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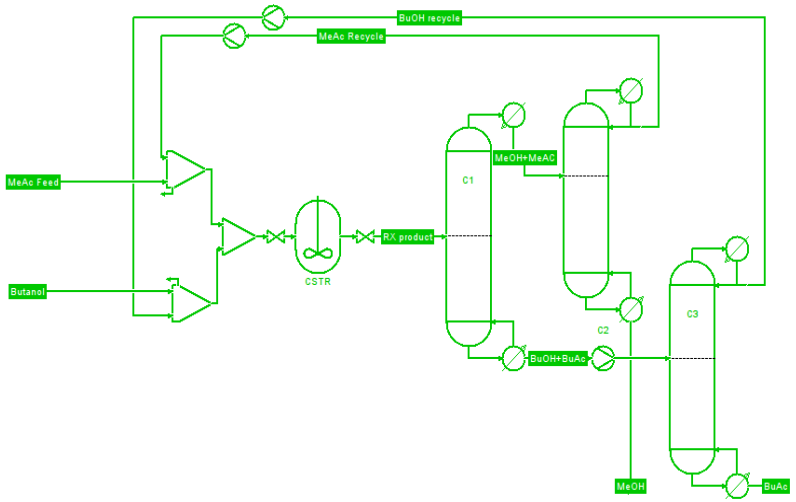
ChemSep
Modeling Separation Processes

Modelling Luyben's Chemical Processes with



COCO+ChemSep

Ross Taylor, Harry Kooijman and Brett Walker

Clarkson University, Potsdam, New York

Jasper van Baten

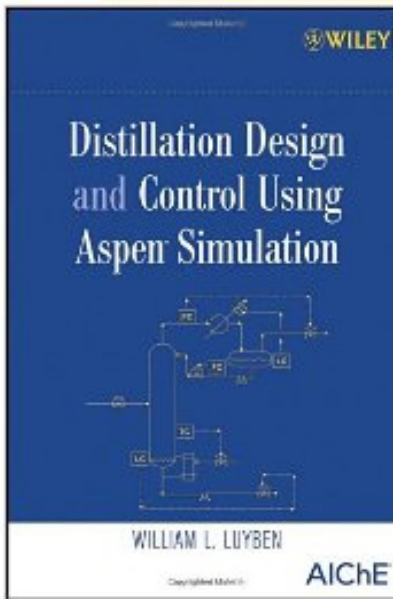
AmsterCHEM, Las Rozas, Spain

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

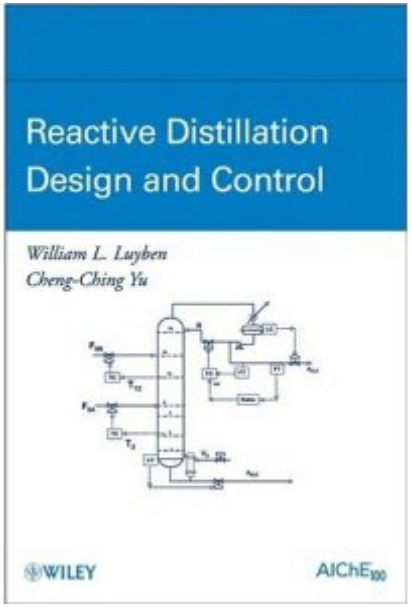
Outline

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

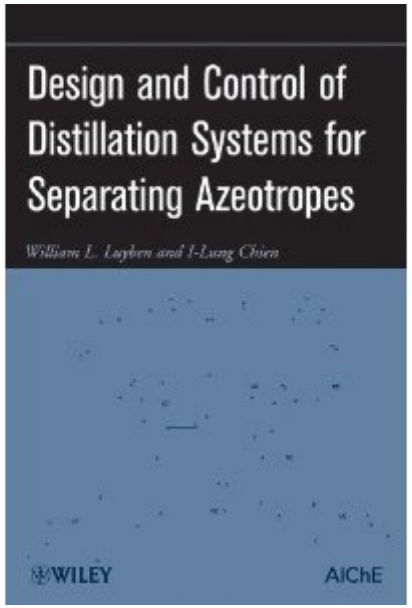
Luyben's Flowsheets



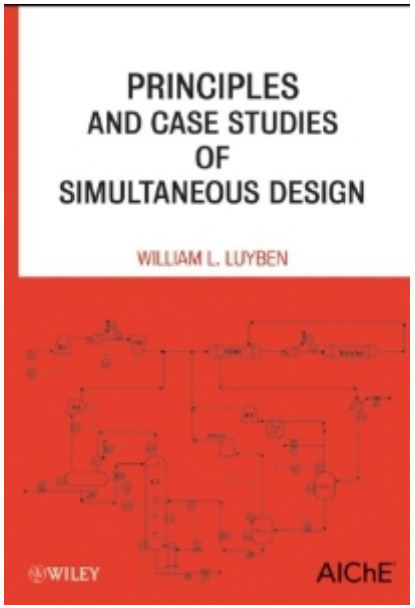
2006



2008



2010



2011

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~~

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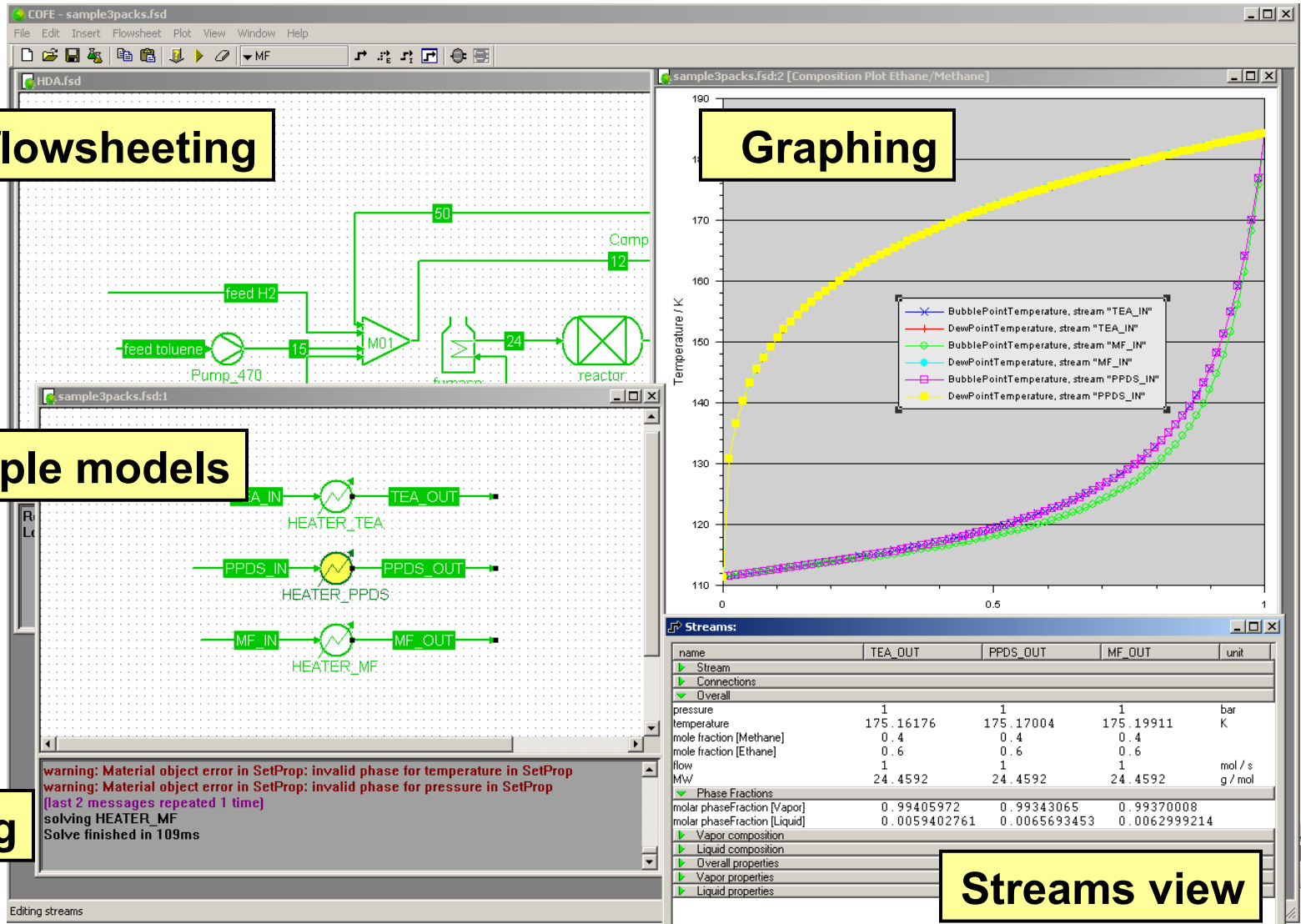
COFE: CAPE-OPEN Flowsheeting Environment



