Liquid-liquid extraction design under uncertainty

ISEC 2014

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Outline

- Motivation
- Framework for the design under uncertainty
- Resource allocation
- Cascaded option trees
- Conclusion

Motivation

- new solvent extraction processes
  - high-viscous media
  - fermentation broths
  - aqueous two-phase systems
- low expertise in design and scale-up
- high uncertainties in knowledge and data

Goal: Optimal resource allocation in design of common and new solvent extraction processes

Uncertainty as supporting information

- uncertainty of input data quantifiable
- uncertainty reducible by process development steps

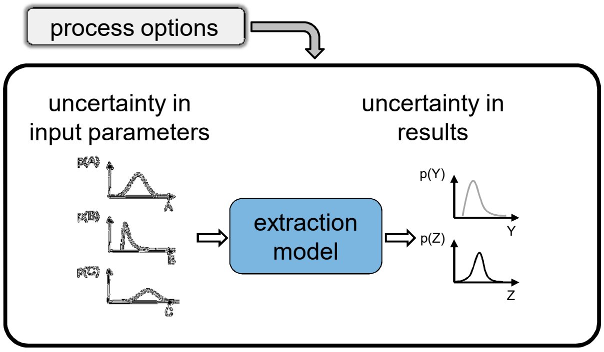
⇒ explicit consideration of uncertainties in all results

⇒ analysis of sensitivities towards uncertainty levels

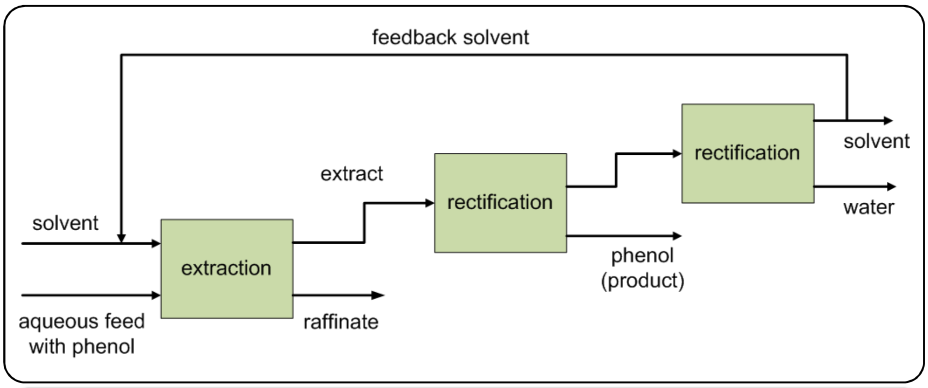
⇒ systematic reduction of uncertainty

- economics as criterion for the selection of best option

Design under uncertainty



Example process

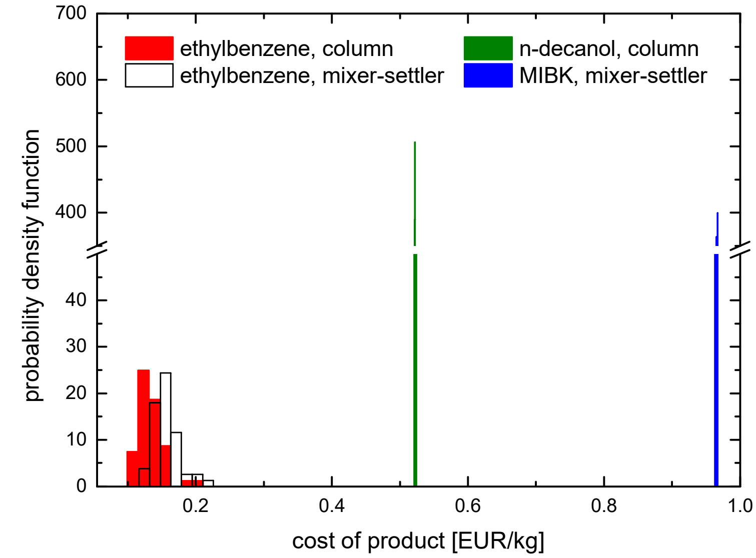


process options:

