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Modelling and simulation of the TAEE synthesis by reactive distillation

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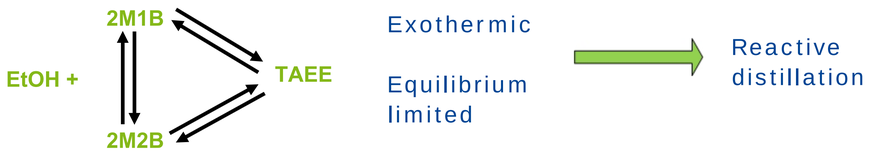
Introduction

Fuel additives

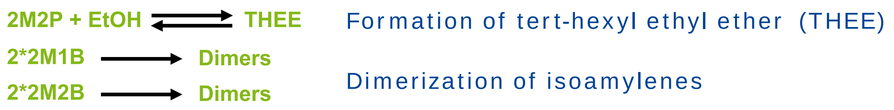
- Tertiary ethers are important additives in gasoline to:
  - Enhance the octane number
  - Improve combustion
  - Reduce emissions
- Methyl-tert butyl ether (MTBE) is the most common ether used in gasoline blending, but:
  - Insufficient supply of Isobutene (limiting reactant in the MBTE synthesis)
  - Groundwater pollution (high solubility of MTBE in water)
- The production of other oxygenated compounds, such as tert-amyl ethyl ether (TAEE) is of present interest, due to:
  - Low solubility in water
  - Removal of reactive olefins from fluid catalytic cracking (FCC)

Chemical system

- TAEE is synthesized by the reactions between the two isomers 2-methyl-1-butene (2M1B) and 2-methyl-2-butene (2M2B) with ethanol (EtOH)



- Stream from FCC was taken as a source of isoamylenes (IA)
- More than 100 components and at least 20 azeotropes
- Examples of side reactions:



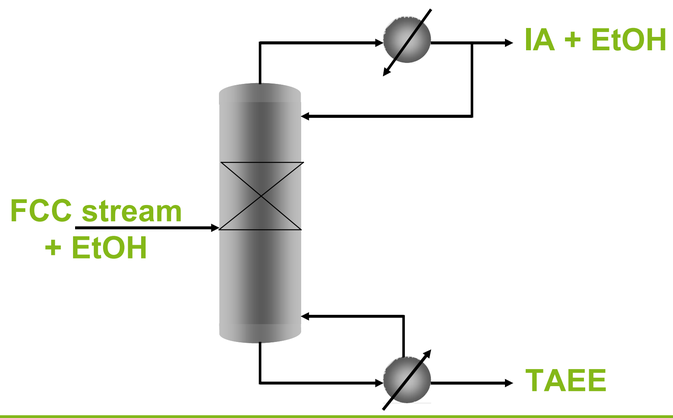
Experiments and Modelling

Experimental setup[2]

Figure 1: TAEE pilot plant

Experimental column setup

Height of reactive section [m]	1 (KATAPAK SP11 with Amberlyst 47
Height of stripping section [m]	2 (MELLAPAK 750Y)
Height of rectifying section [m]	1 (MELLAPAK 750Y)
Column diameter [mm]	200
Feed location	Bottom of the reactive section
Feed rate [mol/h]	380
Pressure [bar]	4
Reflux ratio	1.71
D/F (mol/mol)	0.79



Model assumptions

- Non-equilibrium stage model based on the Maxwell-Stefan approach
- Pseudohomogeneous (reaction only in the liquid phase)
- Non-idealities of the liquid phase were described with the UNIFAC method
- Hydrodynamics and mass transfer were taken into account by using packing specific correlations[a, b, c]
- 18 components and 6 reactions are considered (TAEE synthesis, dimerization of isoamylenes and formation of THEE)
- Kinetics were taken from literature[d]
- An existent model[e] in Aspen Custom Modeler® was modified in order to consider the TAEE synthesis

[a] Rocha J. A., Bravo J. L., Fair J. R., Ind. Eng. Chem. Res. 32 (1993) 641–651
[b] Rocha J. A., Bravo J. L., Fair J. R., Ind. Eng. Chem. Res. 35 (1996) 1660–1667
[c] Brunazzi E., Viva A., INSERT project, 2006
[d] Linnekoski J. A., Krause A. O., Rihko L. K., Ind. Eng. Chem. Res. 36 (1997) 310-316
[e] Klöker M., Kenig E. Y., Hoffmann A., Kreis P., Gorak A., Chem. Eng. Proc. 44 (2005) 617–629

