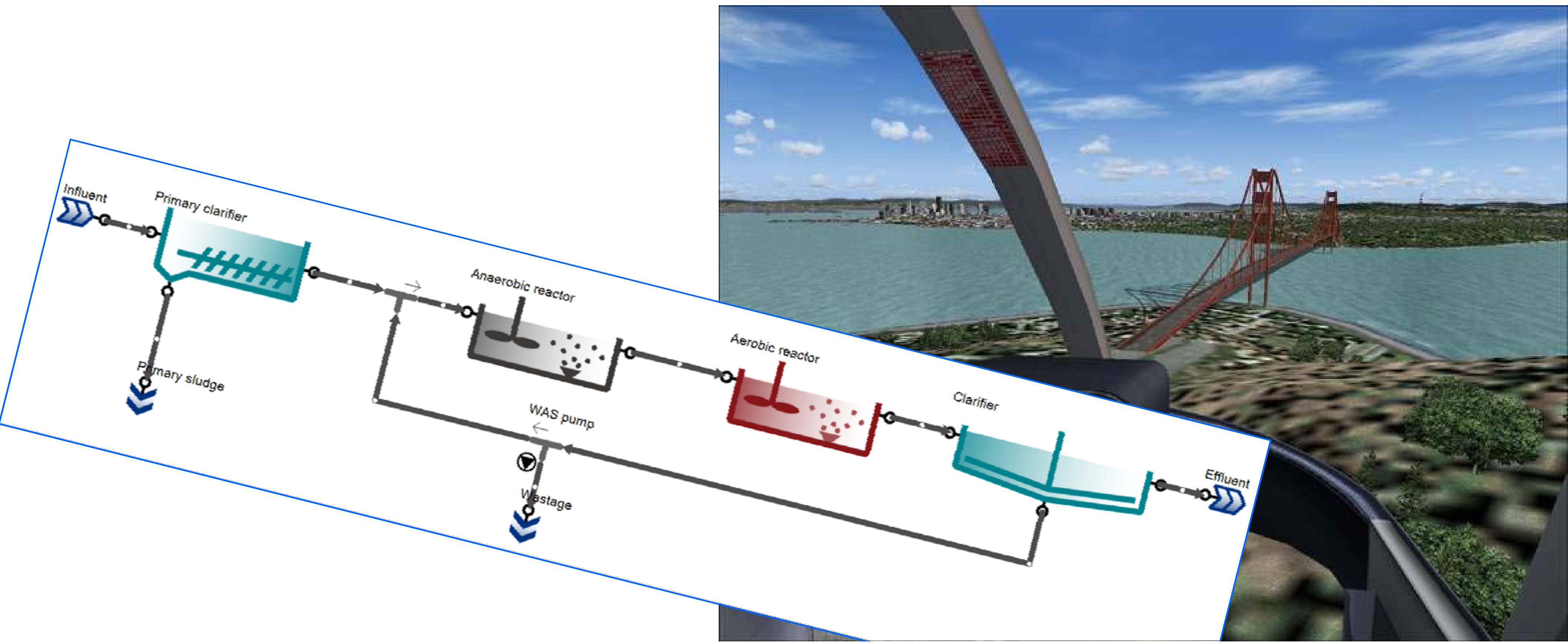
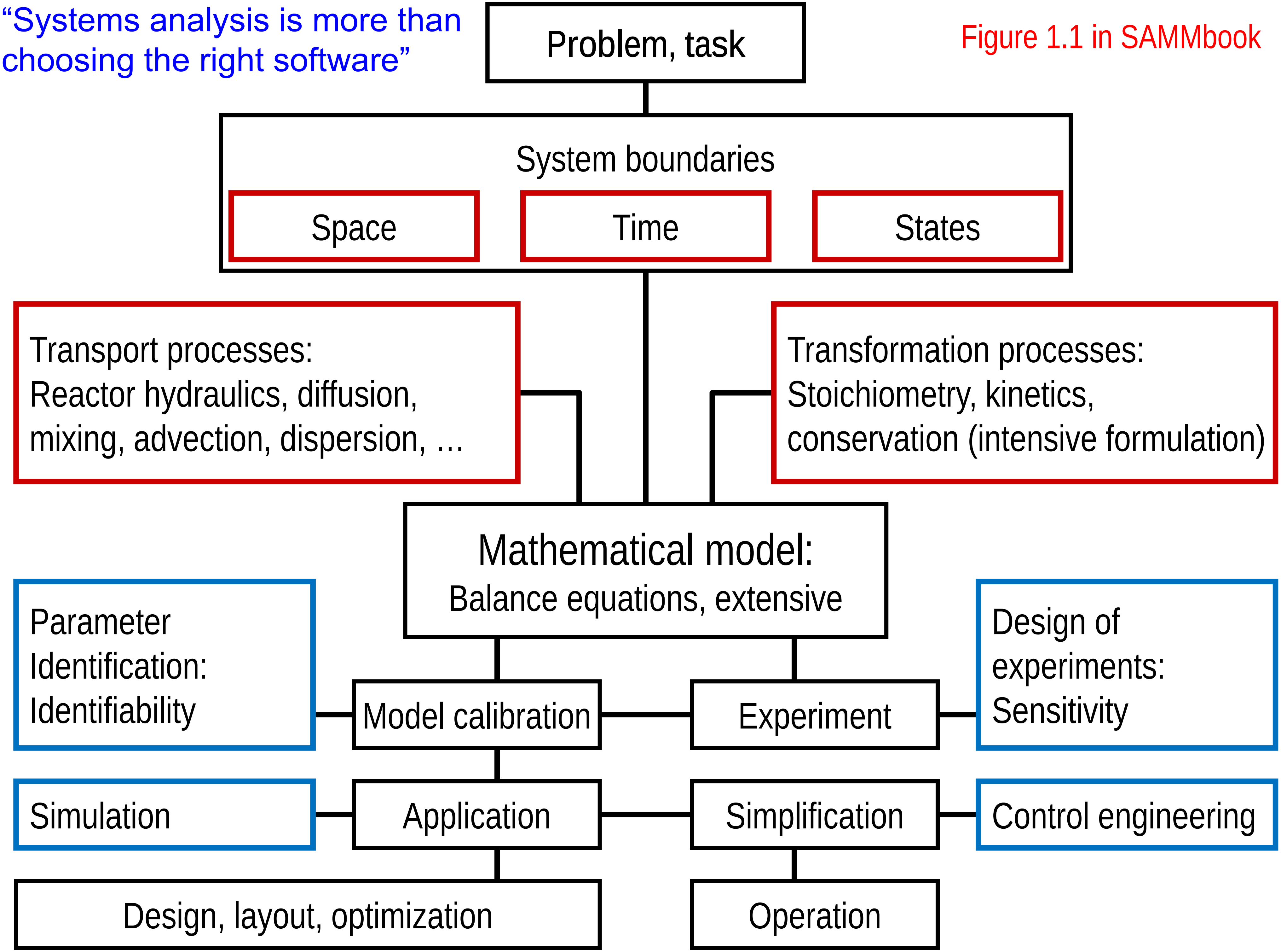
What is a simulation?

