APM2013

The Advanced Process Modeling Forum

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Model-based design and optimization of distillation trains

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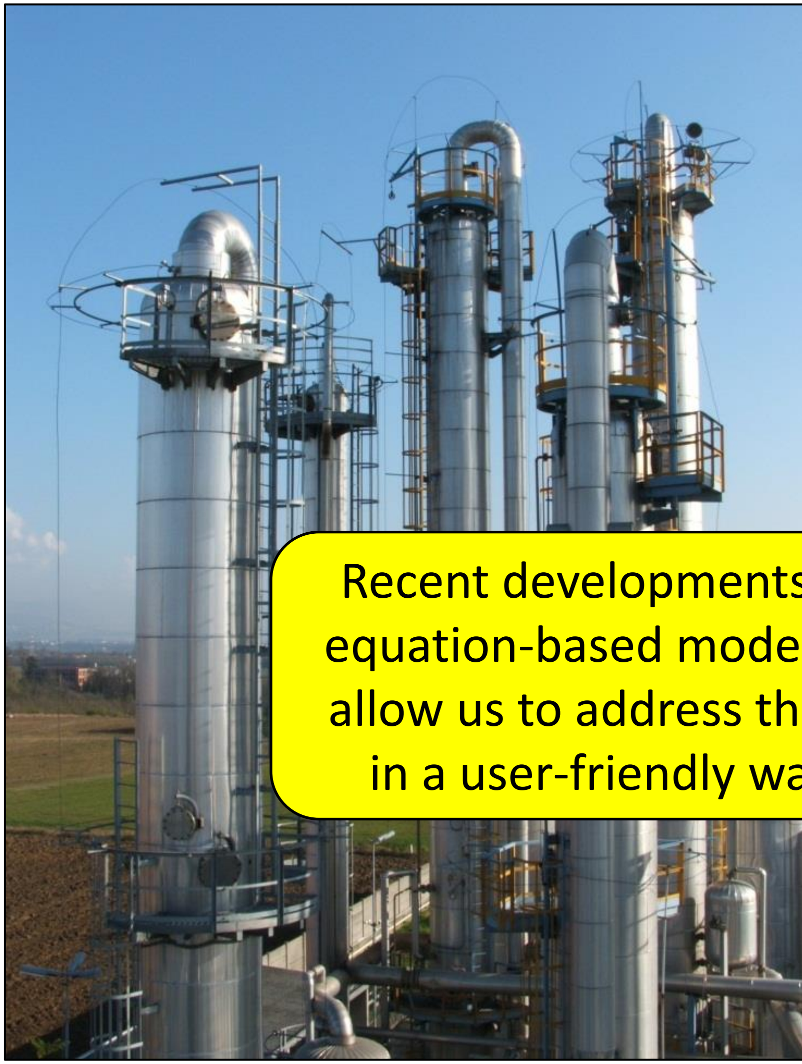
Continuous distillation

- Most frequently used unit operation for separation
- Low thermodynamic efficiency
- Costly to build and operate

Continuous distillation



Recent developments in equation-based modeling allow us to address these in a user-friendly way

- Role of **modeling** in distillation process design is well-established
  - Sequential-modular tools in use for >30 years
- Some problems remain challenging
  - Easy customization (e.g. new concepts, costing)
  - Converging recycles
  - Inverse problem statements (e.g. product purity)
- We can now go beyond simulation
  - Optimizing design and operation simultaneously

Equilibrium tray column model

gPROMS Product Family

General Mathematical Modeling

Model Builder

Sector-focused Modeling Tools

Chemicals & Petrochemicals

PML: SS
PML: DY

Process Builder

AML: GLC
AML: BCR
AML: ...T
AML: ...BR
AML: ...CR

Life Sciences & Fine Chemicals

gCRYSTAL
gSOLIDS
gCOAS

Power & CCS

gCCS
gFUELCELL

Oil & Gas

gFLARE

Materials Modeling

Multiflash
OLI
gSAFT

Model Deployment Tools

gO:Run
gO:Run XML
gO:CAPE-OPEN
gO:MATLAB
gO:CFD

The gPROMS platform

Equation-oriented modeling & solution engine

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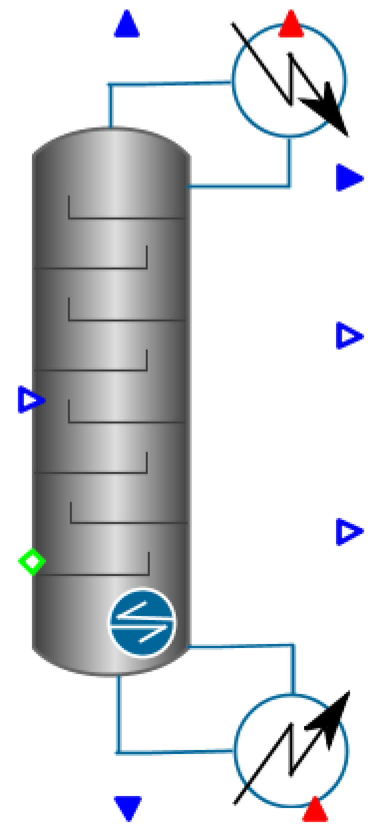
Equilibrium tray column model

