

UNCERTAINTY ANALYSIS

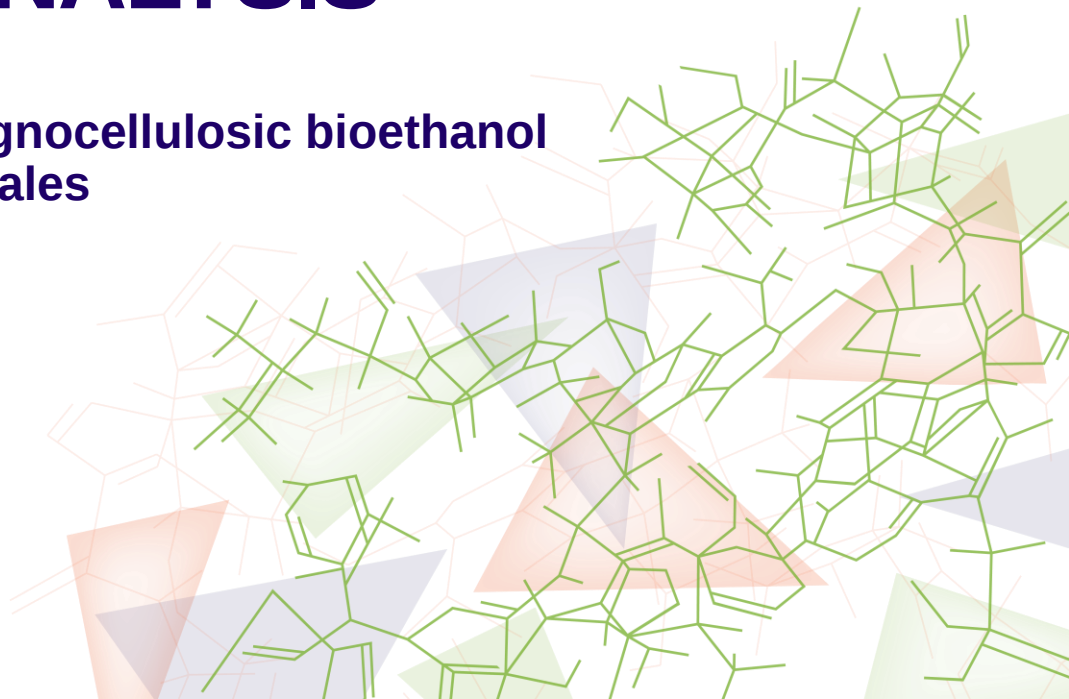
A tool to consistently evaluate lignocellulosic bioethanol processes at different system scales

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Rickard Fornell

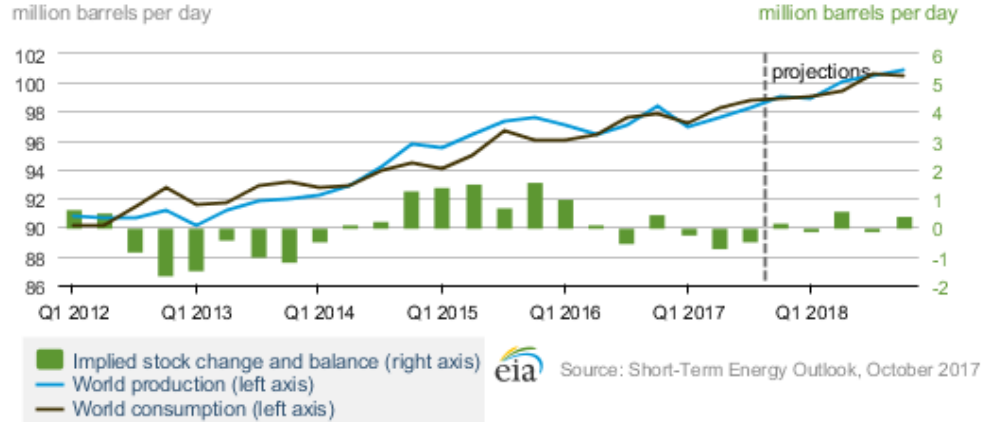
Matty Janssen

Carl Johan Franzén



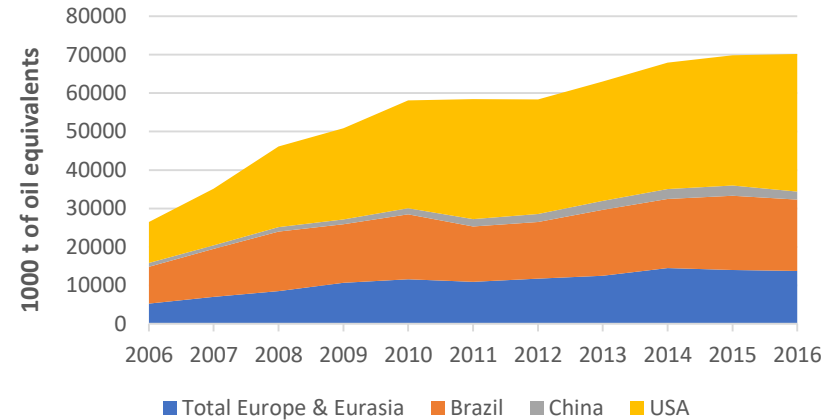
Bioethanol – The current situation

World liquid fuels production and consumption balance



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

Biofuels production worldwide

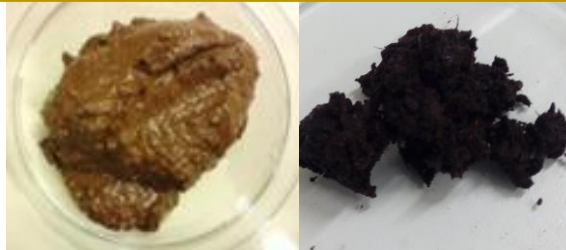


BP (2017): BP Statistical Review of World Energy 2017;
<https://www.bp.com/content/dam/bp/en/corporate/pdf/energy-economics/statistical-review-2017/bp-statistical-review-of-world-energy-2017-full-report.pdf>; retrieved: 13.10.2017