- Simulation implements a mathematical model of a system.
- It allows us to perform virtual (non physical) experiments and to arrive at results, which are transferable to reality.



“Systems analysis is more than choosing the right software”

Figure 1.1 in SAMMbook



Calibration

What to do if the model does not fit reality?

Reality

Model

$$\frac{dS}{dt} = \frac{1}{\theta_H}\left(S_{in} - S\right) + r_S$$

$$\frac{dX}{dt} = \frac{1}{\theta_H}X_{in} - \frac{1}{\theta_X}X + r_X$$

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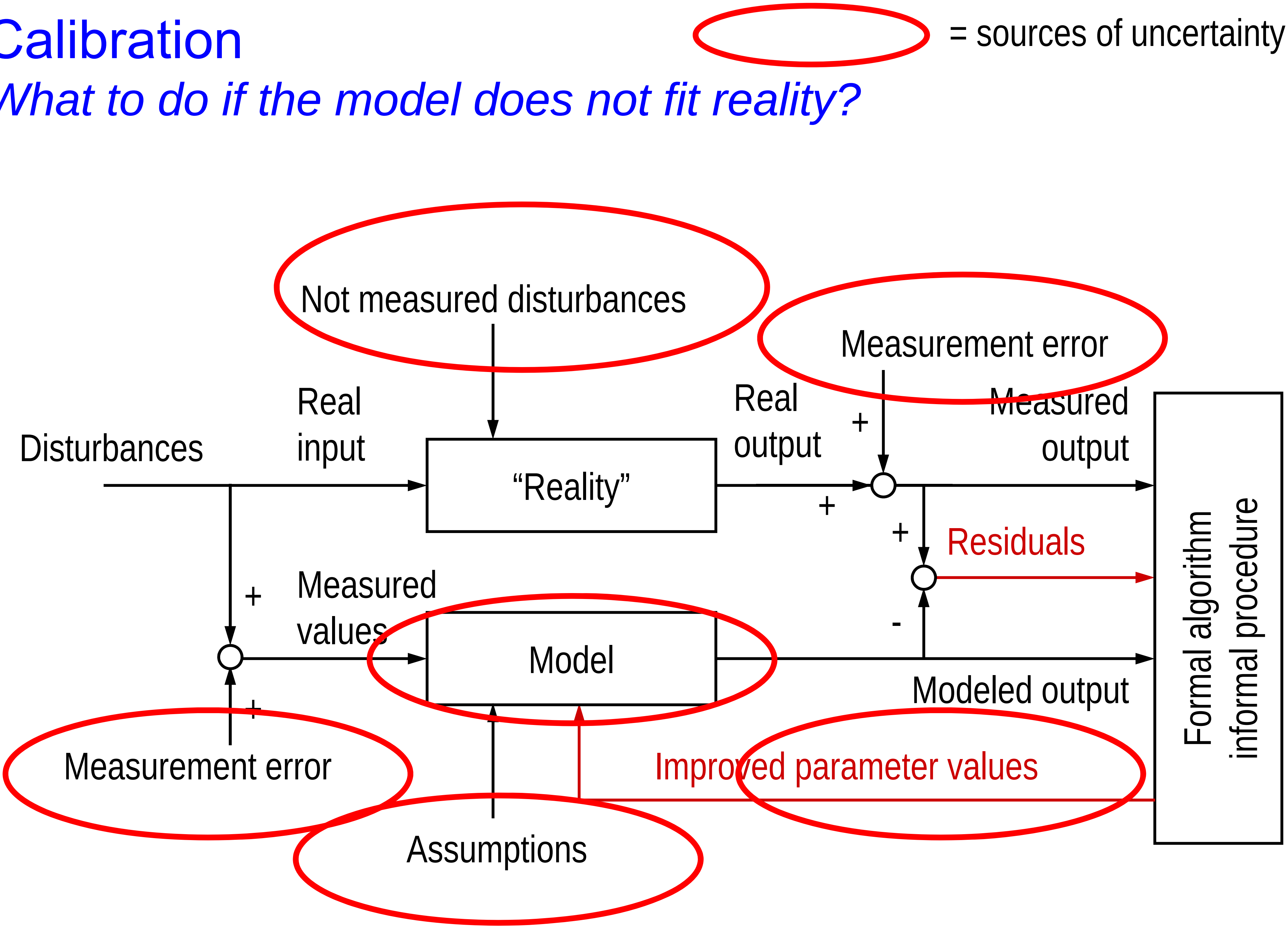
Calibration

