UNCERTAINTY ANALYSIS

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

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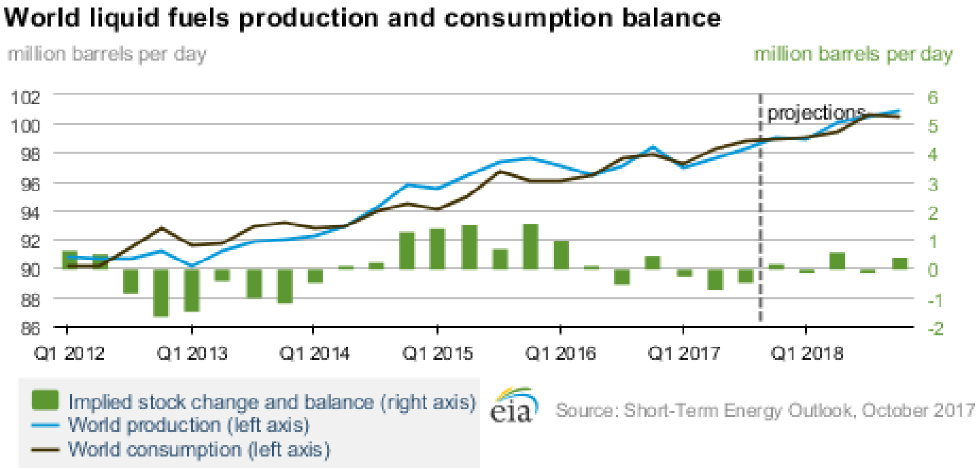
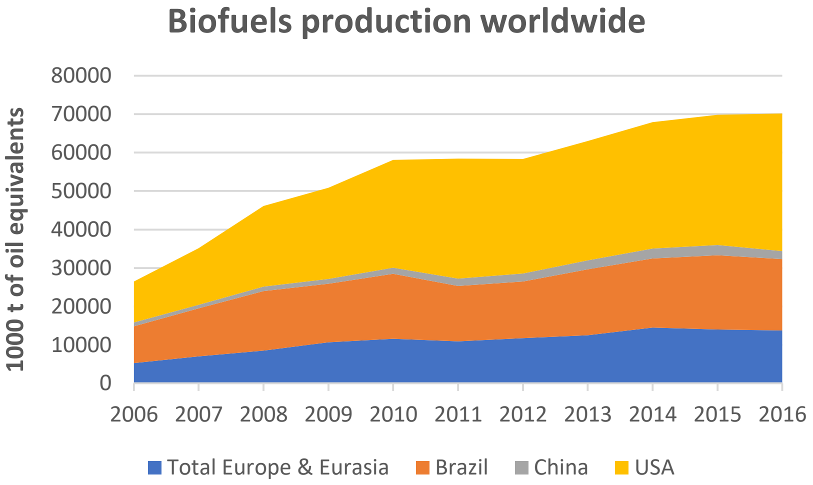
Bioethanol – The current situation





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

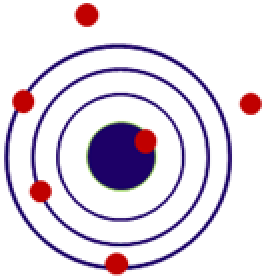
- Turbidity
- Inhomogeneties
- Lack of sensor equipment for online measurements
- Uncertain measurements