Challenges in lignocellulosic processes

Measurement challenges

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

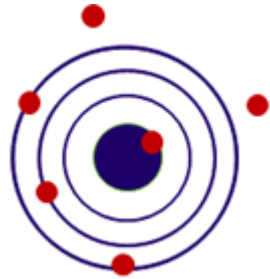


Instable processes

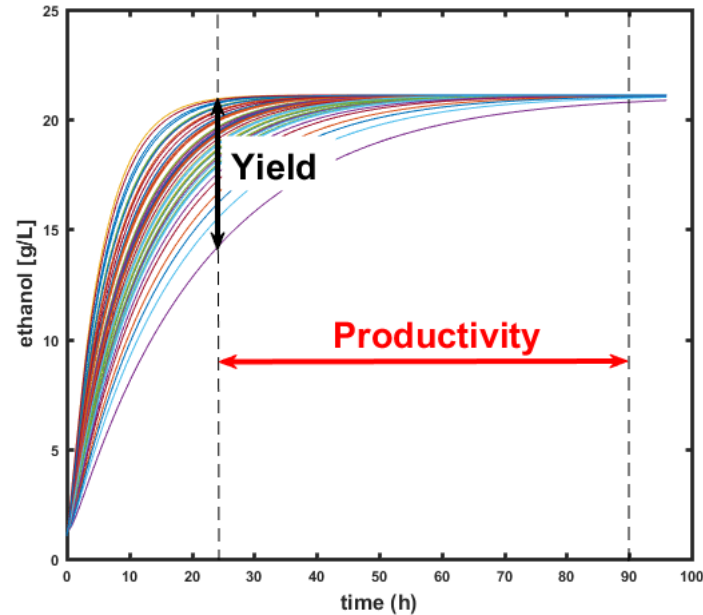
**Lack of mechanistic
knowldge**

**Suboptimal process
design**

Challenges in lignocellulosic processes

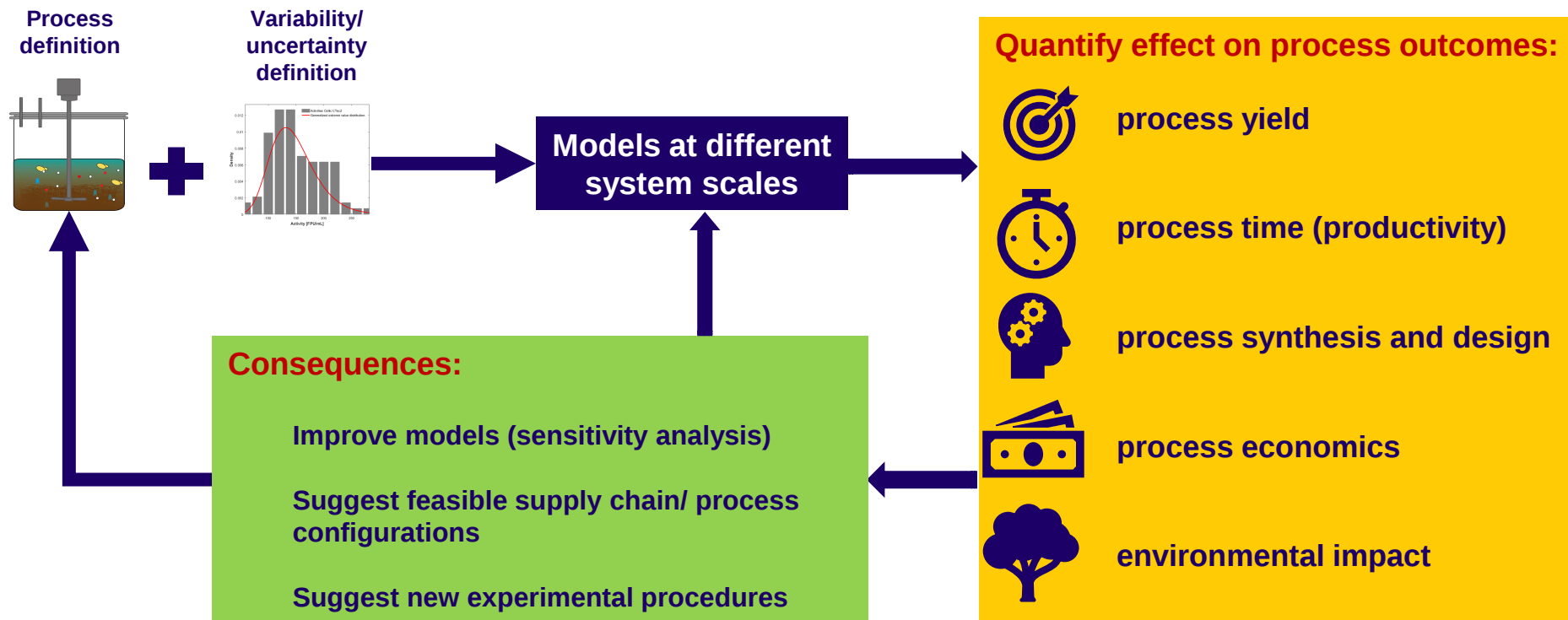


Variability

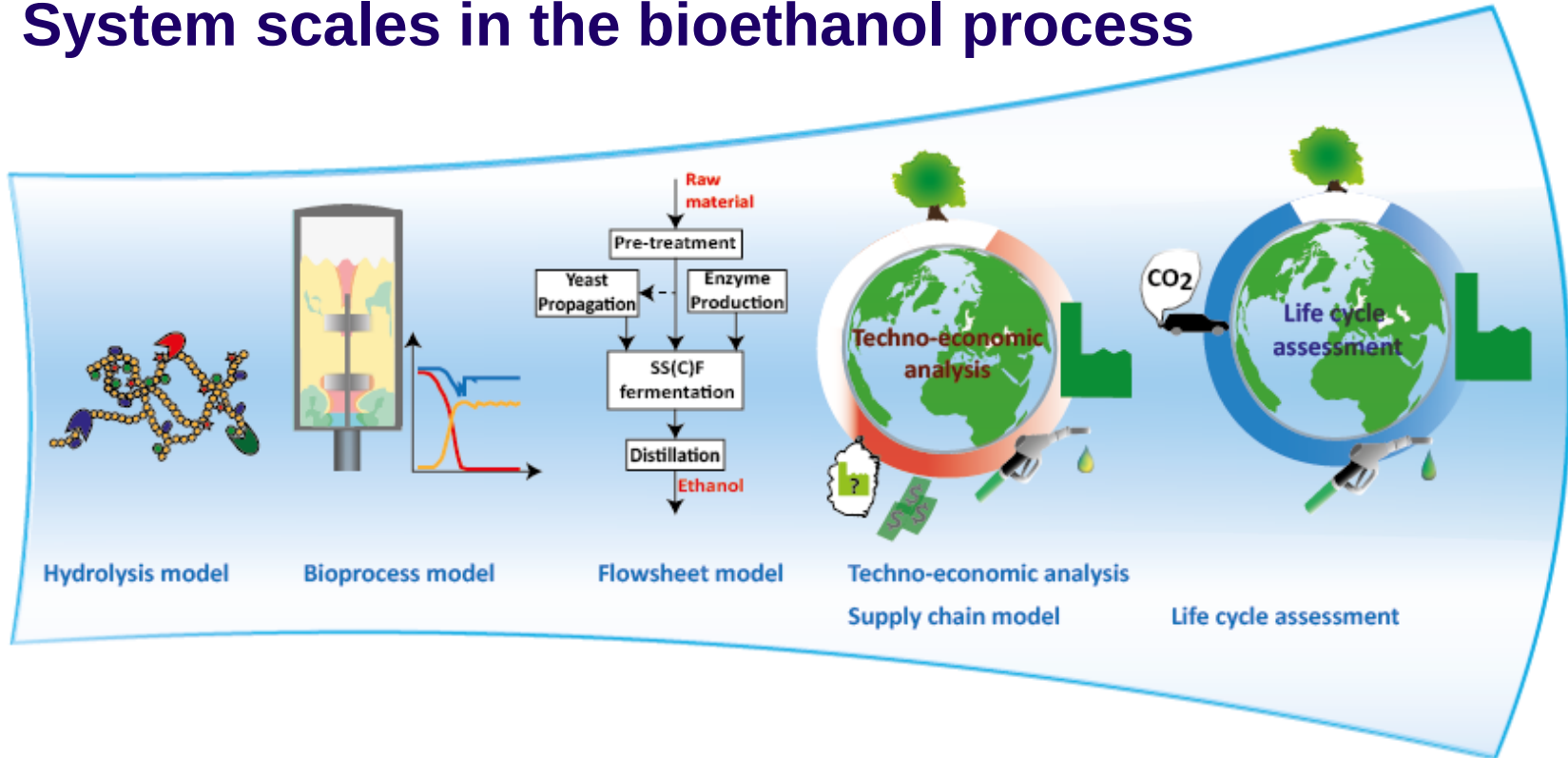


Economics

Multi-scale uncertainty analysis- Methodology