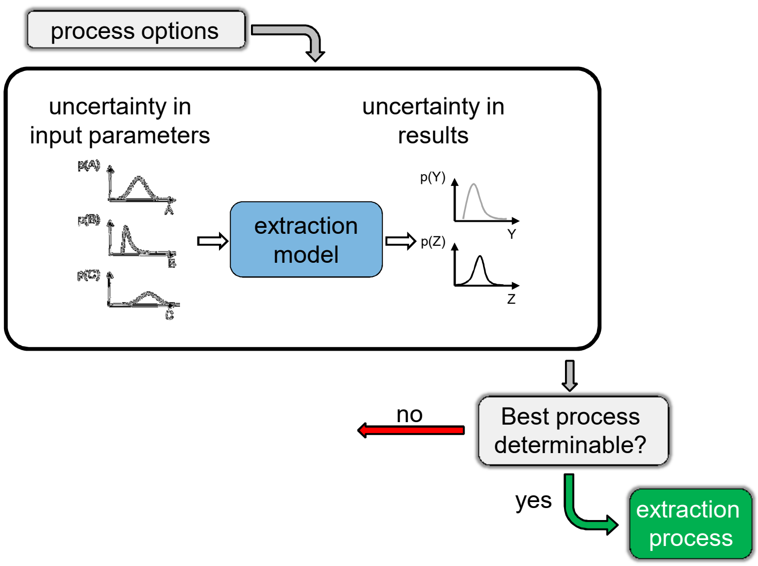
solvent
ethylbenzene
n-decanol
methyl isobutyl ketone (MIBK)

device
mixer-settler
column

Economics of various options



Design under uncertainty



modKL as distinctness measure

- modified Kullback-Leibler distance
- modification for symmetry: $\text{modKL}_{12}=\text{modKL}_{21}$
- comparison of distribution $p(x)$ and $q(x)$:

$$m(x)=\frac{1}{2}(p(x)+q(x))$$

$$\text{mod KL}=\int_{-\infty}^{\infty}\frac{1}{2}p(x)\ln\frac{2p(x)}{(p(x)+q(x))}dx+\int_{-\infty}^{\infty}\frac{1}{2}q(x)\ln\frac{2q(x)}{(p(x)+q(x))}dx$$

$p(x)=q(x)$:

$\text{mod KL}=0$

$p(x)\neq q(x)$:

$\text{mod KL}=\ln 2\approx 0.69$

value of modKL	distinctness
0	identical
modKL < 0.65	slightly different
≥ 0.65	strongly different
0.69	totally different

Berkelmans, I., 2010: *Development and Application of a Framework for Technology and Model Selection Under Uncertainty.* Massachusetts Institute of Technology

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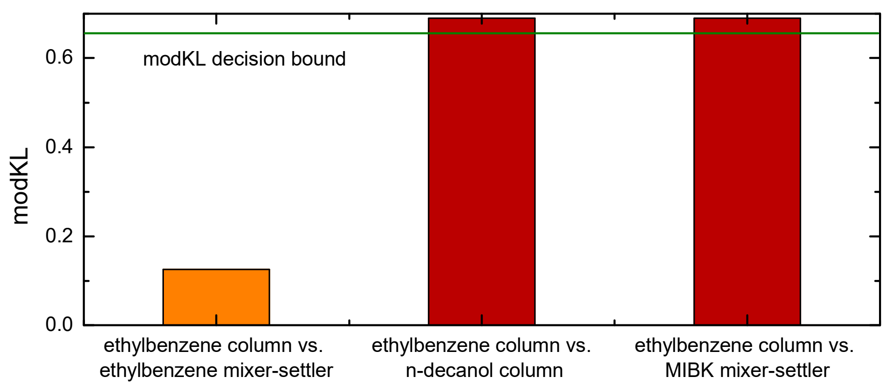
Comparison of processes



