Material Flow Analysis and Life Cycle Assessment

TECHNISCHE UNIVERSITÄT DARMSTADT

2. Unit: Models and modelling

SS12

Prof. Dr. Liselotte Schebek
Fachgebiet Industrielle Stoffkreisläufe
Institut IWAR

2. Unit: Models und modelling

Methods of systems analysis

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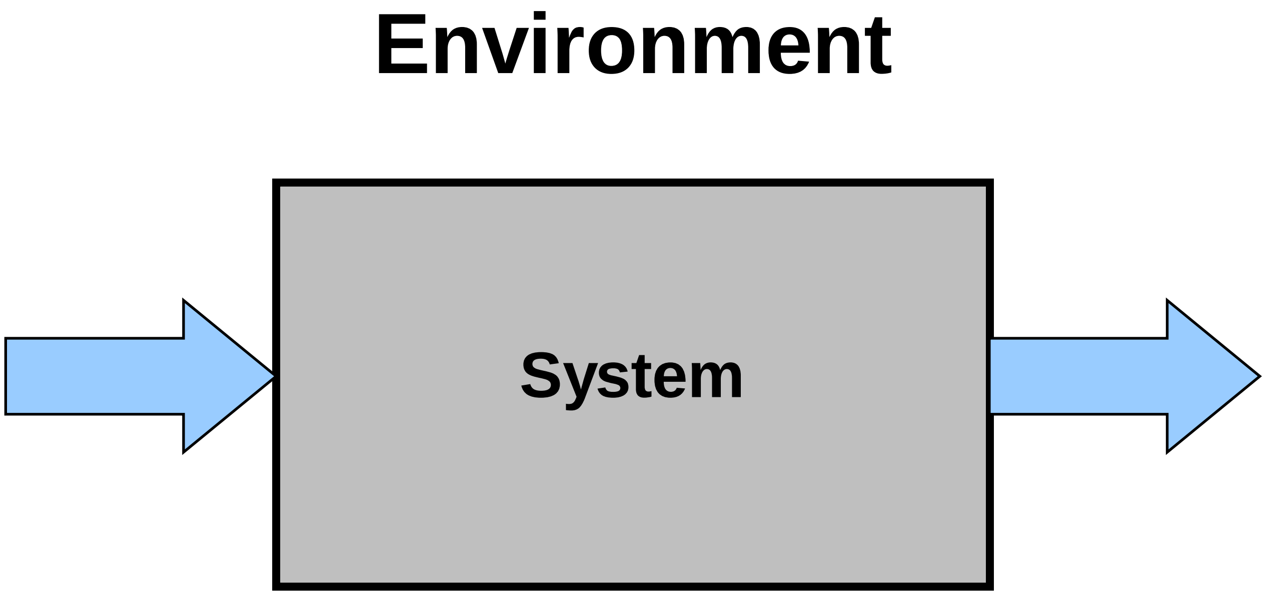
- ... model the reality for a system frame defined by an observer
- ... represent reduced and abstracted descrptions of reality
- ... are used to get new insights about the properties and behavior of the defined system; also about future developments in the context of scenario development
- ... are used in many forms in natural sciences, engineering, economics and information technology

System (I)



System (II)

Definition according to DIN 19226 regulation and control technology:

- *„A system is an array of objects given in a regarded context that are related to each other. This array is* separated from its sourrounding by certain specifications
- [DIN 19226, Part1: 1994]

Definition of systems

A system is an excerpt from a real environment and is described by the system boundaries :

- Geographically : region, river basins, lakes, etc.
- Politically/economically : Germany, EU25, construction sector
- Organizational: company, location
- Technological: process, machine
- Natural Science: chemical reaction

Model (I)

The term "model"

- is derived from the Latin word Modellus - scale (or Italian modello).
- is used in different scientific disciplines for both qualitative and quantitative "descriptions " of reality; i.e. a "model" represents a simplified excerpt of reality.

- Models reduce real systems to major basic relationships.
- A model must reflect both the structural and the inherent features of the original in a sufficiently precise manner.

Model (II)

<u>However:</u>

- Original and model can not totally resemble each other. A model is therefore not a copy of the real system, but merely acts as a “spectacle” for its assessment [Imboden und Koch 2003].
- It is “in principle impossible“ for the modeler to perceive the objective reality [Marquardt 1995]. The creation of a model is therefore associated with a multi-stage process of the loss of realism.
- The sum of subjective effects on the model design leads to a loss of objectivity.

cited by :
Jens Warsen: Validierung von Stoffflussdaten in der Ökobilanz durch Daten aus dem öffentlichen Berichtswesen
Dissertation, TU Darmstadt 2009, WAR-Bericht 203

Simulation

Simulation (= computer simulation)

- It is based on a **model** that describes the problem and the system adequately.
- A model for the simulation represents a description of the system in the form of mathematical equations. The development of a new model is called **modelling**.
- The model parameters can be adjusted or varied ("**scenarios**"). The results of the **simulation** (calculation) are used for conclusions on the behaviour of the system as well as for the solution of the problem.