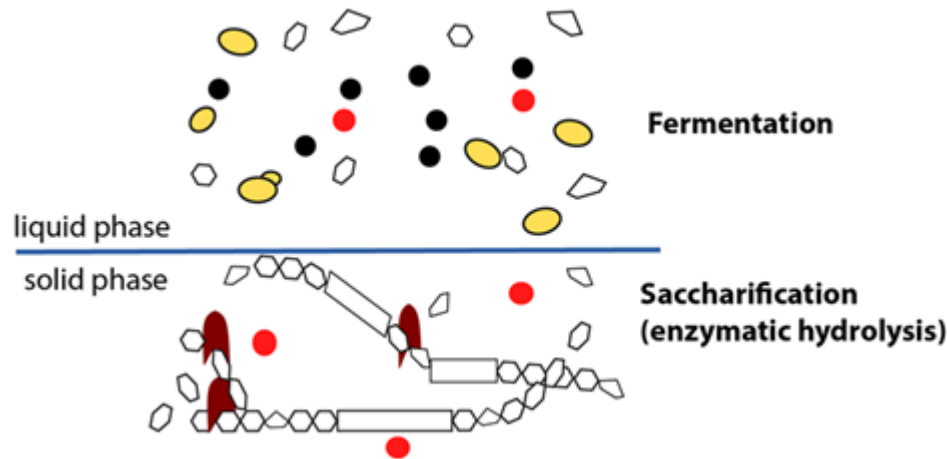


System scales in the bioethanol process



Macro-molecular scale	Bioprocess scale	Factory scale	Global scale	Global scale
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The bioprocess model

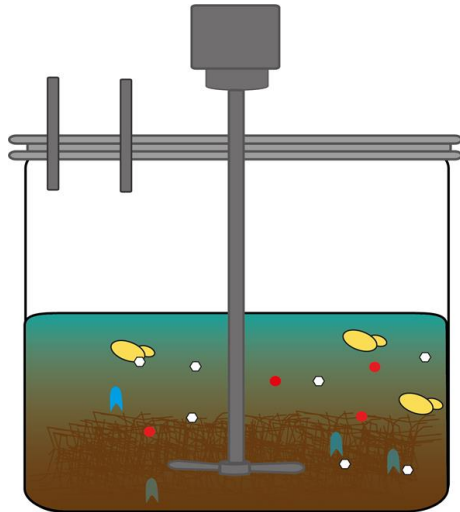


- **Enzyme adsorption:** second order kinetics
- **Hydrolysis inhibited** by glucose and ethanol
- Ethanol dependent **cell death**
- **Ethanol formation** only yield dependent

