APM2013

The Advanced Process Modelling Forum

17-18 April 2013, London

Model-based design and optimisation of distillation trains

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gPROMS Product Family

PSE

General Mathematical Modelling

Model Builder

Sector-focused Modelling Tools

Chemicals & Petrochemicals

Process Builder

AML: GLC

ML: BCR

ML: T

ML: BR

ML: CR

Life Sciences & Fine Chemicals

gCRYSTAL

gSOLIDS

gCOAS

Power & CCS

gCCS

gFUELCELL

Oil & Gas

gFLARE

Materials Modelling

Multiflash

OLI

gSAFT

Model Deployment Tools

gO:Run

gO:Run XML

gO:CAPE-OPEN

gO:MATLAB

gO:CFD

gPROMS

The gPROMS platform

Equation-oriented modelling & solution engine

gPROMS ProcessBuilder

- Drag-and-drop flowsheeting & graphical model configuration
- Steady-state & dynamic simulation & optimisation
- (Optional) custom modelling capability

- **Standard Model Libraries**
  - PML:SS
  - PML:DY

- **<u>New</u> developments:**
  ***not* "evolution" of existing PML**
  - solution robustness
    - separate, interoperable, steady-state & dynamic libraries
    - leverage gPROMS platform developments (e.g. initialisation procedures)
    - simplified connection structure
      - reversible flow only where essential
  - enhanced engineering content

- **Advanced Model Libraries (optional)**
  - Reaction
    - AML:FBCR
    - AML:TBR
    - AML:BCR
    - AML:FT (MT), AML:FT (SL)
  - Separation
    - AML:GLC

- **Proprietary/third-party model libraries**

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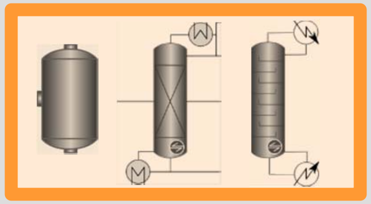
Overview

- PML:SS and PML:DY content overview
- Workflow for distillation column modeling
  - Construct flowsheet and configure column
  - Design, costing and optimization
- Distillation trains
  - C2 and C3 splitter
  - Air Separation Unit
- Conclusions

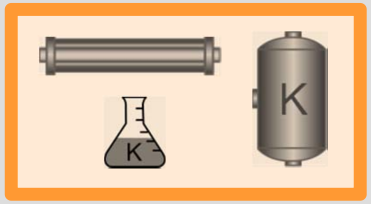
I. Separation

Separation	PML:SS	PML:DY
Component splitter	☑	
Flash drum	☑	☑
Decanter	☑	☑
3-phase separator	☑	☑
Distillation column (tray, equilibrium)	☑	☑
Distillation column (tray, rate-based)	☑	☑
Distillation column (packed-bed, rate-based)	☑	☑
Distillation column (reactive)	☑	☑
Adsorption bed (PSA, TSA)		☑
Membrane separator	☑	☑

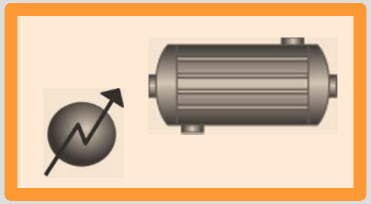
Separation



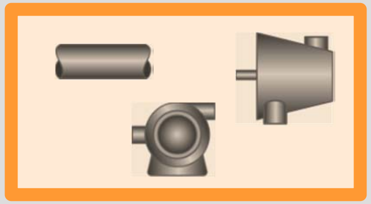
Reaction



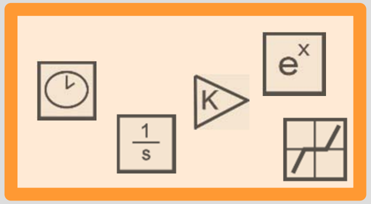
Heat exchange



Flow transportation



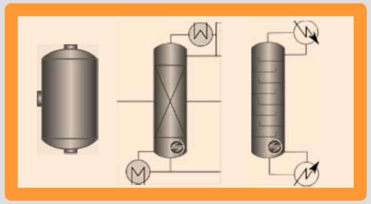
Instrumentation and control



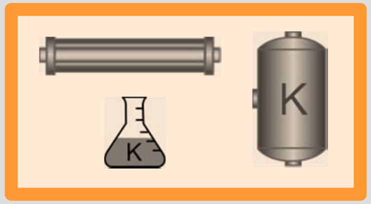
II. Reaction

Reaction	PML:SS	PML:DY
CSTR (conversion)	☑	
CSTR (Gibbs reactor)	☑	☑
CSTR (kinetic & equilibrium reactions)	☑	☑
PFR (kinetic & equilibrium reactions)	☑	☑
Reaction mechanisms: ▪ Arrhenius ▪ Langmuir-Hinshelwood ▪ Michaelis-Menten ▪ User specified	☑	☑

