Liquid-liquid extraction design under uncertainty

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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
Liquid-liquid extraction design under uncertainty

Example process

process options:
- solvent
  - ethylbenzene
  - n-decanol
  - methyl isobutyl ketone (MIBK)
- device
  - mixer-settler
  - column
Economics of various options

![Graph showing probability density function of cost of product for different extraction options](image)

**Design under uncertainty**

- **Process options**
- **Uncertainty in input parameters**
- **Extraction model**
- **Uncertainty in results**

- No best process determinable?
- Yes extraction process

*Liquid-liquid extraction design under uncertainty*
modKL as distinctness measure

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

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

\[
modKL = \int_{-\infty}^{\infty} \frac{1}{2} p(x) \ln \left( \frac{2p(x)}{p(x) + q(x)} \right) dx + \int_{-\infty}^{\infty} \frac{1}{2} q(x) \ln \left( \frac{2q(x)}{p(x) + q(x)} \right) dx
\]

- \( p(x) = q(x) \):
  - modKL = 0
  - value of modKL: 0
  - distinctness: identical
- \( p(x) \neq q(x) \):
  - modKL = ln2 \approx 0.69
  - value of modKL: \( \approx 0.69 \)
  - distinctness: totally different

<table>
<thead>
<tr>
<th>modKL</th>
<th>distinctness</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>identical</td>
</tr>
<tr>
<td>( &lt; 0.65 )</td>
<td>slightly different</td>
</tr>
<tr>
<td>( \geq 0.65 )</td>
<td>strongly different</td>
</tr>
<tr>
<td>0.69</td>
<td>totally different</td>
</tr>
</tbody>
</table>


Comparison of processes

Comparison of processes between ethylbenzene column vs. ethylbenzene mixer-settler, ethylbenzene column vs. n-decanol column, ethylbenzene column vs. MIBK mixer-settler.

Liquid-liquid extraction design under uncertainty
Economics of remaining options

Liquid-liquid extraction design under uncertainty

Design under uncertainty

process options

uncertainty in input parameters

extraction model

optimal resource allocation

Best process determinable?

yes

no

Best process
determinable?

extraction process

literature

experiment

modeling

probability density function

cost of product [EUR/kg]

0.00 0.05 0.10 0.15 0.20 0.25 0.30

0 10 20 30

column
mixer-settler
ethylbenzene
modKL: 0.12

Liquid-liquid extraction 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

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Change of modKL values

- original modKL-value
- determination of density of solvent settling time distribution coefficient
- modKL decision bound

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New distribution after analysis

![Graph showing probability density function for cost of product (EUR/kg) with two data sets: column and mixer-settler for ethylbenzene, modKL: 0.69.]

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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

Liquid-liquid extraction design under uncertainty
Clear summary of design steps

- cascaded option tree

**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.

**Liquid-liquid extraction design under uncertainty**

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