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

Consequences:
- Improve models (sensitivity analysis)
- Suggest feasible supply chain/process configurations
- Suggest new experimental procedures

Quantify effect on process outcomes:
- Process yield
- Process time (productivity)
- Process synthesis and design
- Process economics
- Environmental impact
System scales in the bioethanol process

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Hydrolysis model | Bioprocess model | Flowsheet model | Techno-economic analysis | Supply chain model | Life cycle assessment
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

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Hydrolysis model
Bioprocess model
Flowsheet model
Techno-economic analysis
Supply chain model
Life cycle assessment
Flowsheet model and techno-economic analysis

Bioprocess model

OLE server

Process yields

VBA

SuperPro Designer
Flowsheet model and techno-economic analysis

SuperPro Designer

Bioprocess model

OLE server

Process yields

Yield definitions, mass balances

Bioreactor chain modelling

Experiments

• Process design
• Reactions
• Scheduling

Analyses

• Utility systems
• Up/downstream units

External sources
Flowsheet model and techno-economic analysis

Bioprocess model

- Process design
- Reactions
- Scheduling
- Utility systems
- Up/downstream units

Experiments

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
  - Process mass balance
  - Process energy balance
  - Techno-economic estimate

- Matlab
  - Kinetic modelling
  - Yields
  - Reactions
  - Design parameters

- Environmental assessment

- OpenLCA
  - Life Cycle 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]
  - Minimum
  - Maximum
  - Mean
  - 5% Percentile
  - 95% Percentile

- Power
- Biogas
- Ethanol
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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