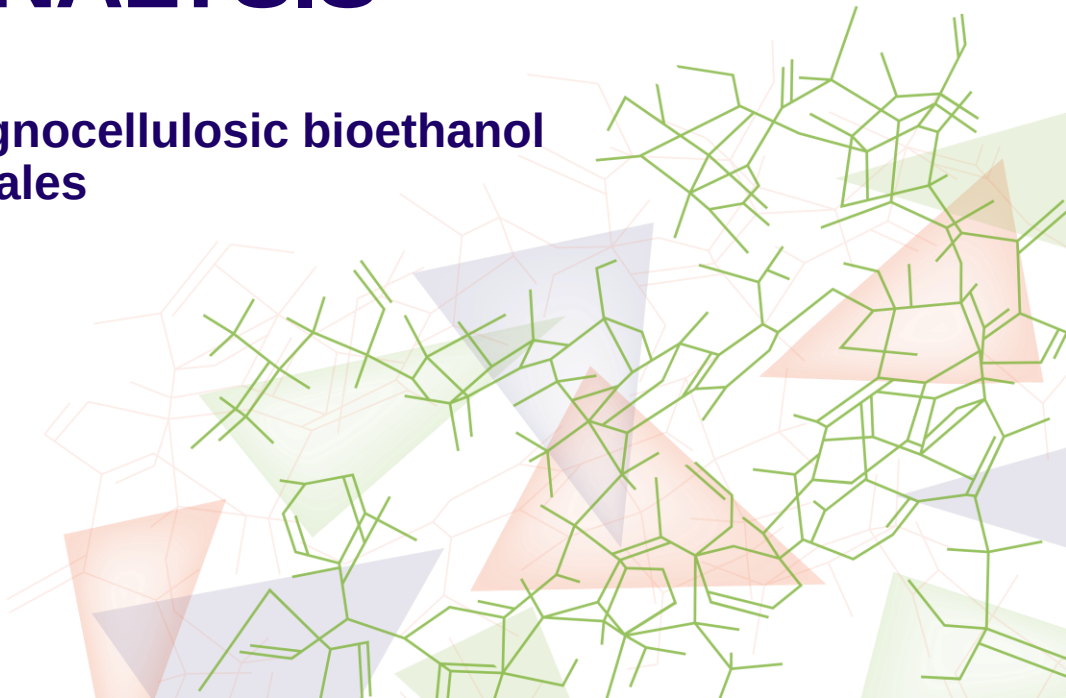
CHALMERS
UNIVERSITY OF TECHNOLOGY

Industrial Biotechnology

# UNCERTAINTY ANALYSIS

## A tool to consistently evaluate lignocellulosic bioethanol processes at different system scales




David Benjamin Nickel

Rickard Fornell

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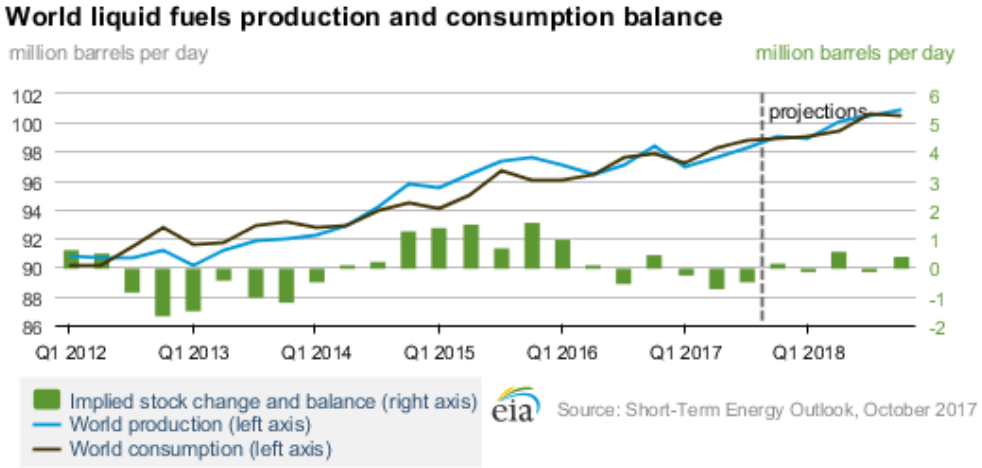
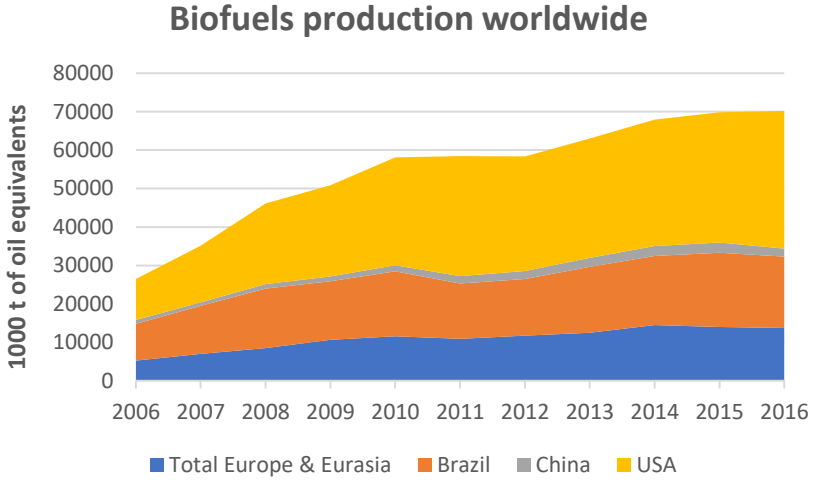
# Bioethanol – The current situation




EIA (2017): Short-Term Energy Outlook, October 2017; https://www.eia.gov/outlooks/steo/pdf/steo_full.pdf, p.13; retrieved: 13.10.2017

BP (2017): BP Statistical Review of World Energy 2017; https://www.bp.com/content/dam/bp/en/corporate/pdf/energy-economics/statistical-review-2017/bp-statistical-review-of-world-energy-2017-full-report.pdf; retrieved: 13.10.2017

# Challenges in lignocellulosic processes

**Measurement challenges**

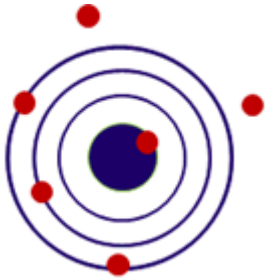
- Turbidity
- Inhomogeneties
- Lack of sensor equipment for online measurements
- Uncertain measurements