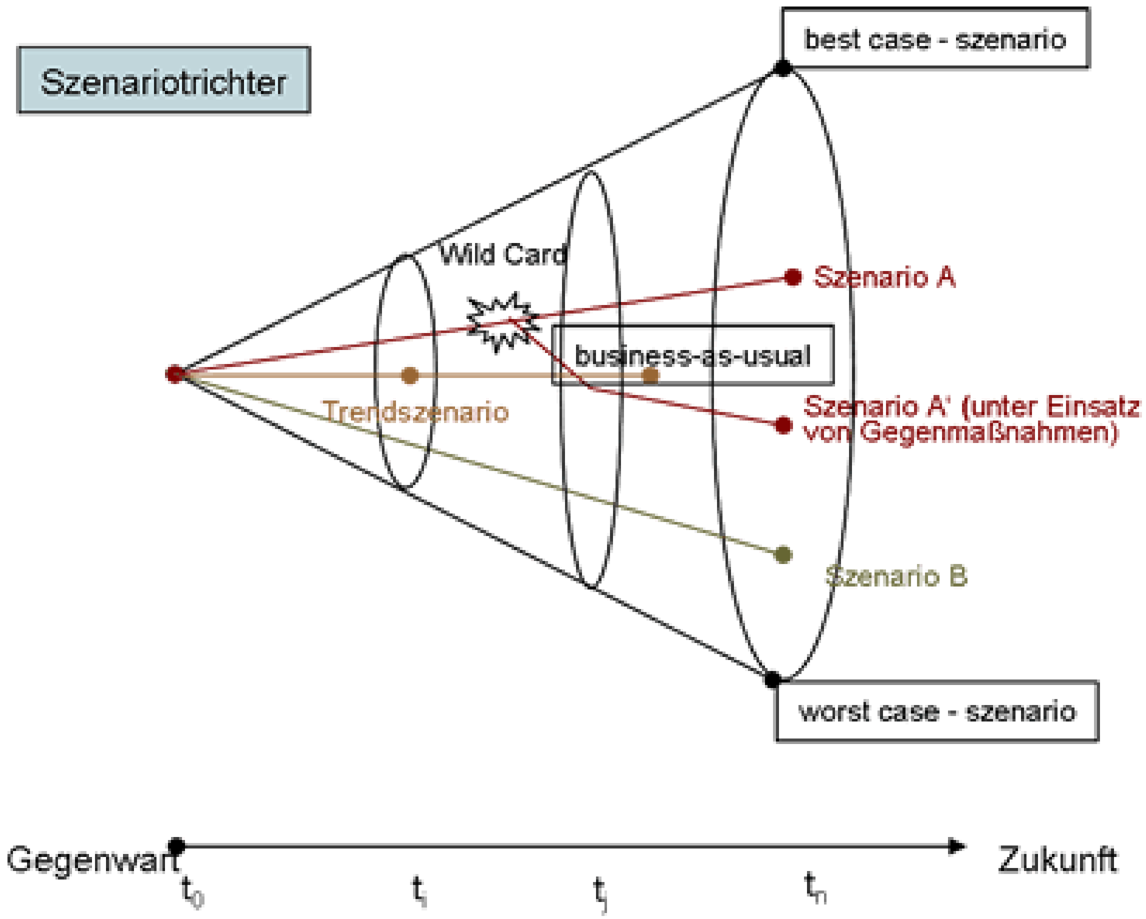
Scenarios (I)

- are descriptions of possible developments in the future.
- describe a future state and the path that leads to this.
- are the quantitative parameters of a model calculation in the framework of a simulation.

- The development of scenarios is usually based on "story-lines“:
  - “Business as Usual“ (BAU)
  - “Worst Case“
  - “Priority for environmental protection measures“ etc.

- serve as preparation of decisions, the development of strategies, the early recognition of developments.

Szenarien (II)



http://www.goldenezeiten.org/texte/M-ZF-Szenario-Technik.htm

Validation

- In principle it must be assumed that the results of a model and that of the original **cannot be identical** [Bossel 1994].

- On the other hand, the sensible use of such information and data is only possible if it can be shown that they constitute a **sufficiently precise reflection** of the real situation [Häuslein 2004].