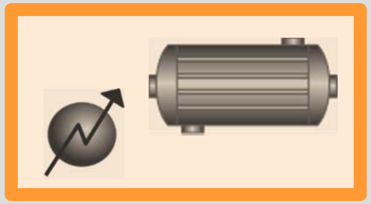
Separation



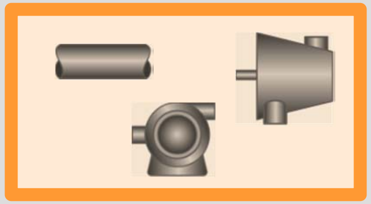
Reaction



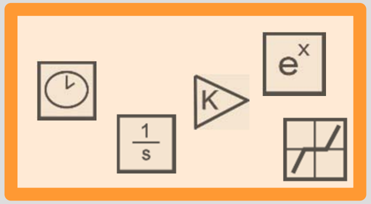
Heat exchange



Flow transportation



Instrumentation and control



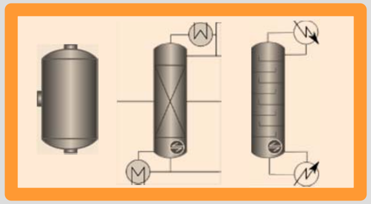
PML:SS and PML:DY overview

III. Heat exchange and flow transportation

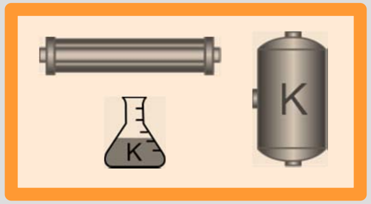
Heat exchange	PML:SS	PML:DY
Heater	☑	☑
Two-stream heat exchanger	☑	☑
Multistream heat exchanger	☑	☑

Flow transportation	PML:SS	PML:DY
Pipe	☑	☑
Compressor section	☑	
Expander	☑	
Valves	☑	☑

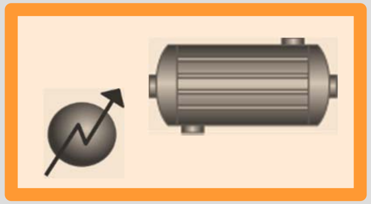
Separation



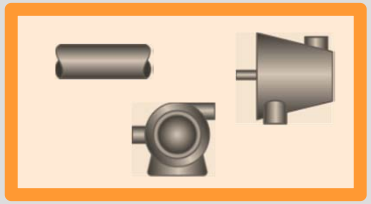
Reaction



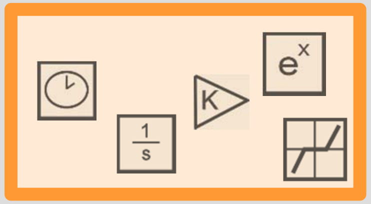
Heat exchange



Flow transportation



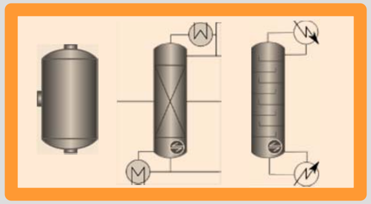
Instrumentation and control



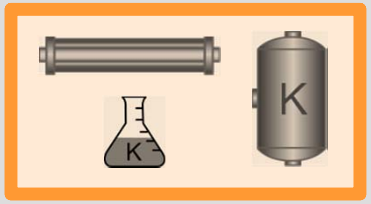
IV. Instrumentation & control

Instrumentation and control	PML:SS	PML:DY
Controllers ▪ Gain, PID	☑	☑
Logic ▪ Switches	☑	
General dynamic behaviour ▪ Transfer function ▪ State-space model		☑
Discrete ▪ Dead zone, hysteresis	☑	☑
Mathematics ▪ Functions, basic operations	☑	
Signal Sources ▪ Constant, ramp, step signal, function generator, time signal	☑	☑
Signal Sinks ▪ Display, plot, X-Y plot	☑	☑
Data ▪ Lookup table, file read, file write	☑	☑

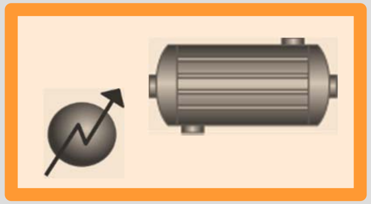
Separation



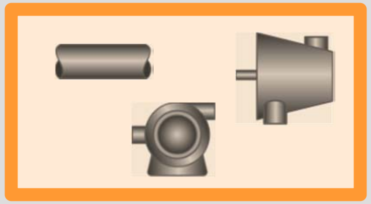
Reaction



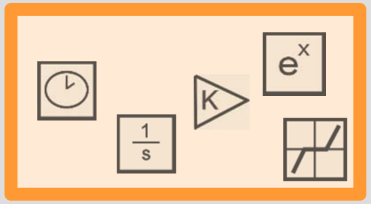
Heat exchange



Flow transportation



Instrumentation and control



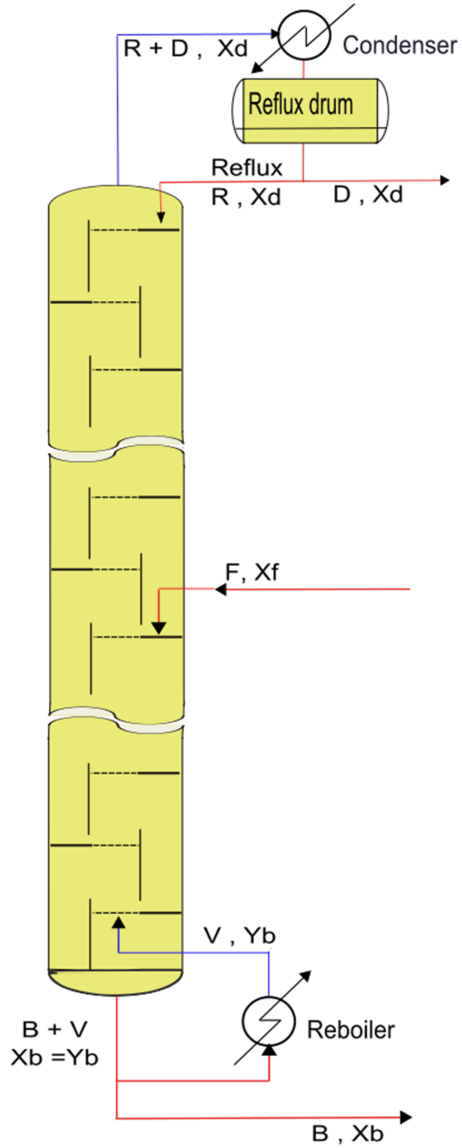
Distillation column optimisation

Distillation column models

- Model basis for trayed column model
  - vapour/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)