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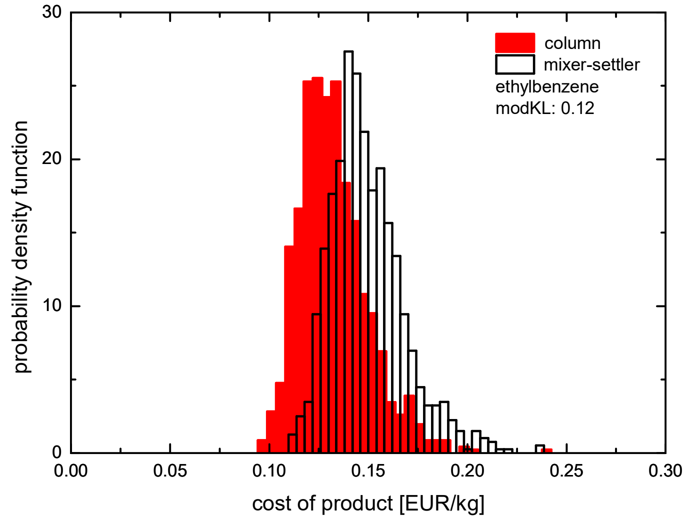
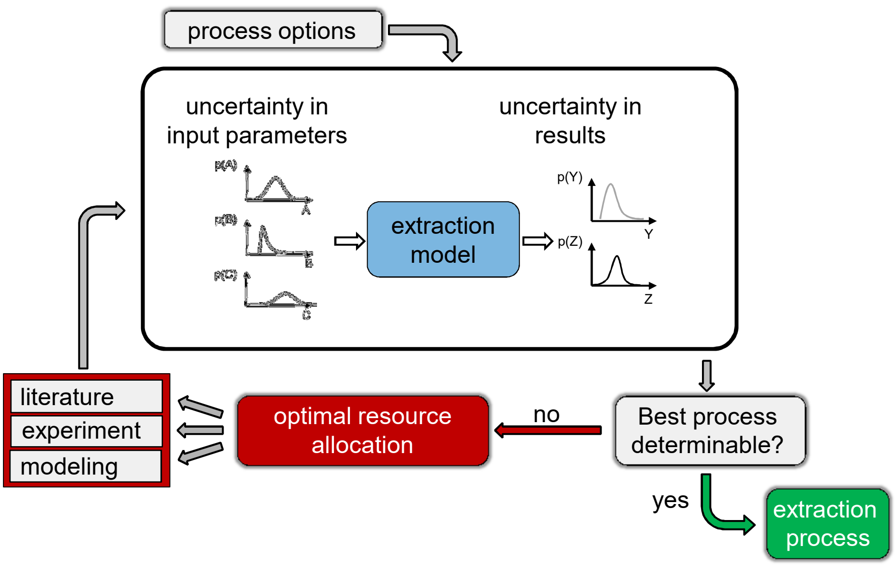
Economics of remaining options