Graphical flowsheeting

Graphing

Multiple models

Logging

Streams view

Introduction to COCO:

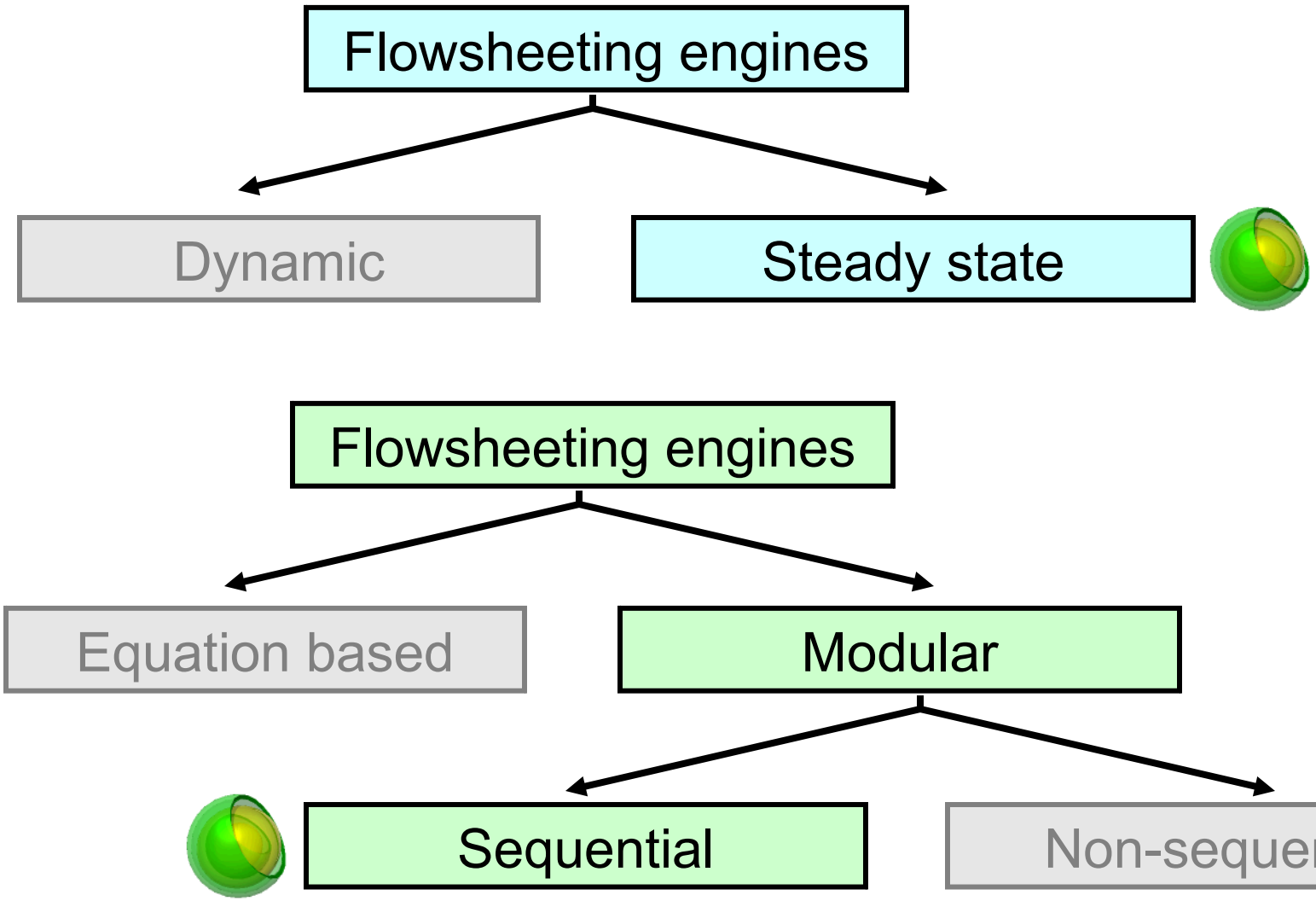
Simulation environment (COFE)

Thermodynamic property package (TEA)

Collection of unit operations (COUSCOUS)

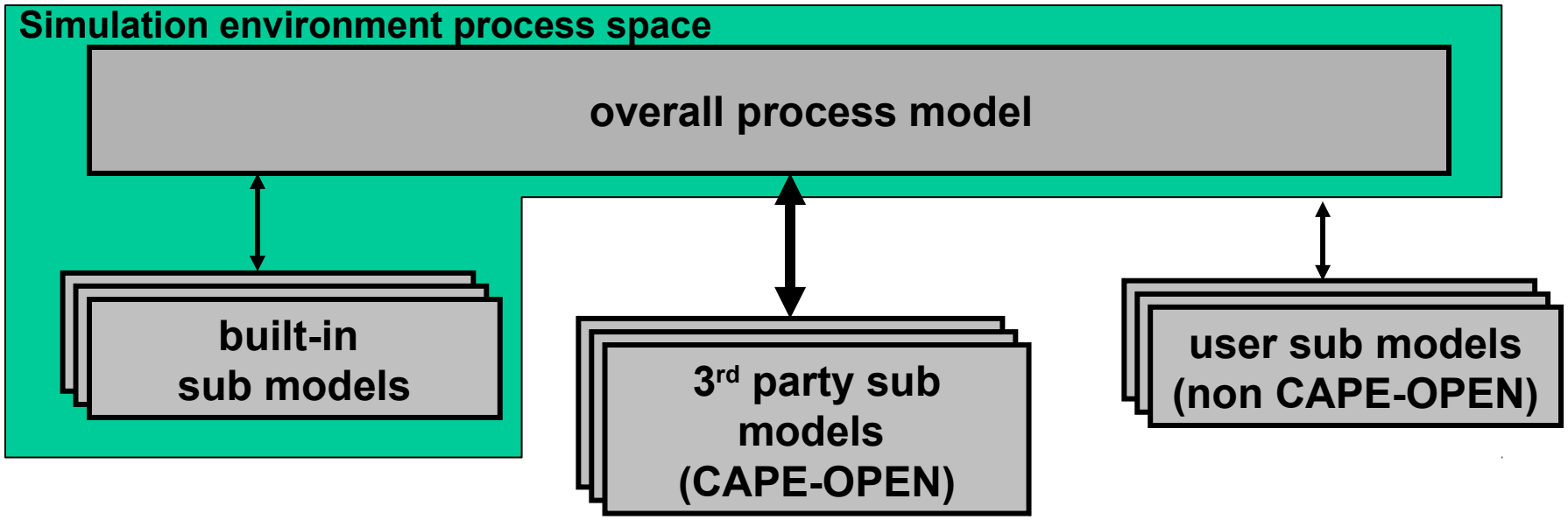
Reaction package (CORN)