- Key assumption: vapor/liquid equilibrium at each stage
  - including reboiler & condenser
  - optional specification of stage efficiencies
- Design calculations
  - column height
  - column diameter
    - determined from flooding limit
- Costing calculations
  - standard equipment cost correlations (Seider & Seader, 2010)
- Built-in Model Initialization Procedures
- Superstructure for design optimization



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Workflow for distillation column modeling

Workflow

Construct flowsheet → Sizing → Costing → Sensitivity + Optimization

1. Construct flowsheet and introduce specifications
    a) Configure material & physical properties
    b) Construct flowsheet
    c) Configure unit models
2. Use design mode for equipment sizing
3. Turn on costing to calculate equipment and operating costs
4. Perform sensitivity and optimization studies

Example #1: Methanol-water separation

- Single column (thermo: NRTL-VLE)

Feed parameters	Value	Units
Composition	50% methanol + 50% water	mol/mol
Pressure	2.4	bar
Temperature	300	K
Flowrate	900	kmol/hr

Column parameters	Value	Units
Number of stages	27	
Feed stage	11	
Boilup ratio	2.3	mol/mol
Reflux ratio	0.55	mol/mol
Top pressure	2	bar
Pressure drop per stage	0.0025	bar

- Video

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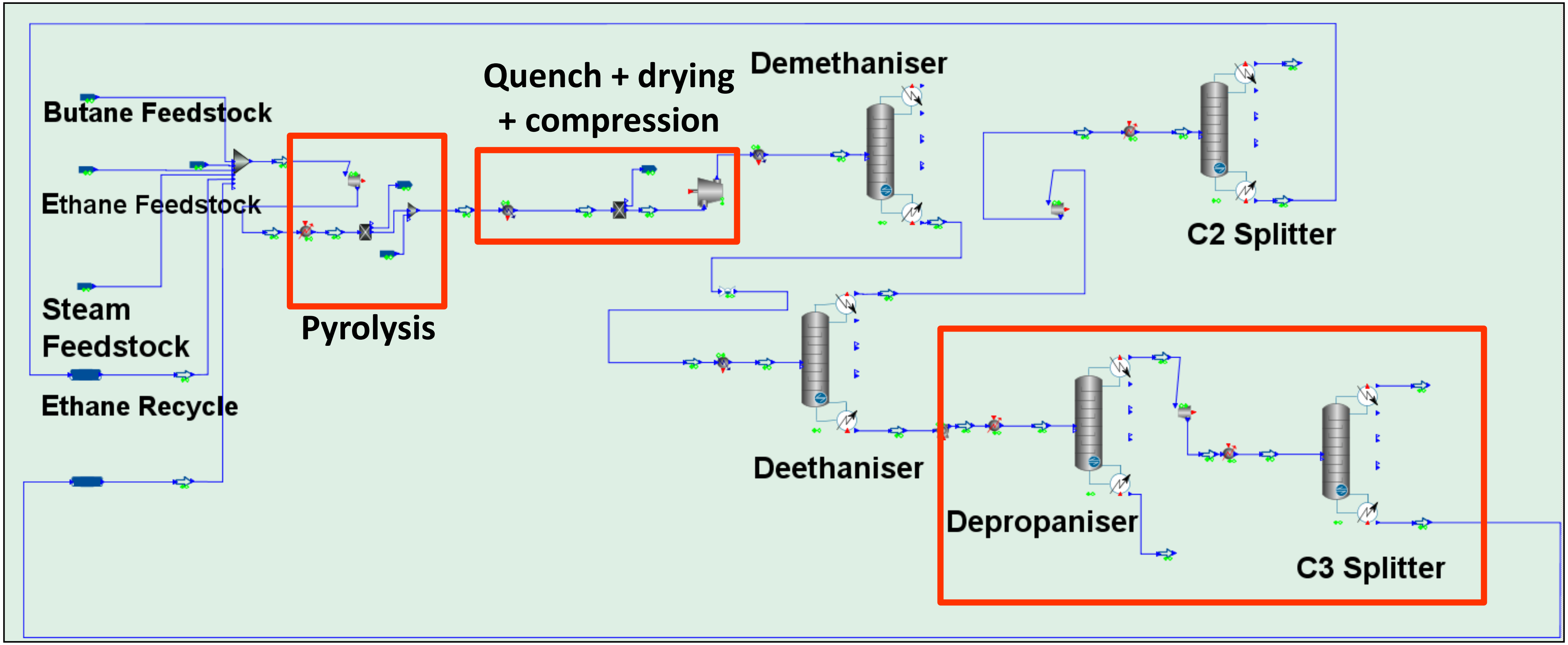
Distillation train modeling

