MULTI-SCALE UNCERTAINTY ANALYSIS

A tool to systematically consider variability in lignocellulosic bioethanol processes
Bioethanol in a circular economy

Usage of **fossil fuels** steadily increasing

ca. 50% is used for transportation

**Bioethanol** sustainable alternative to fossil fuels
Variability in the bioethanol process

Raw materials

- Location
- Harvest time
- Composition of biomass
- Storage

Measurement and control

- High turbidity
- Local viscosity differences
- Solid compounds in liquid mixture
- Complex chemical reaction system
Effect of variability on process

Integrate variability in process development at different scales!
Multi-scale uncertainty analysis – results & objectives

Process definition + Variability/uncertainty definition → Models at different system scales

Quantify effect on process outcomes:
- process yield
- process time (productivity)
- process synthesis and design
- process economics
- environmental impact

Consequences:
- Improve models (sensitivity analysis)
- Suggest feasible supply chain/process configurations
- Suggest new experimental procedures
System scales in the bioethanol process
The bioprocess

- Fermentation
- Saccharification (enzymatic hydrolysis)

- enzyme
- non-accessible lignocellulose parts
- sugars
- inhibitors
- ethanol
- yeast cells
The bioprocess/ hydrolysis model

- Macro-kinetic model consisting of
  - 8 differential equations
  - 4 explicit algebraic equations

- Numerical solution in MATLAB using ode15s solver for stiff problems

Simulation results for selected state variables for a batch process at demo plant (10m³) scale
System scales in the bioethanol process

<table>
<thead>
<tr>
<th>Macro-molecular scale</th>
<th>Bioprocess scale</th>
<th>Factory scale</th>
<th>Global scale</th>
<th>Global scale</th>
</tr>
</thead>
<tbody>
<tr>
<td>describe enzyme action</td>
<td>describe bioprocess</td>
<td>describe process integration</td>
<td>describe cost and profits</td>
<td>describe environmental impact</td>
</tr>
<tr>
<td>maximize hydrolysis yield</td>
<td>develop bioprocess</td>
<td>develop process synthesis and design</td>
<td>develop supply chain</td>
<td>develop process based on environmental impact</td>
</tr>
<tr>
<td>develop enzyme cocktail</td>
<td>perform optimal experimental designs</td>
<td>perform optimal control</td>
<td>select economically best process alternative(s)</td>
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</table>
Flowsheet model and techno-economic analysis

Bioprocess model

OLE server

VBA

Process yields

SuperPro Designer
Flowsheet model and techno-economic analysis

Bioprocess model

OLE server

Process yields

VBA

Yield definitions, mass balances

Experiments

• Process design
• Reactions
• Scheduling

Analyses

• Utility systems
• Up/downstream units

External sources

SuperPro Designer

Bioreactor chain modelling
Flowsheet model and techno-economic analysis

Bioprocess model

- Process design
- Reactions
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- Utility systems
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Experiments

- Process design
- Reactions
- Scheduling

Analyses

External sources

Pinch analysis
Flowsheet model– the outputs

mass/energy balances to:

- Techno-Economic Estimates
- Supply chain analysis
- Life cycle analysis
System scales in the bioethanol process
Life cycle assessment

- Calculates the potential environmental impact of ethanol production

- Inputs:
  - Database
  - Bioreactor model
  - Flowsheet model

- Software: openLCA
Data flow between scales

- **Excel/VBA**: Data node
- **Superpro Designer**: Process simulation
- **OpenLCA**: Life Cycle Assessment
- **Matlab**: Kinetic modelling
  - Yields
  - Reactions
  - Design parameters
- **Process mass balance**
- **Process energy balance**
- **Techno-economic estimate**
- **Environmental assessment**
Variability in enzymatic activities – a case study

Step 1: Data collection

Step 2: Distribution fit

- Generalized extreme value distribution
Variability in enzymatic activities – a case study

Step 3: Propagation in bioprocess model

Step 4: Techno-economic assessment

Lower heating value [MW]

- Power
- Biogas
- Ethanol

<table>
<thead>
<tr>
<th></th>
<th>Minimum</th>
<th>Maximum</th>
<th>Mean</th>
<th>5% Percentile</th>
<th>95% Percentile</th>
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<tbody>
<tr>
<td>Biogas</td>
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<td>Ethanol</td>
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The multi-scale concept:

- includes variability assessment in early process development

- allows to determine stable process configurations

- allows for multi-objective optimization

- shall allow to determine optimal experimental conditions to perform model validation experiments

- Ongoing: Include life cycle assessment in calculations
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