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Optimisation Based Design of Membrane Assisted Hybrid Separation Processes Using an Evolutionary Algorithm

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Introduction

Motivation

Design of energy efficient distillation processes for the separation of non-ideal multicomponent mixtures

- **Conventional separation methods:** extractive, heteroazeotropic or pressure swing distillation
  - High capital costs
  - Low energy efficiency
- **Innovative process concept:** membrane assisted hybrid processes
  - Strong synergies due to interactions between both unit operations
    ➡ Overcoming limitations of stand-alone processes
  - Lack of general design methodology and in-depth understanding of complex interactions
    ➡ Significant economical potential hardly exploited in industry

Development of a reliable methodology for the optimisation based design of hybrid separation processes

Chemical system

- Production of acetone by dehydrogenation of isopropyl alcohol (IPA)
- Separation of ternary azeotropic system acetone-IPA-water
- Potential use of membrane:
  - To cross the distillation boundary (Fig. 1)
  - To separate the close boiling binary mixtures at high organic concentrations (Fig. 2)

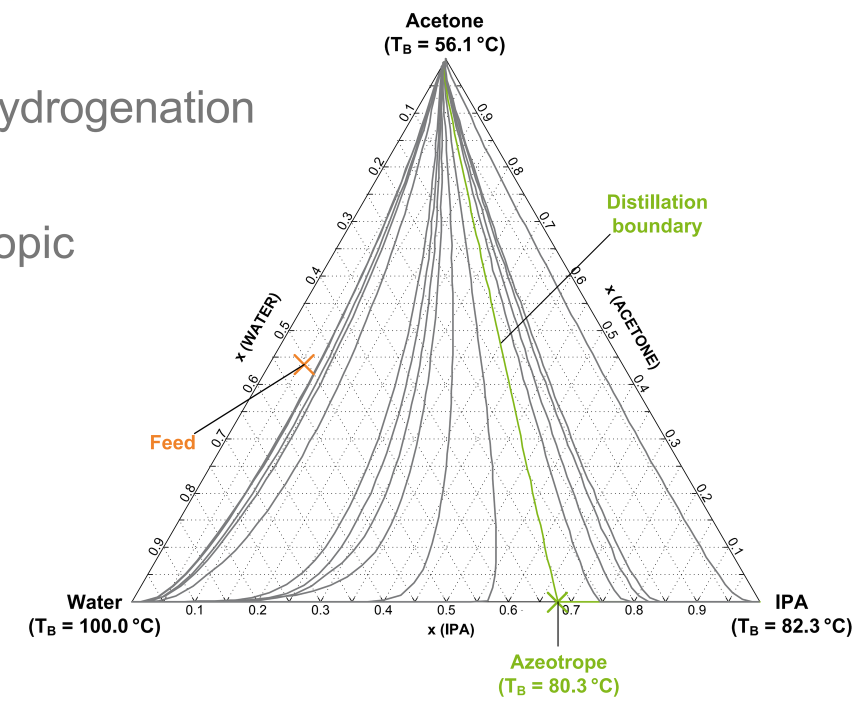


Fig. 1: Residue curve map for ternary system acetone-IPA-water at p = 1 atm

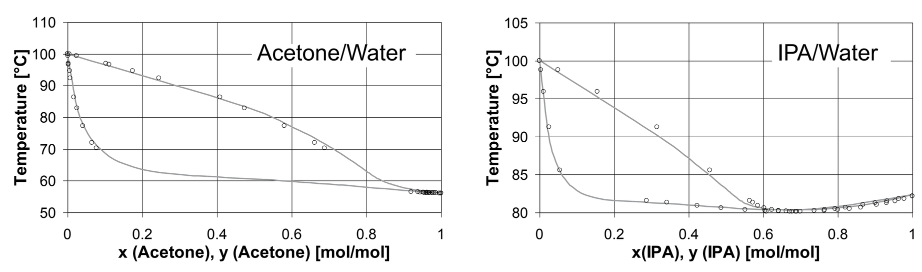


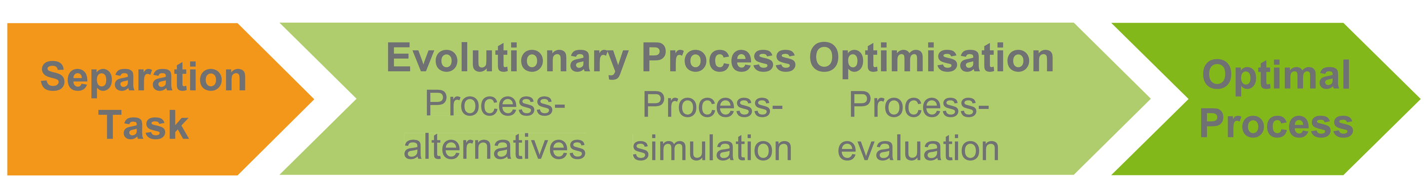
Fig. 2: Binary VLE at p = 1 atm. Lines: Data from Aspen Properties® using NRTL-RK; Symbols: experimental data