**Instable processes**

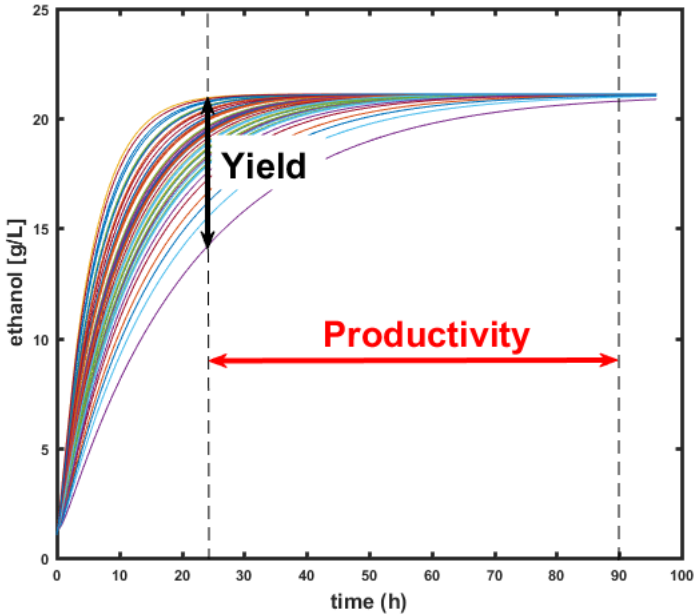
**Lack of mechanistic knowldge**

**Suboptimal process design**

# Challenges in lignocellulosic processes



Variability

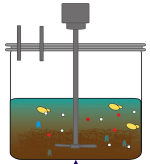


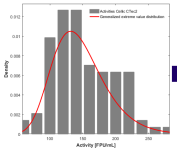

Economics

# Multi-scale uncertainty analysis- Methodology

Process definition

Variability/ uncertainty definition





**Models at different system scales**

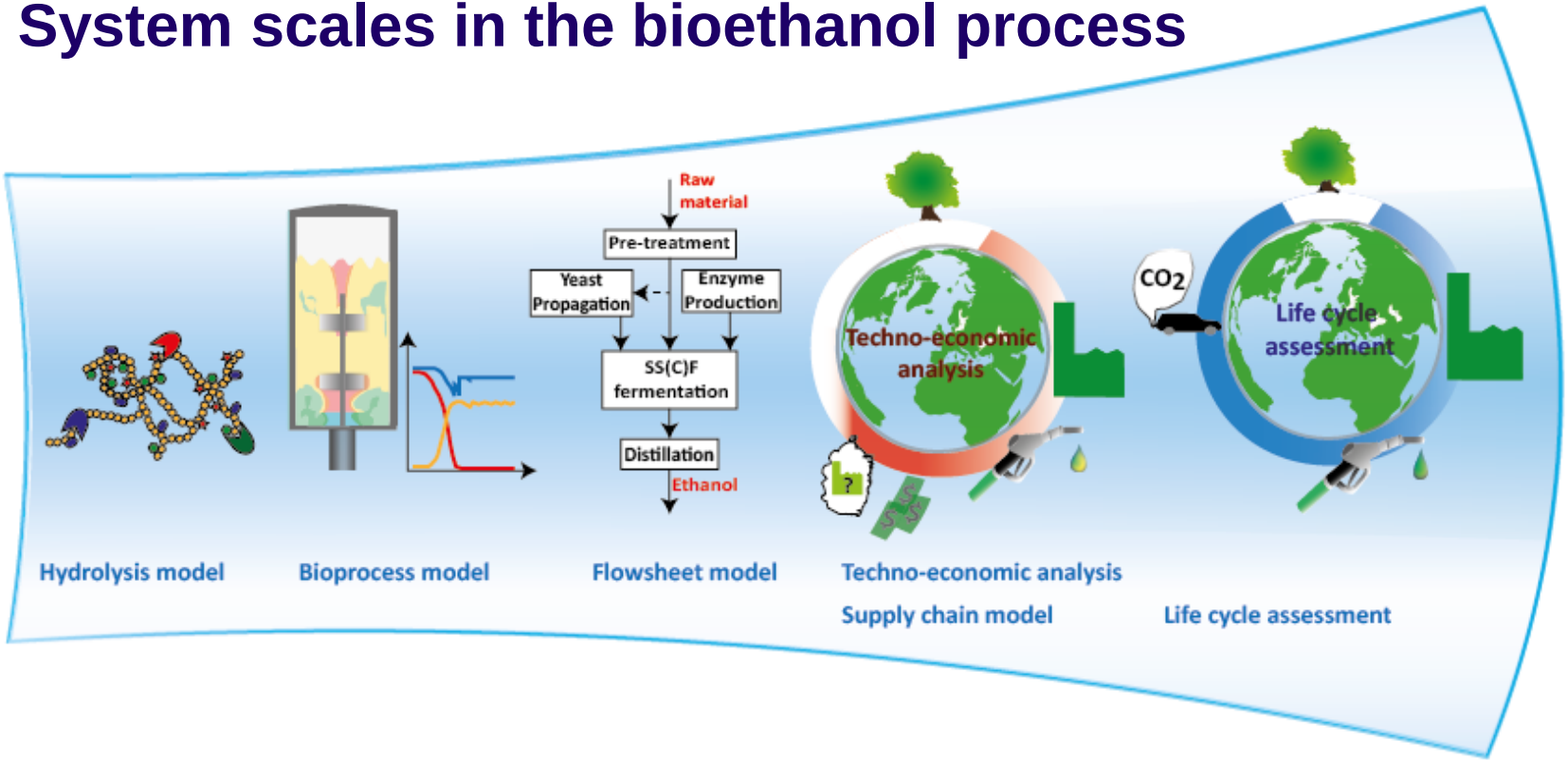
**Quantify effect on process outcomes:**

- process yield
- process time (productivity)
- process synthesis and design
- process economics
- environmental impact