Instable processes

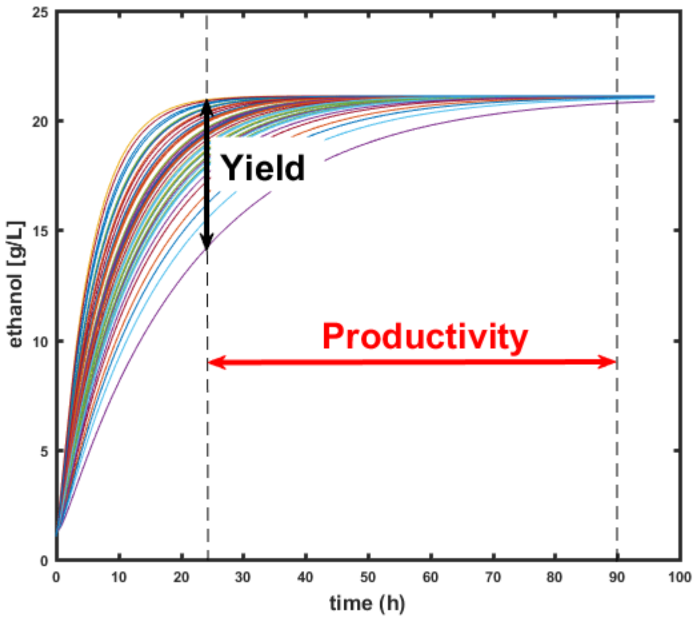
Lack of mechanistic knowldge

Suboptimal process design

Challenges in lignocellulosic processes



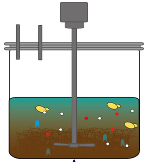
Variability



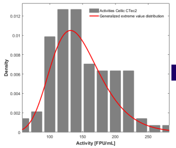
Economics

Multi-scale uncertainty analysis- Methodology

Process definition



Variability/ uncertainty definition



Models at different system scales

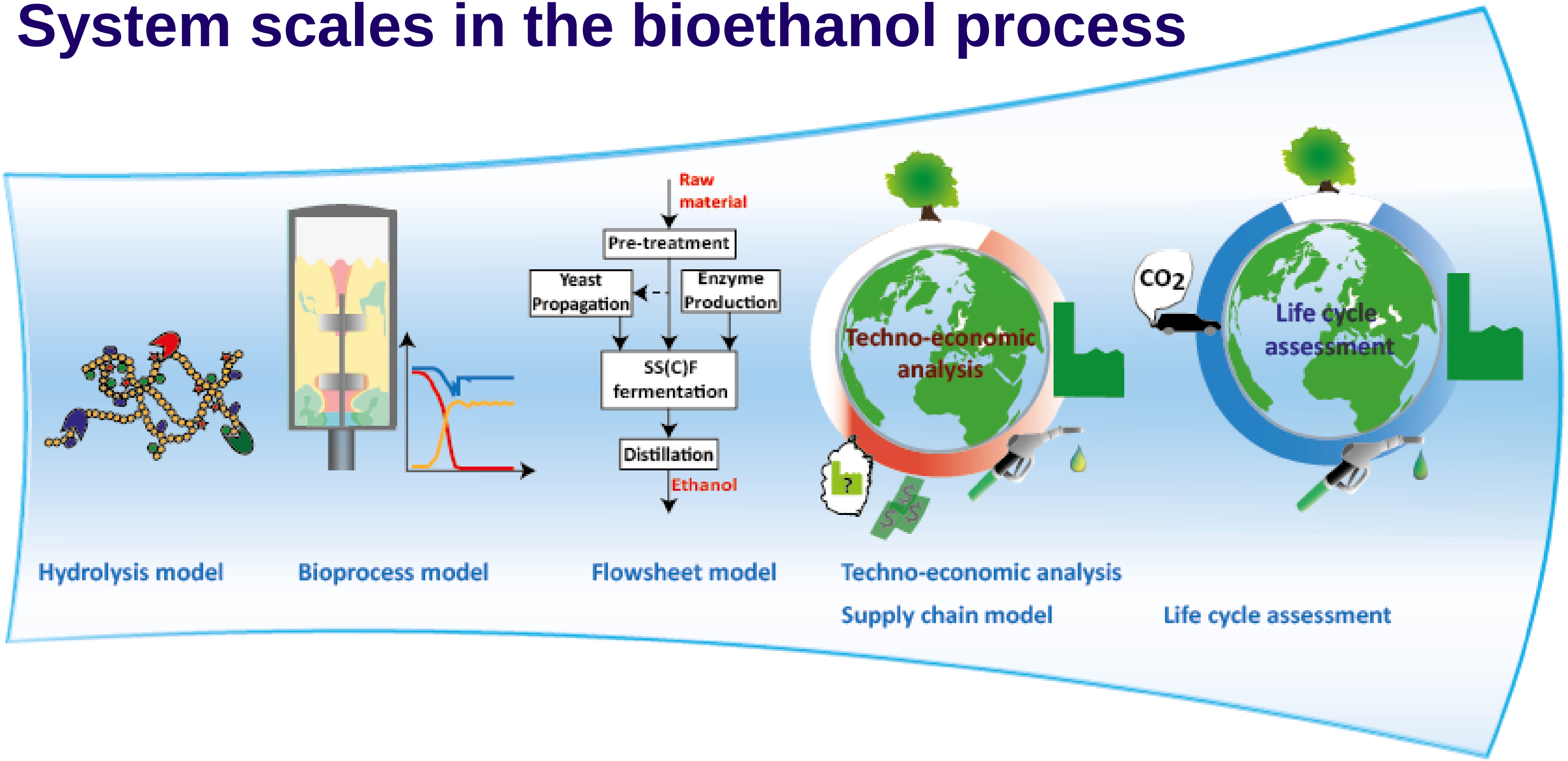
Quantify effect on process outcomes:

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

Consequences:

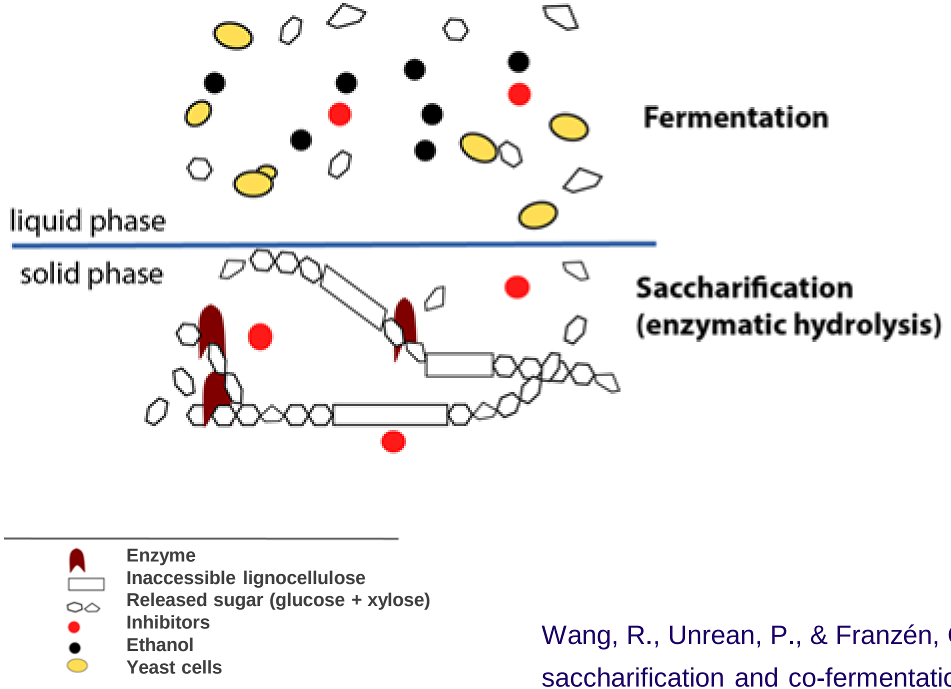
- Improve models (sensitivity analysis)
- Suggest feasible supply chain/ process configurations
- Suggest new experimental procedures