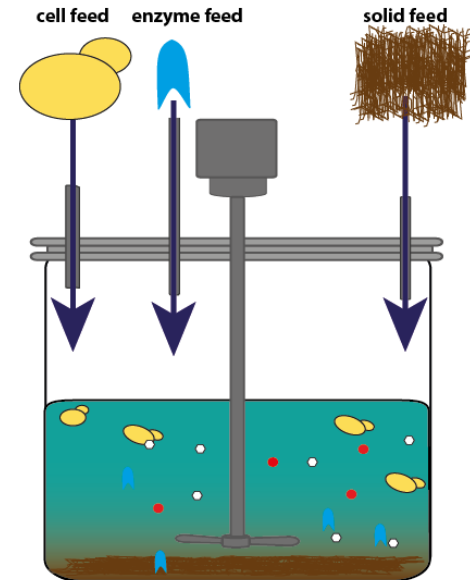
Wang, R., Unrean, P., & Franzén, C. J. (2016). Model-based optimization and scale-up of multi-feed simultaneous saccharification and co-fermentation of steam pre-treated lignocellulose enables high gravity ethanol production. *Biotechnology for biofuels*, 9(1), 88

The bioprocess - Process alternatives

Batch process

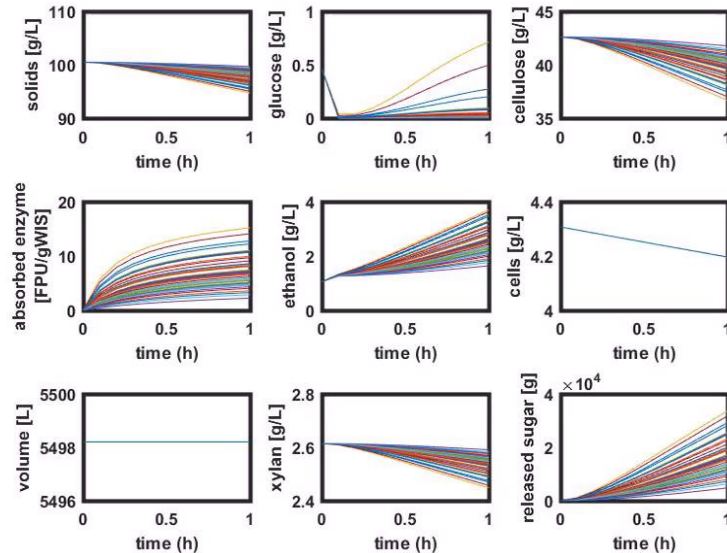


Multi-feed process

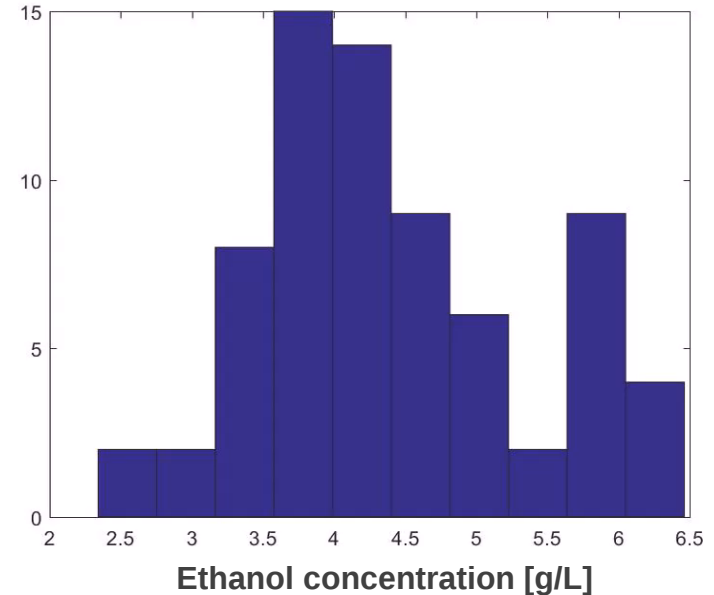


The batch process – Asymptotic stability

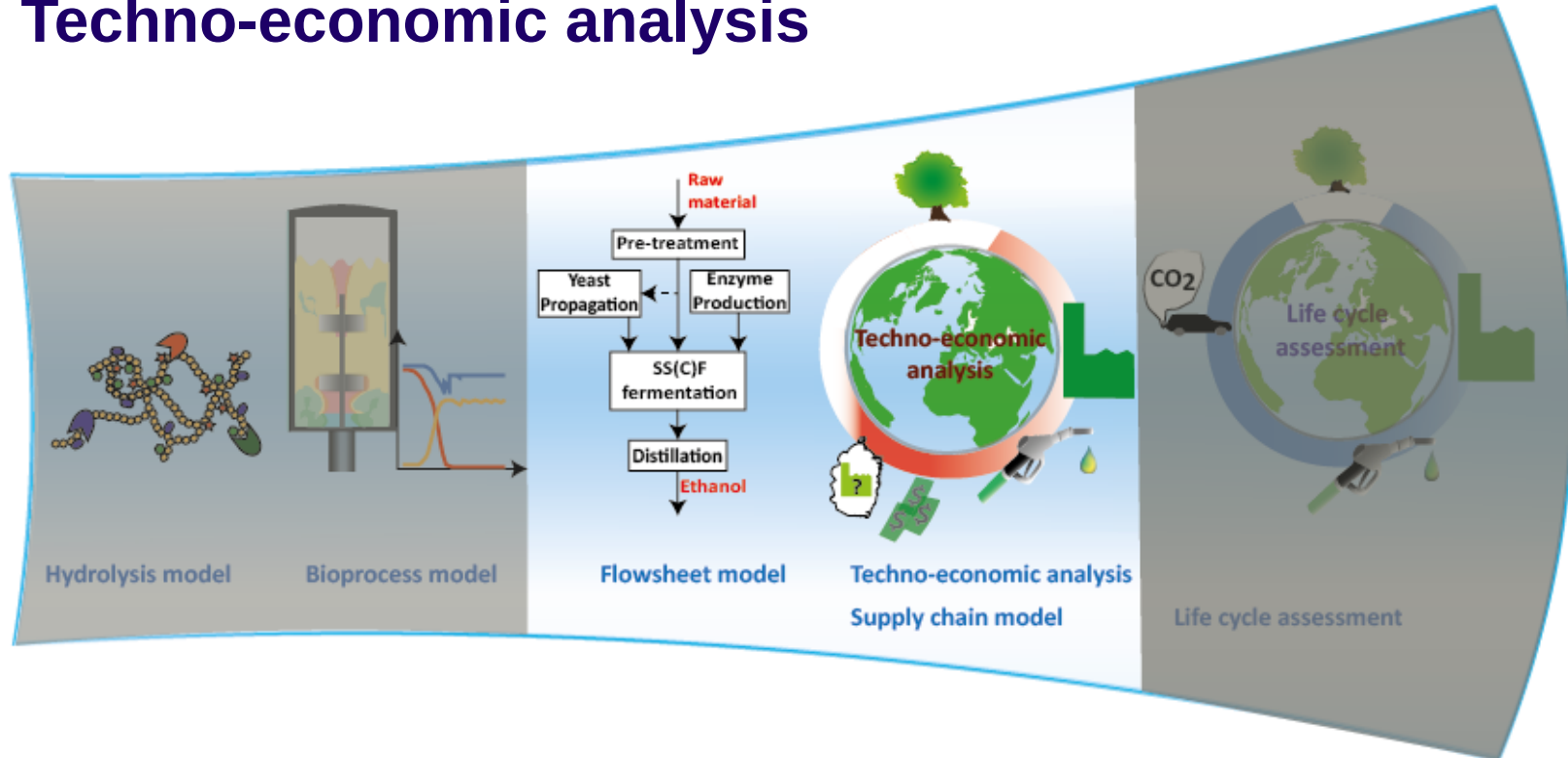
Simulation of batch process



Histogram of ethanol conc. at each simulation time

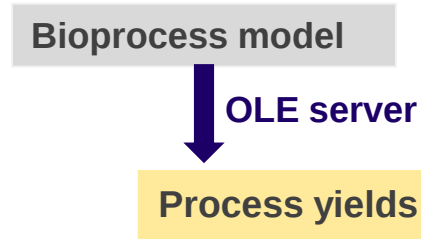


Techno-economic analysis



	Factory scale	Global scale	
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Flowsheet model and techno-economic analysis



VBA

SuperPro Designer

FERMENT-1 (Continuous Stoich. Fermentation) in P-33

Oper. Cond's | Volumes | Reactions | Vent/Emissions | Labor, etc. | Description

Reaction Data

Name: Hydrolysis cellulose Parallel ? ☐

Reaction Limiting Comp.: Cellulose

Conversion Achieved: 74.00 %

Reaction Progress

☐ Set Conversion: 93.00 %

Based on: ☐ Reaction Limiting Component

☐ Ref. Comp.: Cellulose

Conversion Achieved: 74.00 %

☐ Calculate to Achieve Target Concentration

0.0000 kg/m³ of (none)

Reaction Heat Ignore ☒

Assume zero reaction heat at the enthalpy calculation reference temperature (0.0 °C).