Example #2: Ethylene plant

- Ethylene process



- Initializes with no user-provided initial guesses

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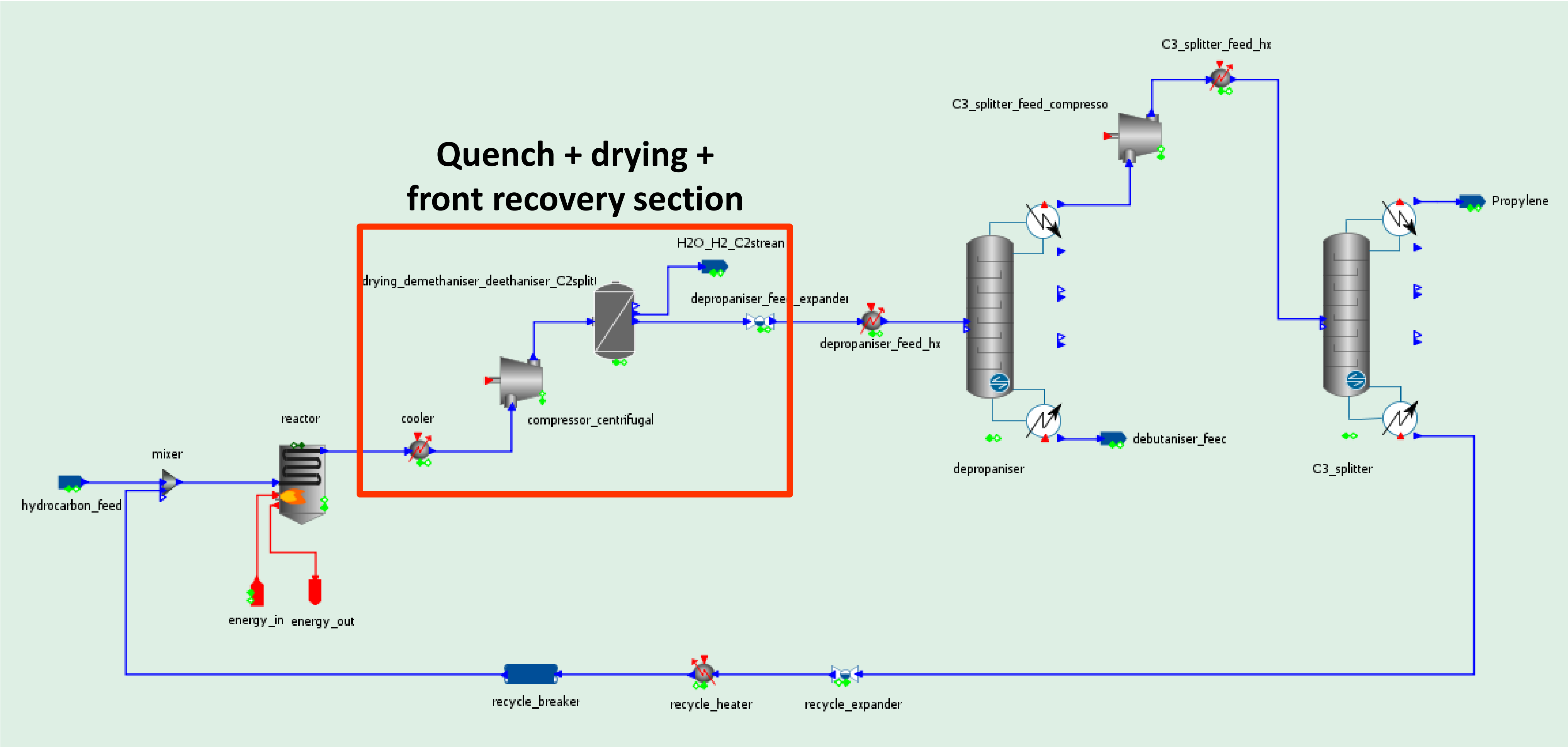
Example #2: Ethylene plant recovery section – 2 columns

- Simplified ethylene process



Example #2: Ethylene plant recovery section – 2 columns

- *Step 1: Construct flowsheet*
- Base case:
  - Ethylene 5.5 x 10^3 t/yr
  - Propylene 3.6 x 10^3 t/yr

Depropanizer parameters	Value	Units
Number of stages	55	
Feed stage	25	
Boilup ratio	3.08	mol/mol
Reflux ratio	1.32	mol/mol
Pressure	16	bar

C3 splitter parameters	Value	Units
Number of stages	200	
Feed stage	100	
Boilup ratio	18	mol/mol
Propylene purity	99.6	%
Pressure	15	bar

- Case initializes with no user-provided initial guesses

Example #2: Ethylene plant recovery section – 2 columns

- *Steps 2-3: Design + Costing*
- Assumptions
  - Tray columns
  - Allowed column flooding 80%
  - Saturated steam 10 bar
  - CW temperature 20 ^{o}C
- Basis for sizing and costing
  - Column diameter based on vapor flowrate
  - Column height based on geometry of tray
  - Column cost based on metal cost
  - Compressor cost based on power consumption
  - HX cost based on area required
  - Operating costs based on CW, steam and power costs

Example #2: Ethylene plant recovery section – 2 columns

- *Steps 2-3: Design + Costing*
- Results

Depropanizer	Value	Units
Column diameter	0.383	m
Column height	46.3	m
Column cost	595 k	$
Operation cost	12 k	$

