Methodology of Mathematical Modeling

A.C.T. Aarts

Technische Universiteit **Eindhoven** University of Technology

Where innovation starts

TU

Contents

- What is Mathematical Modeling?
- Aims of Mathematical Modeling
- Mathematical Modeling Cycle



Mathematical Modeling

What is a Mathematical Modeling?





• What is a model?

<u>Simplified</u> representation of <u>certain</u> aspects of a <u>real</u> system, capturing the <u>essence</u> of that system

• What is a mathematical model?

Model created using <u>mathematical concepts</u> (variables, operators, functions, inequalities,...)



First-Principle Models

based on physical laws (e.g. Newton's second law)

descriptive, explaining

material parameter values often not known (measurements)

Stochastic Models

based on distributions, averages (e.g. risk models)

capable to deal with random phenomena,

hard to distinguish relations

Empirical/data Models based on (historical) patterns, data (e.g. Moore's law)

not explaining, relations based on reality

- Descriptive vs. stochastic
- Continuum vs. discrete
- Qualitative vs. quantitative



Mathematical Modeling





- Forming of mental image of situation being modeled
- Symbolizes the problem
- Using concepts & analogies

Conceptual thinking Creativity Simplification



Mental Image: example



Optimise production line;

Can buffers be removed/reduced?



Mental Image: example



What is the effect of age & medicine on blood pressure ?





People Involved

Problem Owner

Mathematician





Non-uniqueness

Simplification:



Non-uniqueness: choice of model depends on

- the form the solution needs to be (problem)
 - accuracy
- availability of data





Simplification: example





- Simplifications (in consultation with Problem Owner)
 - 1. Core is bending:
 - <u>1D thin-beam</u> bending:
 - 2. Rubber layer is compressed:
 - 1D-model: empirical law:

$$\frac{d^2}{dz^2} \left(E I \frac{d^2 u_{\rm b}}{dz^2} \right) = p$$

$$u_{\rm c} = ap^b$$



Non-uniqueness





What is the chance on 6?

Model based on

1. measurements

2. mechanical balance laws



Outcome



Back to real world:

Recommendations

based on

- qualitative results
- quantitative results





- Mathematics
- Creativity
- Conceptual thinking
- Communication skills





Contents

- What is a Mathematical Modeling?
- Aims of Mathematical Modeling
- Mathematical Modeling Cycle



Aims

- Investigate behaviour and relation of elements of problem
- Consider all possibilities, evaluate alternatives, exclude impossibilities
- Verification against measurements; result to be used in other operating regimes
- Optimization
- Facilitate design and proto-typing
- Substantiate decisions



Mathematical Modeling Cycle



2009

niversity of Technology

Mathematical Modeling Cycle: example



- 1. Produce faster
- 2. Use other polymer material (which is cheaper)

Maintain same mat quality





Step 1: Specify the Problem

- What is background of the problem, its history and its causes.
- What do we want to know?
- Why is one interested in solving the problem? What are the limitations of the current practice?
- What is the solution needed for? What is the purpose of solving the problem?
- What are the constraints to solving the problem?
- Who needs a solution?
- What is the impact/benefit of solving the problem?
- What problem is solved if one has found an answer?
- How will the outcome be judged?
- What form does the solution need to have? What do you communicate to the Problem Owner?--
- How would you implement the solution?
- Are there other related problems?
- What are the sources of facts and data, and are they reliable?





Step 1: Specify the Problem: example

- Rotating drum is also oscillating
- Quality can be characterized by
 - filament diameter in mat
 - amount of attachment of filaments in mat
 - width of coils on drum
- Cheaper polymer material has larger viscosity
- Data of polymer material are available:
 - measurements of shear viscosity and mass density: not accurate
- Data of diameter measured along filament are available
- Form of solution: trends of end-diameter
 - in terms of process/material parameter,
 - based on computer simulation program



Step 2: Create a mental image

- What are the operative processes at work?
 - What needs to be determined for solving the problem?
 - What are the main features, which ones are relevant and which ones are not?
 - What is the relation between the main features?
 - Which features do change?
 - What is controllable in the problem?
 - What are the conditions?
 - What are the relevant timescales and dimensions of the problem?
 - What kind of material is considered, and what is characteristic of that material?

Simplification



Assumptions





Step 2: Create a mental image

Assumptions

made in real world

- whether or not to include certain features, and why
- about the relationships between features,
- about their relative effects.

In collaboration with Problem Owner

• level of detail,

Decisions:



Step 2: Create a mental image: example



die-swell

coiling

- polymer is molten, cools down
- begin velocity and diameter at spinneret known
- die-swell, just below spinneret hole
- filament diameter in mat = diameter @ position of coiling
- low velocities: falling under gravity
- thin filament

Assumptions:

- at coiling position: no influence of surface
- neglect temperature effects
- resistance against stretching

Step 3: Formulate Mathematical Model

Translate relationships of metaphor

into

mathematical terms

Mathematical Model:

- Input and Output
- Constants
- State variables
- Independent variables
- Domain

chnische Universitei

Boundary / initial / constraint conditions



September

2009

PAGE 25

Step 3: Formulate Mathematical Model: example



Balance of momentum:

Mass balance:

Material behaviour:

State variables: V, D

Boundary conditions:

 $z = 0, \quad z = H:$

Input parameters:





Step 4: Solve Mathematical Model



- Analytically
- Numerically

make equations dimensionless

such that computations with order-1 numbers



Step 4: Solve Mathematical Model: example

Boundary value problem; numerically, dimensionless



Step 5: Interprete Solution



Retraction of conceptual leap from mathematical world to real-world problem





Step 5: Interprete Solution: example



 $D_{\text{end}} = D_{\text{end}} (\Phi, \rho, \eta, H, D_0)$



Step 6: Compare with Reality



- Validation of model
- Extraction of model parameters
- Extension to other operating regimes

Model insufficient for solving problem



Accuracy of measurements



Step 6: Compare with Reality

Extraction of material/process parameters:



Step 7: Use Model to Explain, Predict, Decide, Desig



- Determine:
 - typical behaviour
 - critical parameters
 - trends
 - dependency on control parameters





Step 7: Use Model to Explain, Predict, Decide, Desig



Recommendations

For an end-diameter of 0.4 mm:

- Increasing the mass flux to 10 gr/min, a falling height is needed of H = 95 cm
- For a polymer with η = 800 Pa s, the mass flux must be limited to 5 gr/min, if H must be smaller than 100 cm



Summary

Mathematical Modeling

- driven by the problem from the <u>real</u> world;
- also includes the <u>interpretation</u> of the solution

Finding an appropriate model is an art:

Mathematical Modeling:

- -conceptual thinking
- -appropriate simplifications

-close collaboration between Problem Owner and Mathematician.





Literature

- Saaty TL and Alexander JM, Thinking with Models, Pergamon, 1981
- Berry JS, Burghes DN, Huntley ID, James DJG Moscardini AO (Eds.), Teaching and Applying Mathematical Modelling, Wiley, 1984
- Houston SK, Blum W, Huntley I, Neill NT (Eds.), *Teaching and Learning Mathematical Modelling*, Albion, 1997



For your modeling project :

- **1.** Why is a mathematical model needed?
- 2. Work out Step 1 of the Mathematical Modeling Cycle: "Specify the Problem"

Hand in with: A.C.T. Aarts (<u>a.c.t.aarts@tue.nl</u>),

Ultimately: Friday 22 October 2010