Fermentation Mass Stoichiometry

162.16 Cellulose + 18.02 Water → 180.15 Glucose

Stoichiometry Balance for Hydrolysis cellulose

Reactants

	Component	Mass Coeff.
1	Cellulose	162.1600
2	Water	18.0150

Total Mass: 180.175

Products

	Component	Mass Coeff.
1	Glucose	180.1570

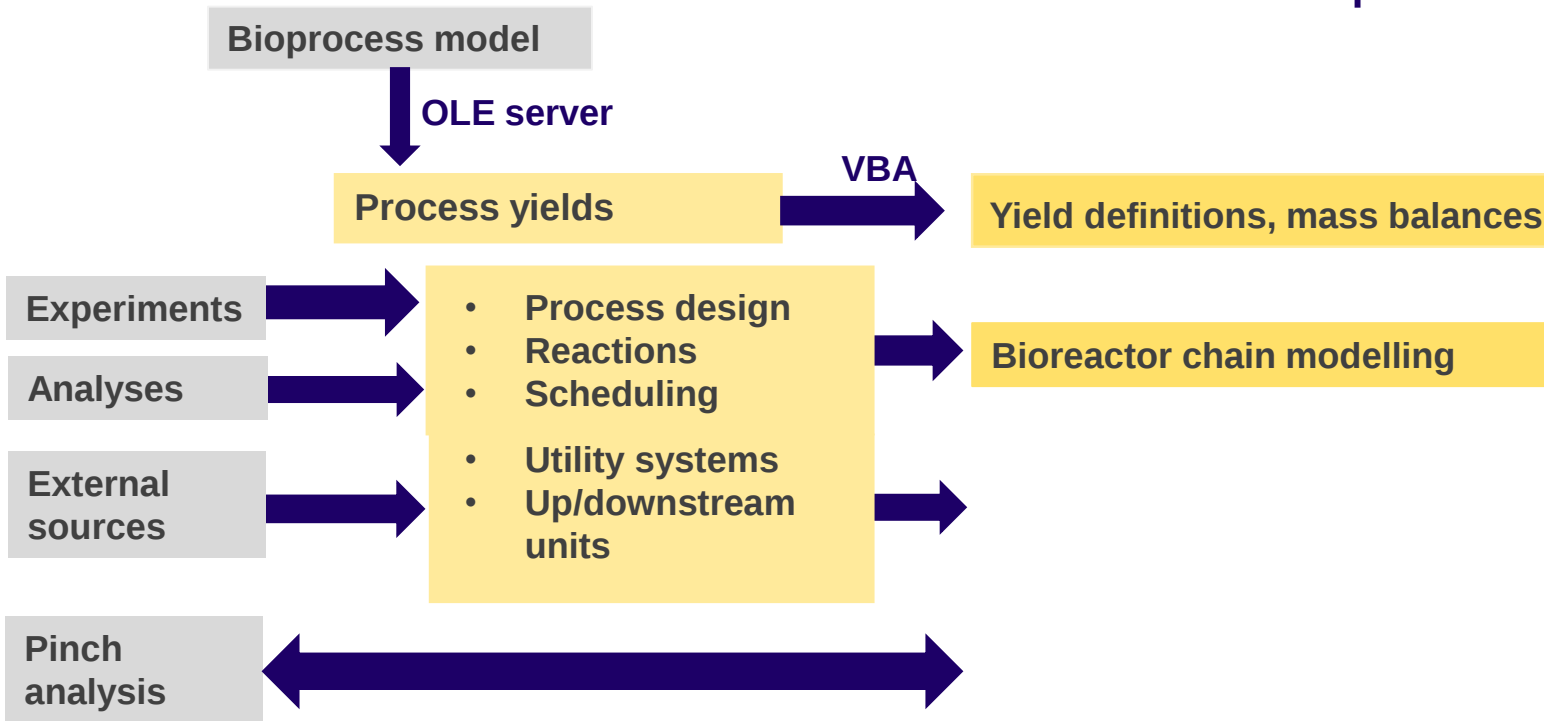
Total Mass: 180.157

Stoichiometric Coefficients: ☐ Mass ☐ Molar

OK Cancel Help

Flowsheet model and techno-economic analysis

SuperPro Designer



Bioprocess model

OLE server

Process yields

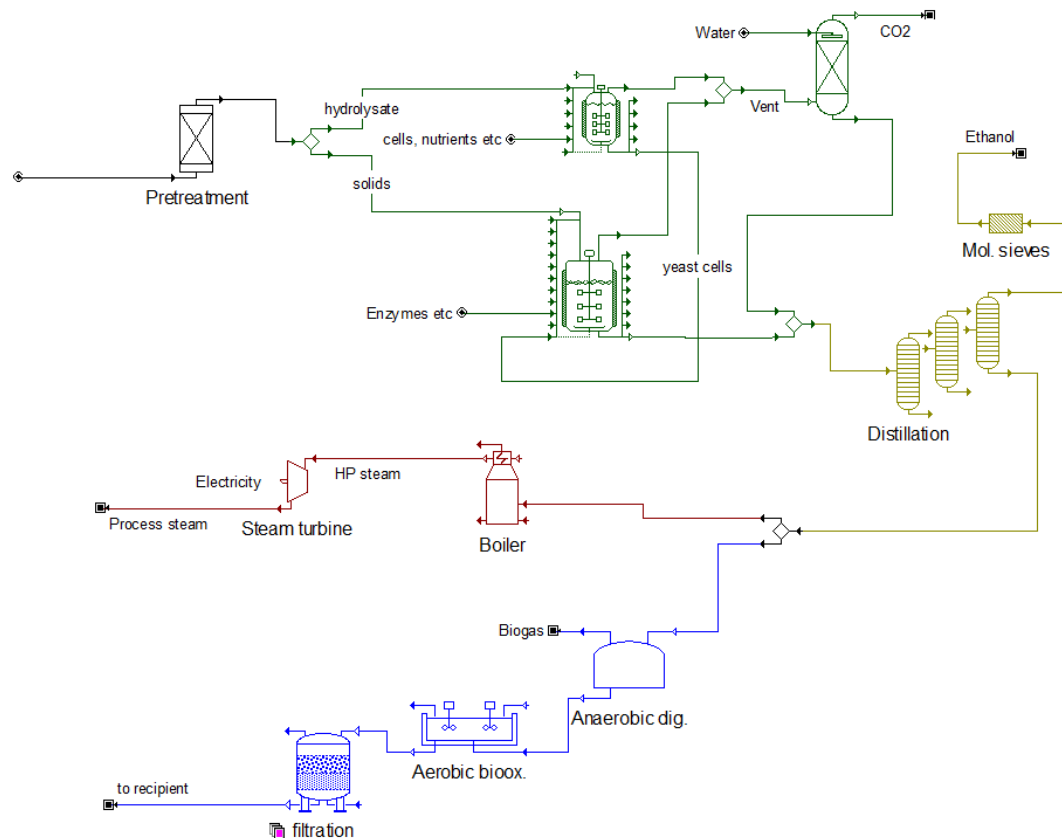
Experiments

Analyses

External sources

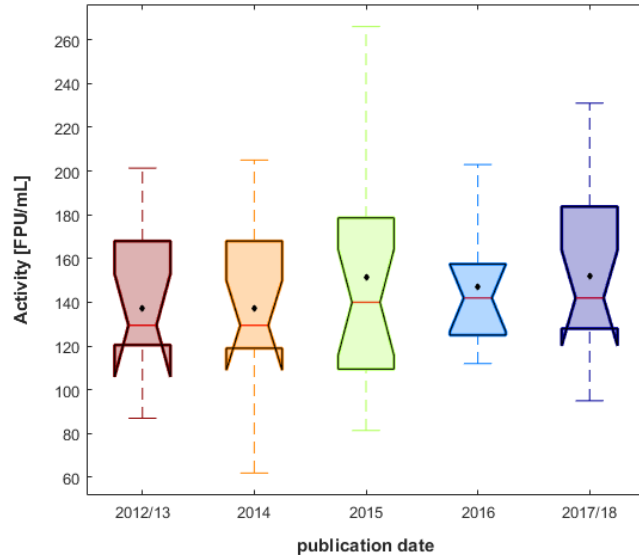
- Process design
- Reactions
- Scheduling
- Utility systems
- Up/downstream units