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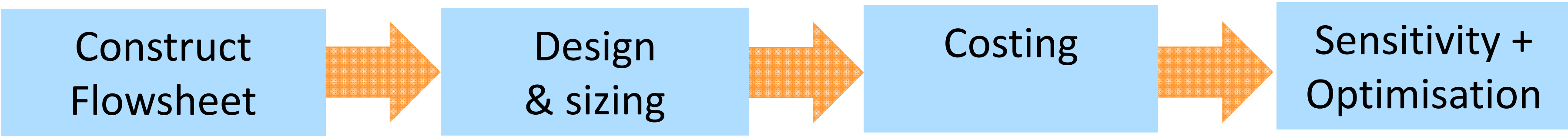
Workflow



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

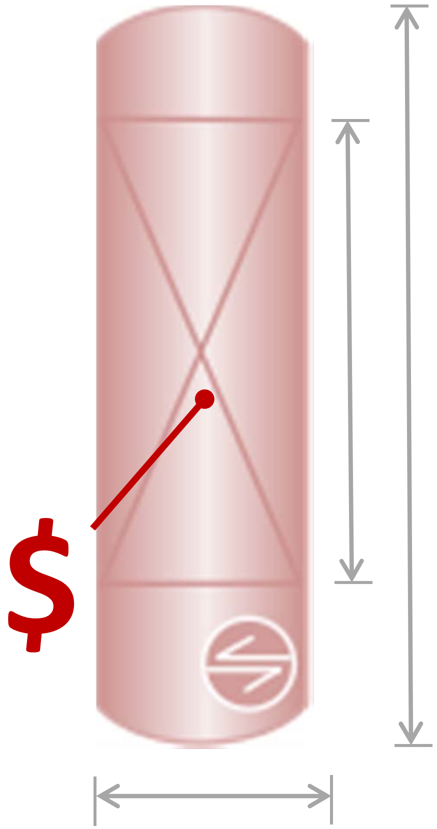
Column parameters	Value	Units
Number of stages	27	
Feed stage	11	
Boilup ratio	2.3	mol/mol
Reflux ratio	0.55	mol/mol
Top pressure	2 bar	bar
Pressure drop per stage	0.0025 bar	bar

- Video

Example #1: Methanol-water separation

- Design equipment
  - "Design" tab of model specification dialog
  - Choose design method and enter geometrical information

Design parameters	Value	Units
Allowed flooding factor	0.85	
Plate spacing	0.8	m
Tray type	Sieve trays	



- Costing
  - "Costing" tab of model specification dialog
  - Choose costing correlation and pricing information
- Video

Example #1: Methanol-water separation

- Operation optimisation

Minimise **reboiler heat duty** subject to:

Quantiy	Constraint	Units
Methanol top purity	>0.99	mol/mol
Top product molar flowrate	>400	kmol/hr

By adjusting

Quantiy	Initial value	Units
Boilup ratio	2.3	mol/mol
Reflux ratio	0.55	kmol/hr

- Video

Example #1: Methanol-water separation

- Design and operation optimisation (Mixed-Integer)

  Minimise **column capital cost** subject to:

Quantiy	Constraint	Units
Methanol top purity	>0.99	mol/mol
Top product molar flowrate	>400	kmol/hr

  By adjusting

Quantiy	Initial value	Units
Number of trays		mol/mol
Feed location		kmol/hr
Boilup ratio	2.3	mol/mol
Reflux ratio	0.55	kmol/hr

- Video

Example #1: Methanol-water separation

- Result operation optimisation

Quantiy	Initial value	Final value	Units
Boilup ratio	2.3	1.97	mol/mol
Reflux ratio	0.55	0.58	mol/mol
Reboiler duty	4.05E7	3.78E7	kJ/hr

- Result design and operation optimisation

Quantiy	Initial value	Final value	Units
Number of trays	27	22	-
Feed location	11	20	-
Boilup ratio	2.3	1.72	mol/mol
Reflux ratio	0.55	0.50	mol/mol
Column capital cost	146000	104700	$