What to do if the model does not fit reality?



Compare: Figure 2.2 and 2.3 in SAMMbook

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Systems analysis

- Based on mathematical models, *Systems Analysis* provides us with methods and tools, which allow us to:
  - Analyze the properties of real world systems and to predict their behavior
  - Plan experiments and design plants and systems
  - Interpret (learn from) data and observations
  - Identify parameters and their uncertainty
  - Compare model structures
  - Quantify error propagation
  - ...

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Important terms

- Intensive properties are independent of the size of a system. We can transfer our experience from one system to another one in the form of intensive information.
  Concentration, temperature, velocity, pressure, …

- Extensive properties depend on the size of a system. They are system specific and cannot be used to transfer experience from one system to another one.
  Volume, flow rate, mass, energy, force, …

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Important concepts

- Dimensions:
  Mass [M], Length [L], Time [T]
  Temperature, Moles, Current

- Units are relative. They are defined within a system of measurement, e.g. the SI system:
  meter, kilogram, seconds, …

Always check the dimensions when you derive an equation and the units when you apply the equation!

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Natural sciences vs. Engineering sciences

- Research in natural sciences tries to identify and leads to understanding the mechanisms which cause the behavior of a natural system:
  How does a system behave or function?

- Engineering sciences have the task of planning, designing, realizing, influencing, controlling, and operating systems. They utilize scientific understanding in order to reach a goal with the least possible cost and effort:
  How can we make a system behave as desired?

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The task of models

- Natural sciences:
  Create and communicate understanding, improve understanding of the real world:
  The model is the goal of the work

- Engineering sciences:
  Models should help to make valid statements with the least effort:
  The model is the means to an end.

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Types of mathematical models

deterministic ↔ stochastic

dynamic ↔ static

spatially continuous ↔ spatially discrete

continuous time based ↔ discrete time based

digital ↔ analog

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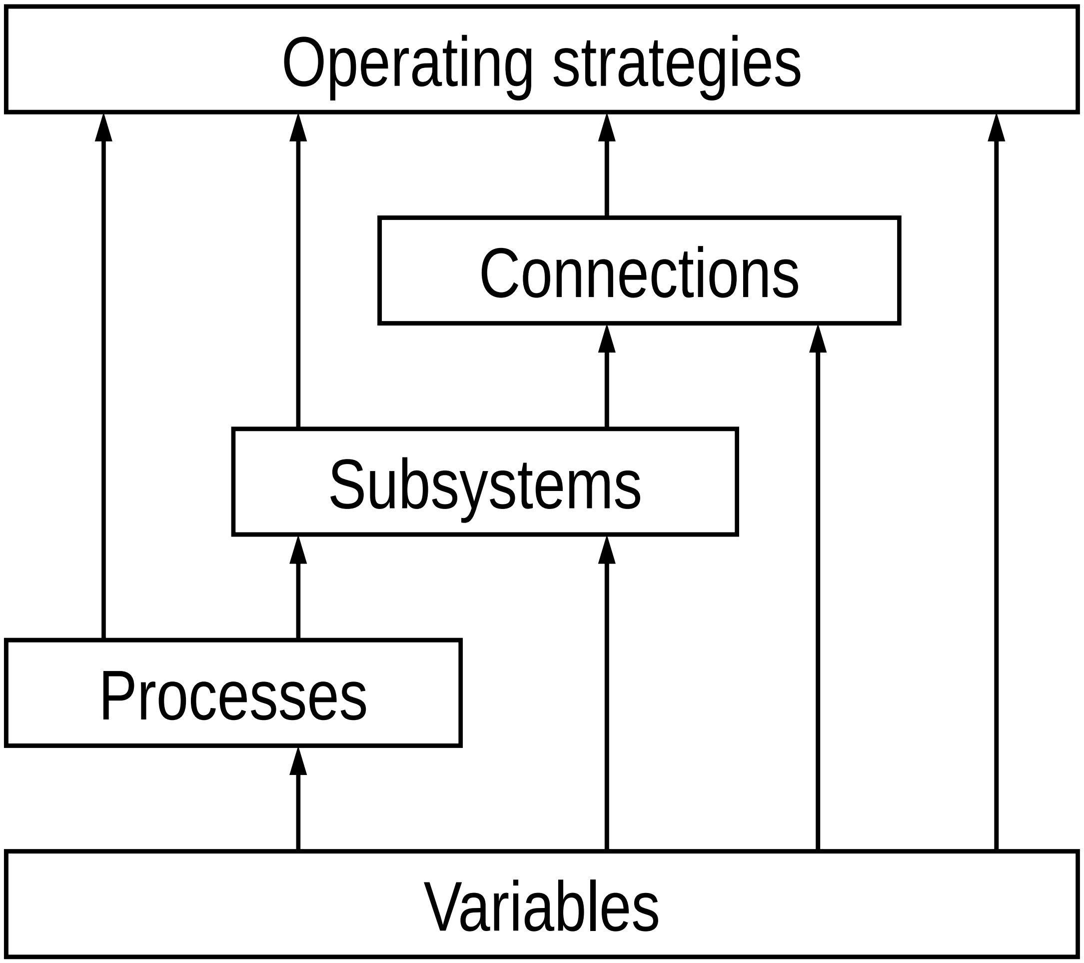
Structural elements of a mathematical model