**Consequences:**

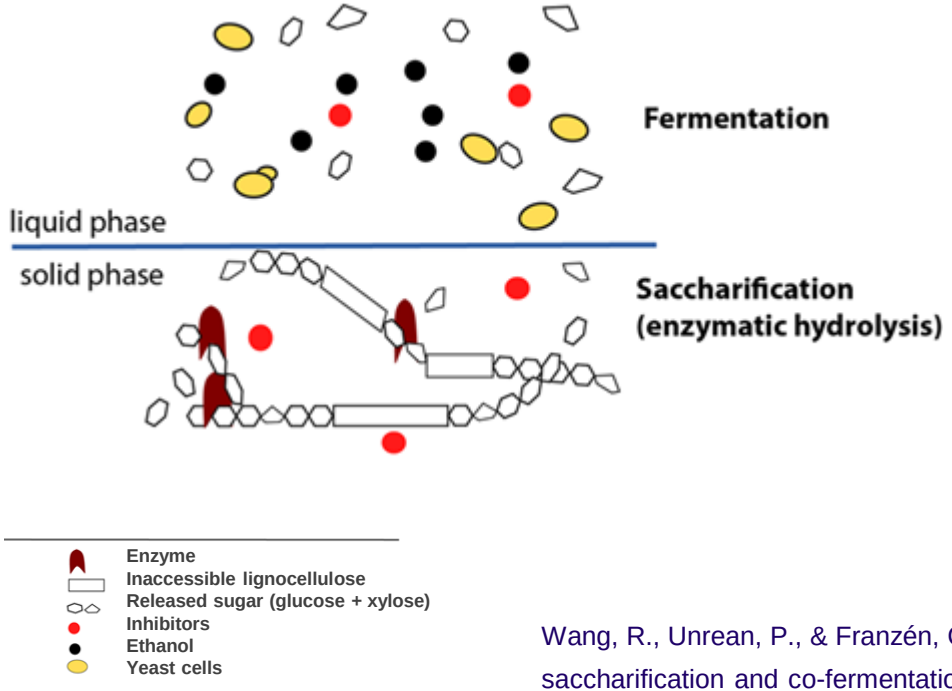
- Improve models (sensitivity analysis)
- Suggest feasible supply chain/ process configurations
- Suggest new experimental procedures

# System scales in the bioethanol process




| Macro-molecular scale | Bioprocess scale | Factory scale | Global scale | Global scale |
|---|---|---|---|---|

# The bioprocess model

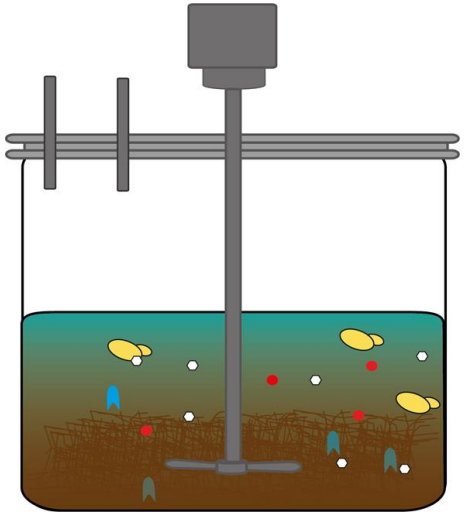



- **Enzyme adsorption:** second order kinetics
- **Hydrolysis inhibited** by glucose and ethanol
- Ethanol dependent **cell death**
- **Ethanol formation** only yield dependent

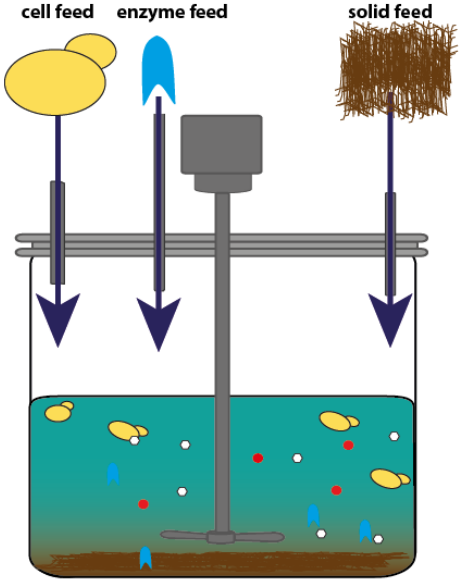
Wang, R., Unrean, P., & Franzén, C. J. (2016). Model-based optimization and scale-up of multi-feed simultaneous saccharification and co-fermentation of steam pre-treated lignocellulose enables high gravity ethanol production. *Biotechnology for biofuels*, *9*(1), 88