Distillation train modelling & simulation

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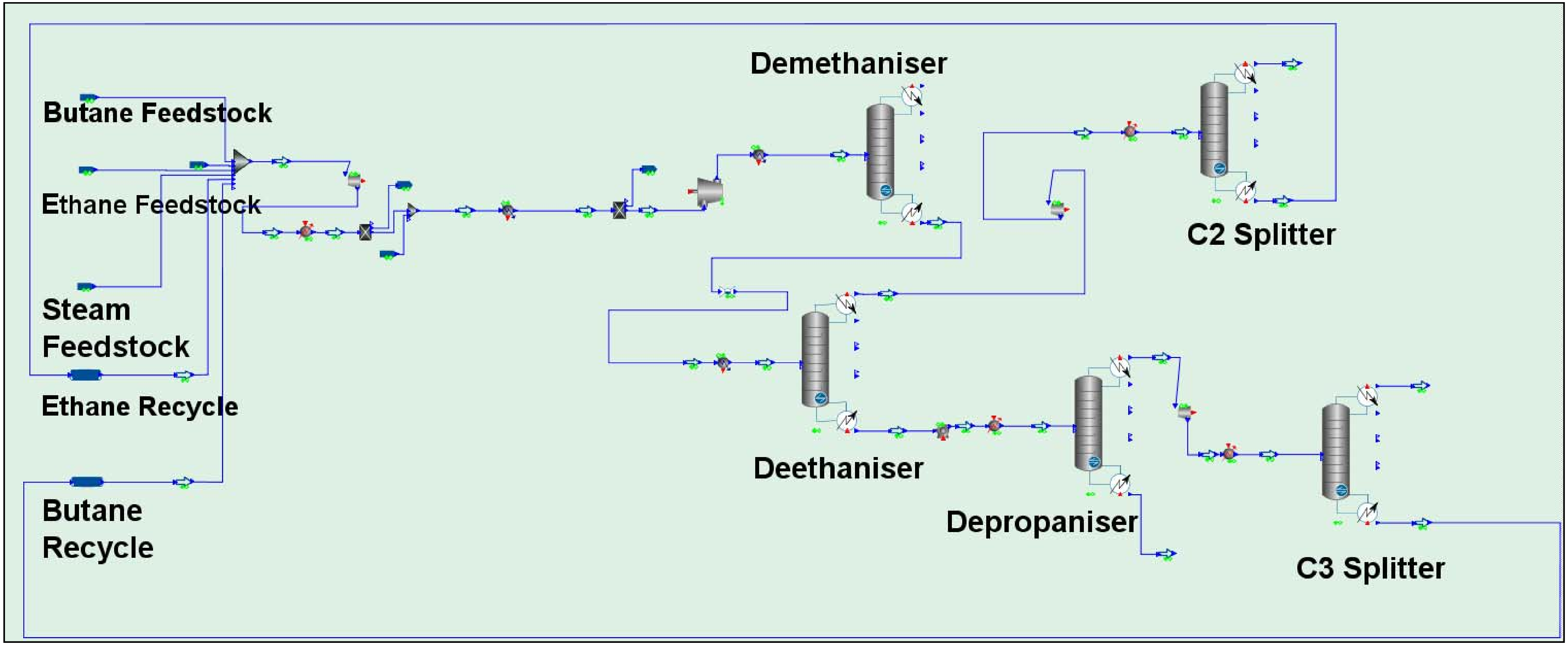
Example #2: Ethylene plant recovery section

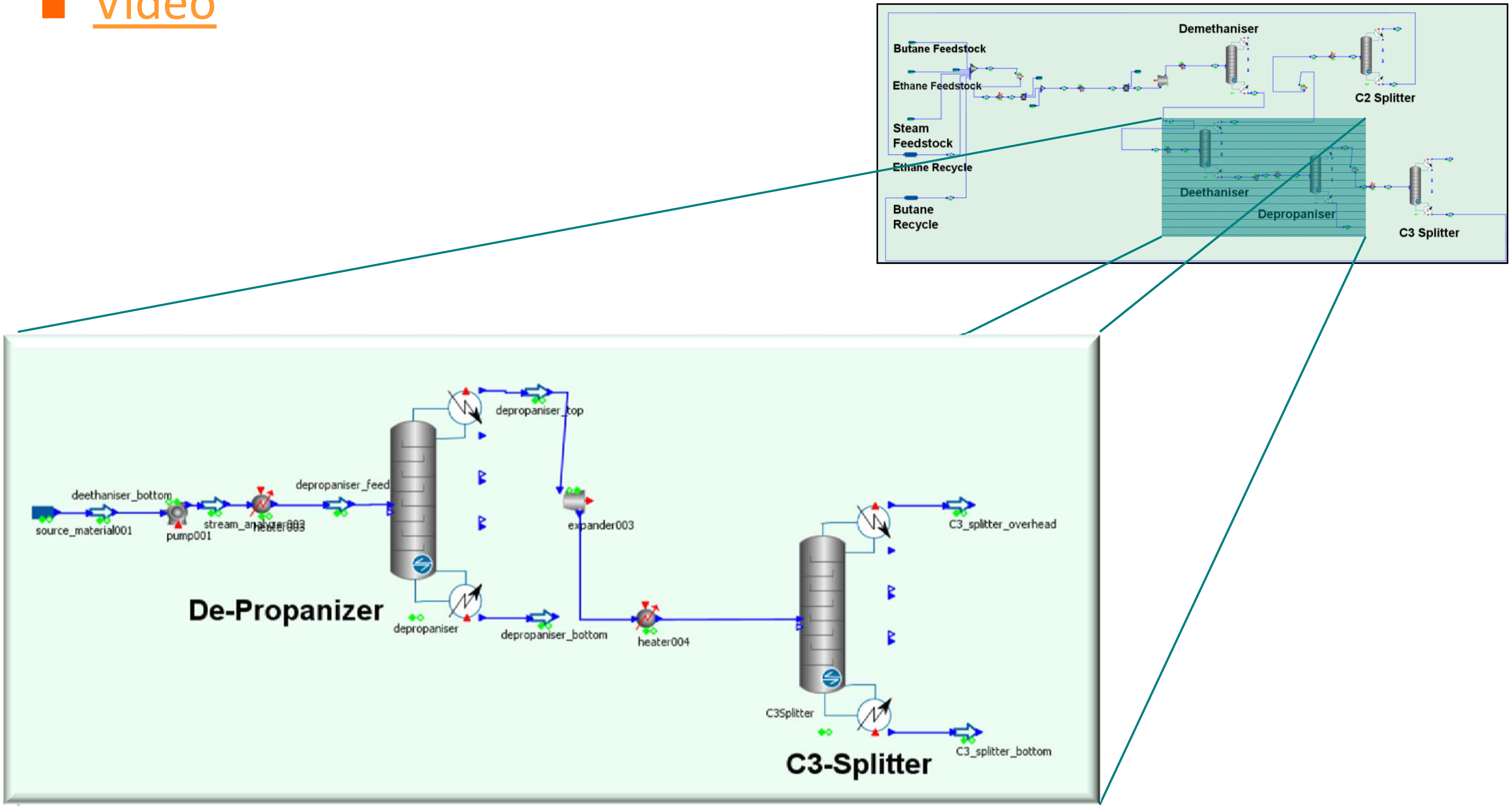
- Physical properties: Ideal gas / Peng-Robinson WoS
- Solution time with no user-provided initial guesses: 37 CPU s (Intel i7 laptop)