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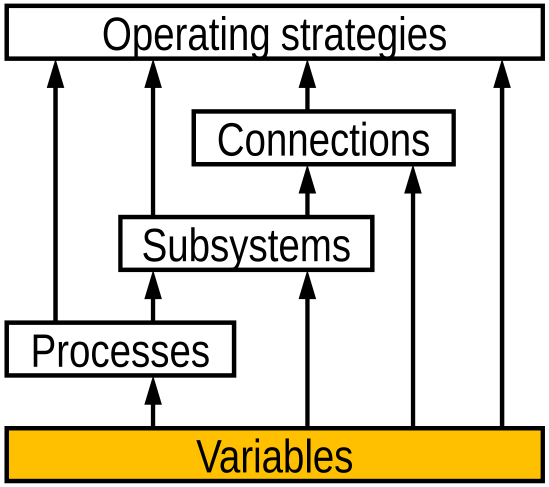
Variables



System variables: Time, space, subsystem
State variables (model output)
Disturbances (model input)
Initial conditions and boundary conditions
Parameters
Data, observations, measurements (analog or digital)

Assign the following to the appropriate type of variable:

- Wastewater composition
- Measured effluent concentrations
- Modeled effluent concentrations
- Oxygen concentration in the reactor
- Oxygen solubility

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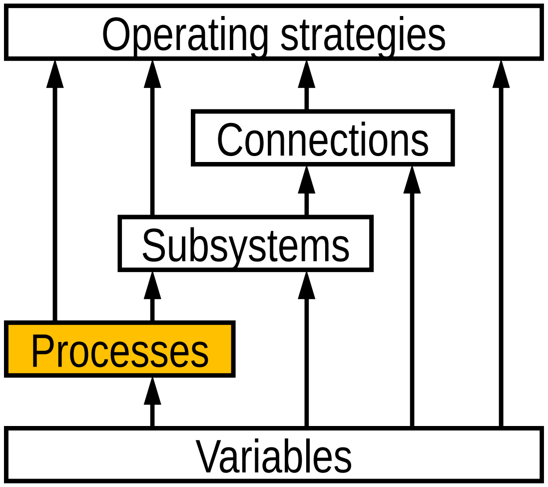
Processes



Accumulation:	Change of inventory, storage
Transport processes:	Diffusion (molecular, turbulent)
	Advection
	Sedimentation / Flotation
	Dispersion
Transformation processes:	Dynamic processes
	Equilibrium processes
Technical processes:	Controlling elements
	Valves, pumps, controllers, …

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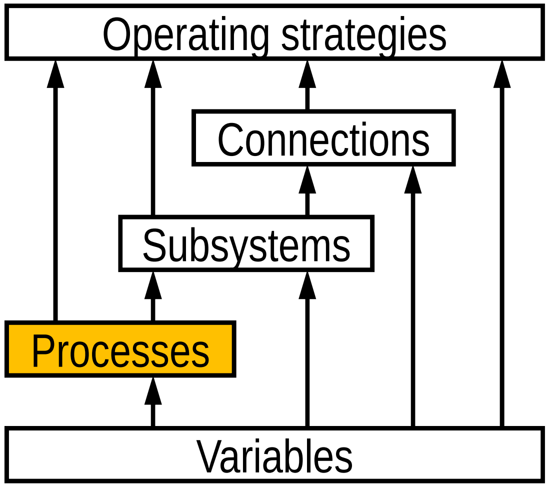
Processes



- Accumulation links state variables over time
- Transport links state variables over space
- Transformation affects state variables at a specific location
- Technical processes are extensive and affect states over large areas, long distances and long time

Reminder: Extensive properties depend on the size of a system. They are system specific and cannot be used to transfer experience from one system to another one.
Volume, flow rate, mass, energy, force, …