➔ The term validation refers to the **verification of the approximation to reality** of a model.

Zitiert nach:
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Validation in the Quality Management

Definition according to ISO 9000: Quality management systems - Fundamentals and terminology

Validation:

Confirmation by the provision of a objective evidence that the requirements for a specific intended use or a specific intended application are fulfilled.

[ISO 9000: 2005] (3.8.5)

objective evidence: this means data…

- *"confirming the existence or truth of something*“; and
- that “*are generated by observation, measurement, test or other means*“.

System, model, simulation

System: An excerpt of the reality described by the system boundaries.

Model: Idealised, simplified association of an excerpt of the reality (a system).

Modelling: creation of a model; in the case of a mathematical model, the description of a system in the form of mathematical equations.

Simulation: to simulate inferences, conclusions, or predictions for a system on paper or the computer

Scenario: depiction of possible future developments for a mathematical model in the form of parameters.

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Types of models for the mathematical representation

Models based on fundamental laws of science :

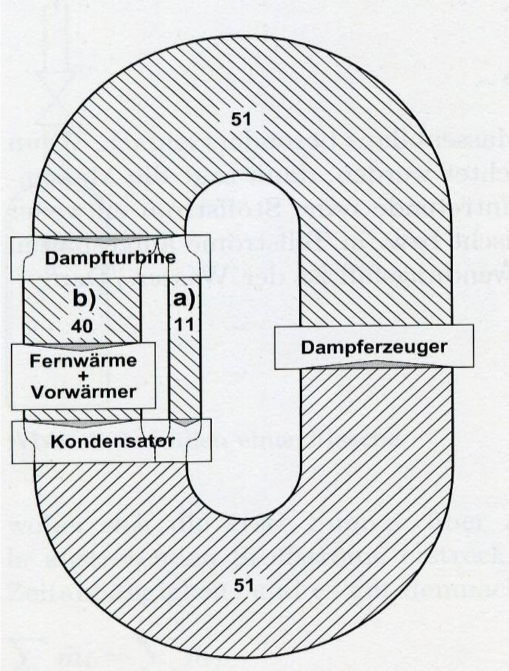
Example: law of mass conservation

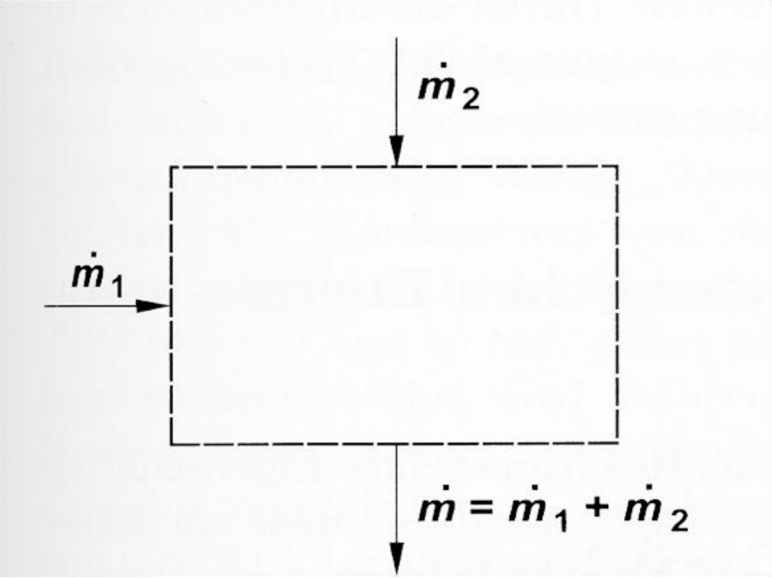
Data models: Management and visualization of data (parameters) **of a system** (purely descriptive)

Example: Geographic Information Systems

Bacchini

Scientific model
Examplel: Material-/Mass balance in process engineering





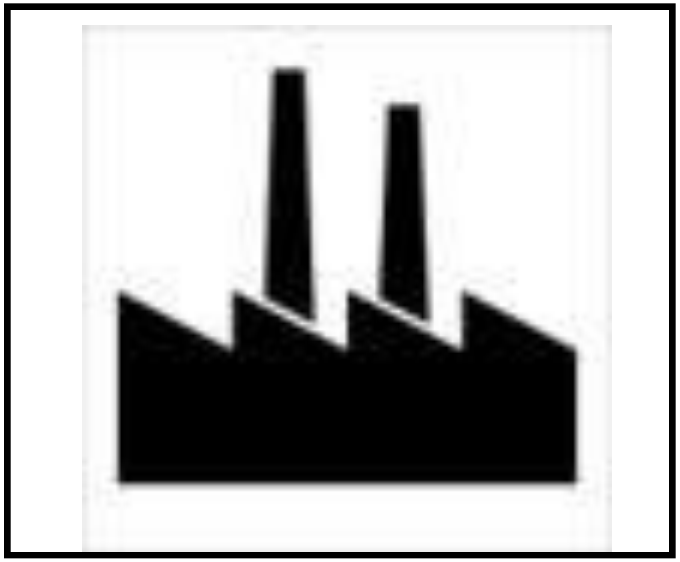
Example: Water-steam cycle of a combined heat and power station