# The bioprocess - Process alternatives

## Batch process

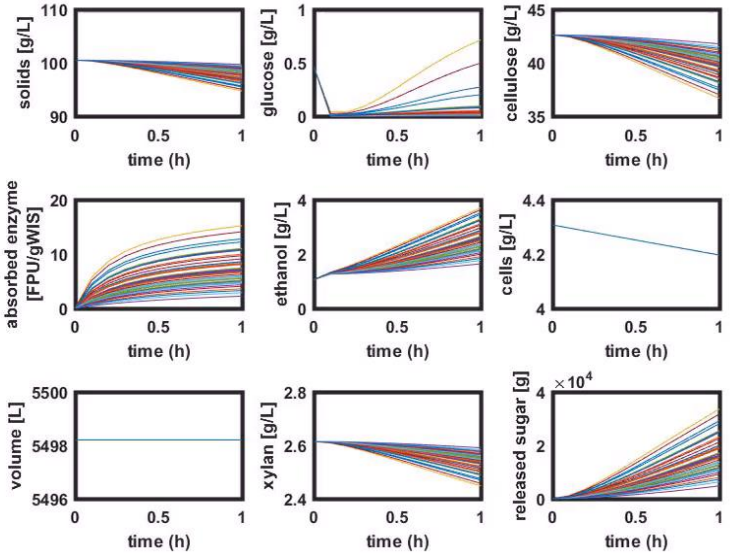


## Multi-feed process

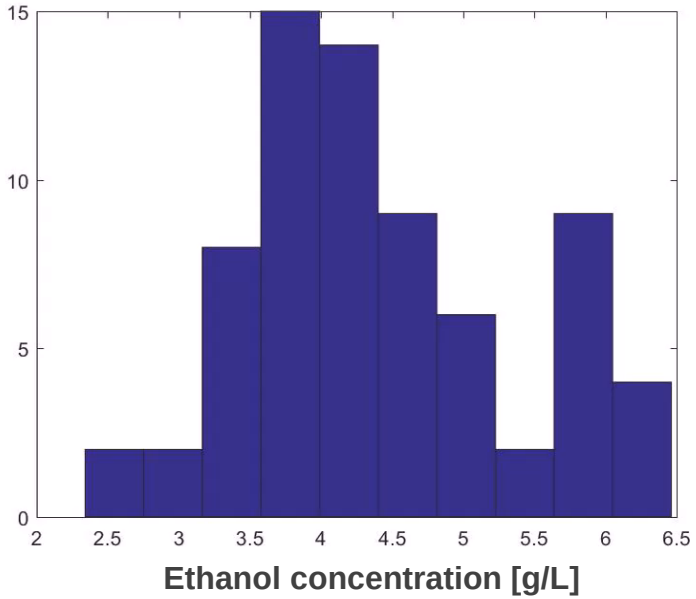


# The batch process – Asymptotic stability

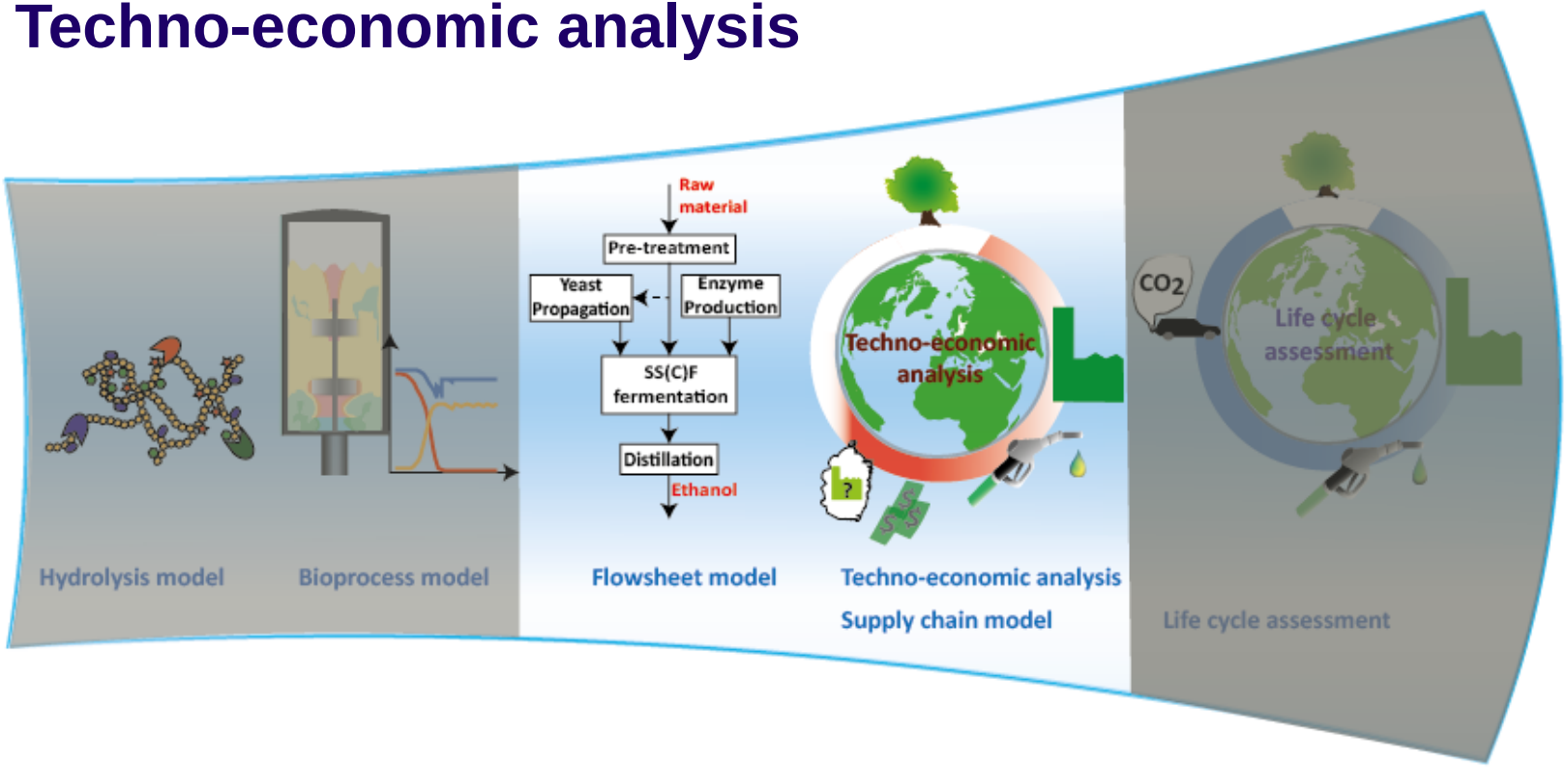
## Simulation of batch process




## Histogram of ethanol conc. at each simulation time



# Techno-economic analysis




| | Factory scale | Global scale | |
|---|---|---|---|

# Flowsheet model and techno-economic analysis

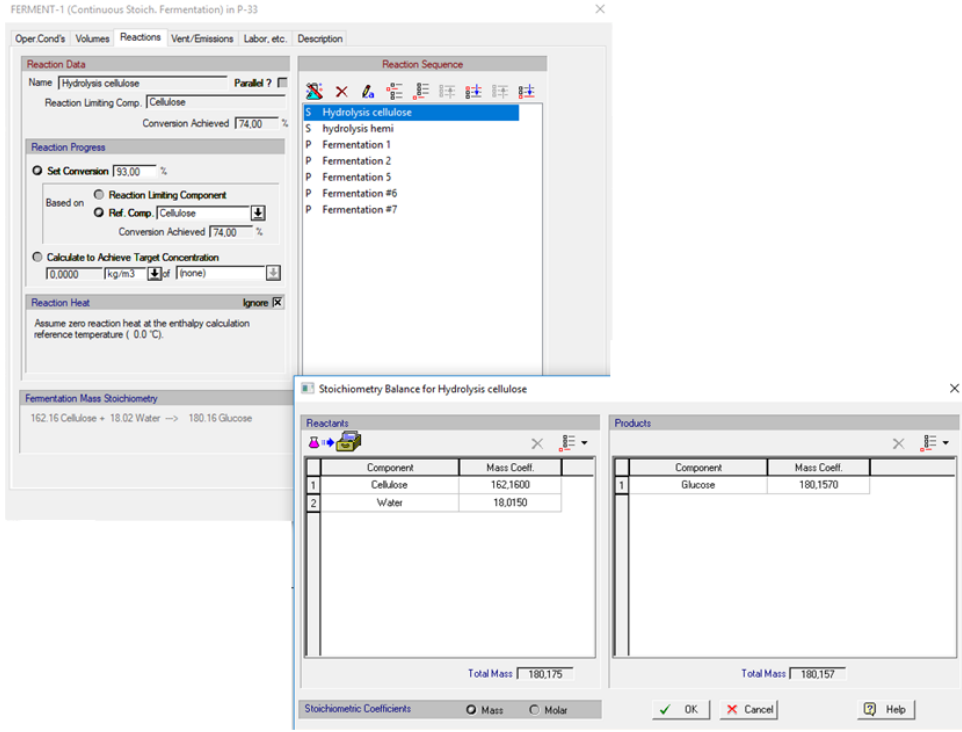
Bioprocess model