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


Flowsheeting engines
Dynamic
Steady state
Flowsheeting engines
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)

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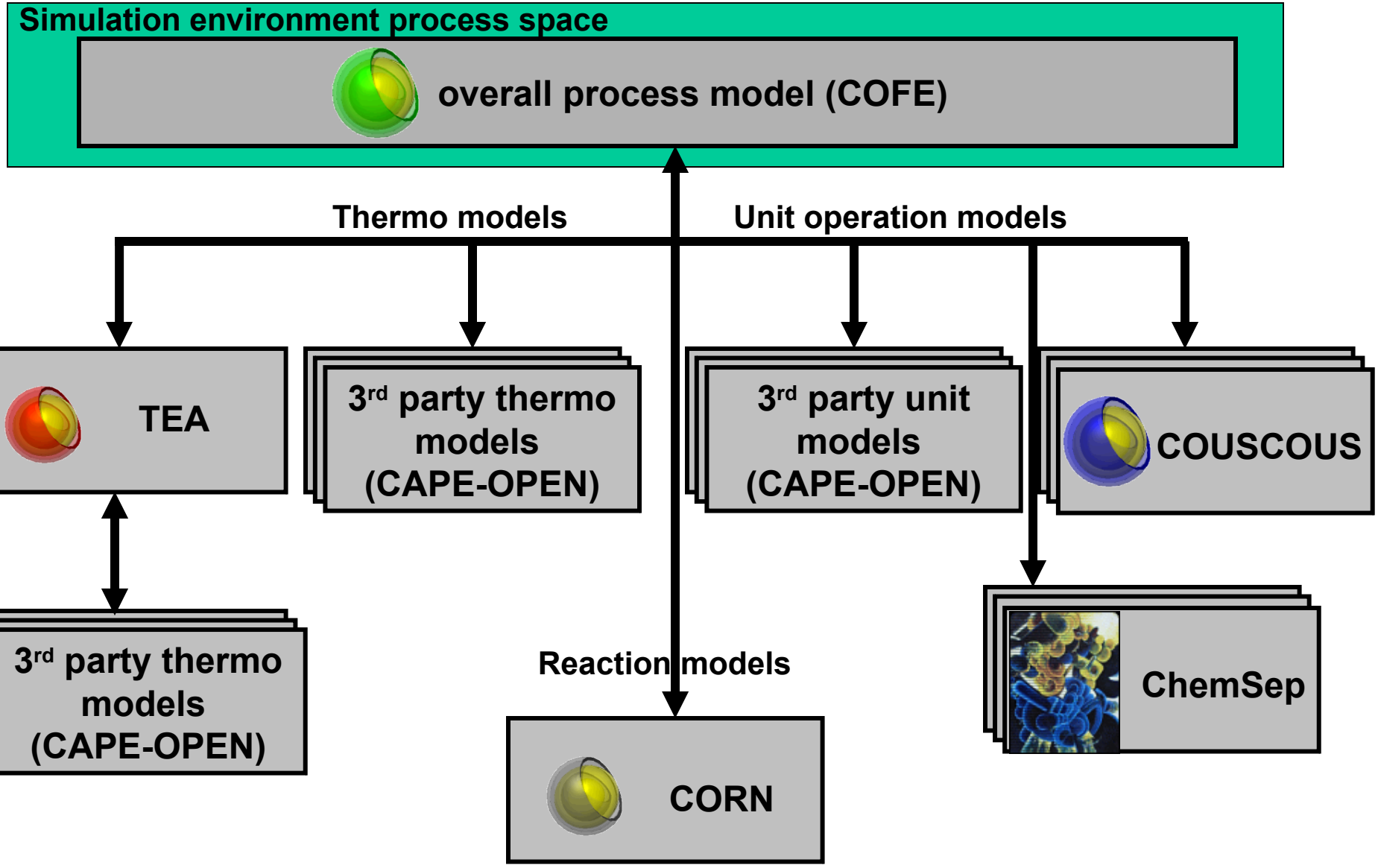
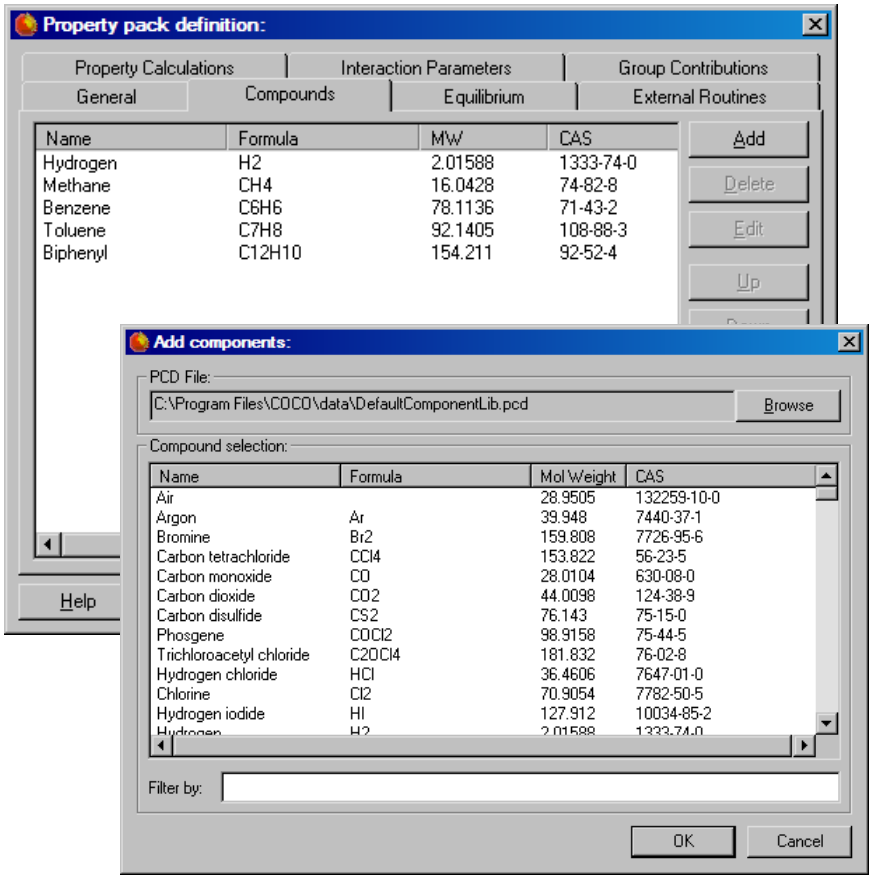
ChemSep
Modeling Separation Processes

