Combination of Optimisation Methods and Material Flow Analysis for the Improvement of Operational Material Use (KOMSA)

The concept and its implementation

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Agenda

• Background: Research project KOMSA – ideas and goals
• An example: The Two-Crude-Oil-Refinery
• Terminology: the standard optimisation model of OR
• Formulation by means of Material Flow Networks
• The framework of the KOMSA optimisation tool
• Solution with the prototype of our software tool
• Conclusions and Outlook

What is KOMSA about?

Material Flow Analysis

• analysis of material flow systems
• assessment of (real) material flows
• improvement analysis

⇒ synthesis: material flow based optimisation

Operations Research

• mathematical = parametric representation of (virtual) system designs/ operation modes
• algorithms to find best feasible solution

KOMSA (1) – Research Questions

• Objectives fit, methods either?
• How to map material flow based optimisation problems with material flow networks (MFN)?
  – advantages? drawbacks?
  – application fields?
• How to optimise an existing MFN?
  Is that always possible?
• Which type of optimisation problem (OP) results?
• What are appropriate algorithms to solve them?
KOMSA (2) – Software Development

- enhance existing material flow modelling software Umberto® → module for algorithmic optimisation
  - formulation of material flow based OP: optimisation cockpit
  - implementation of appropriate algorithms
  - link to existing optimisation packages
- conserve experimental modelling approach of Umberto
  - flexibility in process specification
- user-friendly model formulation
  - adaptation of material flow network concept

KOMSA (3) – Application

- industrial partners: increase resource efficiency
  - Ciba speciality chemicals, Lampertheim
  - Hanomag Hardening Center, Hannover
- develop exemplary cases for optimisation module
  - test software
  - guidelines for future users
- description of potential application fields

What next...

- a small example for a material flow based OP
- framework of the KOMSA tool
- how to solve the material flow based OP using the tool
- some ideas on using material flow networks to formulate OPs

An example: the “Two crude oil” refinery

- fictitious refinery in Hamburg
- processes two different crude oils
  - from Venezuela 3000t/d
  - and from Saudi-Arabia 3000t/d

- and produces:
  - Gasoline
  - Jet fuel
  - Lubricants
The company’s objectives

- **meet demand (constraints)**
  
<table>
<thead>
<tr>
<th></th>
<th>Lower limit [t/d]</th>
<th>Actual output [t/d]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Gasoline</td>
<td>2.000</td>
<td>2.100</td>
</tr>
<tr>
<td>Jet fuel</td>
<td>1.500</td>
<td>1.800</td>
</tr>
<tr>
<td>Lubricants</td>
<td>500</td>
<td>1.500</td>
</tr>
</tbody>
</table>

- **minimise costs (objective)**
  
<table>
<thead>
<tr>
<th></th>
<th>Saudi</th>
<th>Venezuela</th>
</tr>
</thead>
<tbody>
<tr>
<td>Price [€/t]</td>
<td>19.25</td>
<td>14</td>
</tr>
<tr>
<td>Transport [€/t*1000km]</td>
<td>0.1</td>
<td>0.1</td>
</tr>
<tr>
<td>Distance [km]</td>
<td>7.500</td>
<td>10.000</td>
</tr>
</tbody>
</table>

How to influence the company’s costs?

- **two crudes**
  - different prices and transport distances
  - differ in chemical composition ⇒ product mix
- **respective quantities of the crudes ⇒ decision variable**

Standard Model of Operations Research

- **objective function**
- 2 decision variables
- (algebraic) constraints
  - inequalities
  - (equations)

```
min \sum_{i} c_i x_i + 15 x_1
s.t. \ 0.3x_1 + 0.4x_2 \geq 2.0
\ 0.4x_1 + 0.2x_2 \leq 1.2
\ 0.2x_1 + 0.3x_2 \geq 0.5
\ x_1 \leq 9
\ x_2 \geq 0
\ x_1, x_2 \geq 0
```

- no start value (actual state of the system) necessary
- decision variables ⇒ degrees of freedom ⇒ ranges!
- constraints ⇒ “interaction”

Two-Crude-Oil as Material Flow Network

- Model variables \( \bar{x} = (j, \tilde{p}, \tilde{x}) \)
  - 6 material flows
  - 0 parameters and stocks
- Causality
  - topology of network
  - transition specifications
- Objective
  - cost accounting

- maps actual state
- model variables ⇒ (calculated) values!
- constraints?
**Different Modelling Paradigms**

- \( \bar{x} = (\bar{j}, \bar{p}, \bar{x}) \) = vector with all model variables
- usually, e.g. LCA: given the functional we obtain a unique \( \bar{x} = \bar{x}(j_0) \)
- **Optimisation**: independent components of \( \bar{x} \) span solution space, search for optimal \( \bar{x}^* \)

⇒ include degrees of freedom (choices) in the model!

**Matching of Concepts**

- Material Flow Model
  - Processes
  - Material flow network
  - Valuation system & Cost accounting
  - Indicators
- **Optimisation**
  - Decision variables \( \bar{x} = (\bar{j}, \bar{p}, \bar{x}) \)
  - Constraints
  - Objective

**The Role of Transitions**

- 6 model variables, 6 decision variables?
- transition specification: equations reduce degrees of freedom!

⇒ Transitions are effectively constraints

**System Enlargement: Include Transport**

- include transport
- add many model variables (~20 material flows, 2 trans.-parameters)
- but: adds no degrees of freedom!

⇒ because: network structure adds constraints!
**Places as Constraints... some Examples**

- \( j_1 = j_2 \) connection 1 DoF
- \( x_{j_1} = j_1 + j_2 \) store 3 DoF
- \( j_1 = j_1 + j_2 \) bifurcation 2 DoF
- \( x_{j_1} = j_1 + j_2 \) merging 2 DoF

**Include Cost-Information**

\( \Rightarrow \) cost accounting: existing feature of Umberto®

**Include additional Constraints**

\( \Rightarrow \) adding constraints: not yet part of Umberto®

**Framework of the KOMSA tool**

- optimisation algorithms
  - Nelder-Mead/Complex
  - Genetic
  - Particle Swarm
- and packages
- complete definition of the OP (objective, constraints,...)
- choose algorithms, set parameters,...
- controls optimisation procedure
**Generation of Objective Function**

- Type of objective
- Automatic generation

**Selection of Decision Variables**

- Selection and explicit constraints
- Logical constraints on several decision variables

**Algorithm and Constraints**

- Check of termination algorithm
- Constraints on dependent decision variables

**Results**

- Values of decision variables
- Objective function
Plot of the results...

Different possible Representations

- Degree of freedom within process
- Degree of freedom within network

Conclusions

- Material flow models (Umberto)
  - are “natural” starting point for parameter optimisation
  - useful for structuring decision problems concerning material flow systems (strong causality, material flows)
  - Efficiency and effectiveness of algorithms ⇔ ease of model formulation
- Simulation-based optimisation approach operational as prototype

Outlook

- Further experiences → test cases!
- Algorithms: Interface to Matlab Optimisation Toolbox
- Role of transitions and places
  - substitutional inputs
  - flexible combined production
  - bifurcations
  - deduce: modelling principles for material flow based OIPs.
Thank you!