OLE server

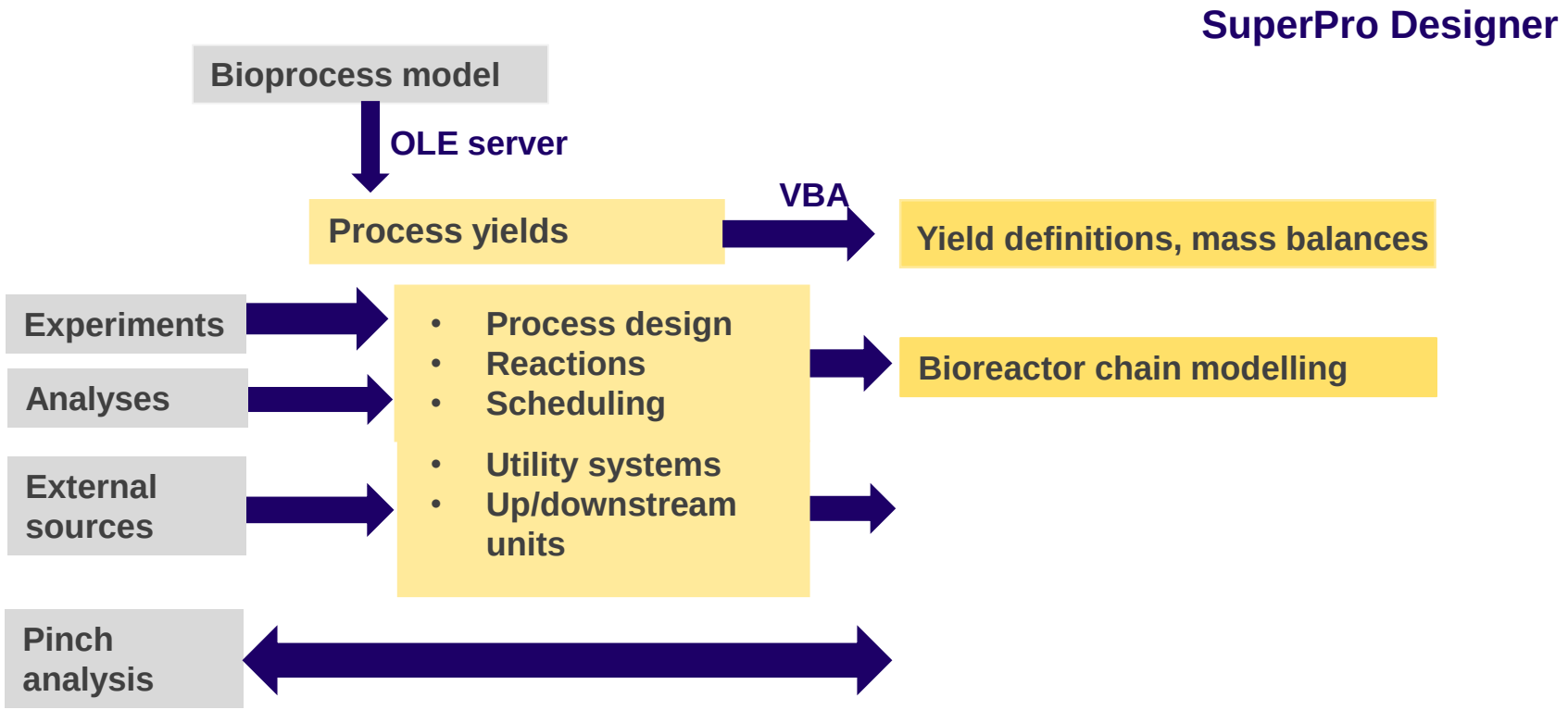
Process yields

VBA

SuperPro Designer



# Flowsheet model and techno-economic analysis



# Flowsheet model and techno-economic analysis

**Bioprocess model**

**OLE server**

**Process yields**

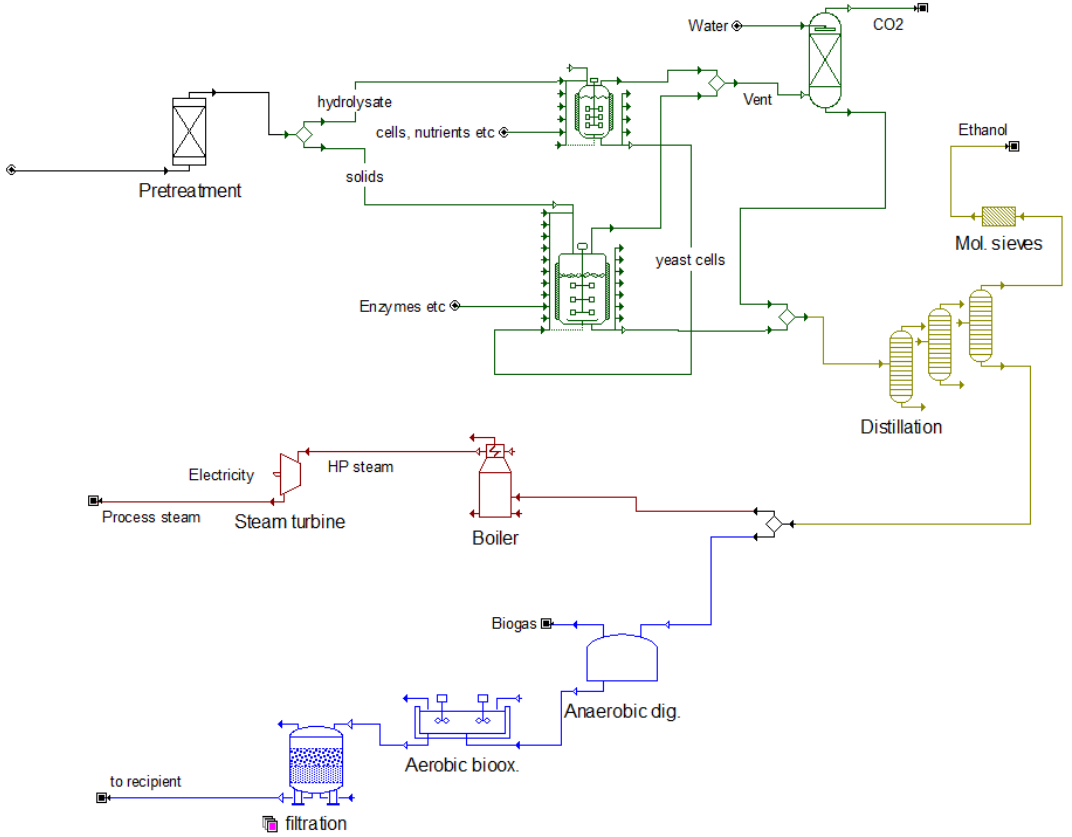
**Experiments**

**Analyses**

**External sources**

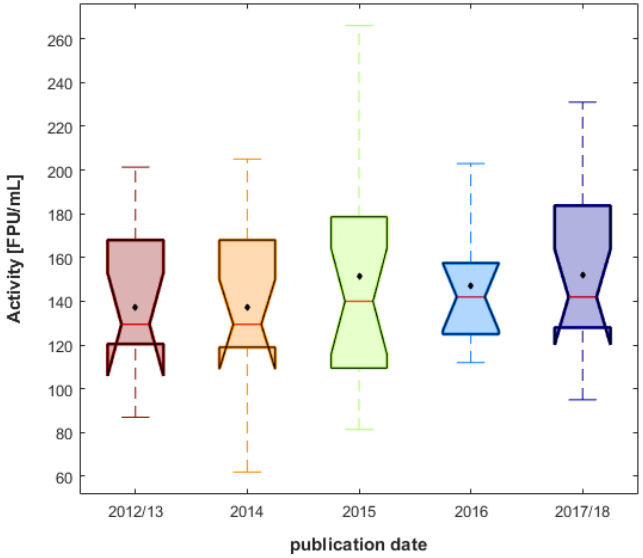
- Process design
- Reactions
- Scheduling
- Utility systems
- Up/downstream units

**Pinch analysis**



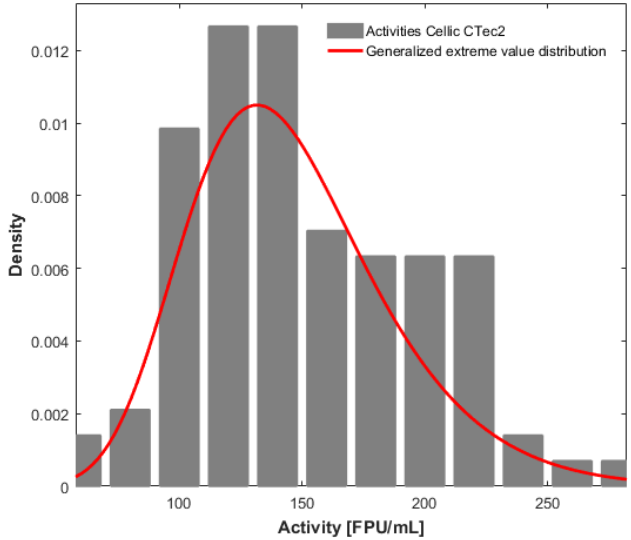