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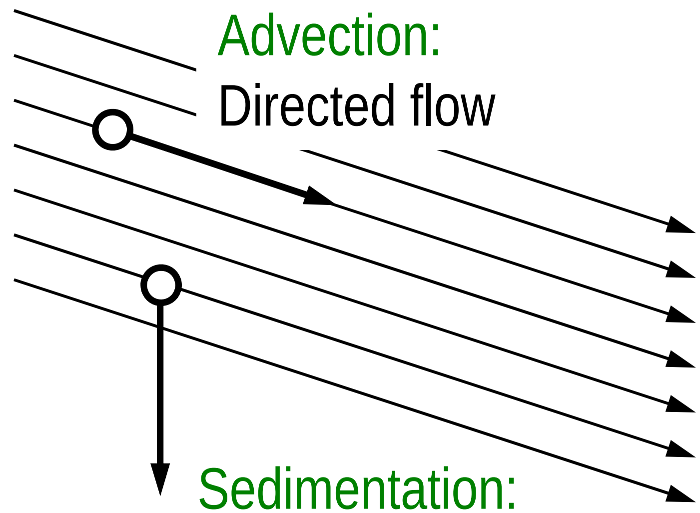
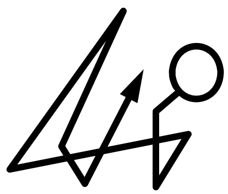
Transport processes

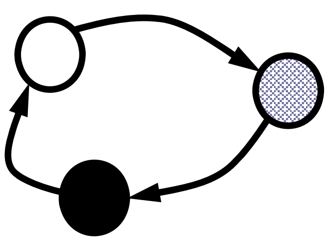


Advection:
Directed flow

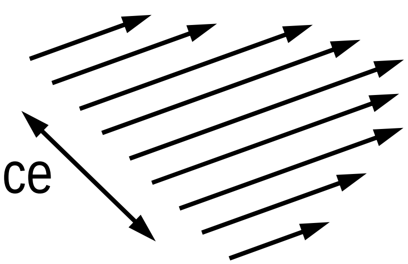


Molecular diffusion:
Random movement
of individual particles,
‚random walk‘, Brownian motion

Sedimentation:
Directed movement
relative to the water



Turbulent diffusion:
Exchange of water parcels



Turbulence

Dispersion:
Advection averaged over
space
(over a velocity profile)

Figure 2.5 in SAMMbook. For details on transport processes see Chapter 4.

Technical processes

- Controlled processes (feed forward, feed back):
  - Aeration
  - Removal of excess sludge
  - Dosing of chemicals
  - Backwashing of a filter bed
  - Opening of a valve
  - Operation of a pump
  - ...

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Transformation processes

- Dynamic process:
  Relative to the observation time, the rate of a dynamic process is of importance:
  → Growth of a population of organisms

- Equilibrium processes:
  The rate of the process is high, forward and backward reactions are nearly equal (very close to equilibrium):
  → Acid – Base equilibrium, pH

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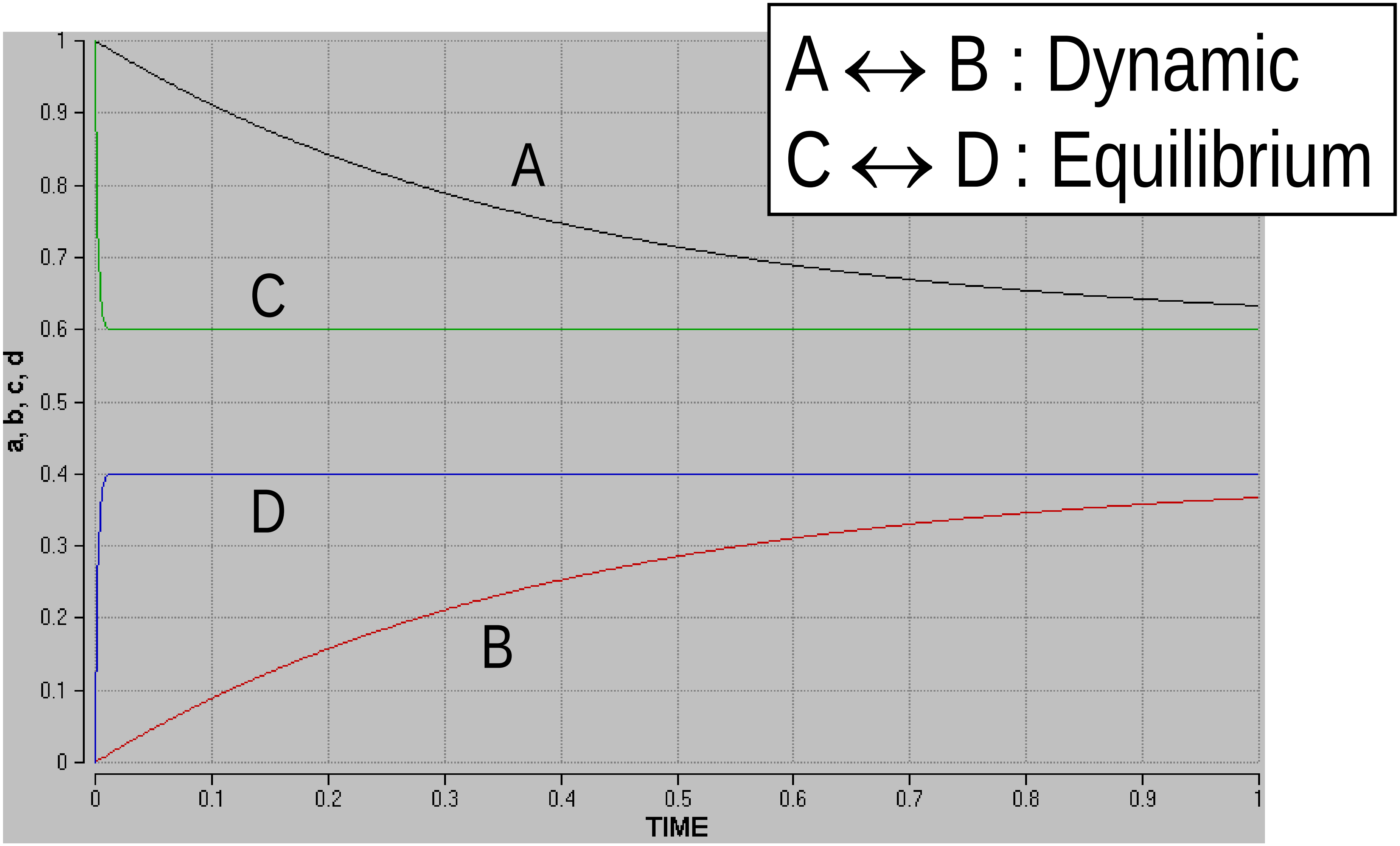
Dynamic and Equllibrium Processes