Pinch analysis

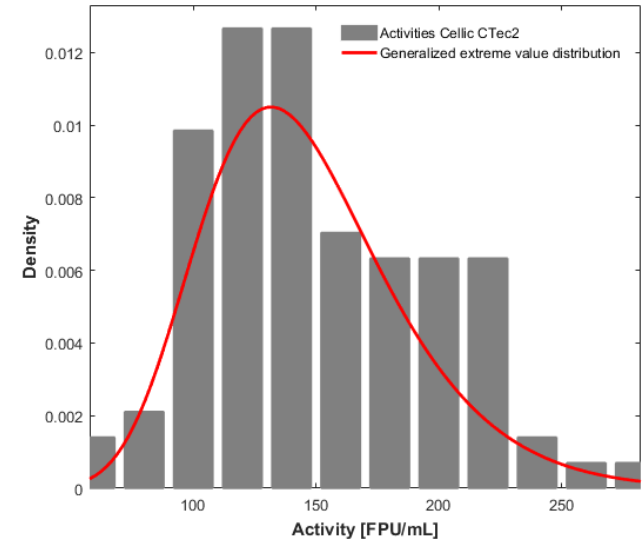


Variability in enzymatic activities – a case study

Step 1: Data collection



Step 2: Distribution fit



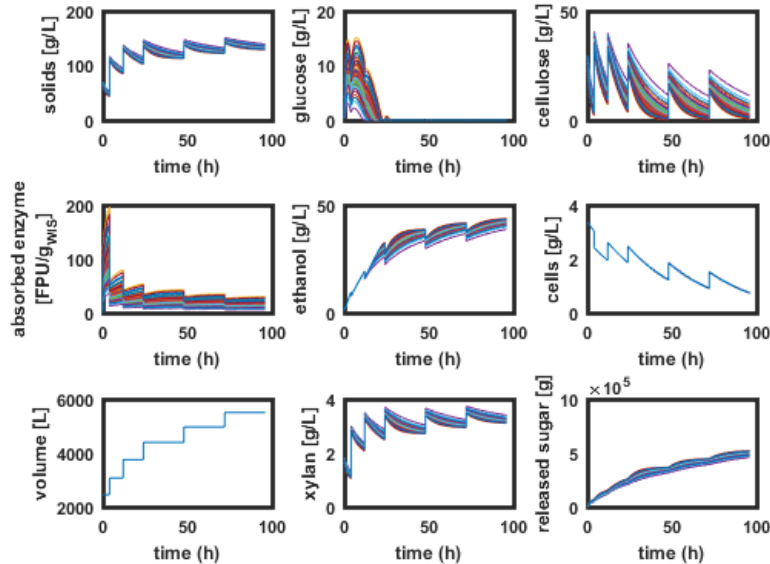
Method

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

- Generalized extreme value distribution

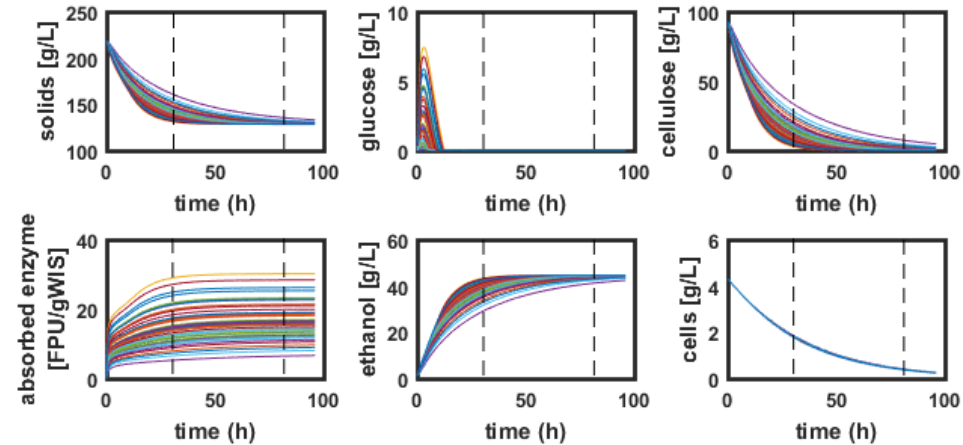
Variability in enzymatic activities – a case study

Propagation in multifeed process



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

Propagation in batch process

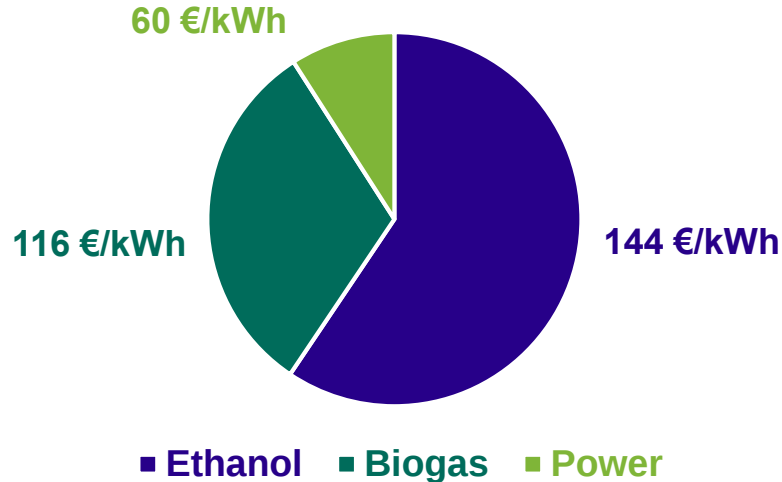


Practically impossible due to mixing and control problems!

