

ProcessNet-Jahrestagung und 32. DECHEMA-Jahrestagung der Biotechnologen  
12.-15.09.2016, Aachen, Germany

# Systematic Downstream Development, Optimization, and Equipment Design for Biobased Products and Processes

Andreas Bednarz, Bettina Rüngeler, Peter Scherübel,  
Markus Schmidt, Andreas Pfennig

[andreas.pfennig@ulg.ac.be](mailto:andreas.pfennig@ulg.ac.be)

Products, Environment, and Processes (PEPs)

Department of Chemical Engineering

Université de Liège

[www.chimapp.ulg.ac.be](http://www.chimapp.ulg.ac.be)

Université  
de Liège



## outline

- challenges for biomass as feedstock
- cascaded option trees
- problems in downstream processing
- example
- conclusions

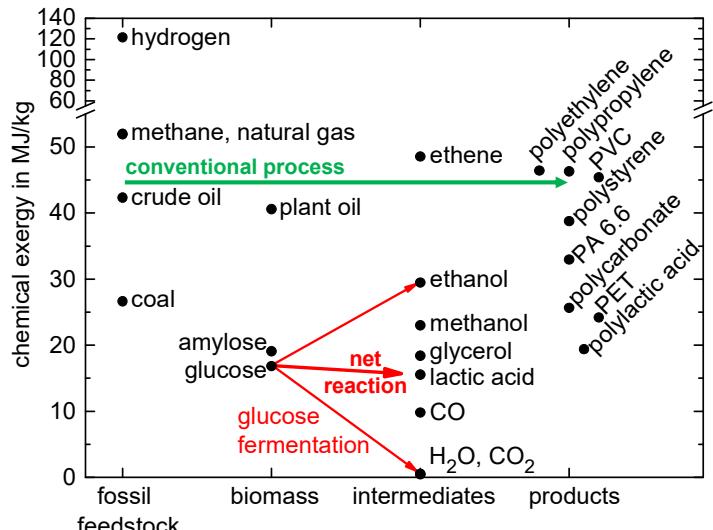
PEPs

CHEMICAL  
ENGINEERING

2 Université  
de Liège



## exergy as measure sorting the options



PEPs

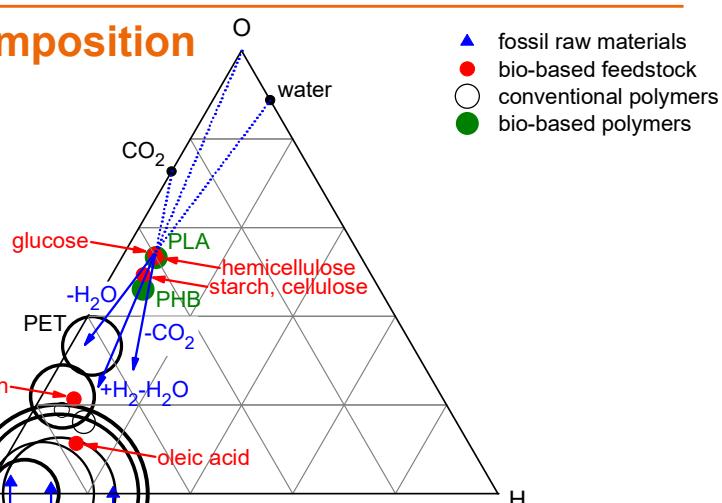
CHEMICAL  
ENGINEERING

3

Université  
de Liège



## COH composition



PEPs

CHEMICAL  
ENGINEERING

4

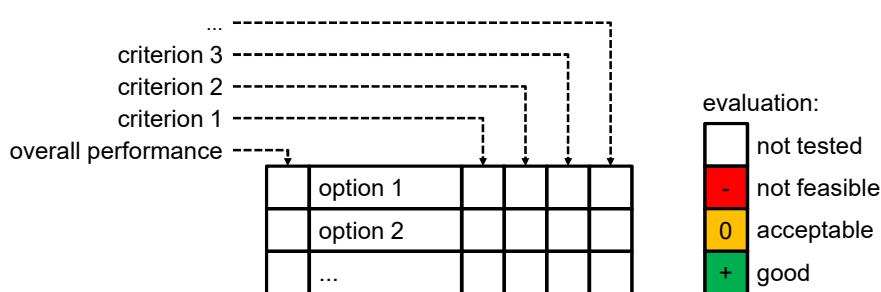
Université  
de Liège



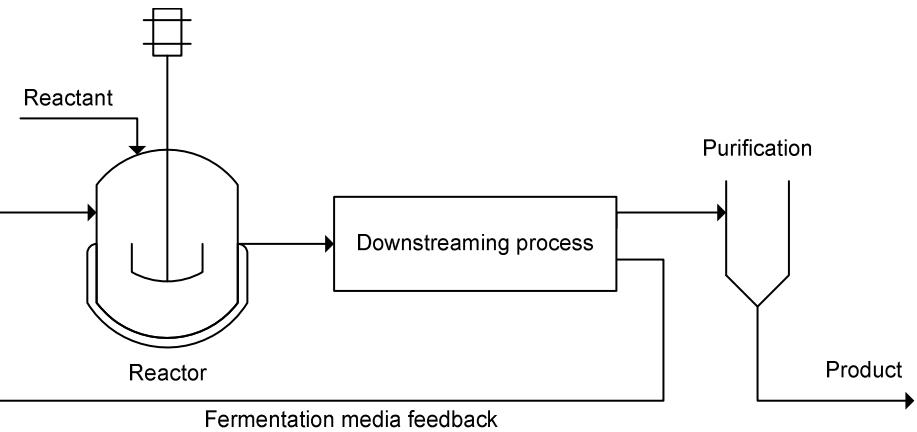
## challenges for biomass as feedstock

- new processes, new chemistry
- higher oxygen content
  - lower vapor pressure
  - higher viscosity
  - solids content
- new thermodynamics
- biotechnological steps
  - separate hydrophilic components from water
  - microbes act as solids

## characterizing options



## general process flow sheet



## cascading the tree

		product concentration			thermal stability			biocompatibility		
		-	distillation	-	-			-		
-		0	solvent extraction	+	+	0	+	0	0	0
+		+	reactive extraction	+	+	+	+	+	+	+
0		0	crystallization	0	0	+	-	-		

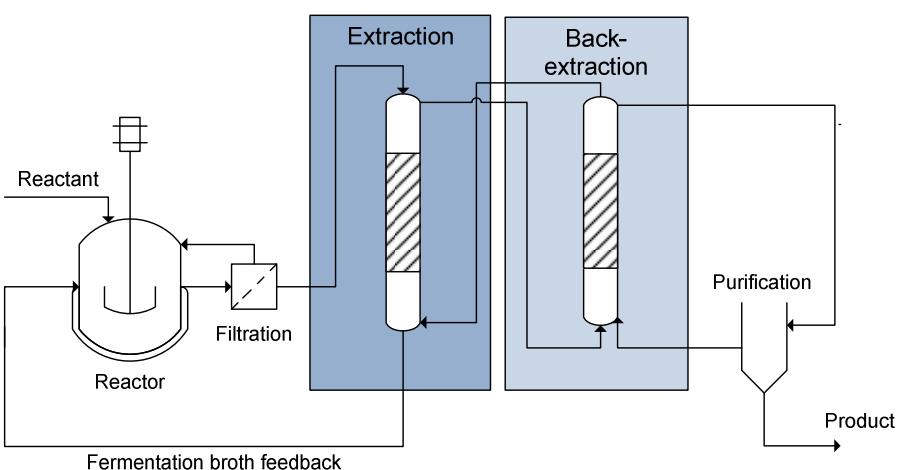
  

		toxicity of auxiliaries			coalescence			equilibrium		
		0	extractant 1	+	0	0	0	+	0	0
+		+	extractant 2	+	+	+	+	+	+	+
-		-	extractant 3	+	-	-	-	-		

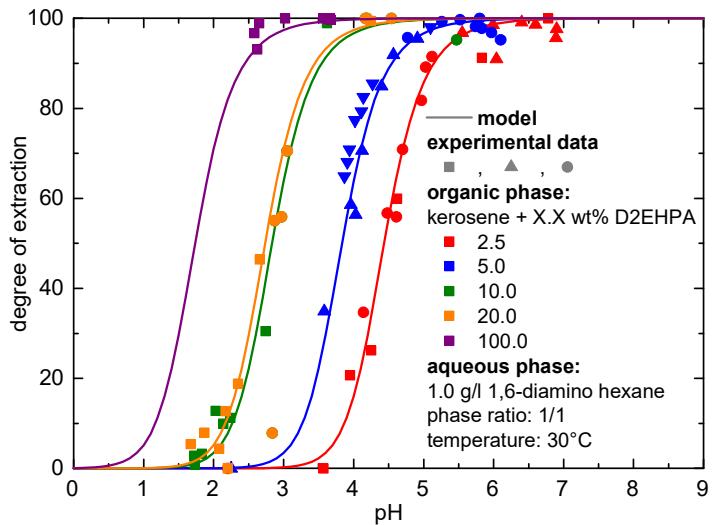
## evaluation of criteria

- expert knowledge
- literature information
- modelling, simulation
- experiment
- ... you name it

## process flow sheet



## basics of reactive extraction



PEPs

CHEMICAL  
ENGINEERING

11

Université  
de Liège



## crud basics



Crud:  
Chalk River Undefined Deposit  
corrosion residual unidentified deposit

S. Ruckes, A. Pfennig, 2010: Untersuchungen zum Einfluss von Mülle auf das Abscheideverhalten organisch-wässriger Stoffsysteme.  
AiF-Abschlussbericht zu Projekt 14997 N

PEPs

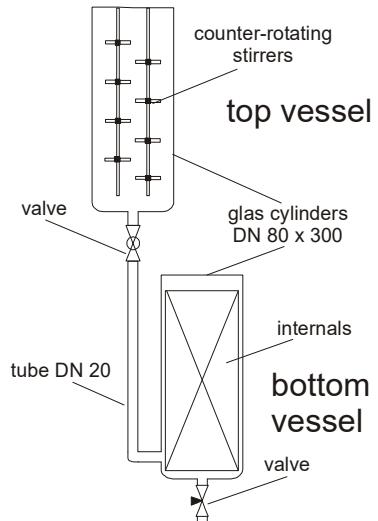
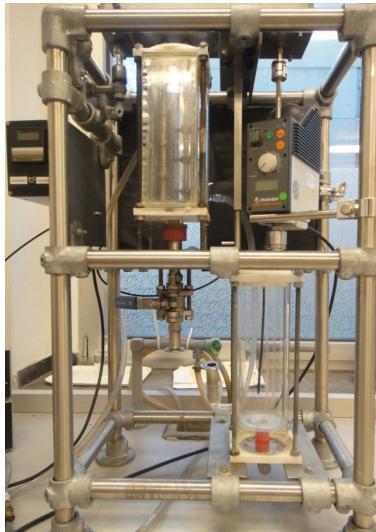
CHEMICAL  
ENGINEERING

12

Université  
de Liège



## standardized lab experiment for settling

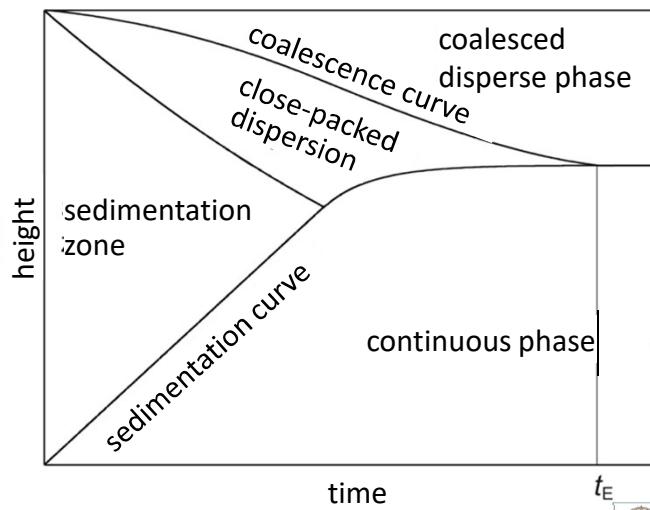
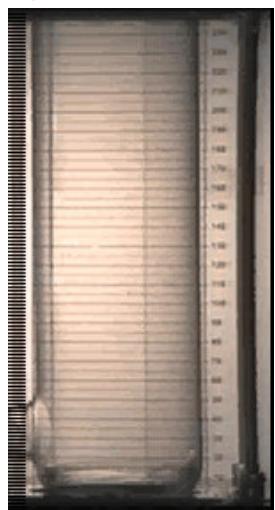


PEPs  
CHEMICAL  
ENGINEERING

13 Université de Liège



## principles of settling

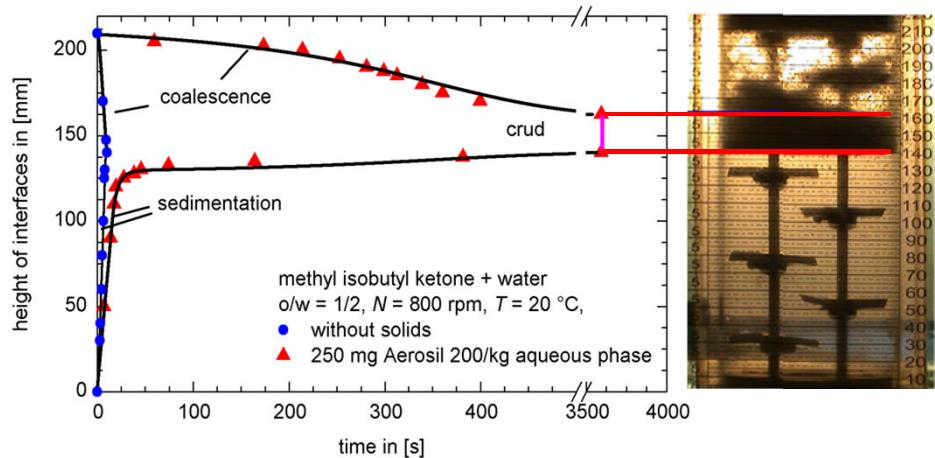


PEPs  
CHEMICAL  
ENGINEERING

14 Université de Liège



## influence of solids in settling experiment



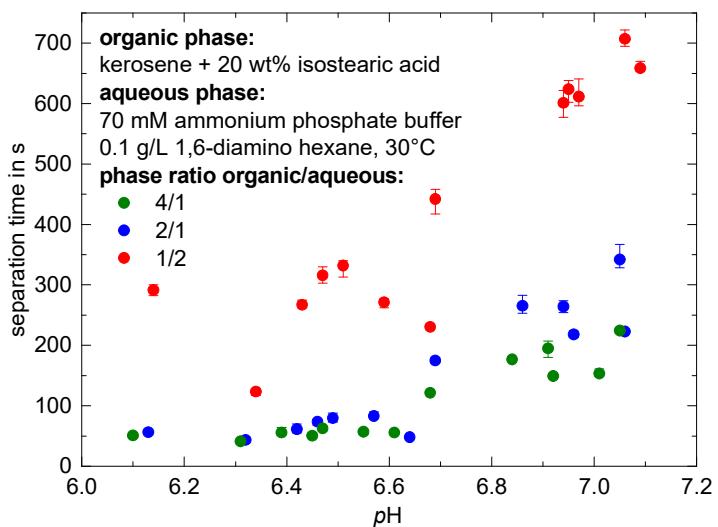
S. Ruckes, A. Pfennig, 2010: Untersuchungen zum Einfluss von Muim auf das Abscheideverhalten organisch-wässriger Stoffsysteme.  
 AIF-Abschlussbericht zu Projekt 14997 N



15 Université de Liège



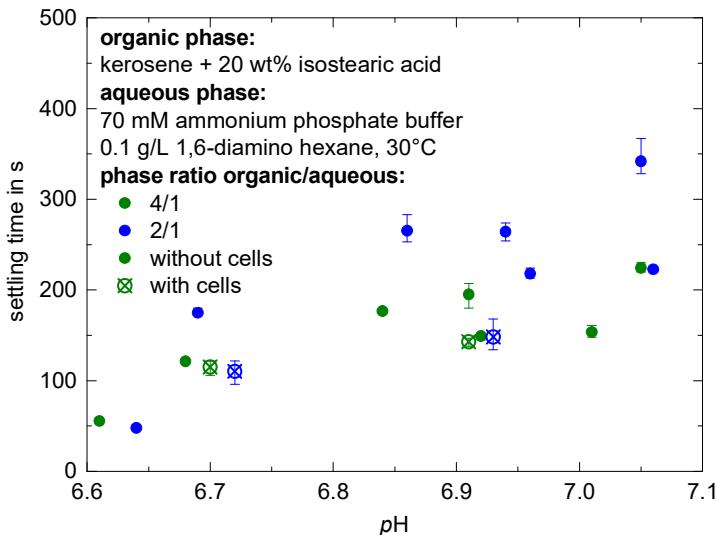
## phase separation



16 Université de Liège



## phase separation with cells

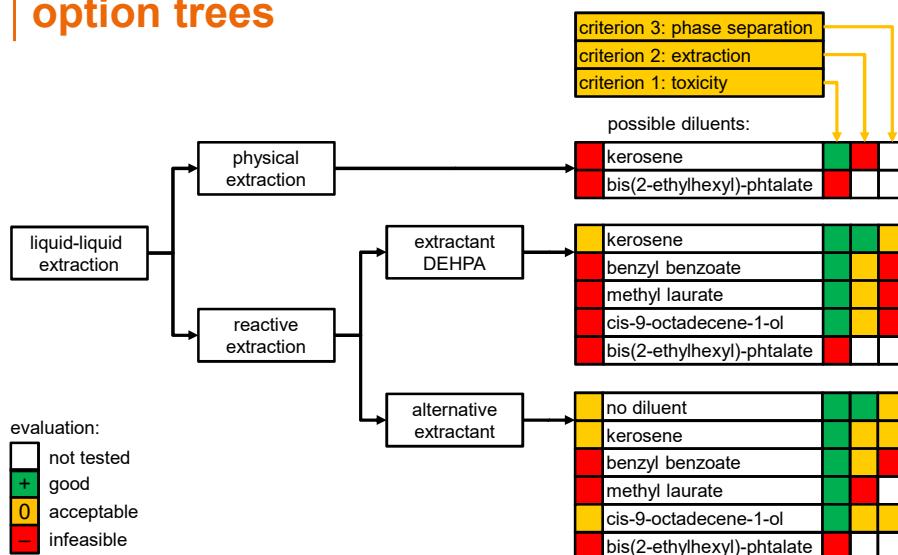


PEPs  
CHEMICAL  
ENGINEERING

17 Université de Liège



## option trees



PEPs  
CHEMICAL  
ENGINEERING

18 Université de Liège



## optimization criteria

- bio-compatible pH
- extractant concentration
  - capacity
  - pH-shift between extraction and reextraction
  - phase separation

## examples for different levels

- overall process options
- principal downstream options
- unit operations
- solvent selection
- direction of dispersion
- operating conditions like pH, phase ratio, etc.
- type of equipment
- ...
- also: modelling approaches, model contributions

## cascaded option trees

- clear book-keeping of options
  - cascading through levels
  - allows very different character of evaluations
  - documentation
- clear view of status also for communication
- clear view of second-best alternatives
- creates prototypes of procedures
- intuitive to use

A. Bednarz, B. Rüngeler, A. Pfennig:  
Use of Cascaded Option Trees in Chemical-Engineering Process Development  
Chem. Ing. Tech. 2014, 86(5), 611–620



21 Université de Liège



## Systematic Downstream Development, Optimization, and Equipment Design for Biobased Products and Processes

Andreas Bednarz, Bettina Rüngeler, Peter Scherübel,  
Markus Schmidt, Andreas Pfennig

[andreas.pfennig@ulg.ac.be](mailto:andreas.pfennig@ulg.ac.be)

Products, Environment, and Processes (PEPs)

Department of Chemical Engineering

Université de Liège

[www.chimapp.ulg.ac.be](http://www.chimapp.ulg.ac.be)

Université  
de Liège



## option tree method

choose starting level of detail

- note all feasible options
- note all relevant critical criteria
- sort criteria by relevance

evaluate options and criteria,  
preferably most critical criteria first

step to next  
level of detail

rank available  
options

at least one  
feasible  
option left?

yes

refinement  
required?

yes

no solution  
possible

solution  
found



23 Université de Liège



## some criteria for bio-downstream design

- extractant selection

- biocompatible physical-extraction system?
- partition coefficient in physical extraction
- biocompatible reactive extraction system.  
reactive extractant, diluent/solvent, modifier
- equilibrium without cells
- equilibrium with cells
- extraction kinetics
- ease of phase separation (column or mixer-settler or none)
- phase separation with cells
- ease of re-extraction (T or pH shift?)
- fate of reactants, minor components, impurities
- ...crud, choice of nutrient system, buffer system,...

- equipment design



24 Université de Liège