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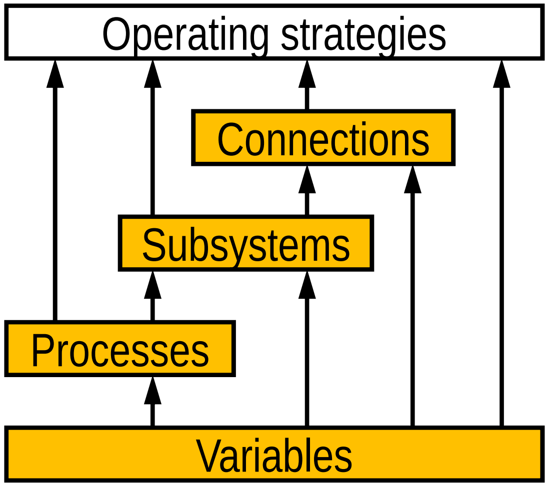
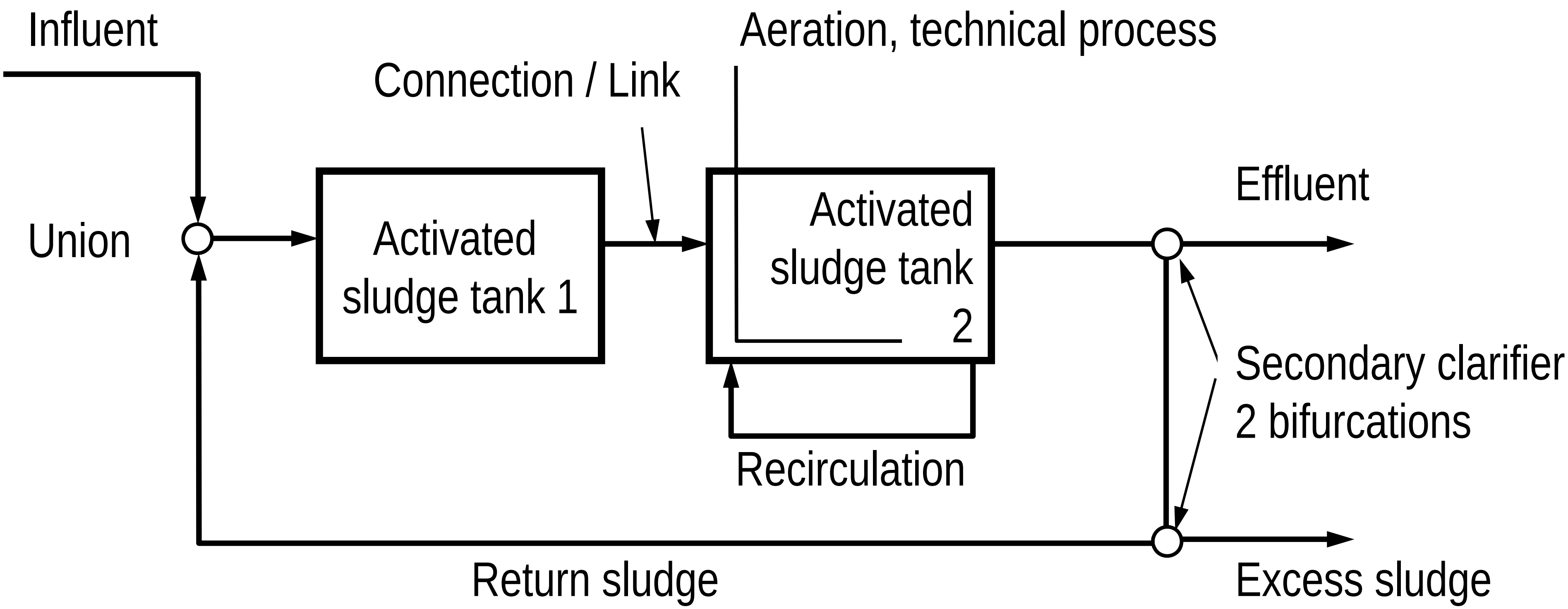
Elements of systems subsystems