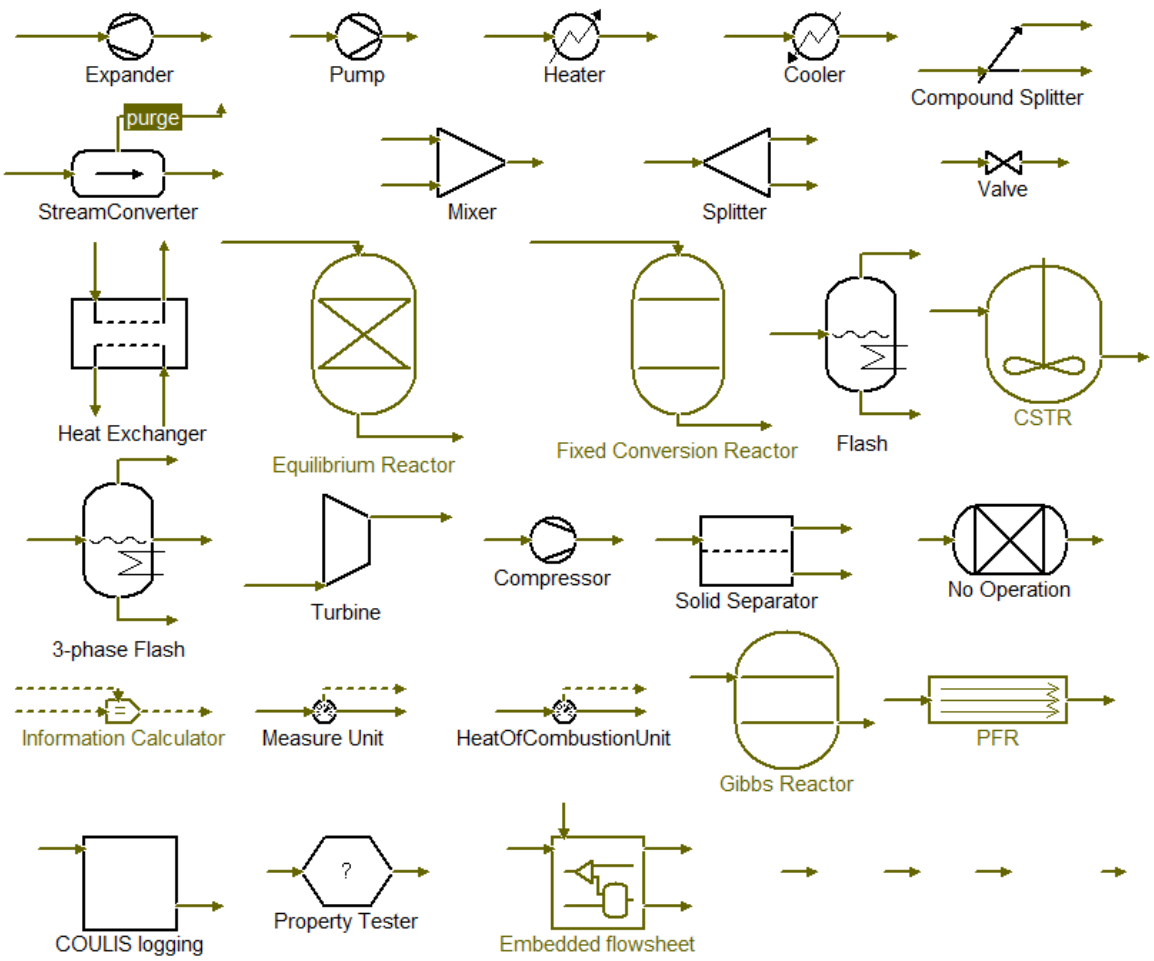


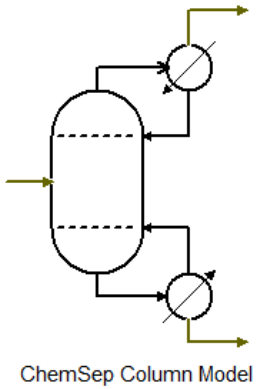
TEA: Thermodynamics for Engineering Applications

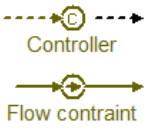
- Pure compound data library (extendible, or use DIPPR)
- 100+ Property calculation methods (25+ different properties)
- Property derivatives
- Support of external property calculation routines and external equilibrium servers