C3 splitter	Value	Units
Column diameter	0.839	m
Column height	173.3	m
Column cost	13,785 k	$
Operation cost	202 k	$

Total annualised costs	Value	Units
Capital cost	5,023 k	$
Operation cost	1,051 k	$
Total	6,074 k	$

Example #2: Ethylene plant recovery section – 2 columns

- *Step 4: Optimization*
- Objective function
  - Minimize total annualized cost
- By adjusting
  - Feed locations
  - No of trays
  - Column pressures
  - Boilup ratio in C3 splitter
  - Boilup and reflux ratio in depropanizer
- Constraints
  - Ethylene and propylene production
  - Propylene recovery
  - HX temperature differences

Example #2: Ethylene plant recovery section – 2 columns

- *Step 4: Optimization*
- Results

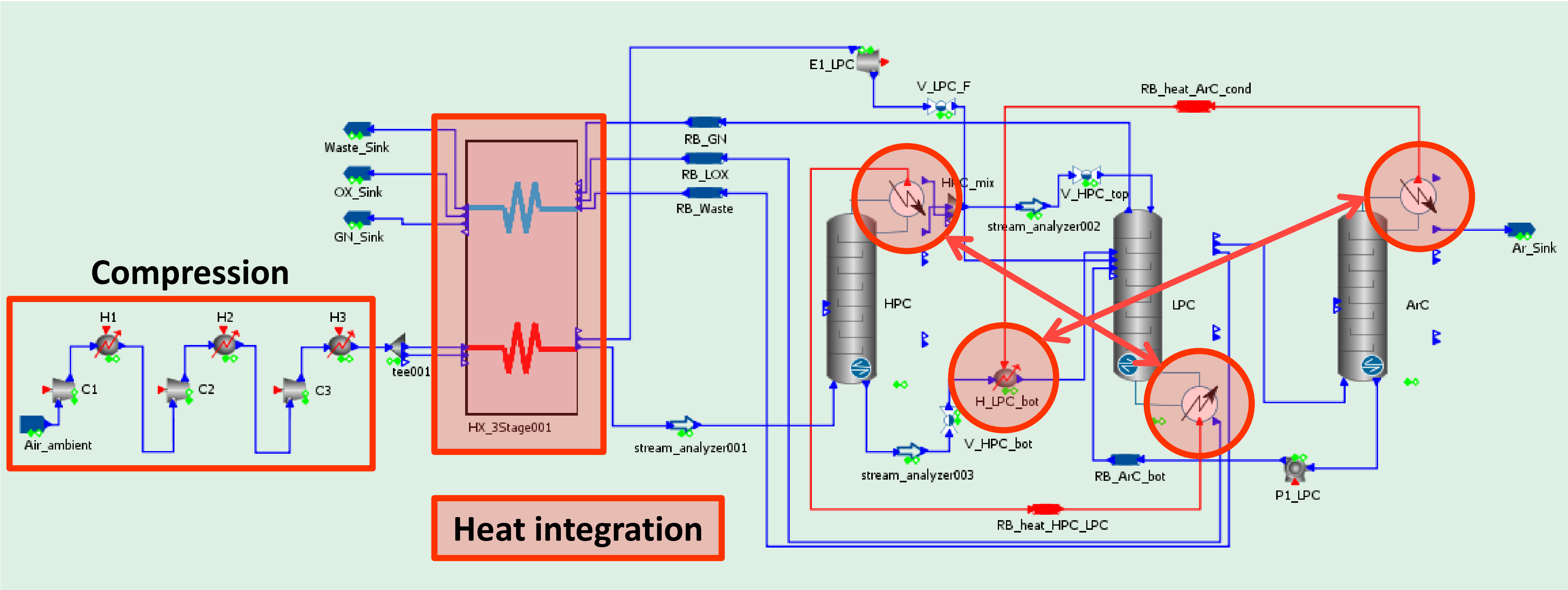
Depropanizer	Initial value	Final value	Units
No. trays	55	11	-
Feed location	25	5	-
Column diameter	0.383	0.482	m
Column height	46.3	7.9	m
Column cost	595 k	68.5 k	$
Operation cost	12 k	21 k	$

C3 splitter	Initial value	Final value	Units
No. trays	200	173	-
Feed location	100	97	-
Column diameter	0.839	1.487	m
Column height	173.3	149.6	m
Column cost	13,785 k	5,707 k	$
Operation cost	202 k	392 k	$

Total annualized costs	Initial value	Final value	Units
Capital cost	5,023 k	2,156 k	$
Operation cost	1,051 k	1,252 k	$
Total	6,074 k	3,408 k	$

Tightly coupled distillation systems

Example #3: Air Separation Unit (ASU)



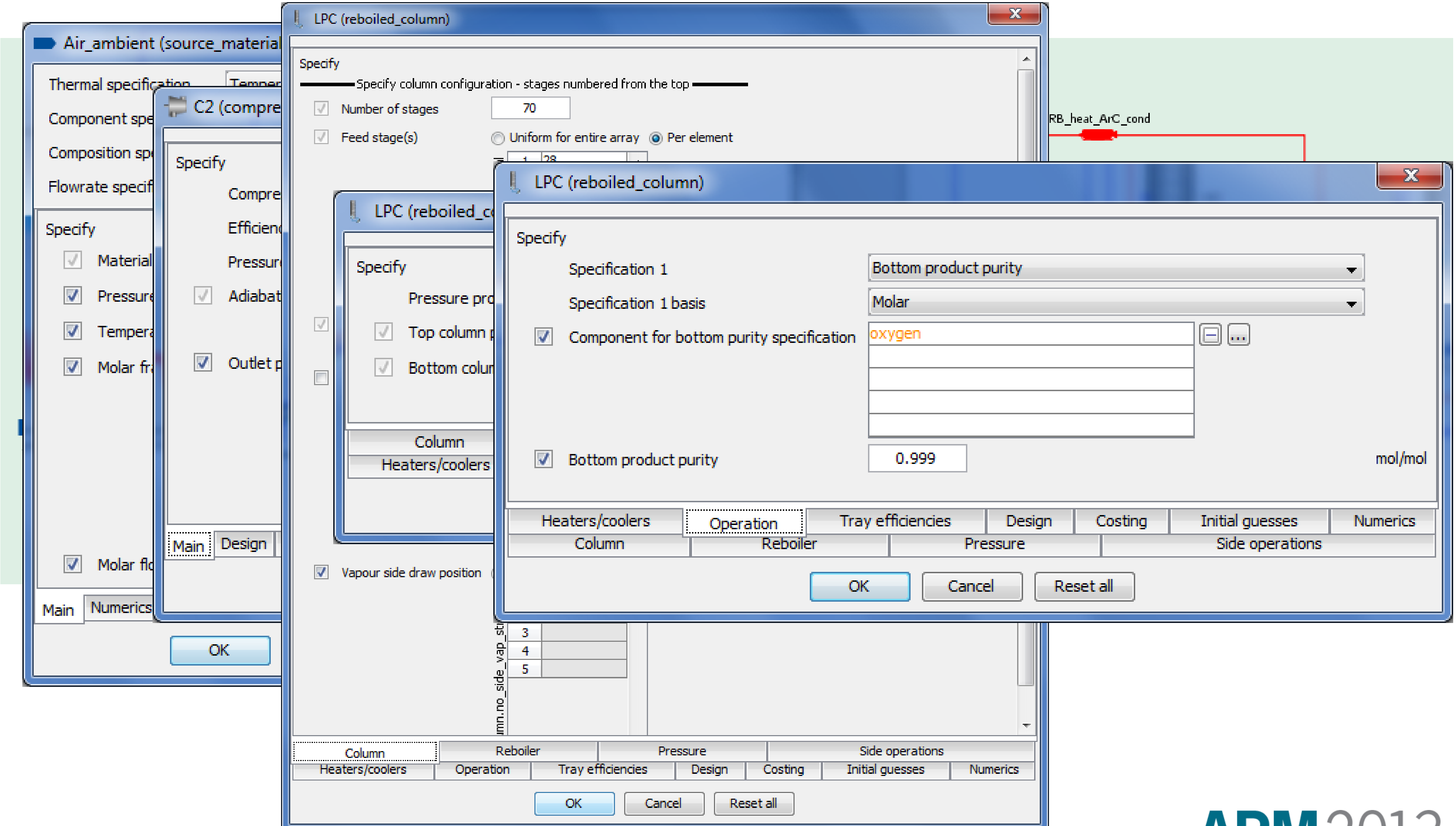
R. Pack, *Integration of Model Based Optimal Design Methods in the Process Modeling Environment gPROMS*, Diploma Thesis, RWTH Aachen 2013

Example #3: Air Separation Unit (ASU)

- *Step 1: Construct flowsheet*
  - Base case
    - Oxygen production — 410×10^3 t/yr
    - Oxygen purity — 99.9 %
    - Impurity in Argon product — 1 ppm

- *Step 2: Design*
  - Column design at 80% flooding

Example #3: Air Separation Unit (ASU)



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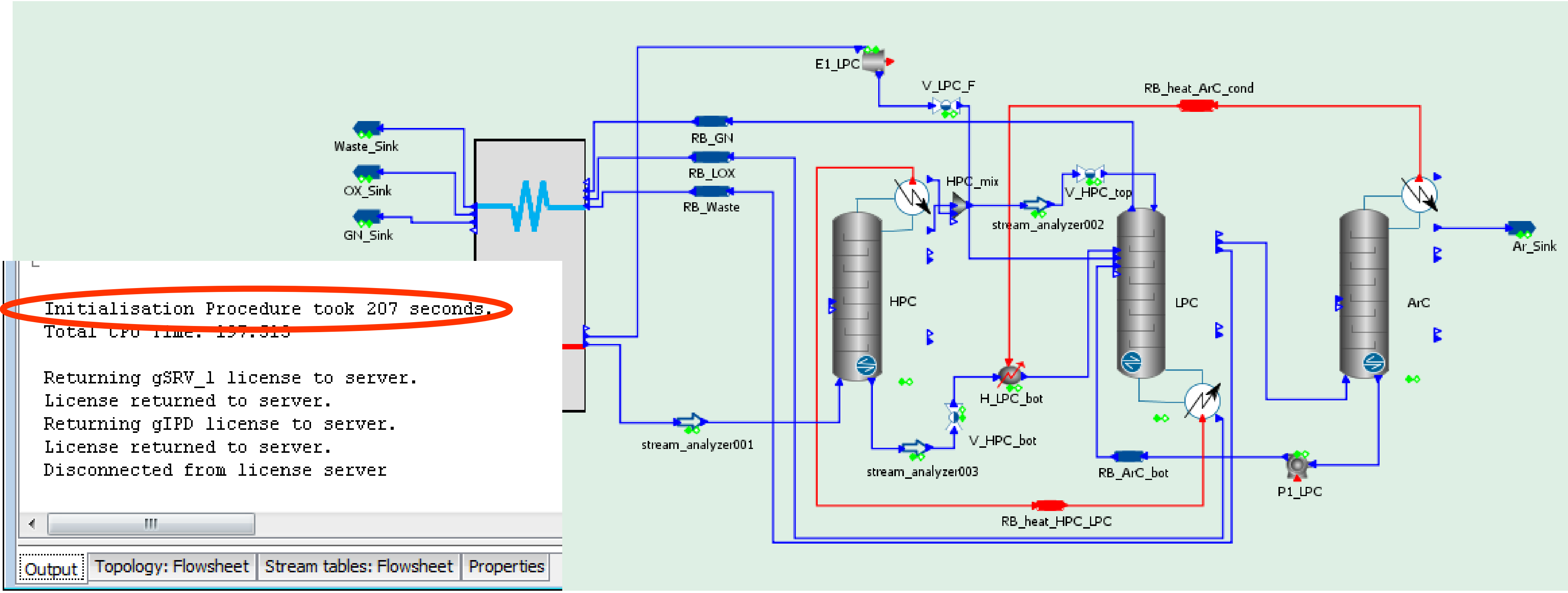
Example #3: Air Separation Unit (ASU)

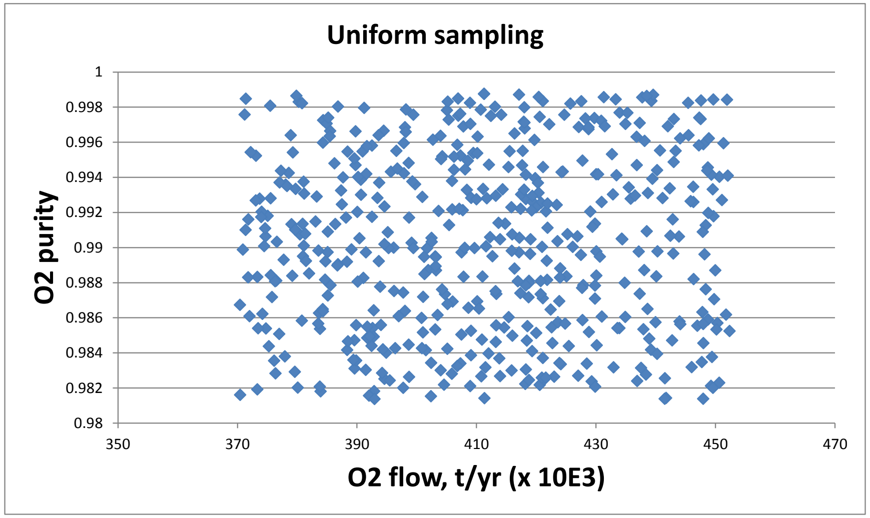


- **Solution with no user-provided initial guesses: 200 CPU s (Intel i7 laptop)**
  - **Subsequent solutions: ~1.5 s**

Example #3: Air Separation Unit (ASU)

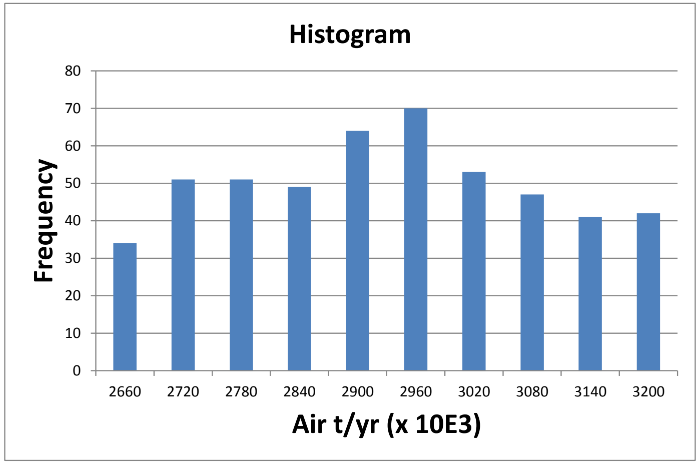
- *Step 4: Sensitivity study*
- What will be the effect of uncertain oxygen demand on the plant operation?
  - Uniform sampling (500 points)
    - Oxygen production +/- 10%
    - Oxygen purity 98.5 – 99.9%
  - Fixed column size
  - Fixed argon product purity

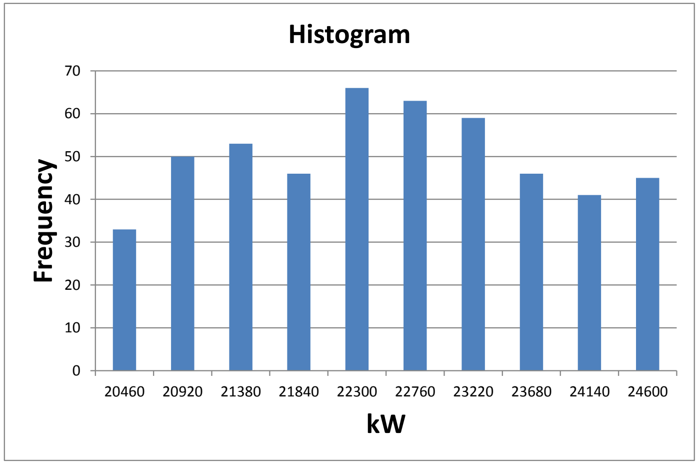
Total CPU time < 15 min

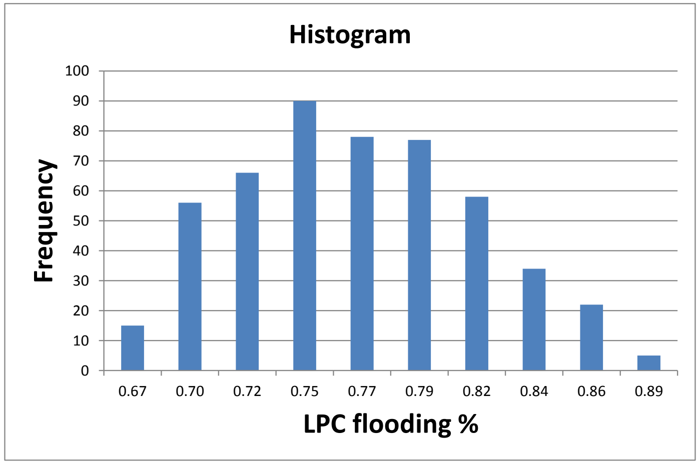


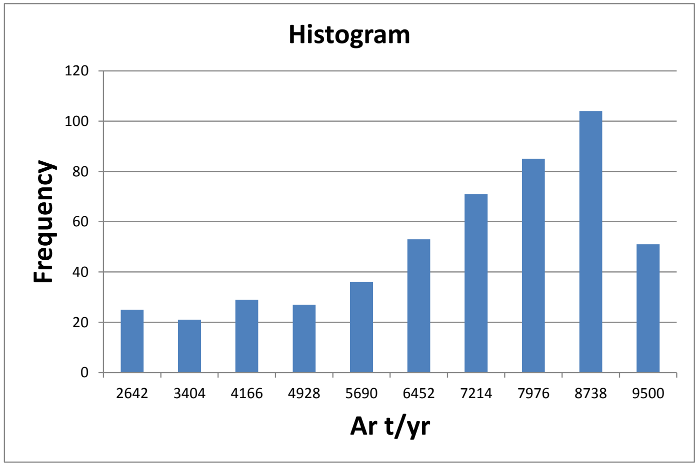
Example #3: Air Separation Unit (ASU)

- *Step 4: Sensitivity study*
- Results









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Conclusions

Summary

Recent developments in equation-based modeling

- Built-in Model Initialization Procedures
- Mixed-integer optimization
- State-of the art models

allow us to address

- Customization (new concepts, costing)
- Converging recycles
- Inverse problem statements
  (e.g. product purity)

and more

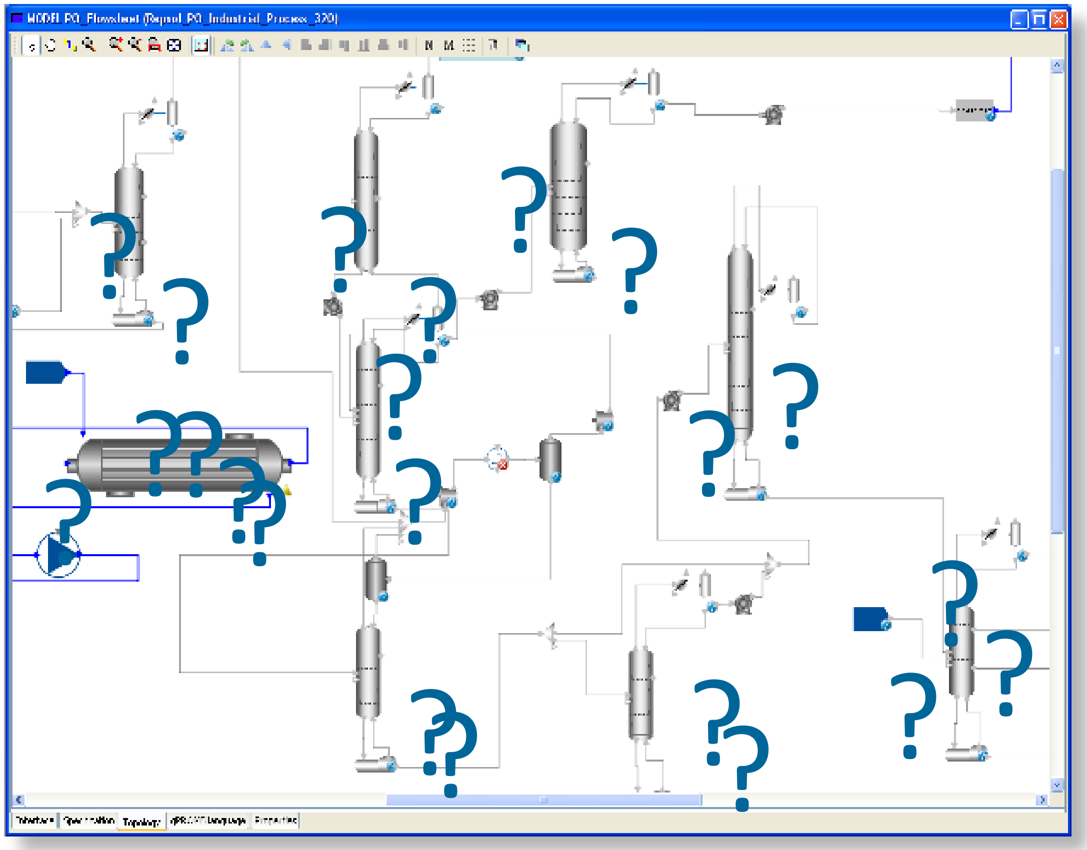
- Optimizing many design aspects simultaneously
- Plant-wide Mixed Integer Optimization

Example 4: propylene oxide production

HPPO: Hydrogen Peroxide route to Propylene Oxide

$$CH_3CH{=}CH_2 + H_2O_2 \rightarrow CH_3\text{-}CH\text{-}CH_2 + H_2O$$

- Plant-wide optimisation
- Detailed multitubular reactor
- Many distillation columns
  - 1 azeotropic
  - 2 reactive
- Two major recycle streams
- Simultaneous optimization
  of design and operation
- \$10M p.a. savings identified



H. Martin Rodriguez, A. Cano, M. Matzopoulos, *Improve engineering via whole-plant design optimization.* Hydrocarbon Processing, December 2010, pp. 43-49

Acknowledgements

- Library development
  - Maarten Nauta
  - Diogo Narciso
  - Robert Pack

- Testing & applications
  - Pedro Chainho
  - Francisco Borralho

Thank you!

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Extra slides

References

- Ethylene recovery:

  - K. Y. Cheung, Site-wide and supply chain optimisation for continuous chemical processes, PhD thesis, Imperial College, 2008

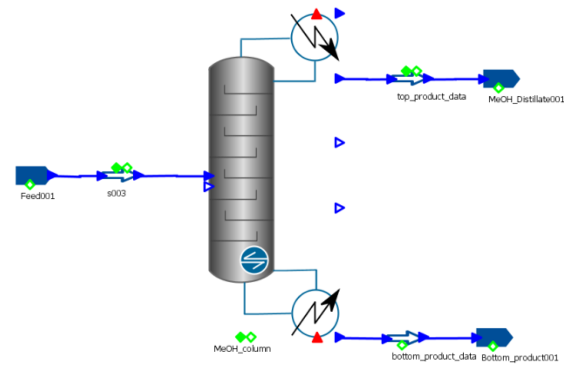
- Air Separation Unit (ASU):

  - R. Pack, Integration of Model Based Optimal Design Methods in the Process Modeling Environment gPROMS, Diploma Thesis, RWTH Aachen 2013

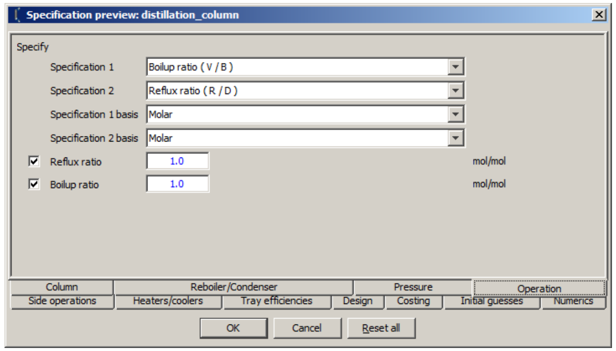
Workflow - Construct flowsheet

- Construct flowsheet

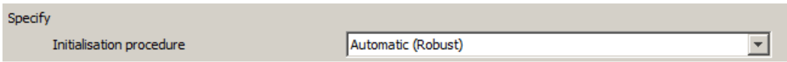
1. Drag-and-drop column model onto flowsheet



2. Configure minimum set of specifications



3. gPROMS takes care of initialization




```
INITIALISATION_PROCEDURE default_initialisation_procedure DEFAULT
# Start Initialisation Procedure Specifications
  USE
      MeOH_column : Init_Flash_Fast_Spec;
  END
# End Initialisation Procedure Specifications
```

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