Variability in enzymatic activities – a case study

TEA of multifeed process

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



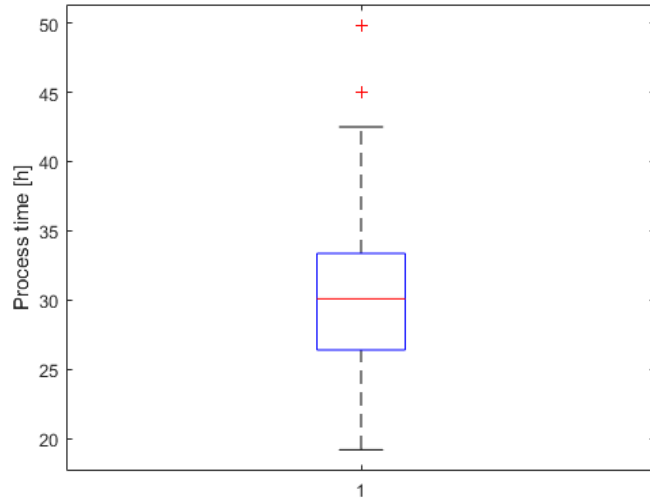
How to improve the multifeed?

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

Variability in enzymatic activities – a case study

The impact of variability on process times in a batch process

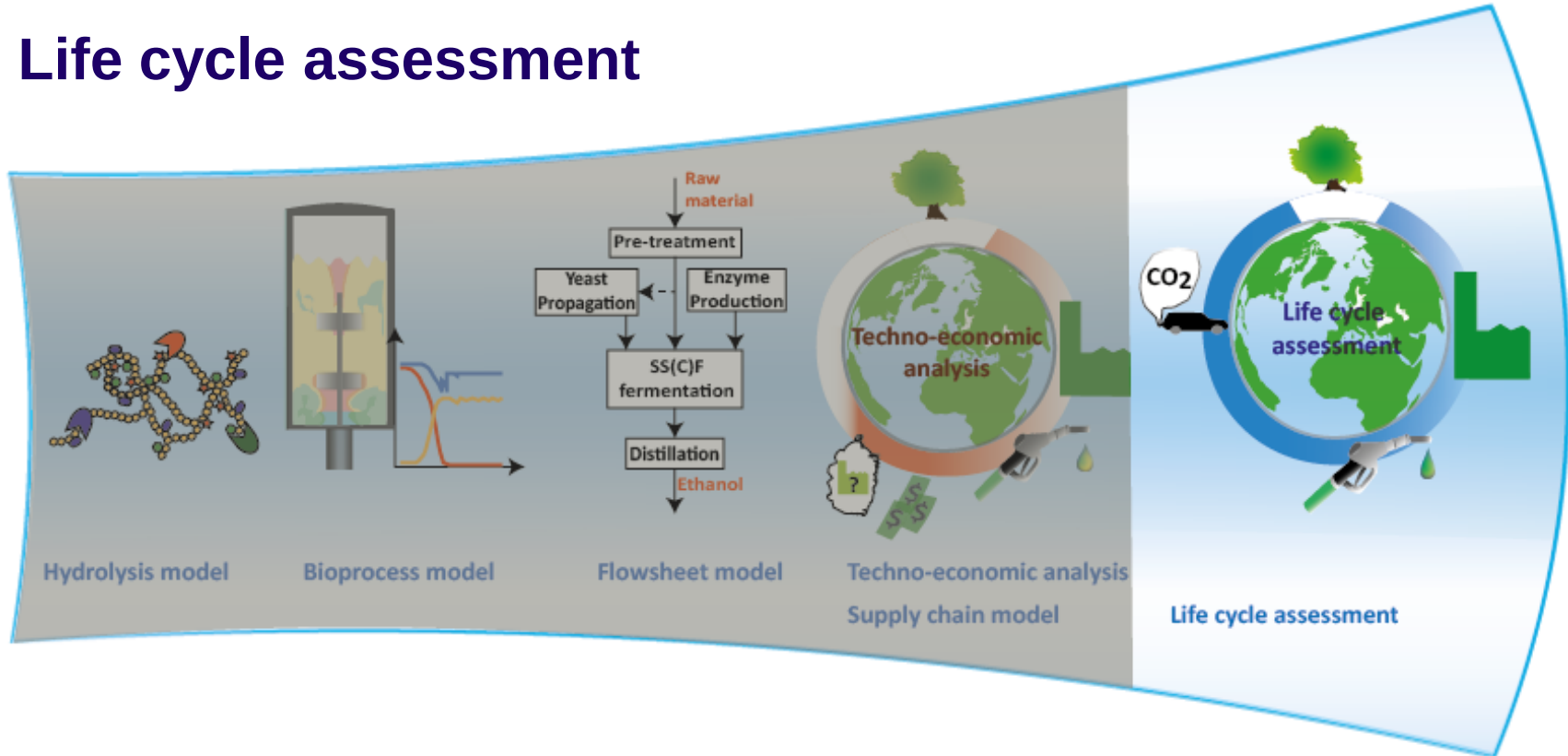
Introduction of process stop criterion: Stop process if $q_{\text{EtOH}} < 0.1$ g/Lh



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
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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