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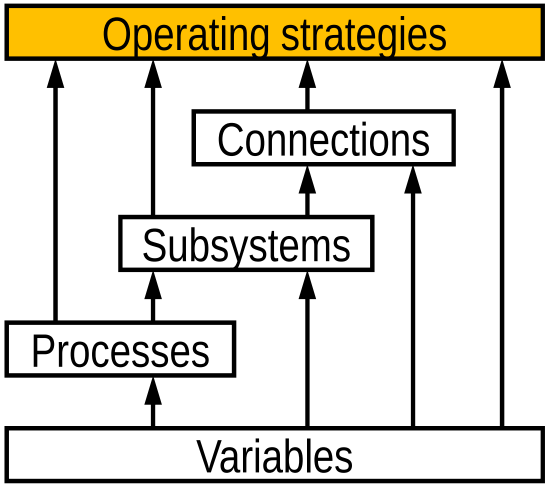
Operating strategies



- Using the degrees of freedom of a system to reach a defined goal

- In an activated sludge system:
  - Maintain a given solids retention time
  - Maintain an activated sludge concentration
  - Maintain an oxygen concentration
  - Optimize nitrification before denitrification
- Maintain the pressure in a water supply system
- Use pumps only during the night, make use of reservoirs

→ Process control

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Calibration, validation, verification

- **Calibration:**
  We adjust the model parameters in order to reach the best possible agreement between model and experiment: Interpolation
- **Validation:**
  We test the validity of the model in view of the question to be answered, which lies in the near field of our experience: Design
  (Validation is a relative procedure)
- **Verification:**
  A verified model is generally valid. We can use it wide outside of our field of experience: Extrapolation
  (Verification is an absolute procedure)

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Compare model prediction with observations

http://www.richardfeynman.com

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Examples

- **Calibrated model:**
  Empirical model to predict time an apple requires to fall from a tree
- **Validated model:**
  Velocity of a falling feather in vacuum and of an apple from a tree
- **Verified model:**
  Newton's law of gravity
- But then came Einstein's general theory of relativity…
- Models in environmental engineering are typically very complex so that they cannot be verified – but calibrated and validated

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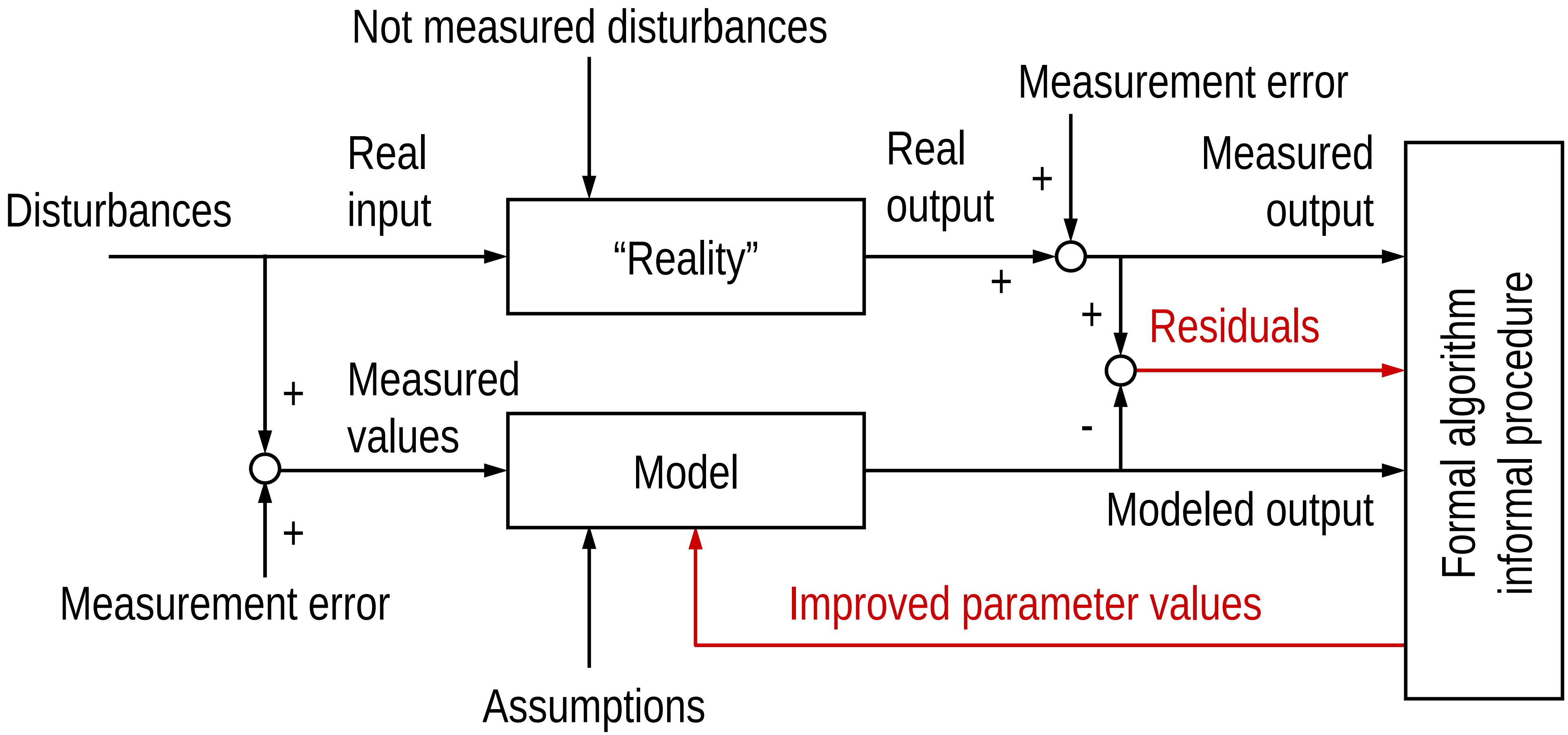
Calibration