Results

Model validation

- Excellent agreement between experiments and simulation (Fig. 2)
- No ethanol and isoamylenes are present in the bottom
- Low mole fraction of TAEE in the bottom (~23 mole %)

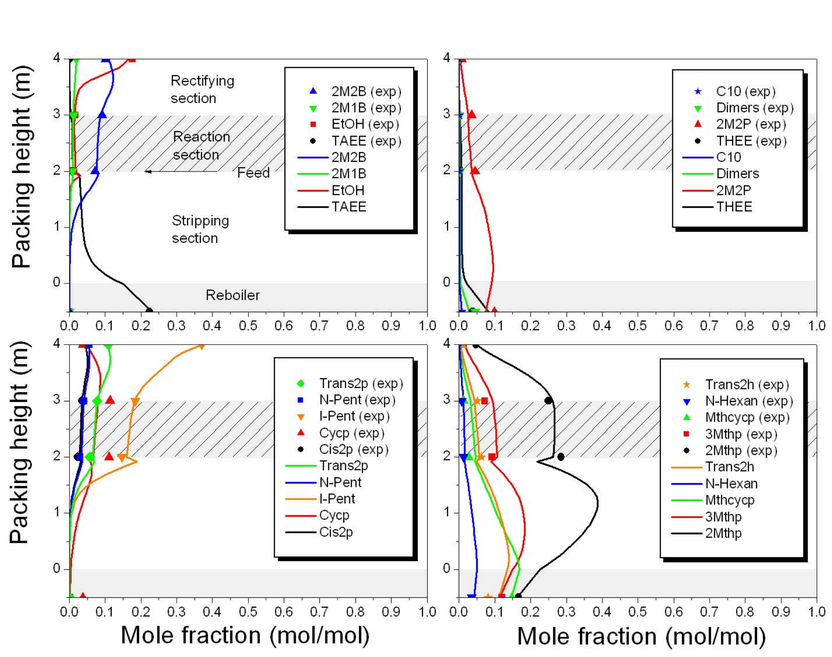


Figure 2: Composition profiles in the liquid phase

Simulation studies

- Optimal operating conditions were found to obtain the highest conversion (around 40%) for the investigated column configuration
- Multiplicity of steady states was found

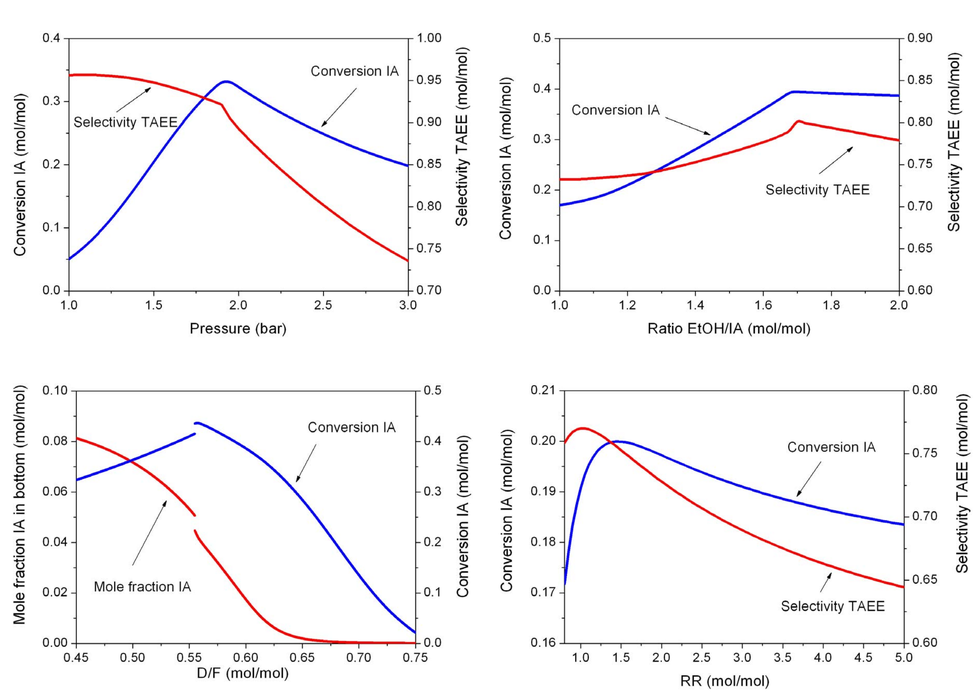


Figure 3: Influence of operating parameters on conversion and selectivity. Pressure = 3 bar, RR = 1.84, D/F = 0.62 (mol/mol), Ratio EtOH/IA =1.16 (mol/mol)

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