# Variability in enzymatic activities – a case study

## Step 1: Data collection




**Method** Ghose, T. (1987). "Measurement of cellulase activities." Pure and applied Chemistry 59(2): 257-268.

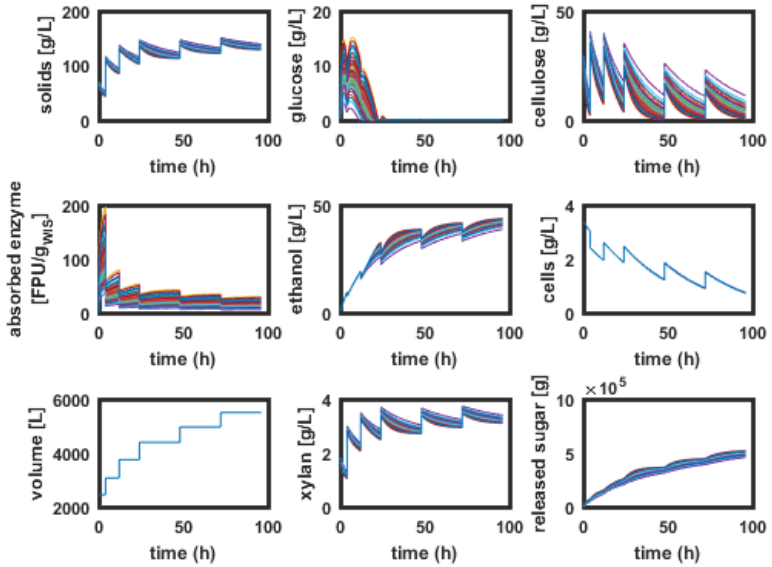
## Step 2: Distribution fit




- **Generalized extreme value distribution**

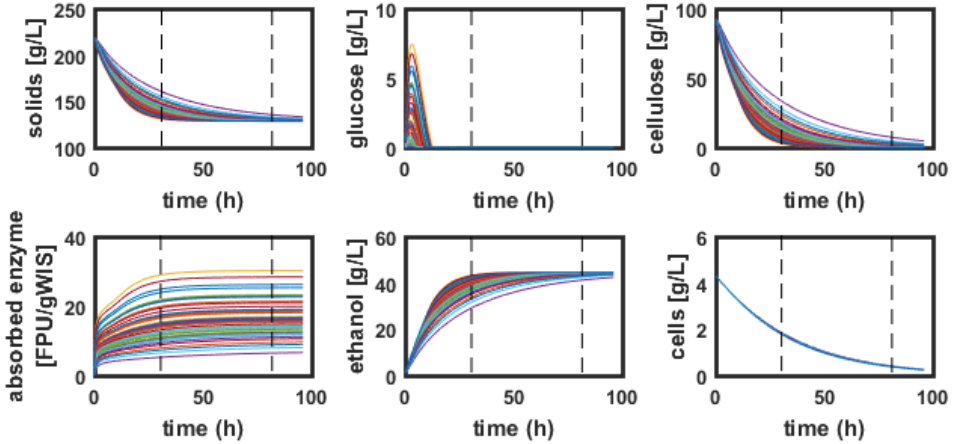
# Variability in enzymatic activities – a case study

## Propagation in multifeed process




Long process, shortage possible. Feeding restricts variability in process time.