Validation

Without adapting the parameters, the deviation between model and experiments (experience) which cover the field of application is small enough

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Validation

…means to make the model valuable.

- The model generates reliable (valuable) results in view of our question or design problem.
- Validation of a model is always relative, never absolute!

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Uncertainty

- Uncertainty characterizes the degree of our ignorance in the description of the behavior of a system.

- Uncertainty has many different sources and its quantification is uncertain itself.

- We can reduce uncertainty with an investment of additional resources
  - More measurements
  - More costly model development
  - …

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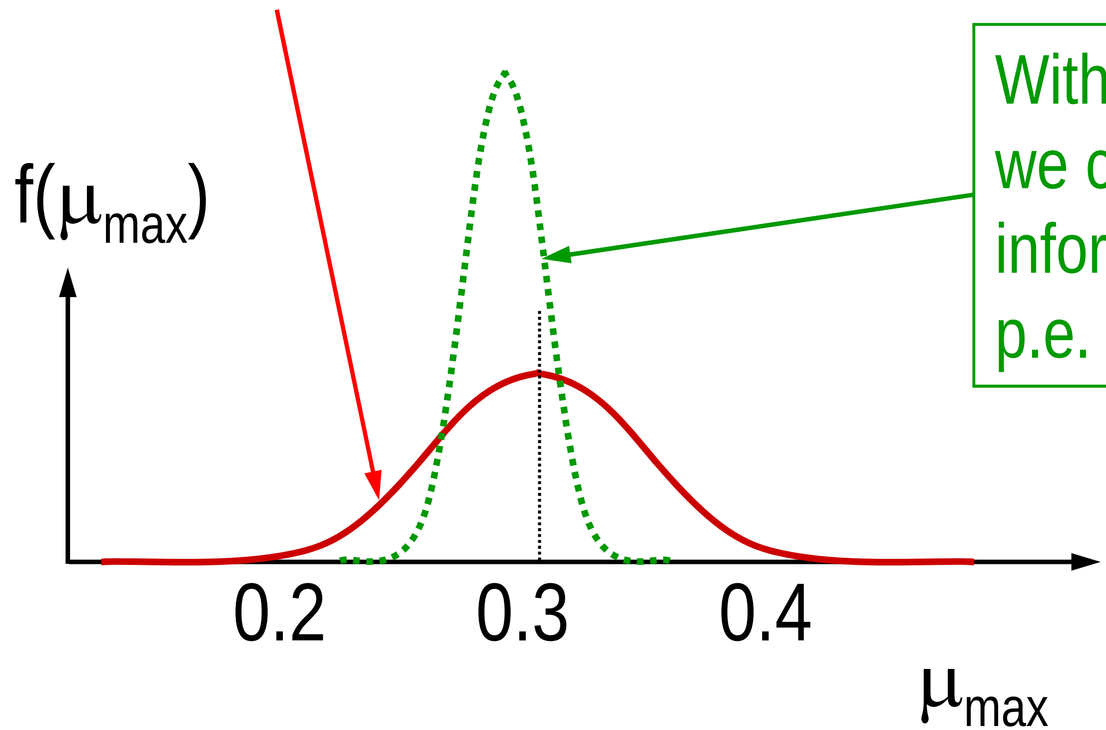
Example: Parameter uncertainty

The maximum growth rate of a microorganism is:

$\mu_{max} = 0.3 \pm 0.03\ d^{-1}$



With additional experiments we can obtain more accurate information,
p.e. $\mu_{max} = 0.029 \pm 0.01\ d^{-1}$

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Variation

- Variation occurs naturally over time and space,
  it cannot be reduced with additional analytical effort.

- We may, however, not know (be uncertain) about the instantaneous, local value of a variable disturbance.

- Examples:
  - Rain intensity
  - Flow of water
  - Temperature
  - Pollutant concentration

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Example: Variation of pollutant load