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

Example #2: Ethylene plant recovery section – 2 columns

- Video



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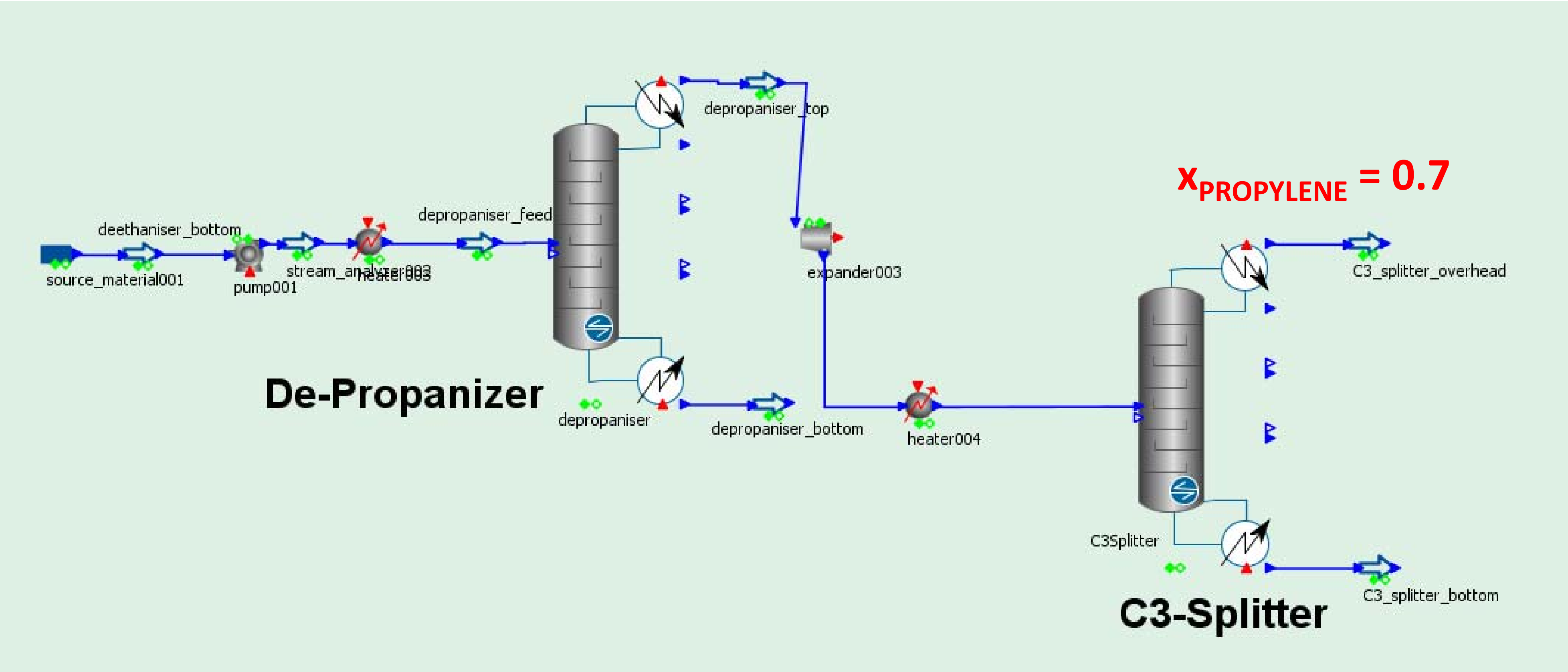
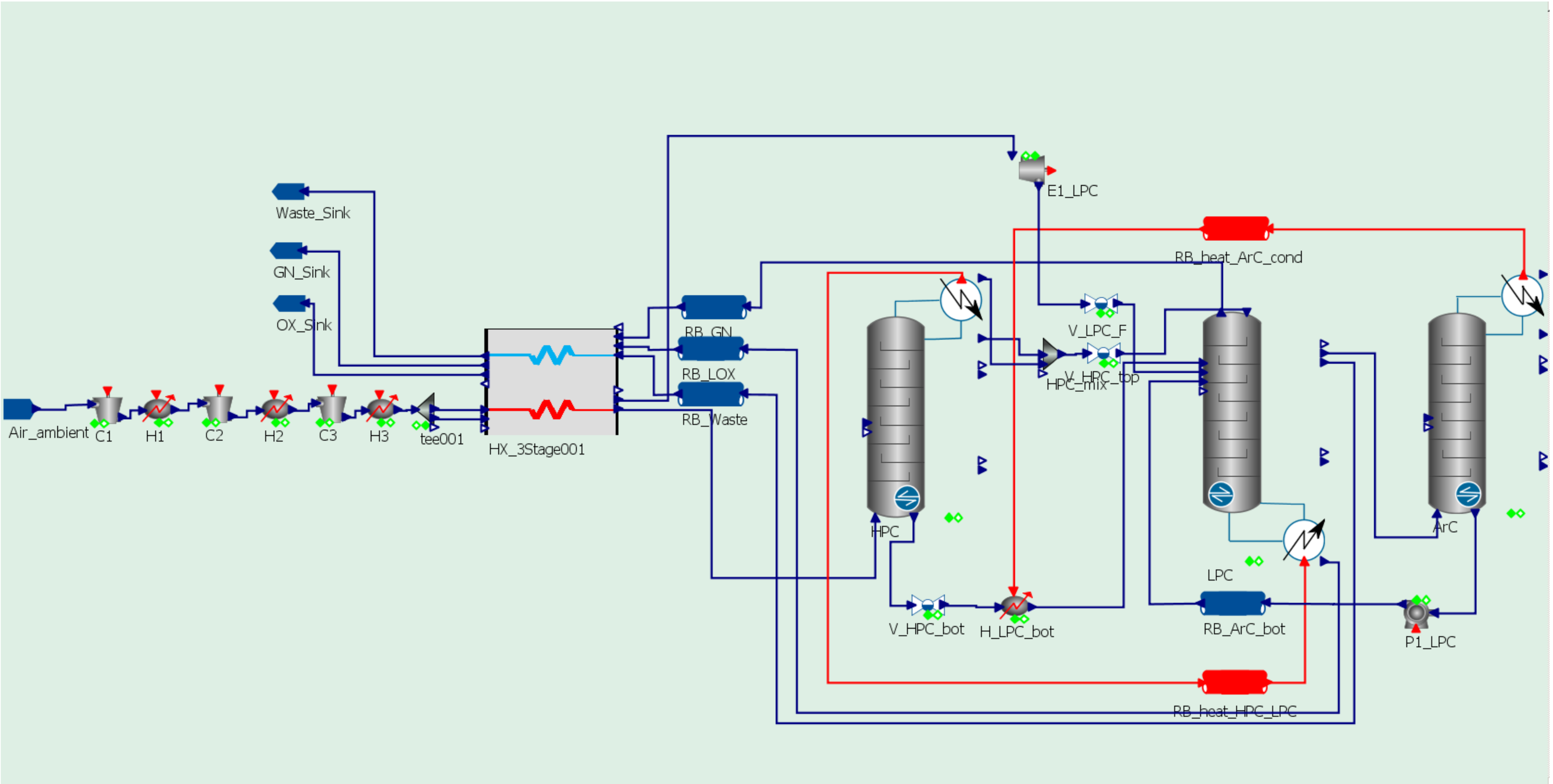
Example #2: Ethylene plant recovery section – 2 columns