## Propagation in batch process

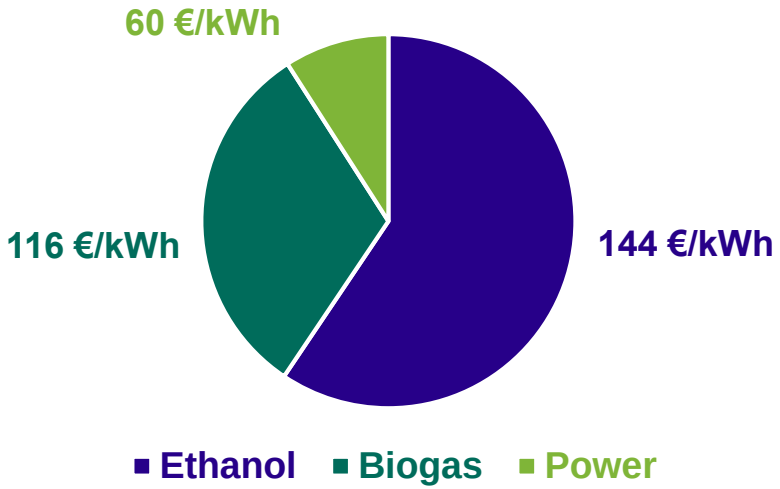



Practically impossible due to mixing and control problems!

# Variability in enzymatic activities – a case study

## TEA of multifeed process

**Products [MW] and value of product [€/kWh]**



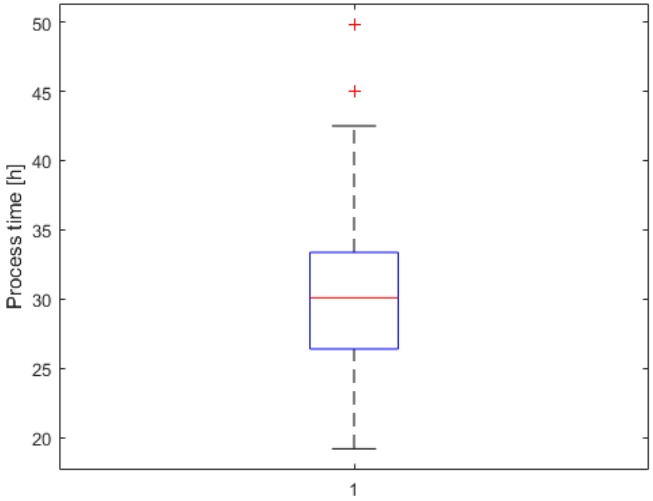

## How to improve the multifeed?

- **Faster additions of solids**
  → estimated saving of process time: ca. 24 h
- **Improve fermentation yield**
  - Simulated to be 0.42 $g_{EtOH}/g_{total\ sugars}$
  - Redirect xylose consumption to ethanol production instead of biogas
  - Methods:
    genetic engineering
    improved preadaptation

# Variability in enzymatic activities – a case study

## The impact of varibility on process times in a batch process

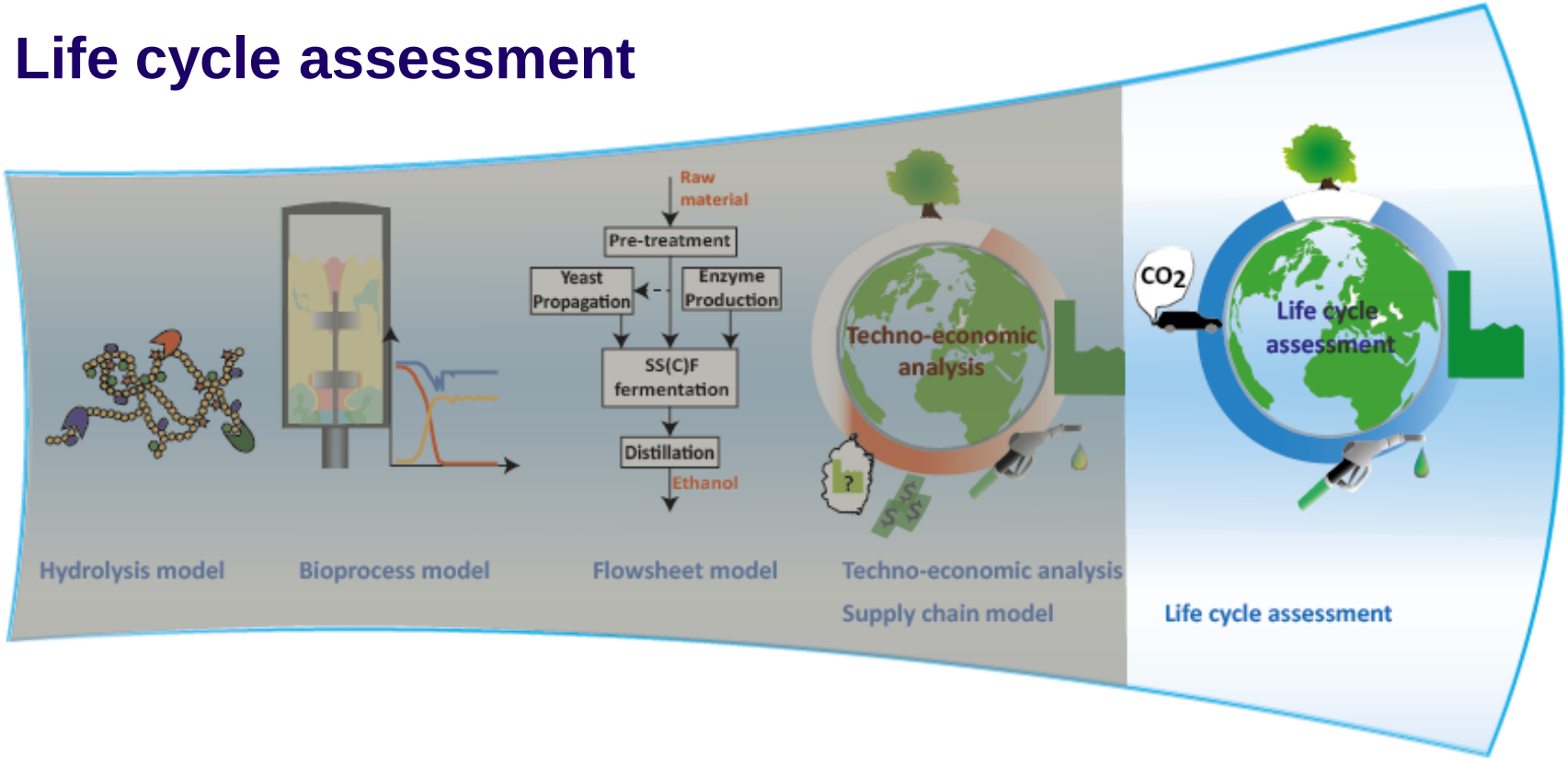
**Introduction of process stop criterion: Stop process if $q_{EtOH}$ < 0.1 g/Lh**