Source: Lucas, Thermodynamik

Example: Waste incinerator

Input:

- waste



Output:

- slag
- fly ash
- exhaust air

How does the heavy metal content of the slag (output) vary when the heavy metal content of the waste (input) alters?

Example: Stoichiometric calculation

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Input:

nitrogen

hydrogen

$$N_2 + 3\ H_2 \leftrightharpoons 2\ NH_3$$

Output:

ammonia

Production of ammonia (Haber-Bosch process)

Which quantity of source materials (input) is required to produce a certain quantity of a product (output)?

Descriptive model: Description of production processes in economics

Data Models: Management and visualization of data (parameters) of a system (purely descriptive)

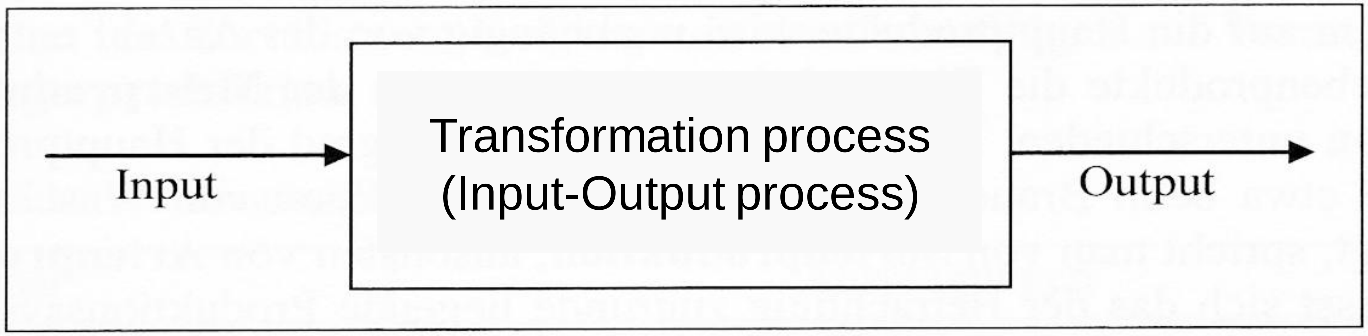


Bild 2.1: Production system or process as an Input-Throughput-Output process

Dyckhoff, Spengler: Produktionswirtschaft – Eine Einführung für Wirtschaftsingenieure

Descriptive model:
Example: Input/Output table of a company

Input/Output table of a leather goods producer

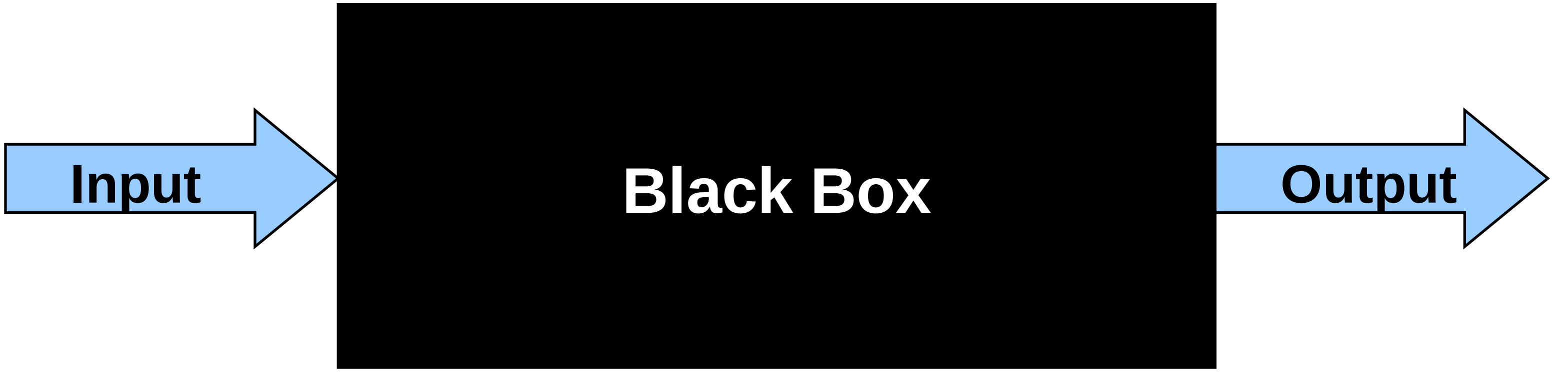
Input			Output
(1) Labour [min]	5000	(4) Shoes [pair]	40
(2) Sewing machine [min]	2500	(5) Bags [unit]	60
(3) Leather [m²]	30	(6) Leather residues [g]	2700