System scales in the bioethanol process



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

The bioprocess model

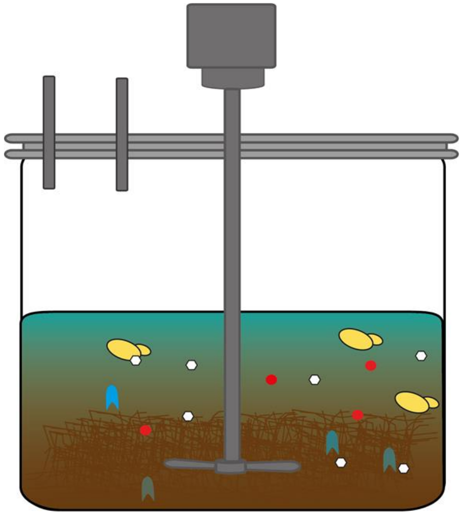


- **Enzyme adsorption:** second order kinetics
- **Hydrolysis inhibited** by glucose and ethanol
- Ethanol dependent **cell death**
- **Ethanol formation** only yield dependent

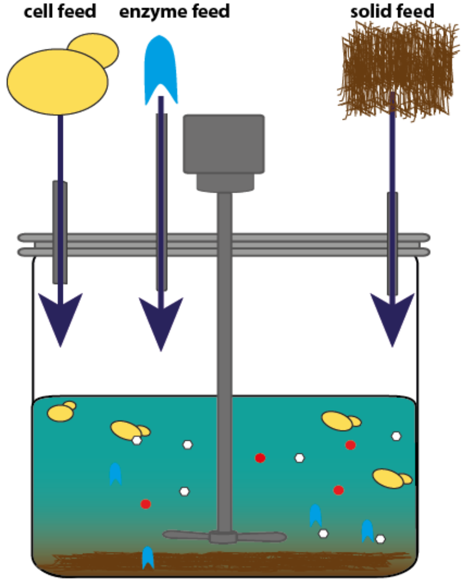
Wang, R., Unrean, P., & Franzén, C. J. (2016). Model-based optimization and scale-up of multi-feed simultaneous saccharification and co-fermentation of steam pre-treated lignocellulose enables high gravity ethanol production. *Biotechnology for biofuels*, *9*(1), 88

