Modelling, synthesis and analysis of biorefinery networks

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KT Consortium Annual Meeting, Helsingør, June 7, 2017
At a glance

- Motivation & objective
- A 3-stage approach to sustainable process design
- Overview of the framework for biorefinery synthesis
  - Generic superstructure representation & model
  - Flexible model formulations
  - Ontology-based data management
  - Fast execution through a user interface
- Application examples
- Overview of problems & applications
- Conclusion
Current situation

World population growth, 1750-2100

Current situation

6-7 x  
Global GDP growth over next ~50 years  
(in constant dollars)

5-6 x  
Production capacity for most commodities  
(steel, chemicals, lumber, etc.)

3.5 x  
Energy demand  
7 x  
Electricity demand

Increase  
Water demand

Increase  
GHG emissions

Source: Sirola, 2012
We need methods to design more sustainable processes

New synthesis-design problems arise from:  
(i) Switch to renewable raw materials (biomass, CO2); 
(ii) Discovery of new technologies (catalysts, solvents, etc.); 
(iii) New design objectives and constraints (sustainability)
Overall sustainable design problem formulation

The decision-making nature of the process design problem makes it an optimization problem

\[ \min_{w, y} \quad C = c^T y + p(w) \]

s.t. \[ r(w) = 0 \]
\[ s(w) + By \leq 0 \]
\[ w \in \mathbb{R}^n, \quad y \in \{0,1\}^l \]

Problems: LP, NLP, MILP, MINLP, Simulation…

Solution strategies: simultaneous, decomposition-based
A 3-Stage approach to sustainable process design

Decomposing the design problem into stages allows to manage the complexity

**Given:** set of feedstock & products

**Find:** processing route

- Define problem
- Generate superstructure
- Mathematical formulation
- Solve optimization problem

Quaglia et al. (2012)

**Stage 1**
Synthesis

**Stage 2**
Design

**Stage 3**
Innovation

**Given:** feasible design (base case)

**Find:** alternative more sustainable design

- Generate sustainable intensified alternatives

Babi et al. (2015)

- Detailed analyses to identify process bottlenecks

Carvalho et al. (2013)

**Given:** processing route

**Find:** feasible design
A 3-Stage approach to sustainable process design

Decomposing the design problem into stages allows to manage the complexity

<table>
<thead>
<tr>
<th>CHARACTERISTIC</th>
<th>Stage 1: Synthesis</th>
<th>Stage 2: Design</th>
<th>Stage 3: Innovation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Number of alternatives</td>
<td>Large</td>
<td>Medium</td>
<td>Small</td>
</tr>
<tr>
<td>Model complexity</td>
<td>Low</td>
<td>High</td>
<td>High</td>
</tr>
<tr>
<td>Data accuracy</td>
<td>Lower</td>
<td>High</td>
<td>High</td>
</tr>
<tr>
<td>Smallest scale</td>
<td>Interval</td>
<td>Unit operation</td>
<td>Phenomena</td>
</tr>
</tbody>
</table>

**Diagram:**
- **Pretreatment**
  - Cassava rhizome
  - HP steam
  - R1: Pretreatment reactor
  - T1: Blowdown tank
  - C1: Centrifuge
  - Off-gas

- **Saccharification**
  - R4: Saccharification reactor

**Phenomena**
- Phase contact
- Reaction
- 2 Phase mixing
- Cooling
A 3-Stage approach to sustainable process design

Decomposing the design problem into stages allows to manage the complexity
A 3-Stage approach to sustainable process design

Focus on Stage 1

Given: set of feedstock & products

Find: processing route

Given: feasible design (base case)

Find: alternative more sustainable design

Currently there is no commercial tool available for process synthesis
Synthesis (stage 1) framework

The objective of stage 1 is to obtain the processing route (including feedstock and products)

1. **Step 1.1: Problem definition**
   - Define **objective**, raw material(s), product(s), location(s)

2. **Step 1.2: Superstructure generation and data collection**
   - Generate **superstructure** (raw materials, products, routes, technologies)
   - Collect **data** (mass & energy balance data, location-dependent data)
   - Check data **consistency**
   - Modify generic **model** (if necessary)

3. **Step 1.3: Solution of the optimization problem**
   - Generate **input** file, solve **optimization** problem in GAMS, generate **output** file
   - Perform post-optimality calculations and interpret **results**

   **Decision**
   - Synthesis objectives met?
   - Yes: Define new scenarios?
   - No: To DESIGN

Synthesis (stage 1) framework

The developed framework is **generic, flexible, ontology-based** and **fast**
**Generic superstructure representation & model**

The Processing Step-Interval Network representation is suitable for a wide range of problems.