Dyckhoff, Spengler: Produktionswirtschaft – Eine Einführung für Wirtschaftsingenieure

2. Unit: Models und modelling

- 2.1 System, model, simulation
- 2.2 Basic principles for modelling Material Flow Systems
- 2.3 Input-Output Balances

Input- und Output Balancing



Balancing

Balancing: Acquisition of all incoming (input) and outgoing (output) flows of a system

Practical applications of balancing

- process inventory: system = prozess
- company‘s inventory: system = company

- „product inventory“ (= Life Cycle Assessment):
  system = “product system“)

Input-Output Balancing of processes

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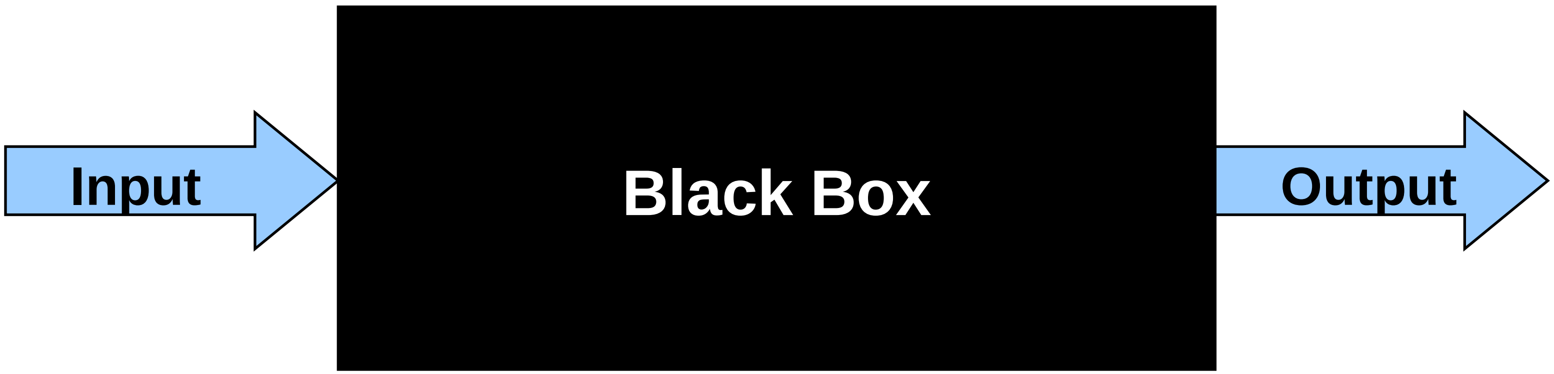
... in natural sciences and engineering:

- mass-/ energy balance

... in economics:

- operational Input-Output Balance

Input- und Output Modellierung



„system“
„process“
„modul“
„transformation“

Input-Output balances and modeling philosophy

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Science Model:

A mass or energy balance is based on the empirical investigation of all known material and energy flows and stocks. Assuming the conservation of mass and energy, missing values are calculated as the difference in the mass balance.

Descriptive Model:

- Particularly for company‘s inventories and processes, it is pracitcally often impossible to draw up a equalised mass and energy balance. The reason for this is that on the one hand the effort for collecting all informations is too great and on the other hand a equalisation is only possible when considering ecologically and environmentally irrelevant materials. This would mean that the effort is too great relative to the obtained information.

Modeling based on fundamental laws of science

- The “system“ is interpreted as a transformation process.
- For this process, input, output and stock values are illustrated based on the law of conversation of mass.
- All material flows can be calculated by means of a few empirically collected material flows by solving linear equations.

Modelling based on a descriptive model

Descriptive model:

- The system is interpreted as a transformation process; No equalised mass and energy balance can be drawn up for this process. Therefore information for incoming and outgoing material flows are empirically determined.
- For the same processes, the assumption can be made that the relation between incoming an outgoing material flows remain constant and can be mathematically represented; it is therefore a linear production function!
- Practically, coefficients are calculated for empirically collected data for material flows that are distinctive for a certain transformation process.