Modelling for Process and Control Design

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Outline

• Motivation
  • Multipurpose Modelling, e.g. Integration of Process & Control Synthesis Exemplified through defining the Control Problem

• Modelling Paradigm for Process & Control Synthesis
  – Didactic Example (from food technology)
  – Workflow for Qualitative Process & Control Synthesis

• Application example on defining the Control Problem
  – Single cell Protein production in U-loop fermentor

• Other Application Examples of Modelling Paradigm
  – Alarm Design (Us et al. (2008))
  – HAZOP assistant (Rossing et al. (2008))

• Conclusions and Research challenges
Process design involves stages such as
1. conceptual process synthesis based upon requirement specifications
2. conceptual design
3. detailed design etc.

To integrate control design into these stages as early as possible involves dealing with control design already from the requirements level.

Thus there is a need to be able to handle integration of process synthesis and control synthesis while developing the process functionality to satisfy the process requirements.

Since conceptual process design is qualitative. Then Integration of Process and Control design may be viewed from a qualitative viewpoint before handling the quantitative aspects.
Levels of abstraction

Representing System Requirements: Objective heteraki

Representing System Knowledge:
• Selection of a proper level of abstraction plays an important role in model building:
  – Spatial structure (the anatomy), many levels of detail possible
  – Behaviour (dynamics), several levels of temporal resolution possible
• Alternatively, levels can be distinguished according to the functional organisation of a system
Modelling Paradigm

• To combine the process requirements to the functional behaviour points to a need for a suitable modelling paradigm!
• With such a modelling paradigm suitable workflows can be formulated!
• How is that accomplished?
  – What is there and what needs to be developed!

  – What else can such a modelling paradigm contribute to CAPE?
Functional modelling

Why the system is there

What the system does

How the system does it

This type of system analysis is means-end analysis or functional modelling which enables causal reasoning. It is based upon theory of actions!

Lind (1994)
Elementary action types

The elementary action types (Von Wright, 1963)

– an attractive basis for the definition of concepts for modelling action functions, e.g. control!
– in direct correspondence to the types of action functions used in control engineering

<table>
<thead>
<tr>
<th>Elementary action</th>
<th>Control action</th>
</tr>
</thead>
<tbody>
<tr>
<td>Produce</td>
<td>Steer</td>
</tr>
<tr>
<td>Maintain</td>
<td>Regulate</td>
</tr>
<tr>
<td>Destroy</td>
<td>Trip</td>
</tr>
<tr>
<td>Suppress</td>
<td>Interlock</td>
</tr>
</tbody>
</table>
Defining the Control Problem

- State the goal(-s), i.e. the functionality for process/plant
- Determine the degrees of freedom (DOF) available in the plant
  - DOF for goal achievement, i.e. actuator variables
  - DOF as disturbances or unassigned
- DOF used for goal achievement become the actuator variables and defines the operating window for the process/plant
- Desirable measurements are pinpointed by considering information provided concerning goal achievement
- Couplings between measurements and actuators is designed, e.g. though inventory control
U-Loop Fermentor

Gas

Recirculated liquid

Suspended gas

Gas Mineral Solution

Harvest

Centrifuge

UF

Steam

Drying

BioProtein

Condensate to boiler
Methylococcus capsulatus

Methane → [Cell Image] → Bioprotein
Oxygen → [Cell Image] → Bioprotein
Ammonia → [Cell Image] → Bioprotein
Minerals → [Cell Image] → Bioprotein
U-Loop representation
Desired Functionality

• Control goal: To achieve high productivity of biomass with high protein content

• This implies that the bioreactor should produce biomass without too high a biomass concentration which would limit oxygen transfer
Degree of Freedom Analysis

<table>
<thead>
<tr>
<th>Equation</th>
<th>No.</th>
</tr>
</thead>
<tbody>
<tr>
<td>PFR equations</td>
<td>$14 \cdot N_d$</td>
</tr>
<tr>
<td>CSTR equations</td>
<td>7</td>
</tr>
<tr>
<td>Mixer equations</td>
<td>5</td>
</tr>
<tr>
<td>Sum</td>
<td>$14 \cdot N_d + 12$</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Variable</th>
<th>No.</th>
</tr>
</thead>
<tbody>
<tr>
<td>PFR variables</td>
<td>$14 \cdot N_d$</td>
</tr>
<tr>
<td>CSTR variables</td>
<td>7</td>
</tr>
<tr>
<td>Mixer variables</td>
<td>5</td>
</tr>
<tr>
<td>Operation variables</td>
<td>$F_{f,l}$, $F_{f,g}$, $F_{res}$, $c_{f,O_2}$, $c_{f,CH_3OH}$</td>
</tr>
<tr>
<td>Sum</td>
<td>$14 \cdot N_d + 17$</td>
</tr>
</tbody>
</table>