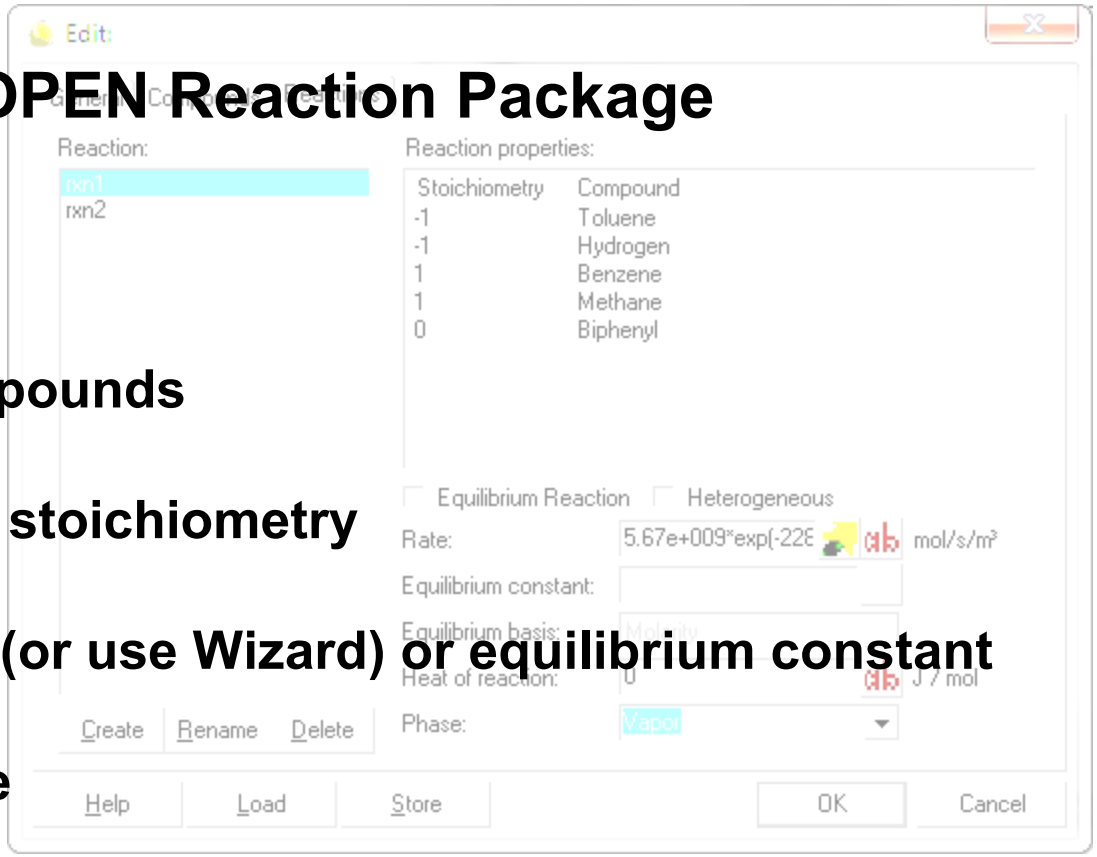
COUSCOUS: Simple unit operations







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

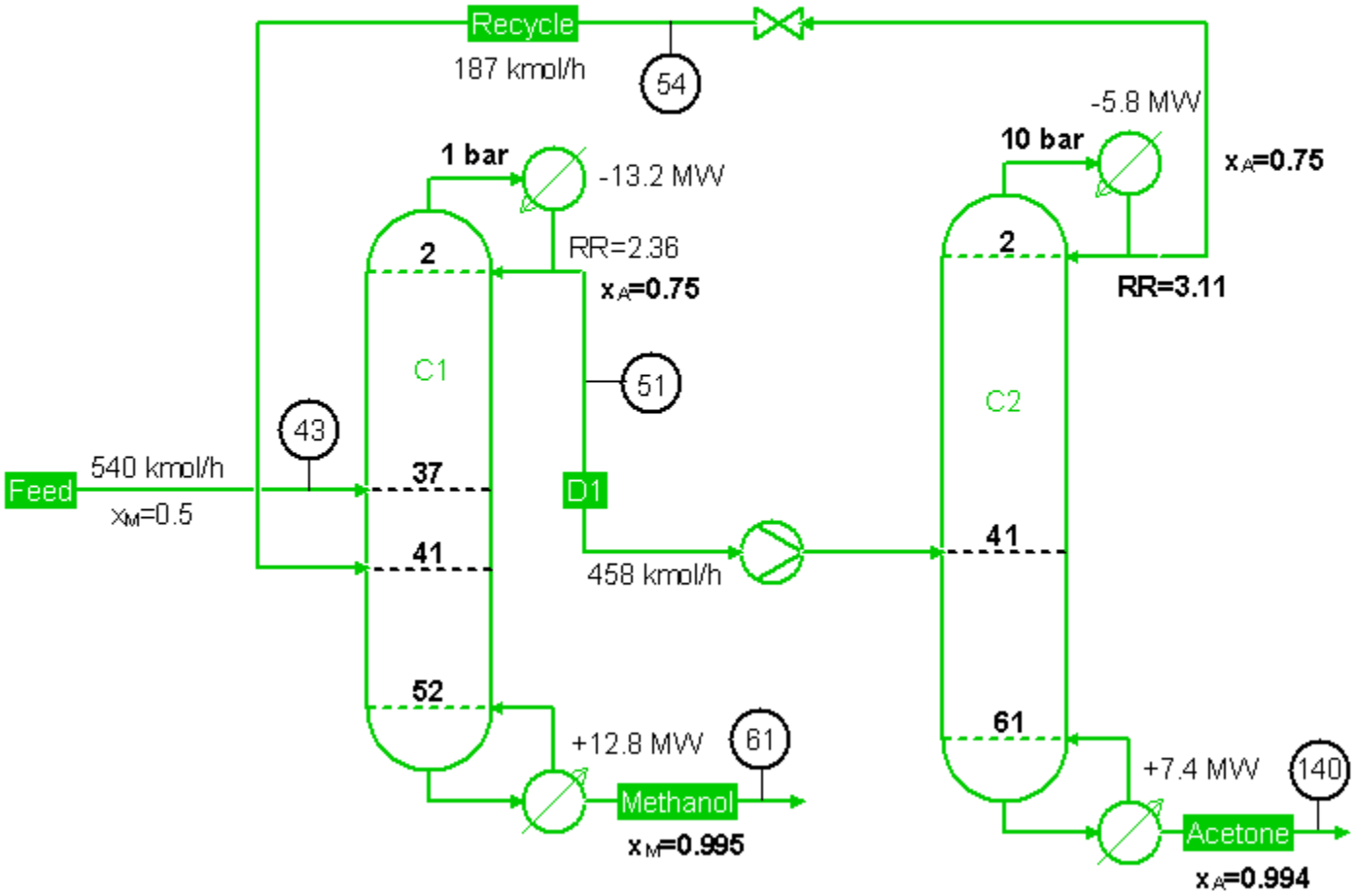
The CAPE-OPEN standard is the de facto standard for interfacing process modelling software components for use in the design and operation of chemical processes. It is based on universally recognised software technologies, such as COM and CORBA. The CO standard is open, multi-platform, uniform and available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

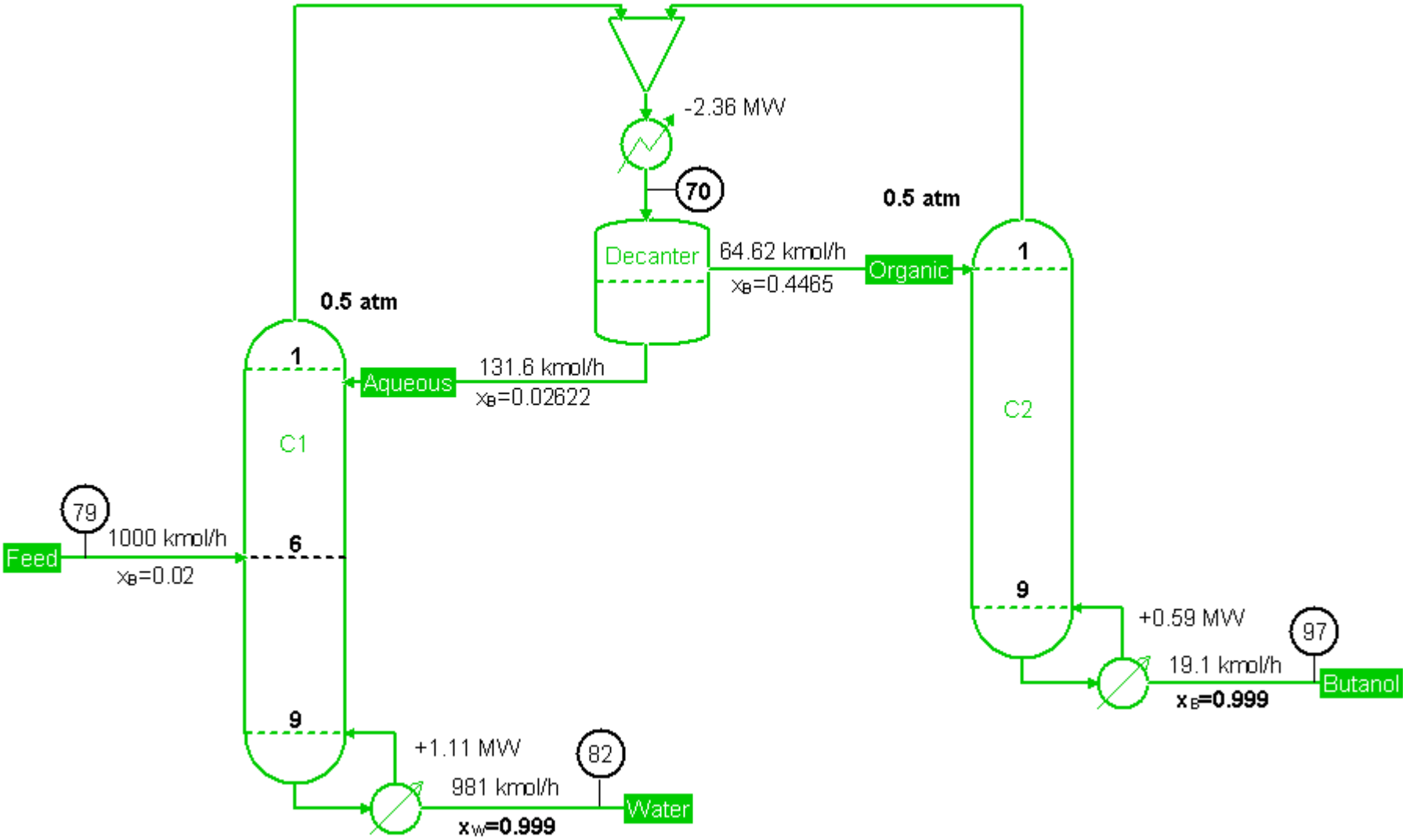
Pressure Swing Distillation of Acetone-Methanol

*Ind. Eng. Chem. Res. (*2008) **47** pp. 2696–2707



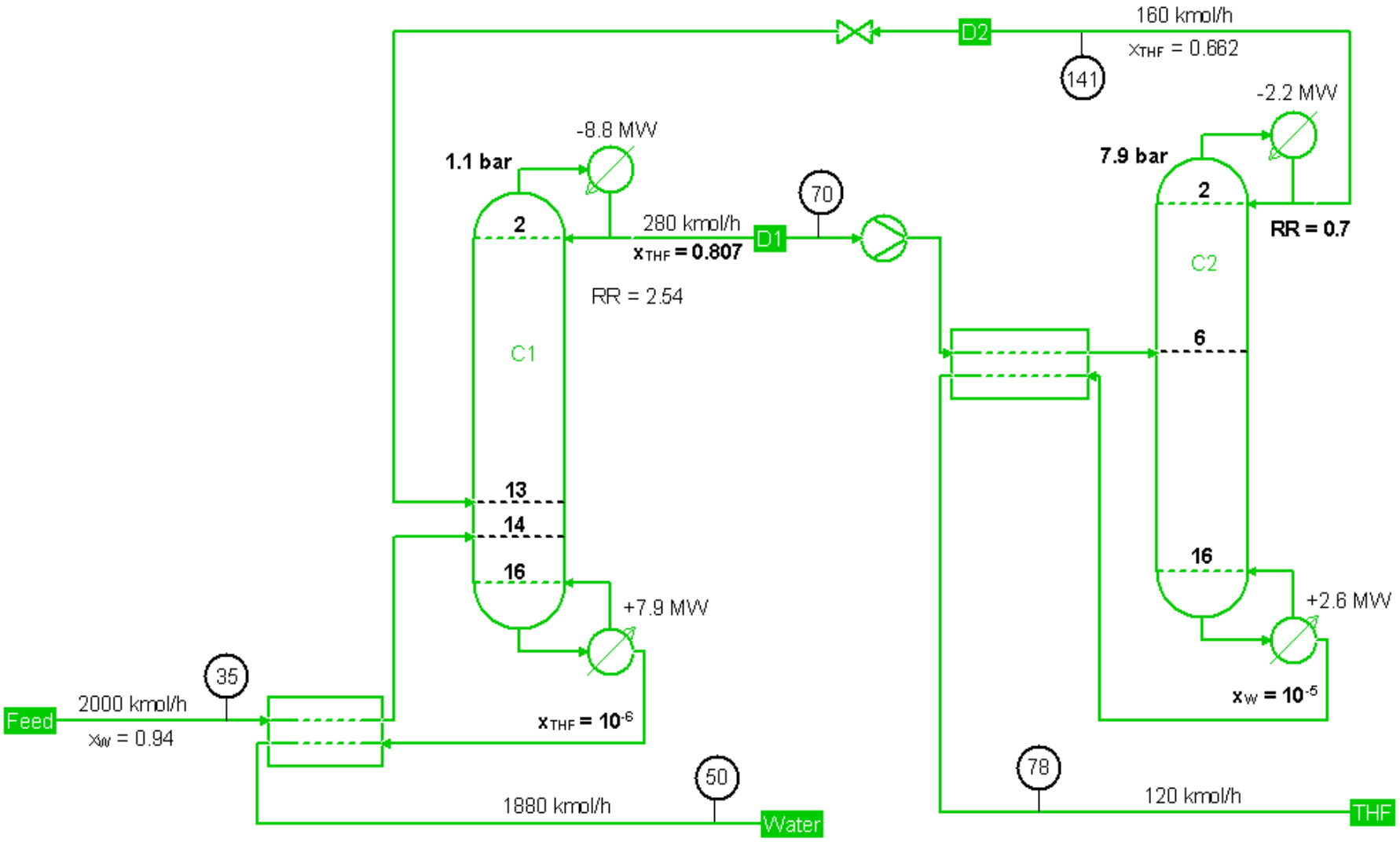
Butanol / Water Separation

Design and Control of Distillation Systems for Separating Azeotropes (2010) / *Energy Fuels* (2008) **22** pp. 4249-4258



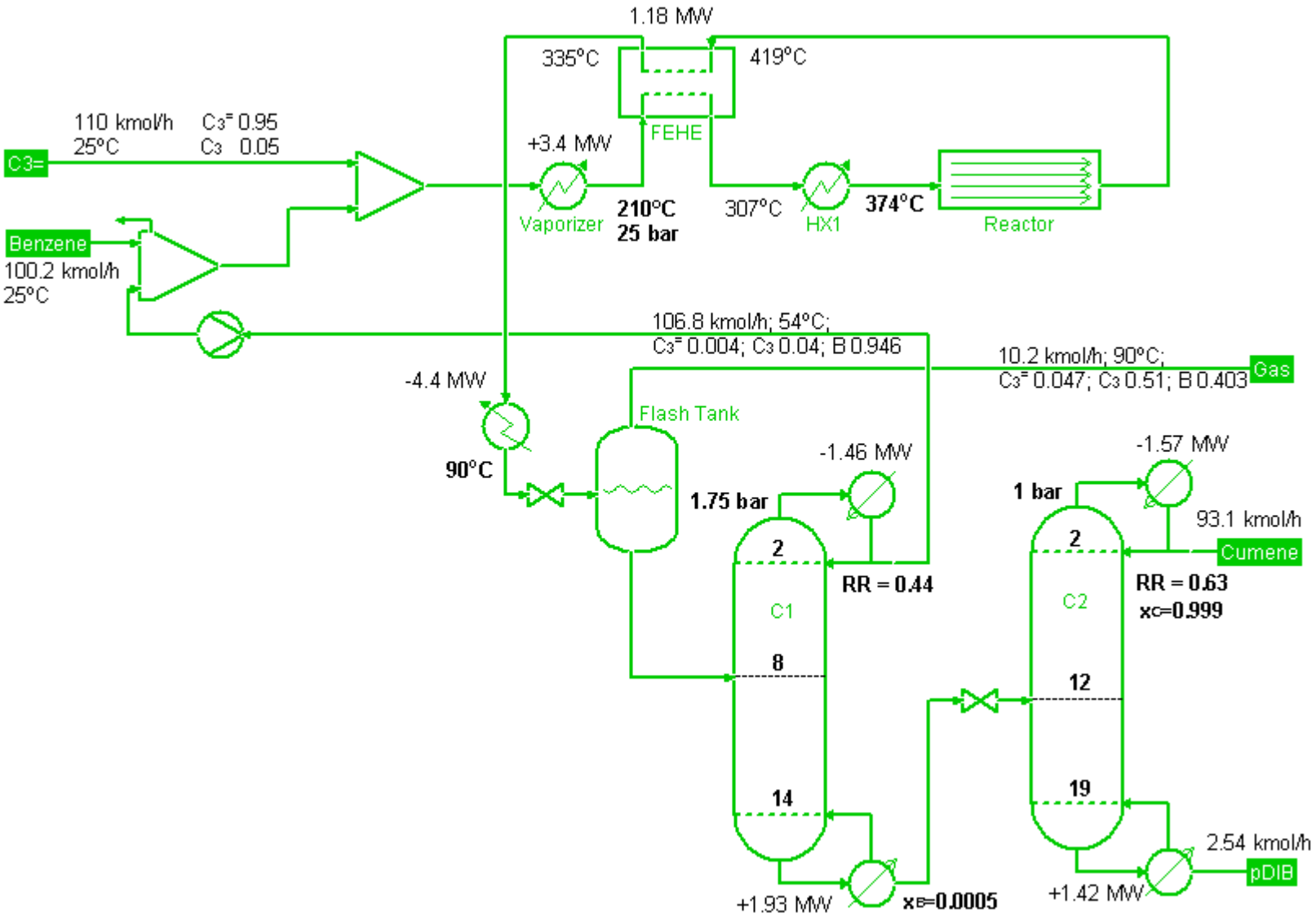
THF / Water Separation with Heat Integration

Design and Control of Distillation Systems for Separating Azeotropes / Ind. Eng. Chem. Res. (2008) **47** pp. 2681-2695



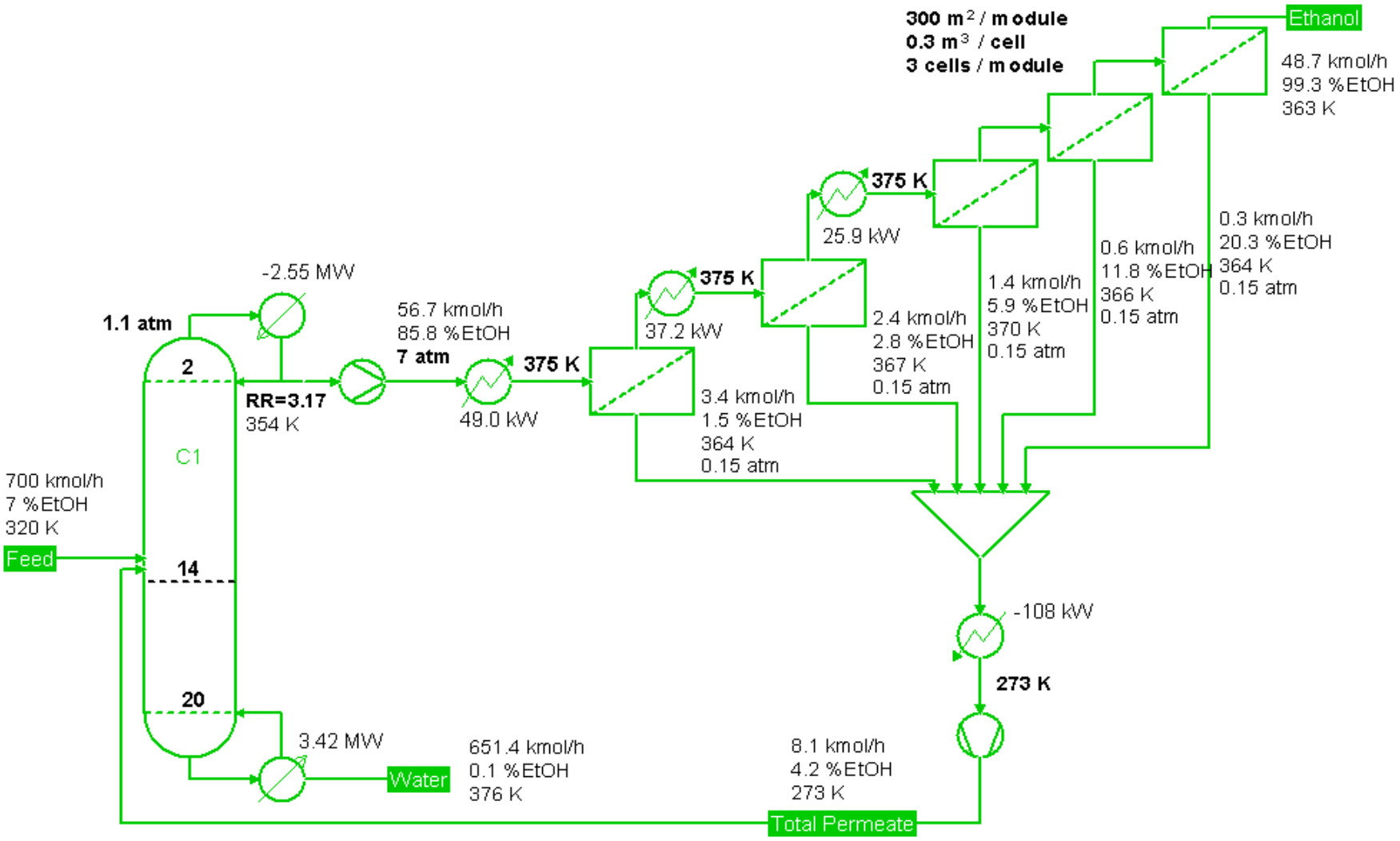
Cumene Process

*Ind. Eng. Chem. Res. (*2010) **49** pp. 719–734



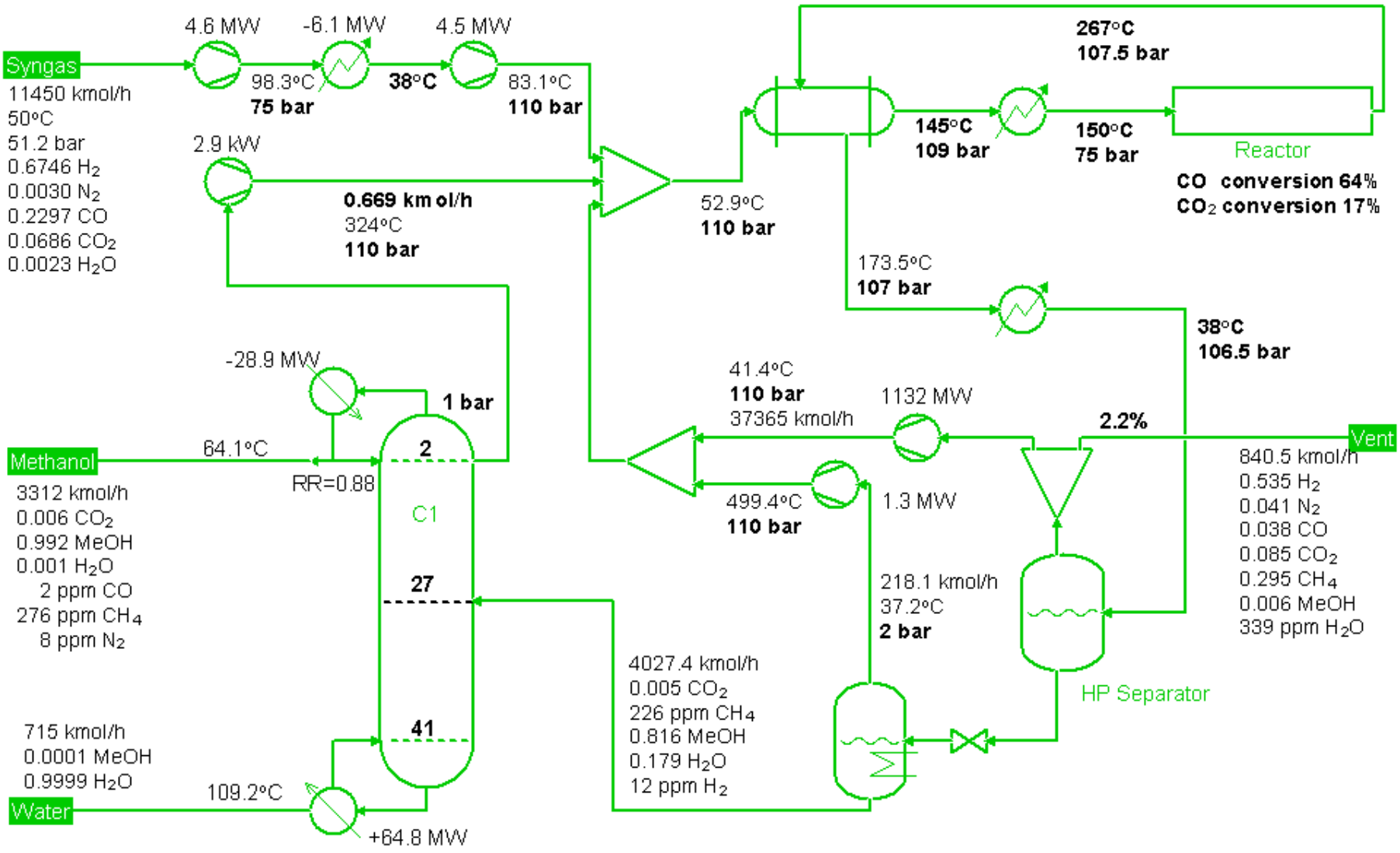
Column/Pervaporation Process for Separating Ethanol/Water

Ind. Eng. Chem. Res. (2009) **48** pp. 3484–3495



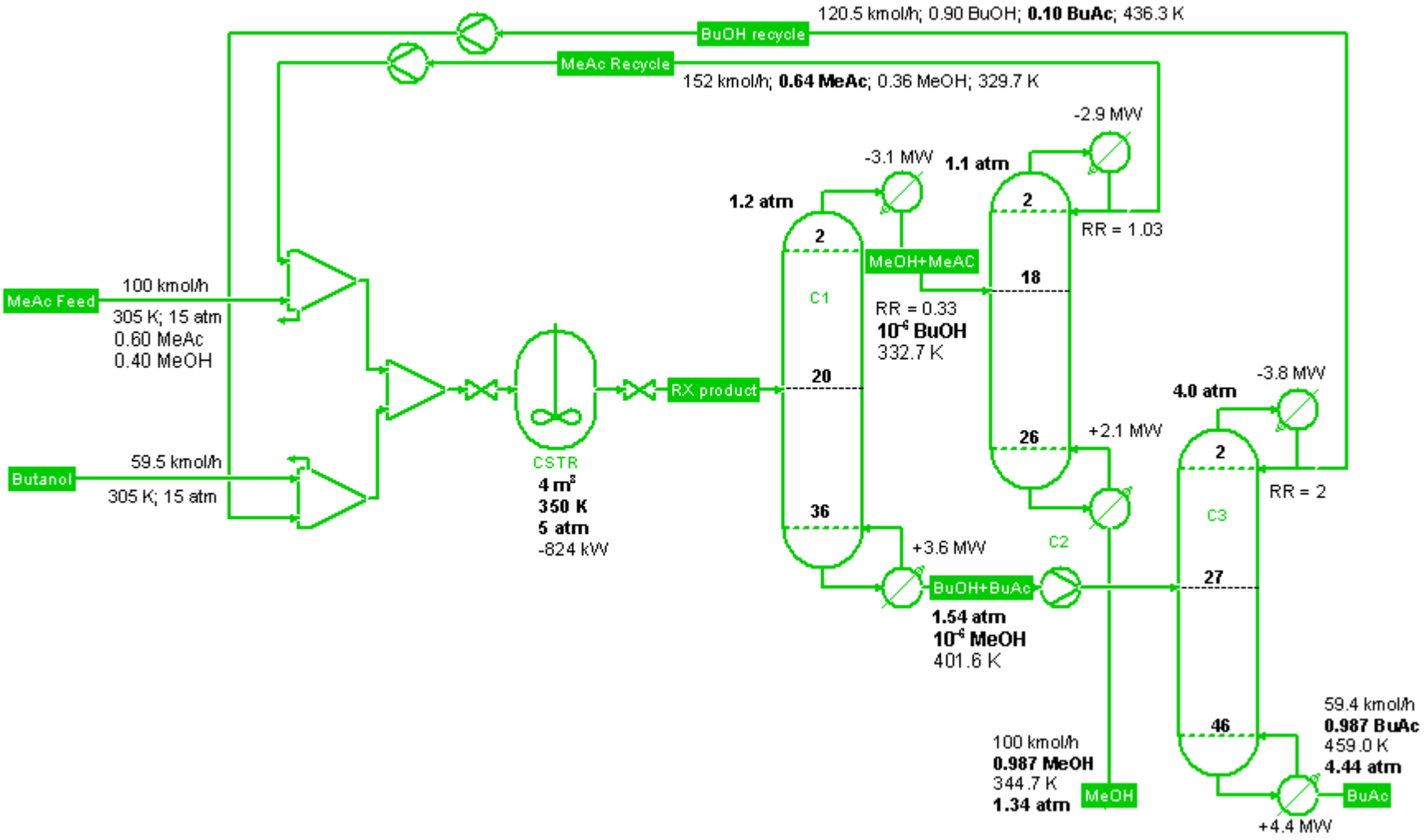
Methanol from Syngas

Ind. Eng. Chem. Res. (2010) **49** pp. 6150–6163



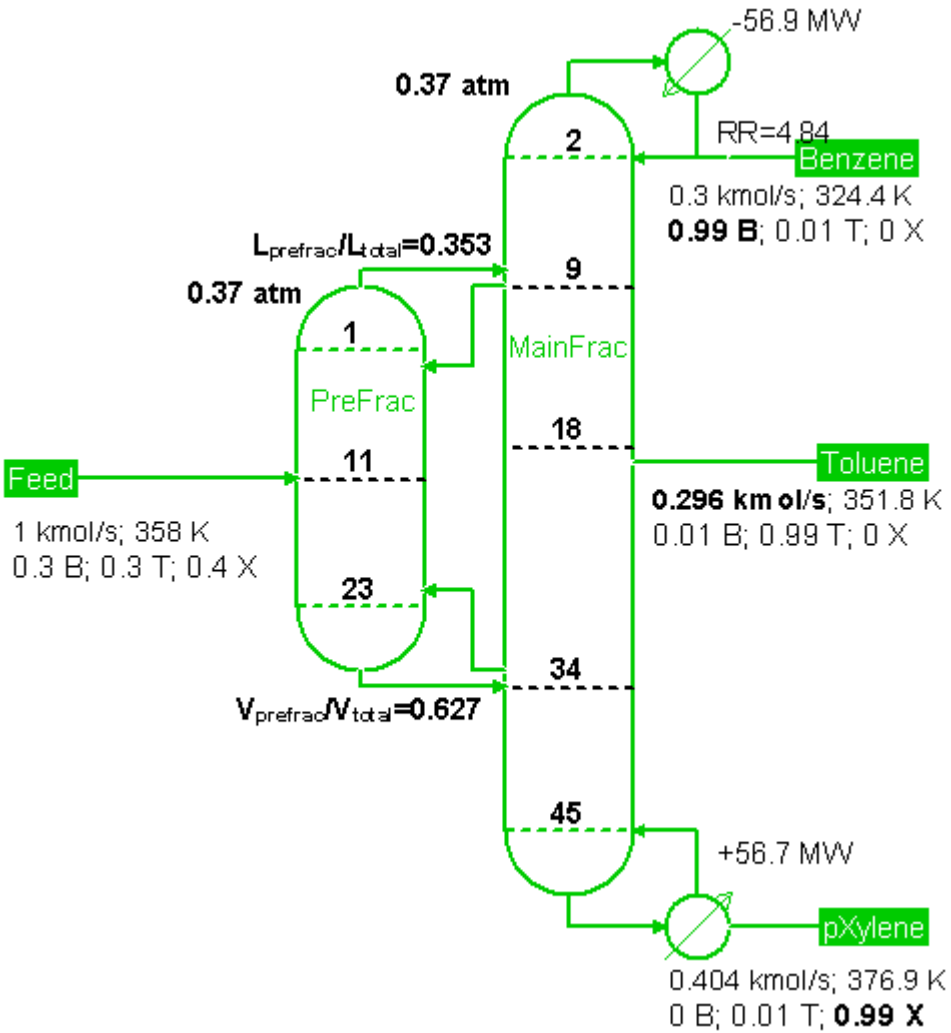
Butyl Acetate

Ind. Eng. Chem. Res. 2004, 43, 8014-8025 ***Ind. Eng. Chem. Res. 2011, 50, 1247-1263***



BTX Divided-Wall Column

Ind. Eng. Chem. Res. (2009) **48** pp. 6034–6049



More Flowsheets

- **Ethyl Benzene (***AIChE Journal*, 2011 **57**, 655)
- **Dimethylether (***Distillation Design and Control using Aspen Simulation***)**
- **Extractive Distillation**
- **Heterogeneous Ternary Distillation (**Alcohol-Water-Entrainer**)**
- **Reactive Distillation of A + B → C + D**
- ***TAME***
- ***Air Separation Unit***
- ***Ethylene Oxide***
- ***Light Ends Unit***

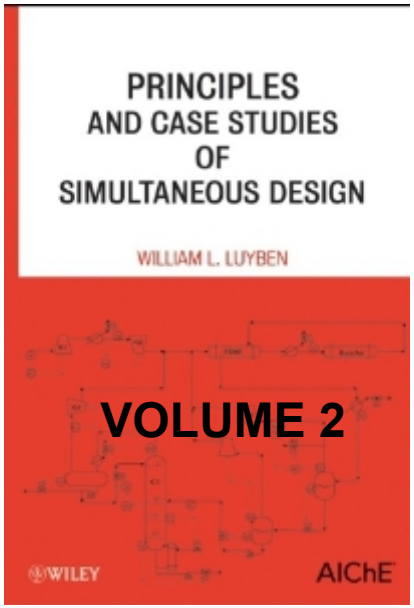
Luyben's Flowsheets with COCO

- 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 needed a databank with more compounds; *ChemSep v6.9 databank extended to 426 compounds + now it is possible to use up to 40 compounds in a column simulation!*
- 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?



2012 / 2013 ?