Approach

Design of hybrid processes

- State of the art:
  - Early decision on process configuration
  - Design approaches mostly based on short-cut methods and simplified models, especially for membrane separation
  - Application of rigorous approaches limited to binary systems

Generic design approach



- Process superstructures for the consideration of all possible process alternatives
- Generic process model with rigorous models for both unit operations
- Simultaneous optimisation of process configuration, dimension of apparatus and operating conditions
- Experimental determination of membrane parameters at lab-scale and experimental validation of hybrid process at pilot-scale

Modelling

- Non-equilibrium stage model of distillation
  - Multicomponent mass and heat transfer
  - Hydrodynamics of column internals considered
  - Calculation of optimal diameter based on correlation of Maćkowiak[1)]
- Detailed model of membrane separation
  - Transmembrane mass transfer based on solution-diffusion model
  - Consideration of all relevant mass transfer resistances

1) J. Maćkowiak, Fluid dynamics of packed columns, Springer-Verlag (2010)

Evolutionary optimisation

- Algorithm based on „modified differential evolution" approach[2)] (Fig. 3)
- Economic objective function (= fitness)

2) R. Angira et al., Chem. Eng. Sci., 61 (2006), 4707-4721

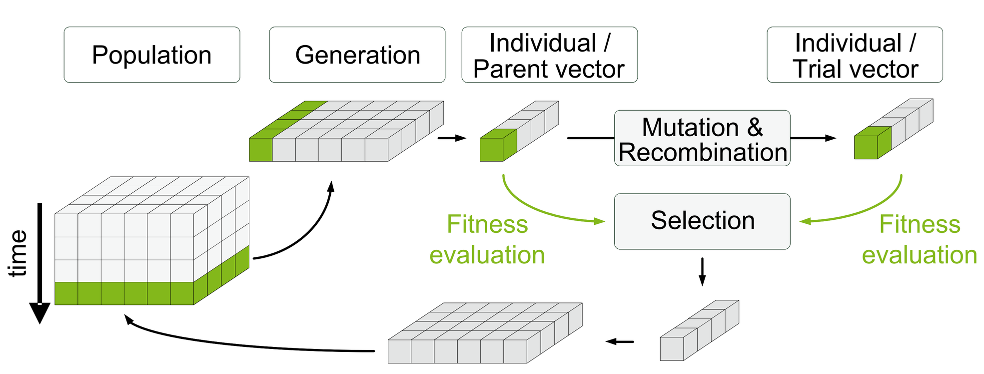


Fig. 3: Simplified flowchart of evolutionary algorithm

Results

Experimental parameter determination

- Pervaporation of IPA-water mixture
- Hydrophilic PVA/PAN membrane (Sulzer Pervap 2201D)
- Membrane area: 162 cm²
- Experimental conditions:
  - $w_{Feed,H2O}$ = 2,5 - 18 wt.%
  - T_{Feed} = 60 - 78 °C
  - p_{Feed} = 2 bar
  - p_{Perm} = 30 mbar
- Model parameters determined for an empirical correlation (Fig. 4)

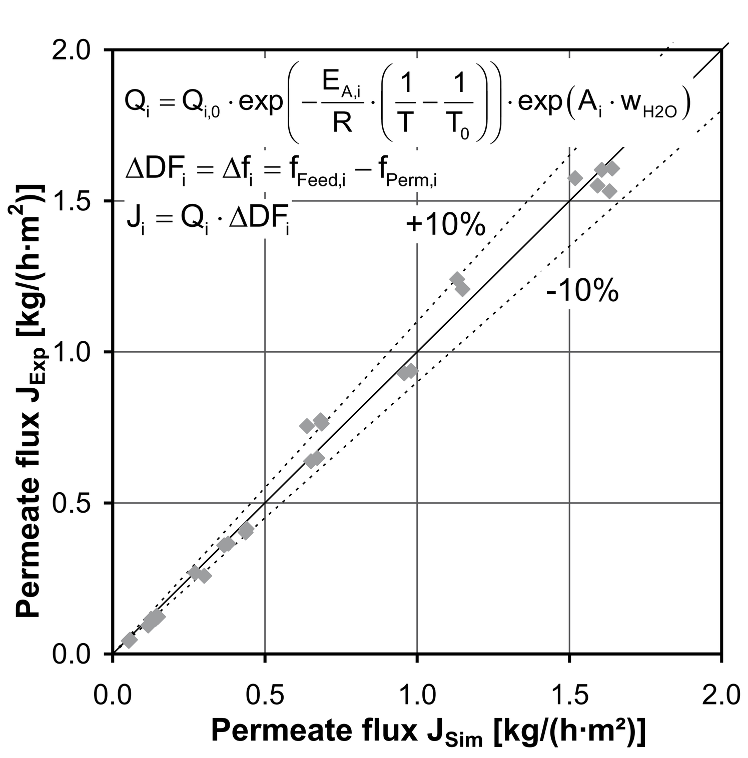


Fig. 4: Parity plot of simulated and measured permeate flux for IPA-water using the empirical correlation

Future work

Future work will focus on the development and optimisation of more complex superstructures, which consider all possible process configurations.

Optimisation of hybrid process

- Hybrid process
  - Packed column (Sulzer BX)
  - Pervaporation module with Sulzer Pervap 2201D
- Simultaneous optimisation of
  - 3 discontinuous and
  - 9 continuous variables (Fig. 5)
- Objective function: costs per ton of purified acetone (CPT)

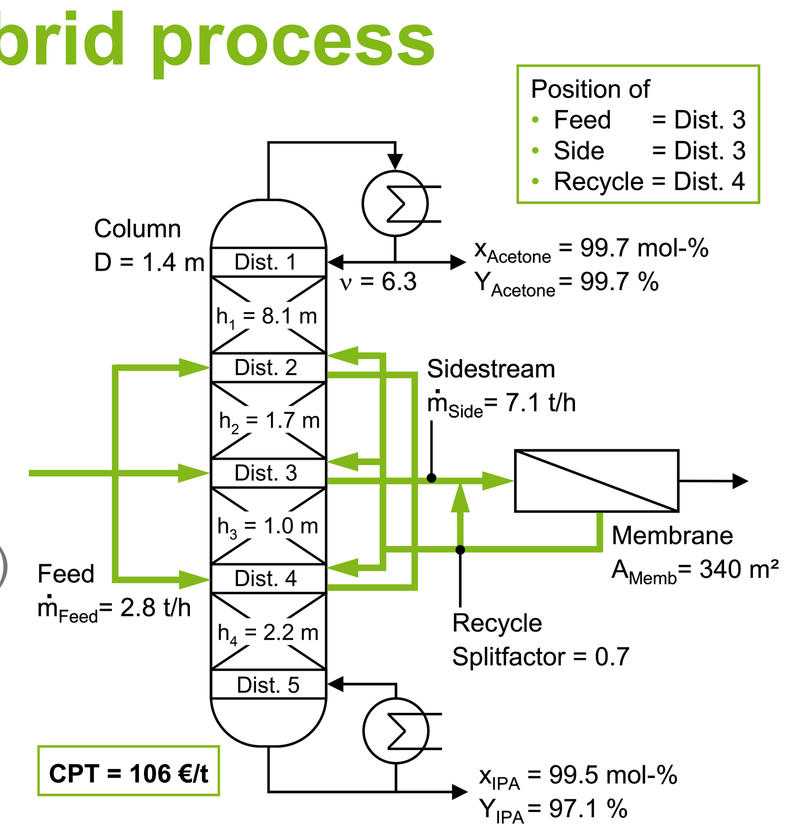


Fig. 5: Superstructure of hybrid process and results of evolutionary optimisation

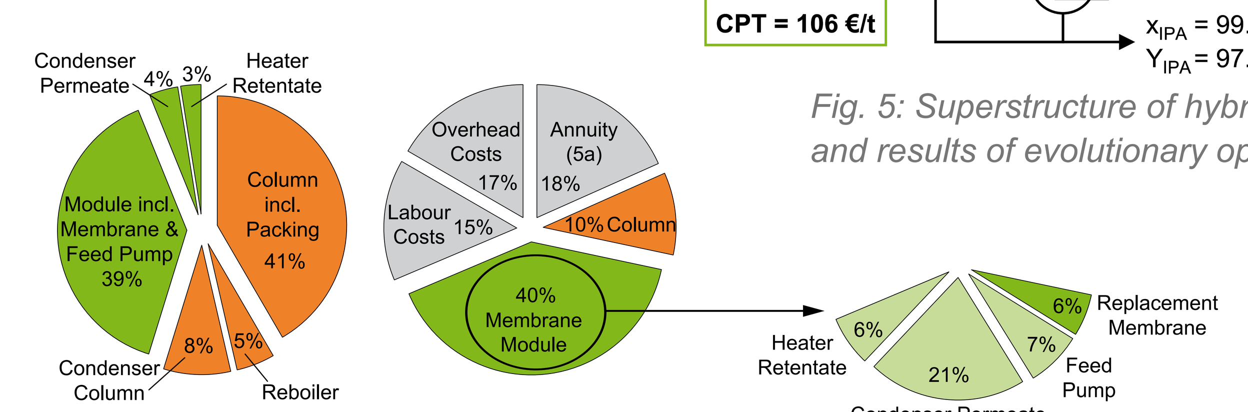


Fig. 6: Distribution of investment costs (left) and operating costs (right) for optimised hybrid process

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