The bioprocess - Process alternatives

Batch process

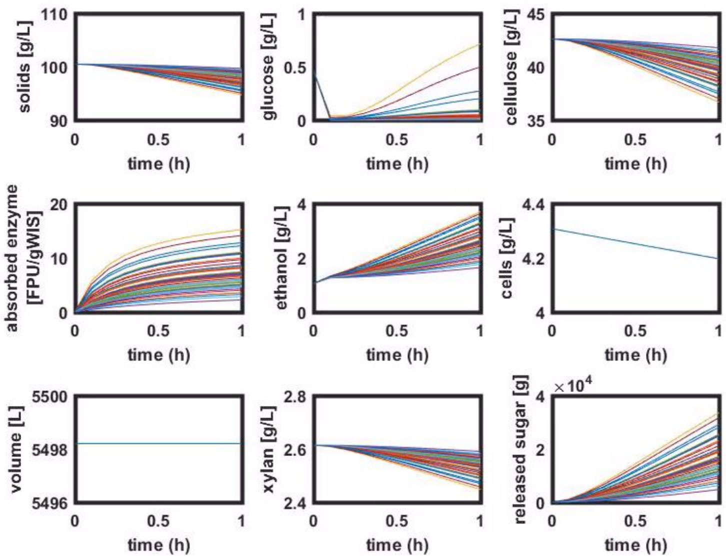


Multi-feed process

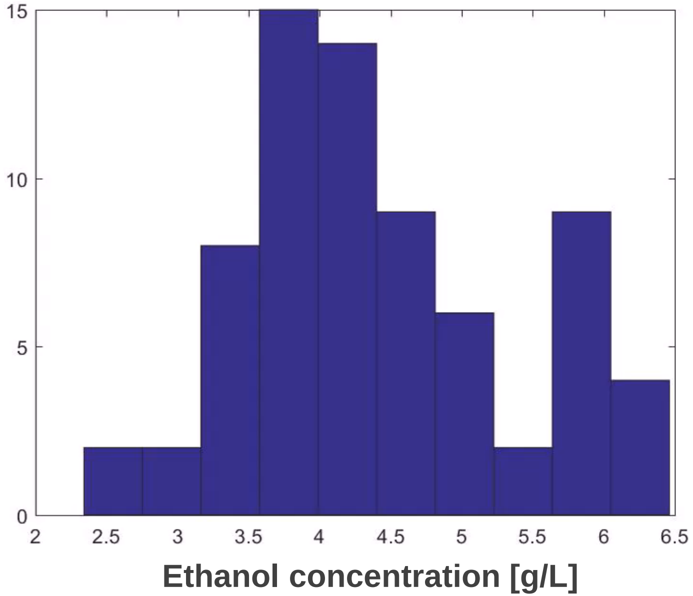


The batch process – Asymptotic stability

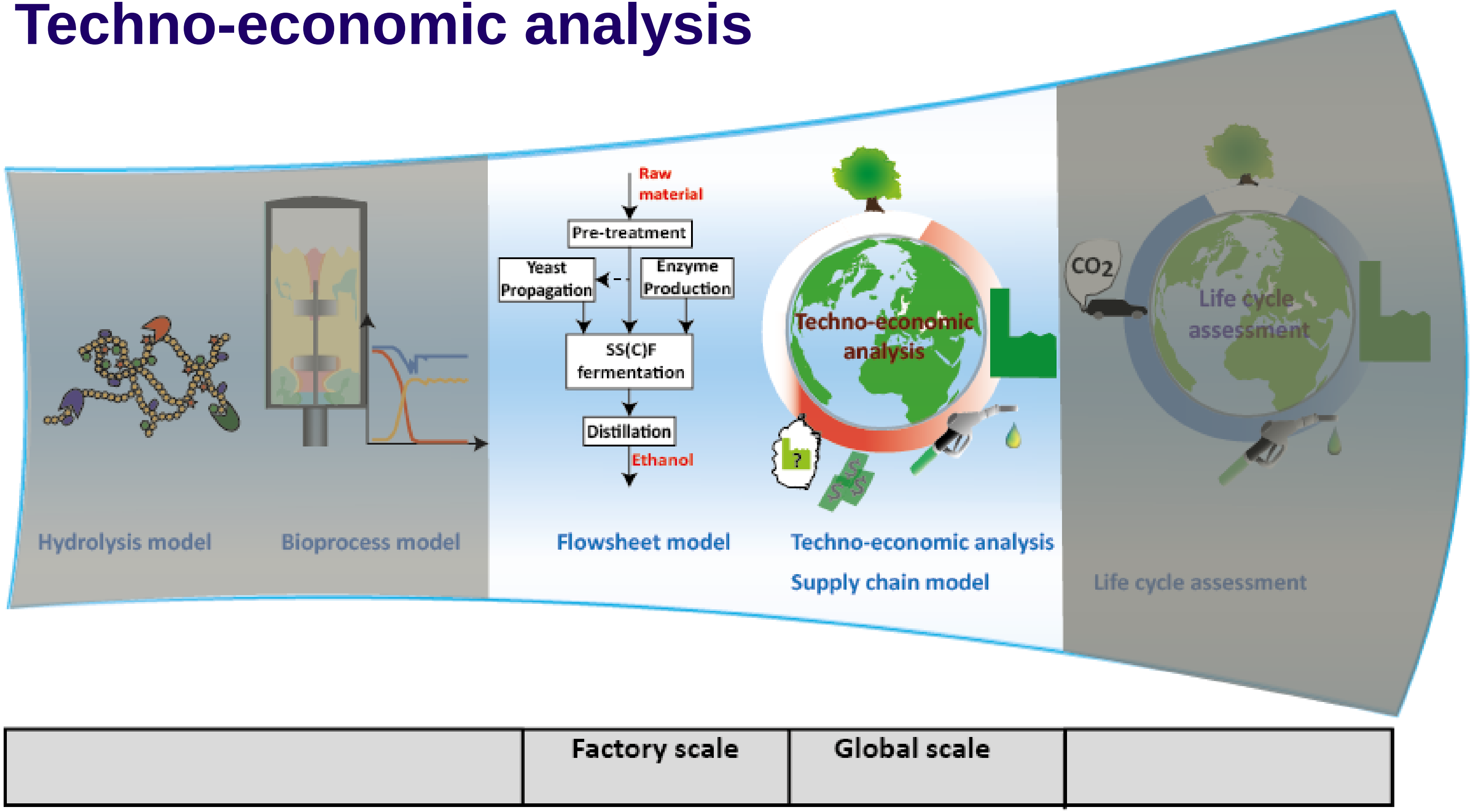
Simulation of batch process



Histogram of ethanol conc. at each simulation time



Techno-economic analysis



Flowsheet model and techno-economic analysis

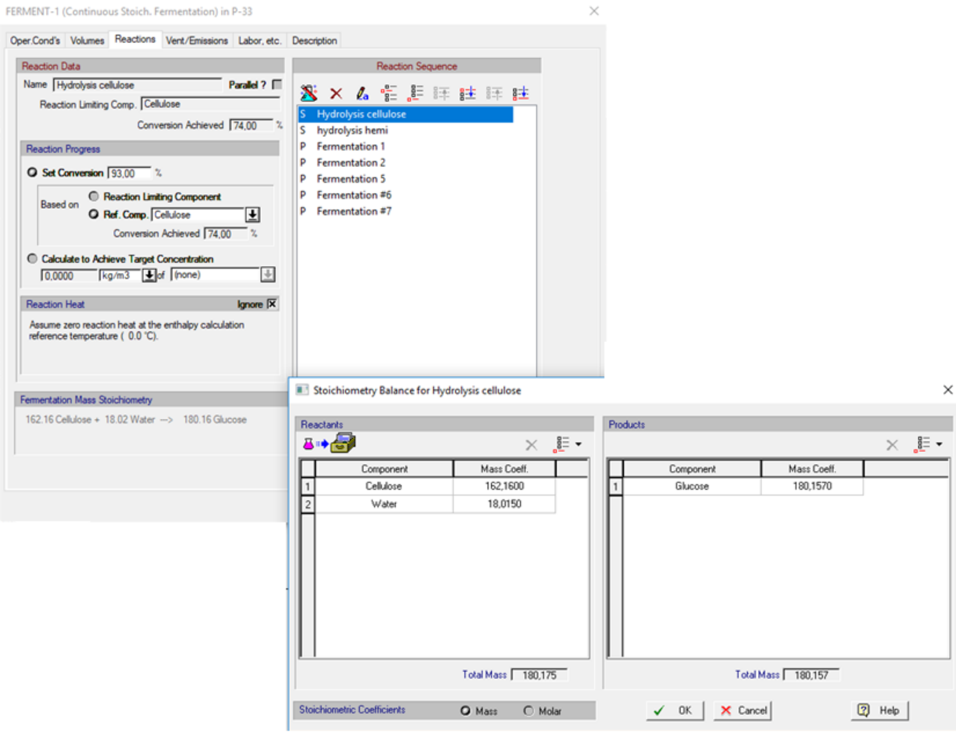
SuperPro Designer

Bioprocess model

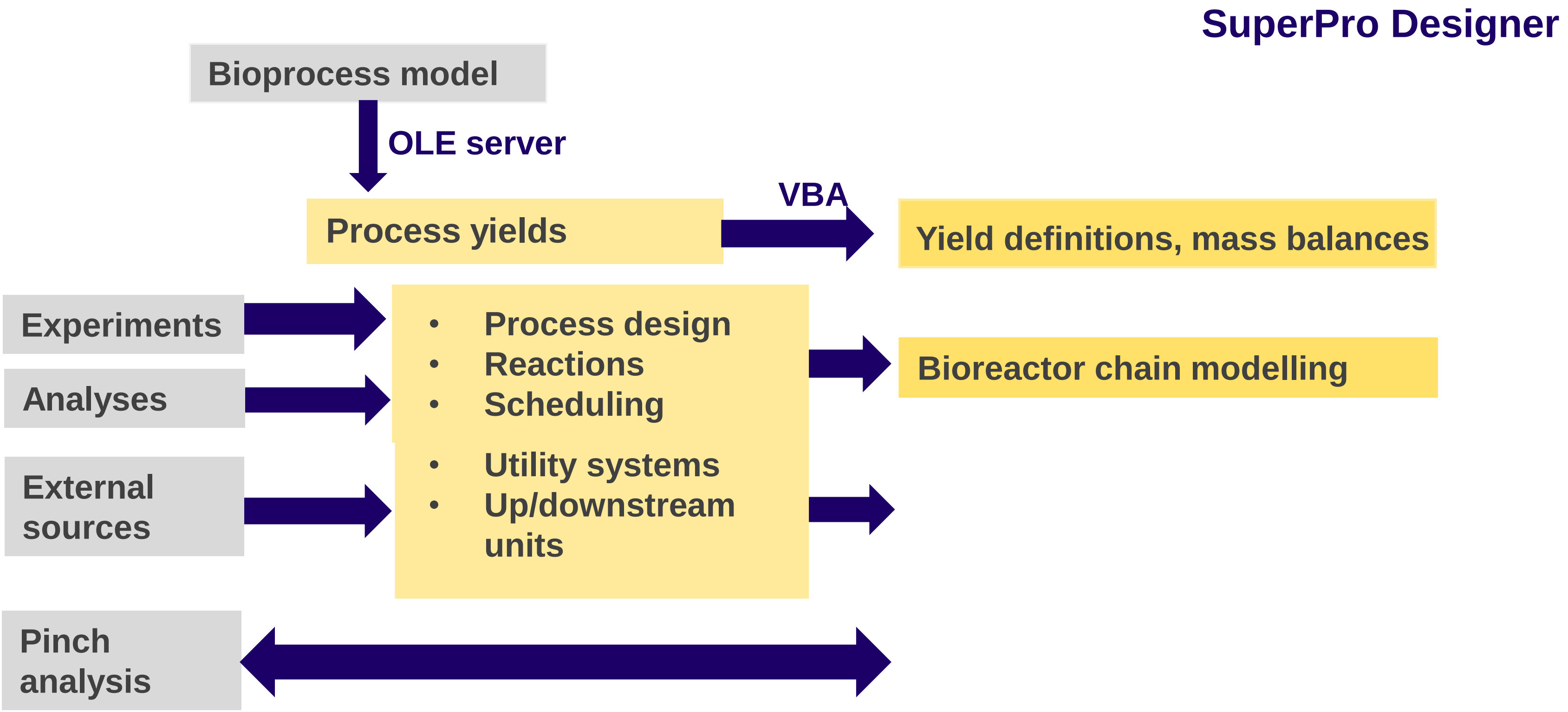
OLE server

Process yields

VBA



Flowsheet model and techno-economic analysis



Flowsheet model and techno-economic analysis

Bioprocess model

OLE server

Process yields

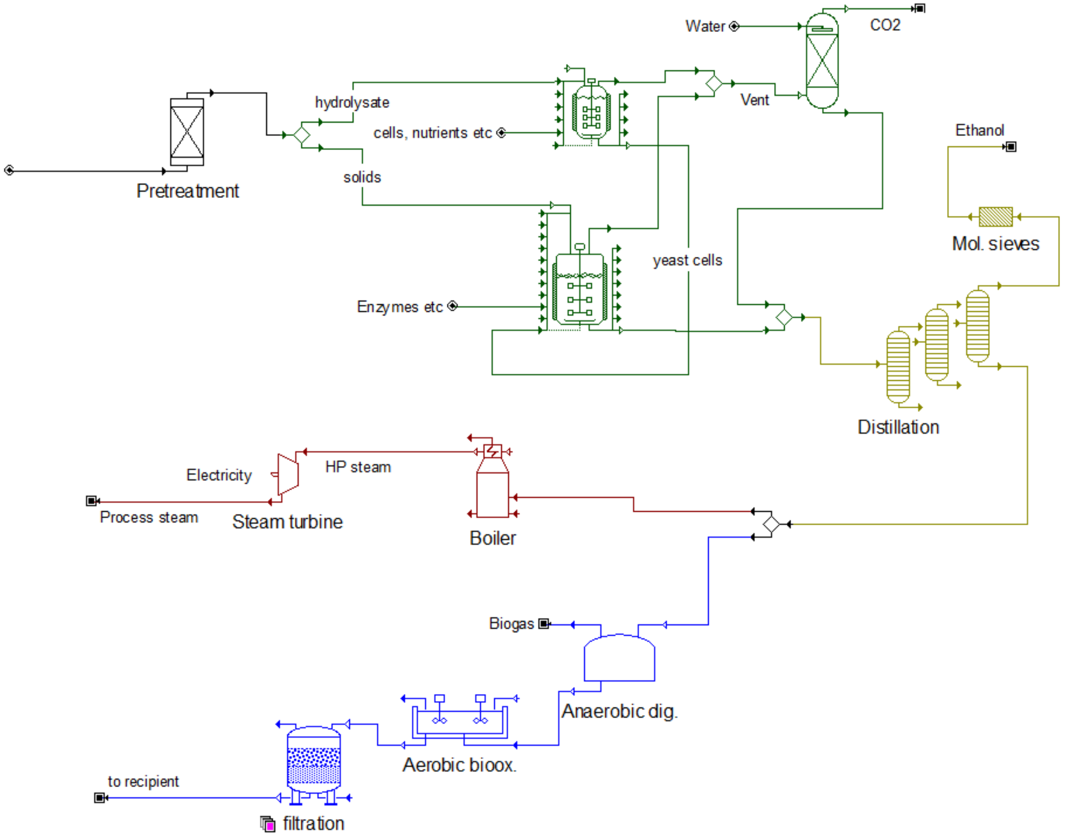
Experiments

Analyses

External sources

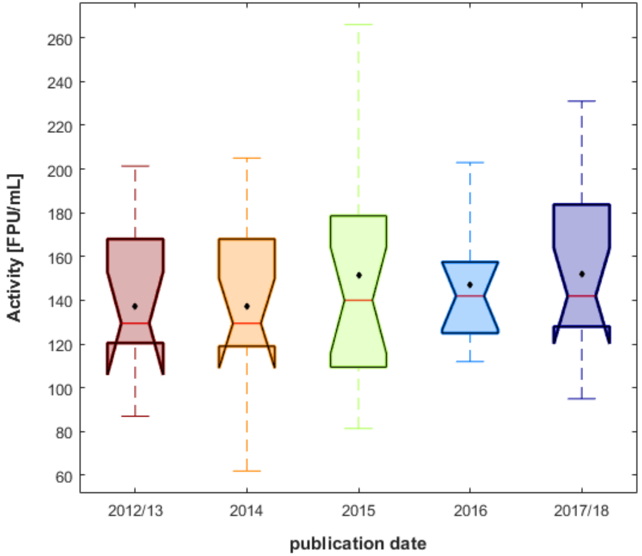
- Process design
- Reactions
- Scheduling
- Utility systems
- Up/downstream units

Pinch analysis



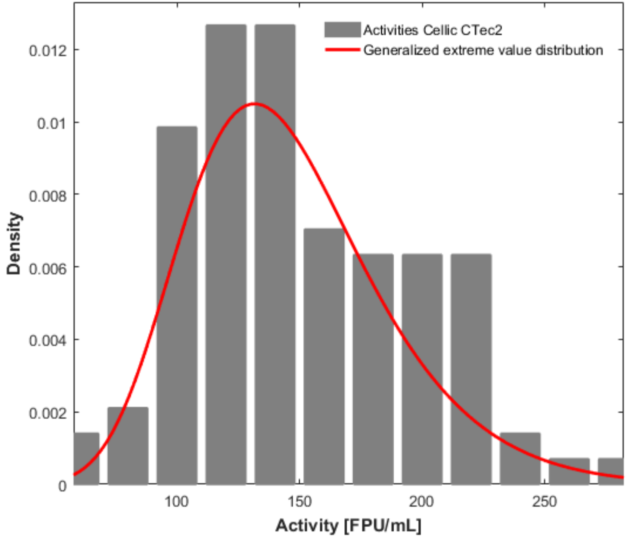
Variability in enzymatic activities – a case study

Step 1: Data collection



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

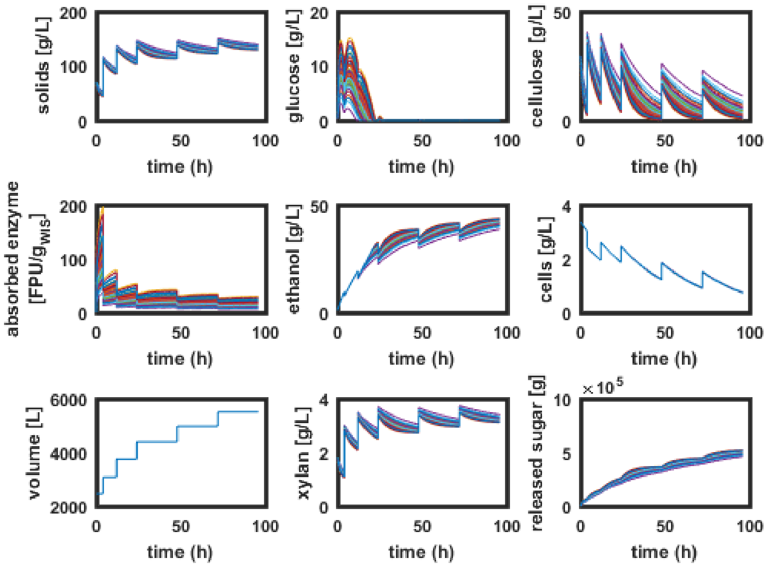
Step 2: Distribution fit



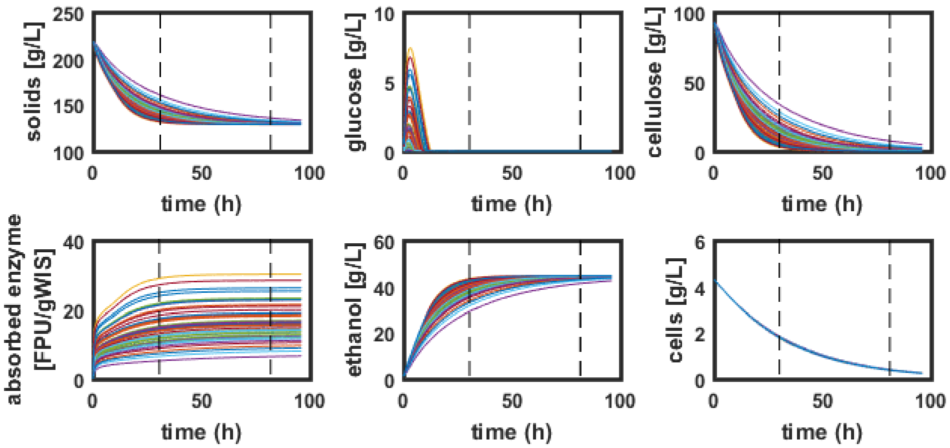
- **Generalized extreme value distribution**

Variability in enzymatic activities – a case study

Propagation in multifeed process



Propagation in batch process



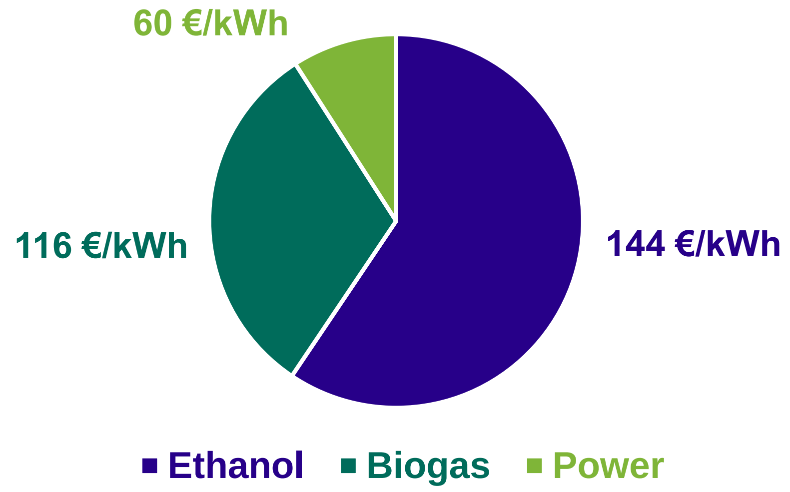
Long process, shortage possible. Feeding restricts variability in process time.

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?