**Resulting differences in process time due to stop criterion**

- **Stop criterion** can be used to execute **online control over solid feed** in **multifeed process**
- Possible directions of **batch process development**:
  - ❑ **Define range of ethanol yields at average (median) process time**
  - ❑ **Optimize process at average (median) process time**

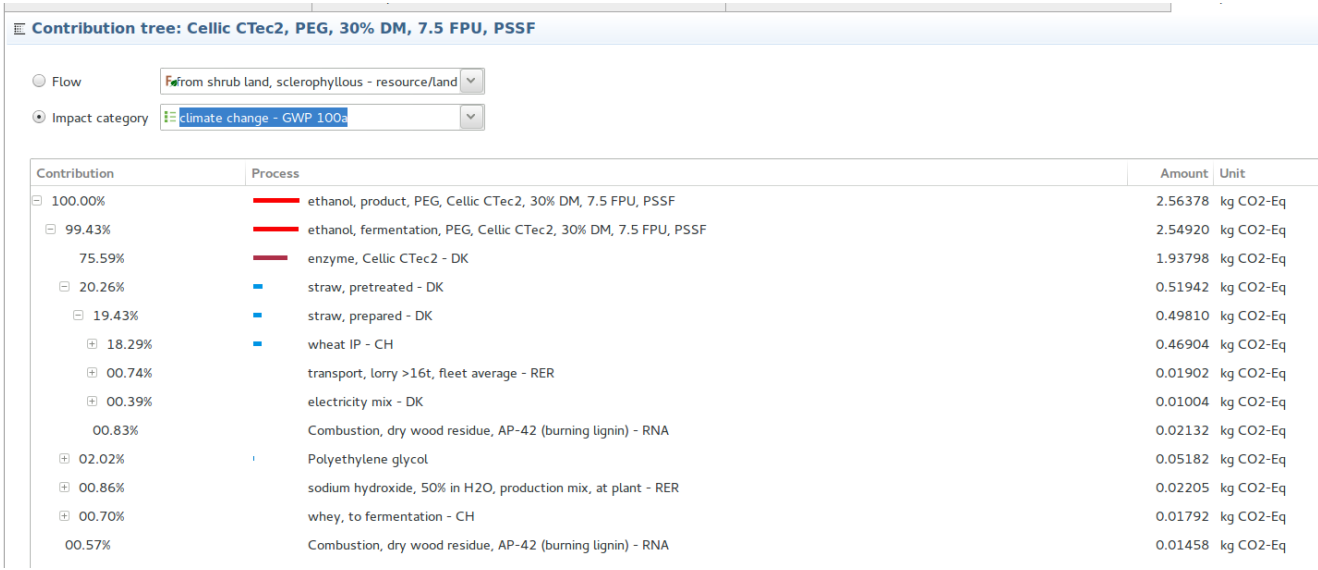
# Life cycle assessment




| | | |
|---|---|---|
| | | Global scale |

# Life cycle assessment

- **Calculates the potential environmental impact of ethanol production**
- **Inputs:**
  - **Database**
  - **Bioreactor model**
  - **Flowsheet model**
- **Software: openLCA**



**Contribution tree: Cellic CTec2, PEG, 30% DM, 7.5 FPU, PSSF**

Flow: from shrub land, sclerophyllous - resource/land

Impact category: climate change - GWP 100a

| Contribution | Process | Amount | Unit |
|---|---|---|---|
| 100.00% | ethanol, product, PEG, Cellic CTec2, 30% DM, 7.5 FPU, PSSF | 2.56378 | kg CO2-Eq |
| 99.43% | ethanol, fermentation, PEG, Cellic CTec2, 30% DM, 7.5 FPU, PSSF | 2.54920 | kg CO2-Eq |
| 75.59% | enzyme, Cellic CTec2 - DK | 1.93798 | kg CO2-Eq |
| 20.26% | straw, pretreated - DK | 0.51942 | kg CO2-Eq |
| 19.43% | straw, prepared - DK | 0.49810 | kg CO2-Eq |
| 18.29% | wheat IP - CH | 0.46904 | kg CO2-Eq |
| 00.74% | transport, lorry >16t, fleet average - RER | 0.01902 | kg CO2-Eq |
| 00.39% | electricity mix - DK | 0.01004 | kg CO2-Eq |
| 00.83% | Combustion, dry wood residue, AP-42 (burning lignin) - RNA | 0.02132 | kg CO2-Eq |
| 02.02% | Polyethylene glycol | 0.05182 | kg CO2-Eq |
| 00.86% | sodium hydroxide, 50% in H2O, production mix, at plant - RER | 0.02205 | kg CO2-Eq |
| 00.70% | whey, to fermentation - CH | 0.01792 | kg CO2-Eq |
| 00.57% | Combustion, dry wood residue, AP-42 (burning lignin) - RNA | 0.01458 | kg CO2-Eq |

# Possible applications of multi-scale uncertainty analysis

## Raw material variation

- Location
- Harvest time
- Composition of biomass
- Storage
- Cultivars
- Pretreatment

## Other

- Optimal process operation time
- Model validation
- Model-based design of experiments

# The multi-scale uncertainty concept:

- Includes variability assessment in early process development
- Allows to determine stable process configurations
- Allows for multi-objective optimization
- Should allow for the determination of optimal experimental conditions to perform model validation experiments

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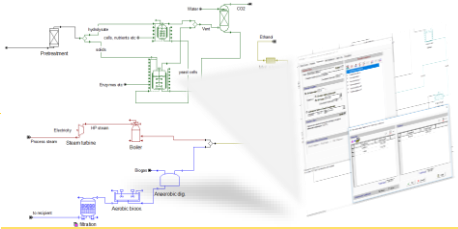
***Funded by:*** Swedish Energy Agency

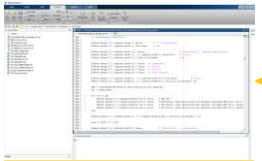
# Data flow between scales

**openLCA**
Life Cycle Assessment



**Excel/VBA**
Data node

**Superpro Designer**
Process simulation



**Matlab**
Kinetic modelling

**Yields**
**Reactions**
**Design parameters**

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

**Environmental assessment**