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Flexible model formulations

The location-dependent model allows the formulation of various relevant scenarios
Flexible model formulations

A subset of top-ranked solutions can be used to find the most suitable for a given case.
Ontology-based data management through databases

Specific databases are built on a common data structure that fits the problem requirements

<table>
<thead>
<tr>
<th>Basic</th>
<th>Material</th>
<th>Process</th>
</tr>
</thead>
<tbody>
<tr>
<td>Component</td>
<td>Feedstock</td>
<td>Step</td>
</tr>
<tr>
<td>Reaction</td>
<td>Product</td>
<td>Location</td>
</tr>
<tr>
<td>Location</td>
<td>Utility</td>
<td>Connection</td>
</tr>
</tbody>
</table>

Data Biorefinery Database

- Components: 71
- Utilities: 4
- Processing steps: 21
- Processing intervals: 102
- Feedstocks: 11
- Products: 9
- Reactions: 63
- Locations: 10

Fast execution through a user interface

Super-O: An interface for formulating and solving synthesis problems using superstructure optimization

Fast execution through a user interface

Super-O: An interface for formulating and solving synthesis problems using superstructure optimization

Synthesis (stage 1) framework

The developed framework is **generic, flexible, ontology-based** and **fast**

- **Model**
  - Superstructure of alternatives
  - Easy to adapt to different applications
  - Library of models and functions
  - Templates for data collection
  - Databases
  - Data structure

- **Interface**
  - User interface
  - Systematic methods & tools
  - Enables data reuse from previously-solved problems

- **Task-based** process model
- **Formulation** that fits various problem types
- **Unique** representation

- **What to produce?**
  - Strategic
  - Fast
  - Generic

- **How to produce it?**
  - Tactical
  - Flexible
  - Ontology-based
What are the possible *problems* and *application areas* for which the synthesis framework can be used?
Application example
Ethanol from biomass

- Which biomass-derived feedstocks can be used?
- Where are they available?
- What are the different routes to convert the feedstocks to the product?
- What are the processing technologies available?
- Is the solution location-dependent?
- Which set of feedstock-topology-location is optimal?
Application examples
Superstructure of alternatives for the biomass-to-ethanol example

## Application examples

Ethanol from biomass: Fixed location vs location-based (constrained to a single location)

<table>
<thead>
<tr>
<th>Location</th>
<th>RM</th>
<th>WADD</th>
<th>PRE</th>
<th>HYD</th>
<th>FERM</th>
<th>BIOR</th>
<th>SEP1</th>
<th>SEP2</th>
<th>PROD</th>
<th>Profit</th>
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</thead>
<tbody>
<tr>
<td>BR</td>
<td>SCB</td>
<td>WADD-ARP</td>
<td>ARP</td>
<td>NREL</td>
<td>FERM</td>
<td>CENTR</td>
<td>BEER</td>
<td>BMIM</td>
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<tr>
<td>CA</td>
<td>WS</td>
<td>-</td>
<td>STEX</td>
<td>NREL</td>
<td>FERM</td>
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<td>CN</td>
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<td>TH</td>
<td>CR</td>
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<td>DA</td>
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<td>CENTR</td>
<td>BEER</td>
<td>BMIM</td>
<td>ETOH</td>
<td>116.03</td>
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<tr>
<td>US</td>
<td>HWC</td>
<td>-</td>
<td>STEX</td>
<td>CONCA</td>
<td>FERM</td>
<td>CENTR</td>
<td>BEER</td>
<td>BMIM</td>
<td>ETOH</td>
<td>47.63</td>
</tr>
</tbody>
</table>

Given

Lowest profit 0 Highest profit

<table>
<thead>
<tr>
<th>RM</th>
<th>WADD</th>
<th>PRE</th>
<th>HYD</th>
<th>FERM</th>
<th>BIOR</th>
<th>SEP1</th>
<th>SEP2</th>
<th>PROD</th>
<th>Profit</th>
<th>Location</th>
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<tbody>
<tr>
<td>CR</td>
<td>-</td>
<td>STEX</td>
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<td>BMIM</td>
<td>ETOH</td>
<td>116.03</td>
<td>TH</td>
</tr>
</tbody>
</table>