- Goal: achieve a specified purity of Propylene at the top of the C3-splitter by adjusting the boil-up ratio of the depropanizer, Video



Tightly coupled distillation systems

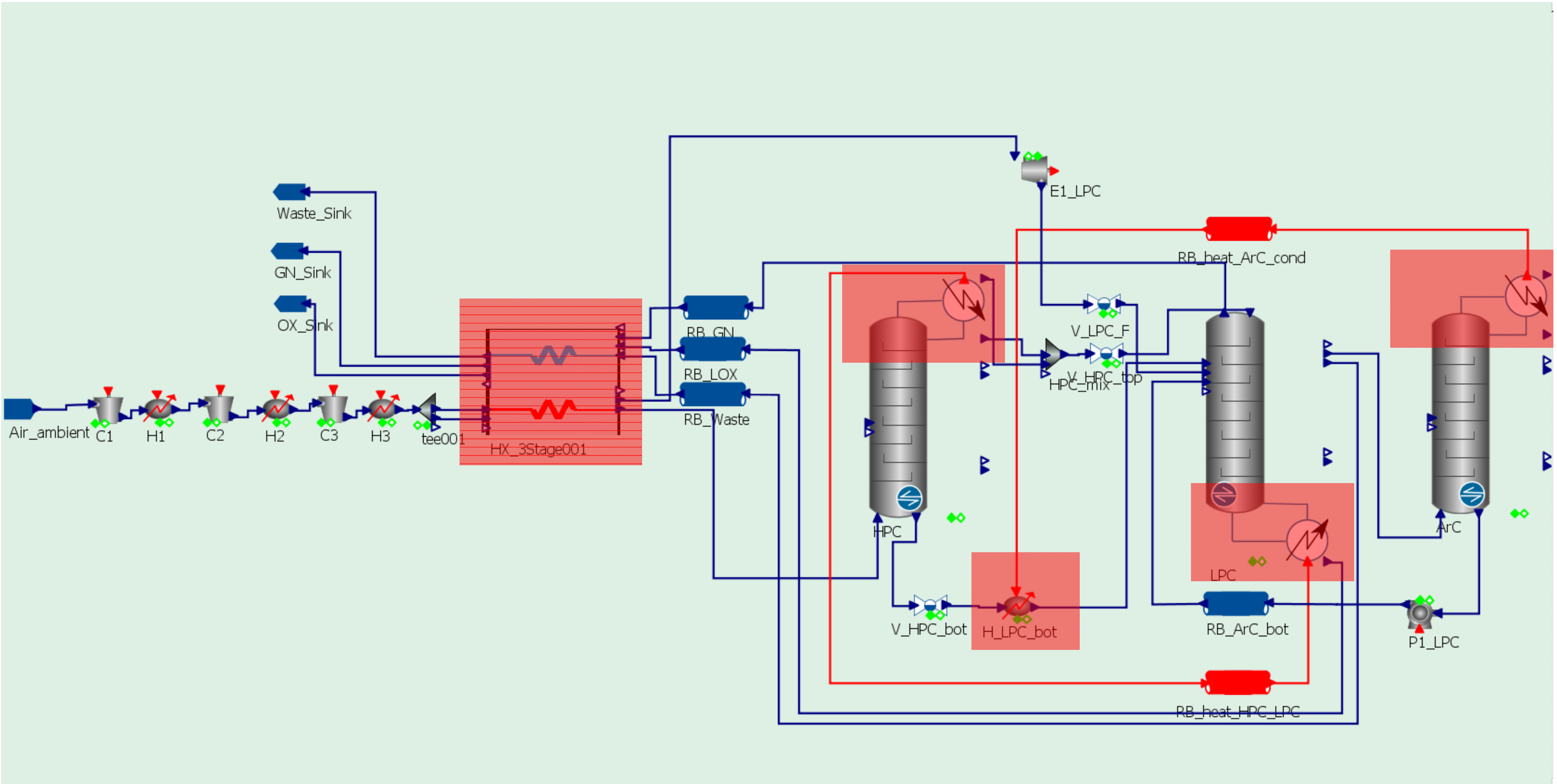
Example #3: Air Separation Unit (ASU)



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)