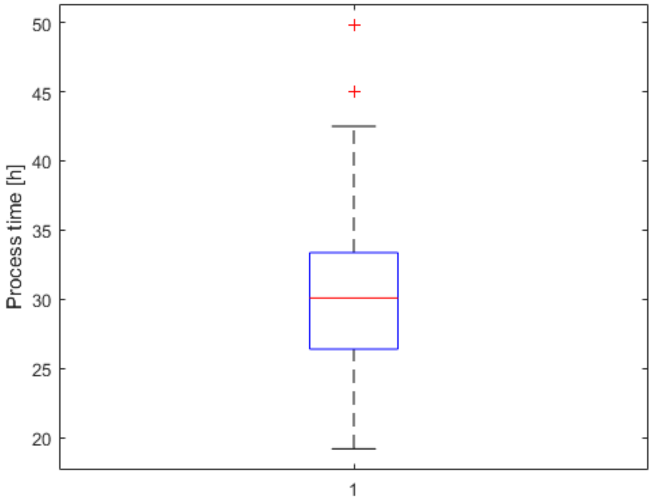
- **Faster additions of solids**
  → estimated saving of process time: ca. 24 h

- **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

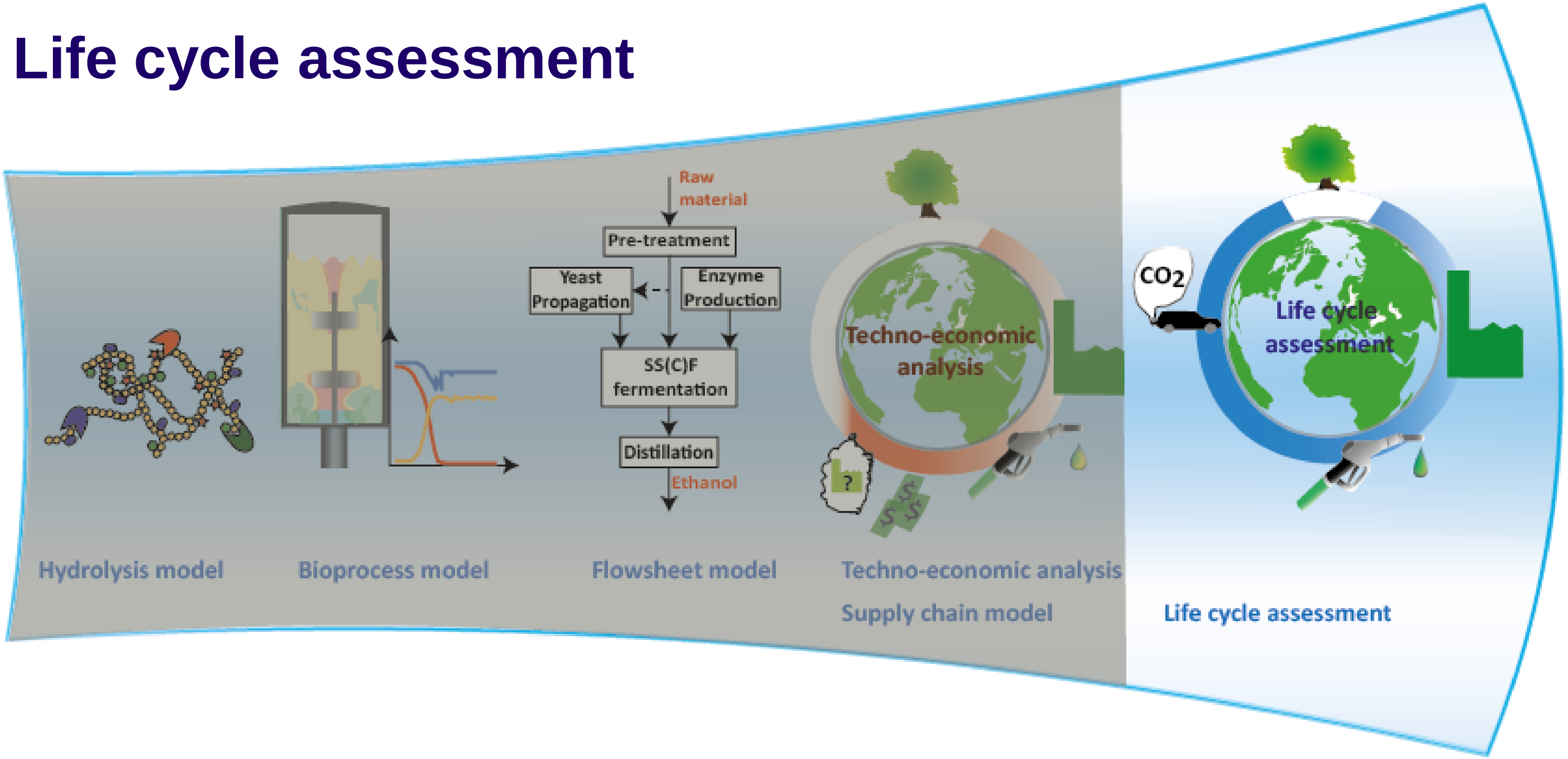
Introduction of process stop criterion: Stop process if q_{EtOH} < 0.1 g/Lh



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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Data flow between scales