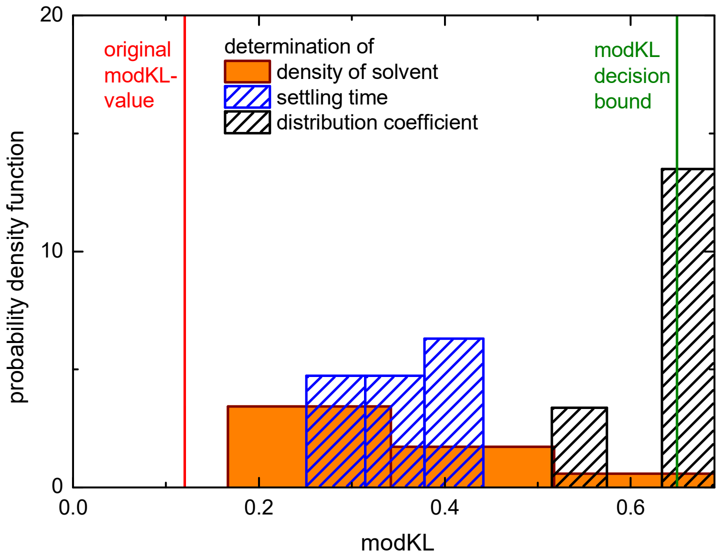
Design under uncertainty



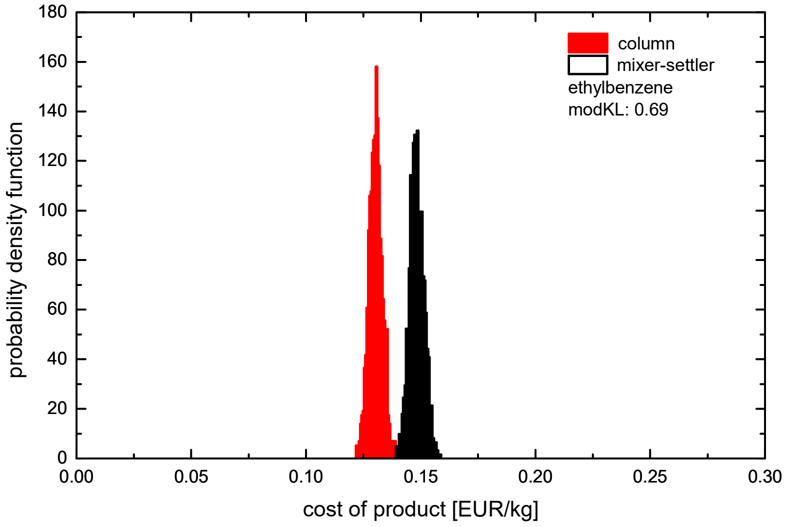
Definition of design steps

- methods for uncertainty reduction
  - literature | experiment | modeling
- reduce uncertainty for input parameters
  - distribution coefficient | density phase 1 | density phase 2 | interfacial tension
  - settling time | viscosity phase 1 | viscosity phase 2 | …
- associated data
  - new uncertainty level | analysis costs

Change of modKL values



New distribution after analysis



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Resource allocation

- How to choose next design step?
  cost – benefit analysis
- cost:
  - cost for research (work and material)
- benefit:
  - reduced uncertainty
  - less risk for decision on best process

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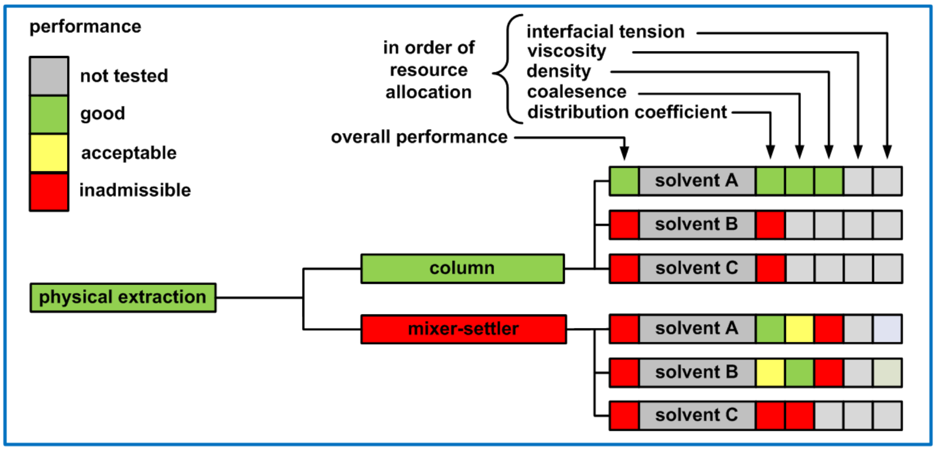
Clear summary of design steps

- cascaded option tree



Bednarz, A., Rüngeler, B., Pfennig, A., 2014: Use of Cascaded Option Trees in Chemical-Engineering Process Development, Chemie Ingenieur Technik 86 (5)

Conclusion

- use of uncertainties as additional information to process
- support for process engineer by systematic resource allocation
- remaining uncertainties at each step of process development visible
- framework for design of solvent extraction under uncertainties

Thank you for your attention.

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