- Physical properties: Peng-Robinson (Multiflash)
- Solution time with no user-provided initial guesses: 21 CPU s (Intel i7 laptop) Video



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Beyond distillation…

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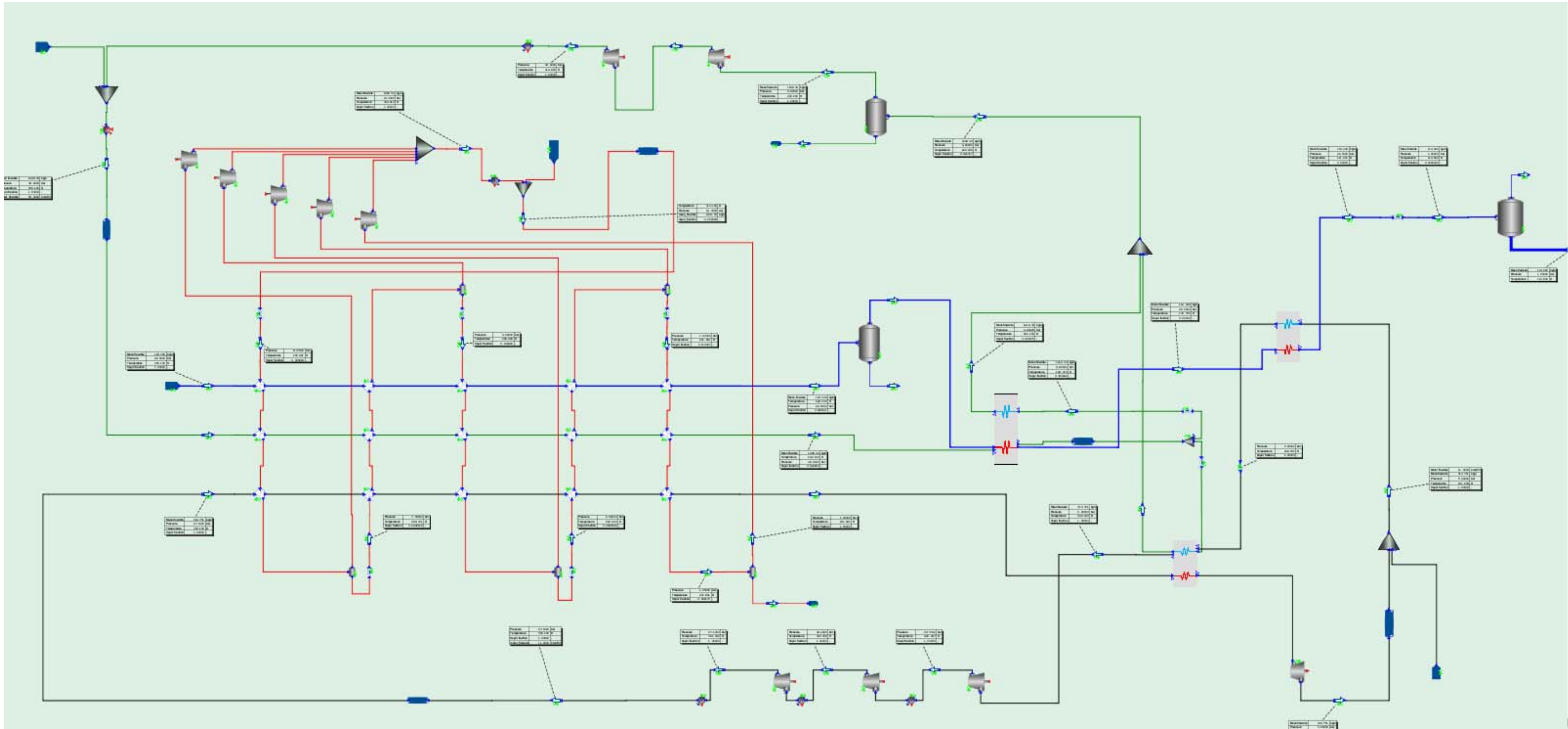
Example #4: C3-MR LNG liquefaction process