- Thus five degrees of Freedom
DOF Analysis

- $F_{f,l} \ c_{f,CH3OH}$ Substrate feed rate and Concentration
- $F_{f,g} \ c_{O2}$ Gas feed rate and concentration
- $F_{res}$ Recirculation rate

$c_{O2}$ constant nearly pure Oxygen
$F_{res}$ is nearly constant to maintain the effect of the static mixers
Thus three degrees of freedom $F_{f,l} \ c_{f,CH3OH}, \ F_{f,g}$ define the operating window

Note the above analysis is based upon qualitative model information. Now let us use a quantitative model to understand the process behaviour.
Stoichiometry

\[ \text{CH}_3\text{OH} + Y_{SN} \ \text{HNO}_3 + Y_{SO} \ \text{O}_2 \rightarrow Y_{SX} \ \text{X} + Y_{SC} \ \text{CO}_2 + Y_{SW} \ \text{H}_2\text{O} \]

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>( Y_{SC} )</td>
<td>0.268</td>
</tr>
<tr>
<td>( Y_{SN} )</td>
<td>0.146</td>
</tr>
<tr>
<td>( Y_{SO} )</td>
<td>0.439</td>
</tr>
<tr>
<td>( Y_{SW} )</td>
<td>1.415</td>
</tr>
<tr>
<td>( Y_{SX} )</td>
<td>0.732</td>
</tr>
</tbody>
</table>

Table: Yield coefficients
U-Loop representation
Kinetics

\[ \mu = \frac{\mu_{\text{max}} c_{\text{CH}_3\text{OH}}}{K_S + c_{\text{CH}_3\text{OH}} + \left(\frac{c_{\text{CH}_3\text{OH}}}{K_l}\right)^2} \cdot \frac{c_{\text{O}_2}}{K_O + c_{\text{O}_2}} \]
Operating Window

\[ c_{gO} \text{ [kg/m}^3\text{]} \]

\[ c_S \text{ [kg/m}^3\text{]} \]

\[ D_{U-Loop} \text{ [1/h]} \]

\[ \text{Productivity [kg/(m}^3\text{ h)}] \]
Biomass range

- Design for optimal biomass concentration
Redefine feed variables

\[ m_{f,S} \in [1.8000; 4.6033] \frac{kg}{h} \]
\[ D_{ULoop} \in [0.0697; 0.2231] \frac{1}{h} \]
\[ F_{f,l} \in [0.0360; 0.1152] \frac{m^3}{h} \]
\[ m_i = c_i \cdot F \]
Design for optimal Biomass Concentration

- Biomass concentration around 20 kg/m$^3$
Control Problem

- Control around a total substrate feed flow rate of 4 kg/h
- Ratio gas addition rate to total substrate feed rate

In addition

- Investigate dynamic interactions and decide on control design paradigm
- Consider control or constraining other nutrient addition rates: Nitric acid and phosphate
Conclusions I

- The control definition procedure relies mainly on qualitative knowledge.
- It is based upon the intended functionality of the process/plant.
- A strong coupling is apparent between process design and control design.
Conclusions II

Functional Modelling provides a unified framework for qualitatively combining:
   Many levels of abstraction, incl. a multilayered granularity
Thus providing potential for Integration of Multiple tasks, incl.:
   Control Problem Definition
   Process & Control Synthesis
   Process & product design incl. Process integration
   Risk management (HAZOP-Assistant)
   Alarm design
   Operator communication etc.

To harvest these potentials then:
Research in functional modelling within the different engineering knowledge domains is necessary!
References

- Rossing; N; Jensen,N.; Lind, M.; Jorgensen, S.B. (2008): ”A Goal Based Methodology for HAZOP Analysis” Accepted for presentation at CSPEC08, Harbin, China.