Application examples
Ethanol from biomass: The output of stage 1 is the processing route (flowsheet)

Application example
Value-added products from sugarcane molasses

*Molasses are a byproduct of sugar production.*

- Which are the potential products?
- What are the alternatives routes and technologies to produce them from the feedstock?
- Which is the optimal product and process topology for Mexico?
Application example
Value-added products from sugarcane molasses

Product sales
Cost of chemicals and utilities
Feedstock cost

\[
\text{max } Z = \sum_{i,kk} (P3_{i,kk} \cdot F_{i,kk}^{\text{out}}) - \sum_{i,kk} (P2_{kk} \cdot R_{i,kk,ss}) - \sum_{i,kk} (P1_{i,kk} \cdot F_{i,kk}^{\text{out}})
\]

- Product sales: 19 M$/a
- Cost of chemicals and utilities: 30 M$/a
- Feedstock cost: 5 M$/a
- Feedstock cost: 6 M$/a
Overview of problems & applications

Synthesis problems in various fields have been solved using Super-O

<table>
<thead>
<tr>
<th>Case (problem type)</th>
<th>Problem size</th>
<th>Model size</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>Network benchmark problem (d)</td>
<td>2 4 12 5 - 2 1</td>
<td>3,476 3,235 (120)</td>
<td>Quaglia et al. (2012)</td>
</tr>
<tr>
<td>Wastewater network (d)</td>
<td>2 6 24 15 - 37 1</td>
<td>112,147 108,742 (74)</td>
<td>Handani et al. (2014)</td>
</tr>
<tr>
<td>Sugarcane molasses biorefinery (b)</td>
<td>1 3 32 12 - 26 1</td>
<td>76,360 73,141 (52)</td>
<td>Bertran et al. (2015a)</td>
</tr>
<tr>
<td>DMC from CO₂ (a)</td>
<td>1 5 16 11 - 7 1</td>
<td>8,546 7,985 (26)</td>
<td>Frauzem et al. (2015)</td>
</tr>
<tr>
<td>Biodiesel biorefinery (d)</td>
<td>3 6 46 27 - 91 1</td>
<td>1,210,227 1,193,507 (182)</td>
<td>Bertran et al. (2015b)</td>
</tr>
<tr>
<td>MeOH, DME, DMC from CO₂ (b)</td>
<td>1 8 13 16 - 14 1</td>
<td>51,373 49,573 (60)</td>
<td>-</td>
</tr>
<tr>
<td>Bioethanol biorefinery (c)</td>
<td>6 1 35 34 3 47 7</td>
<td>175,383 162,798 (1,330)</td>
<td>Bertran et al. (submitted)</td>
</tr>
</tbody>
</table>

NF: number feedstocks, NP: number products, NI: number intervals, NC: number components, NU: number utilities, NR: number reactions, NL: number locations, NEQ: number equations, NV: number variables, NDV: number discrete variables
Overview of problems & applications

The framework is applicable to a number of problem types across various application areas

<table>
<thead>
<tr>
<th></th>
<th>Process synthesis</th>
<th>Supply chain</th>
<th>Feed/product selection</th>
<th>Plant allocation</th>
<th>Equipment selection</th>
<th>Process retrofit</th>
<th>Blending</th>
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</thead>
<tbody>
<tr>
<td>Chemical processes</td>
<td>✪</td>
<td></td>
<td>✪</td>
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<td>Biorefineries</td>
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<td>✪</td>
<td>✪</td>
<td>✪</td>
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<td>Oil &amp; Gas</td>
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<td>Pharma processes</td>
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<tr>
<td>CO₂ utilization</td>
<td>✪</td>
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</tr>
<tr>
<td>Wastewater management</td>
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</tr>
</tbody>
</table>
An international collaboration network

How to convert biomass feedstock into valuable chemicals, energy and fuels?

ProBioRefine

4th Workshop on ProBioRefine
Mexico, December 14-15 2017

Source: www.probiorefine.com
Conclusions

• A **framework** for biorefinery process synthesis using superstructure optimization has been developed.

• The **framework** is generic, flexible, ontology-based and fast to execute.

• The **associated methods and tools** are: superstructure representation, generic process model, data management system.

• The **generic model** allows different formulations covering a wide range of problems and applications and providing location-dependent solutions.

• **Multiple solutions** can be obtained for a given problem & scenario, ordered by value of the objective function.

• A **software implementation** of the framework is available (Super-O).
Thank you for your attention