- Physical properties: GERG-2008 Equation-of-State (Multiflash®)
- LNG cooled by three refrigeration loops: N_2, propene, Mixed Refrigerant
- Unit operations: MX heat exchange, V-L separation, compression, expansion
- Solution time with no user-provided initial guesses: 15 CPU s (Intel i7 laptop)



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Conclusions

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Focus

- gPROMS ProcessBuilder: new product focused on
  - chemicals/petrochemicals applications
  - engineering users
    - Tier-II organisational deployment

Tier I	Tier II	Tier III	Tier IV
First-principles modellers (“custom modelling”)	Drag-and-drop flowsheeting using model libraries	“Non-modellers” requiring access to model-based calculations	Models embedded in online/real-time systems
Primarily R&D	R&D Engineering	Engineering Operations Commercial	Operations

Content

- Comprehensive model libraries
  - standard: PML:SS and PML:DY
  - optional: Advanced Model Libraries (AMLs)
- Extensible via
  - use of proprietary/third-party model libraries
  - (optional) custom modelling
- Physical properties: Multiflash + gSAFT

gPROMS ProcessBuilder

- Taking full advantage of gPROMS Platform developments
  - Model Initialisation Procedures
  - enhanced usability
  - error-free problem specification
  - units of measurement
  - . . . .

- Release timetable
  - PML:SS now available for beta-testing
  - gPROMS ProcessBuilder v1.0: December 2013
    - based on gPROMS Platform v4.0

Acknowledgements

- Library development
  - Rodrigo Blanco
  - Diogo Narciso
  - Robert Pack

- Testing & applications
  - Pedro Chainho
  - Francisco Borralho

Thank you!

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The Advanced Process Modelling Forum

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

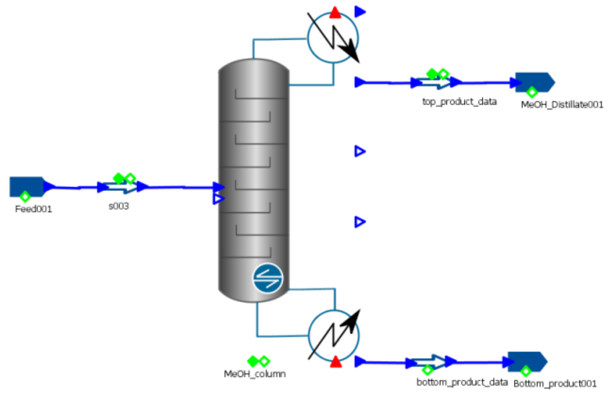
- LNG liquefaction:

  - Shahrooz Abbasi Nezhad, Bezhan Shabani and Majid Soleimani, Thermodynamics Analysis of Liquified Natural Gas (LNG) Production Cycle in APCI Process, Journal of Thermal Science, vol.21 , No.6, Pages 564-571 , 2012.
  - Abdullah Alabdulkarem, Amir Mortazavi, Yunho Hwang, Reinhard Radermacher, Peter Rogers, Optimization of propane pre-cooled mixed refrigerant LNG plant, Applied Thermal Engineering, Volume 31, Issues 6–7, Pages 1091-1098, May 2011.
  - R. A. Mark Julian Roberts, Hybrid cycle for the production of LNG, US Patent no 6,308,531, 2011.

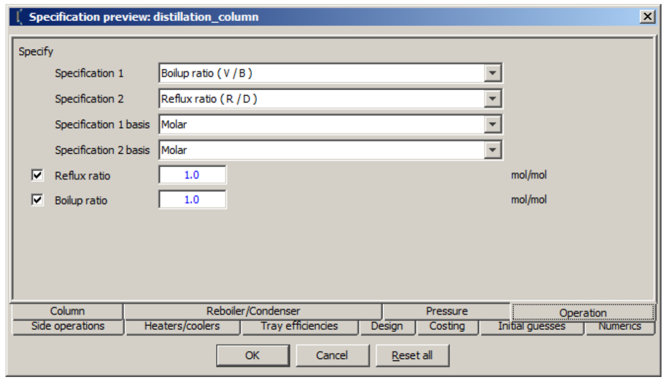
Workflow - Construct flowsheet

- Construct flowsheet

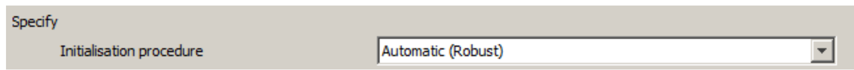
1. Drag-and-drop column model onto flowsheet



2. Configure minimum set of specifications



3. gPROMS takes care of initialisation




```

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

```

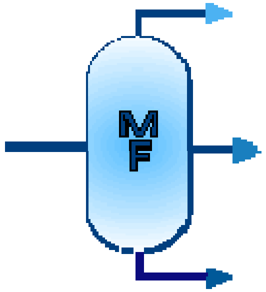
Workflow – Sensitivity study and optimisation

- