Modelling Luyben's Chemical Processes with COCO + ChemSep

Ross Taylor, Harry Kooijman and Brett Walker
Clarkson University, Potsdam, New York

Jasper van Baten
AmsterCHEM, Las Rozas, Spain

AICHE Meeting October 18, 2011 (paper 215d) Distillation Honors Session William Luyben
Outline

- Luyben's Flowsheets
- Introduction to COCO
- What is CAPE-OPEN?
- Example flowsheets
- Lessons learned
Luyben's Flowsheets

- **Class D: Distillation Only**
  - Columns, heat exchangers, recycle
  - *NO (separate) reactors*

- **Class C: Complicated Flowsheets**
  - Columns, heat exchangers, recycle
  - *Chemical reactors*
  - *Other unit operations*
Luyben's Flowsheets

- **Class D: Distillation Only**
  - Pressure Swing Azeotropic Distillation
  - Extractive Distillation
  - Heterogeneous Binary/Ternary Azeotropes
  - Reactive Distillation

- **Class C: Complicated Flowsheets**
  - Cumene Process
  - Butyl Acetate Process
  - Ethanol – Water with membrane unit
Luyben's Flowsheets (with Aspen Simulation)

- Analysis
- Steady State Design
- Optimization
- Process Dynamics
- Control
Luyben's Flowsheets with COCO

- Analysis
- Steady State Design
- Optimization
- Process Dynamics
- Control
COFE: CAPE-OPEN Flowsheeting Environment

- Graphical flowsheeting
- Graphing
- Multiple models
- Logging
- Streams view
Introduction to COCO:

Simulation environment (COFE)

Thermodynamic property package (TEA)

Collection of unit operations (COUSCOUS)

Reaction package (CORN)

Download COCO: http://www.cocosimulator.org/
Flowsheeting engines

Dynamic

Steady state

Equation based

Modular

Sequential

Non-sequential
COFE: CAPE-OPEN Flowsheeting Environment

- Breaking recycles by automatic tearing
- Solving recycles by hybrid Newton / Wegstein approach, using reparameterization
- Support for multiple material types, with selection for thermo and sub-set of compounds
- Material, energy and information streams
Simulation environment process space

- overall process model
  - built-in sub models
  - 3rd party sub models (CAPE-OPEN)
  - user sub models (non CAPE-OPEN)
Simulation environment process space

overall process model (COFE)

Thermo models

TEA

3\(^{rd}\) party thermo models (CAPE-OPEN)

3\(^{rd}\) party thermo models (CAPE-OPEN)

Unit operation models

3\(^{rd}\) party unit models (CAPE-OPEN)

3\(^{rd}\) party unit models (CAPE-OPEN)

Reaction models

CORN

ChemSep

COUSCOUS
• Pure compound data library (extendible, or use DIPPR)

• 100+ Property calculation methods (25+ different properties)

• Property derivatives

• Support of external property calculation routines and external equilibrium servers
COUSCOUS: Simple unit operations
CORN: CAPE-OPEN Reaction Package

• Create reaction package
  • Define or import compounds
  • Define reactions with stoichiometry
  • Define reaction rates (or use Wizard) or equilibrium constant
  • Define reaction phase

• Insert reaction package into simulation

• Assign reaction package to reactor unit operation
Who/What is CAPE-OPEN?

CPI

Software vendors

Academic institutions

Other members

The CAPE-OPEN standard is the de facto standard for interfacing process modelling software components for use in the design and operation of chemical processes. It is based on universally recognised software technologies, such as COM and CORBA. The CO standard is open, multi-platform, uniform and available free of charge.
Luyben's Flowsheets

- Pressure Swing Distillation of Acetone – Methanol
- Butanol / Water Separation
- THF / Water Separation with Heat Integration
- Cumene Process
- Column / Pervaporation Membrane Process (Ethanol / Water)
- Methanol from Syngas
- Butyl Acetate
- BTX Divided-Wall Column
Pressure Swing Distillation of Acetone-Methanol


Feed 540 kmol/h  $x_M=0.5$

Recycle
187 kmol/h

1 bar
10 bar

-13.2 MW
-5.8 MW

RR=2.36
RR=3.11

C1
C2

$R=0.75$
$R=0.75$

54
51
61

43
41

458 kmol/h

+12.8 MW

Methanol

$x_M=0.995$

Acetone

$x_A=0.994$

$540 \text{ kmol/h}$ $x_M=0.5$ $187 \text{ kmol/h}$ $R=2.36$ $x_A=0.75$ $R=3.11$ $x_A=0.75$ $-13.2 \text{ MW}$ $-5.8 \text{ MW}$ $54$ $51$ $61$ $43$ $41$ $458 \text{ kmol/h}$ $+12.8 \text{ MW}$ Methanol $x_M=0.995$ $+7.4 \text{ MW}$ Acetone $x_A=0.994$
Cumene Process

Methanol from Syngas


Syngas
11450 kmol/h
50°C
51.2 bar
0.6746 H₂
0.0030 N₂
0.2297 CO
0.0686 CO₂
0.0023 H₂O

4.6 MW
-6.1 MW
4.5 MW
98.3°C 75 bar
38°C
83.1°C 110 bar

2.9 kW
0.669 kmol/h
324°C
110 bar

-28.9 MW
1 bar
64.1°C
RR=0.88

3312 kmol/h
0.006 CO₂
0.992 MeOH
0.001 H₂O
2 ppm CO
276 ppm CH₄
8 ppm N₂

715 kmol/h
0.0001 MeOH
0.9999 H₂O

267°C 107.5 bar
145°C 109 bar
150°C 75 bar
173.5°C 107 bar
38°C 106.5 bar

218.1 kmol/h
37.2°C
2 bar

718.4 kmol/h
0.005 CO₂
226 ppm CH₄
0.816 MeOH
0.179 H₂O
12 ppm H₂

4027.4 kmol/h
0.005 CO₂
226 ppm CH₄
0.816 MeOH
0.179 H₂O
12 ppm H₂

499.4°C 110 bar
1.3 MW

Vent
840.5 kmol/h
0.535 H₂
0.041 N₂
0.038 CO
0.085 CO₂
0.295 CH₄
0.006 MeOH
339 ppm H₂O

Reactors
145°C 109 bar
150°C 75 bar

HP Separator
More Flowsheets

- Dimethylether (*Distillation Design and Control using Aspen Simulation*)
- Extractive Distillation
- Heterogeneous Ternary Distillation (Alcohol-Water-Entrainer)
- Reactive Distillation of $A + B \rightarrow C + D$
- TAME
- Air Separation Unit
- Ethylene Oxide
- Light Ends Unit
Luyben's Flowsheets with COCO

- Analysis
- Steady State Design
- Optimization
- Process Dynamics
- Control
Some Lessons Learned

- Luyben's chemical processes can be modeled in steady state using COCO
- Some of Luyben's design specs need to be altered
- Results may differ – largely due to (slightly) different thermo
- Use of “make-up mixer” makes flowsheets much more robust to solve
- Use fixed conversion reactor before incorporating reaction kinetics
- To be useful in teaching design COCO/ChemSep need a databank for more compounds than exists at present; databank extended for Luyben flowsheets + use up to 40 compounds in ChemSep v6.9 columns!
- COCO no more difficult to learn to use than UNISIM Design (UD)
- COCO useful in mass and energy balances class where simple component splitter models and conversion reactors are typical
Luyben's Flowsheets: Can we please have some more?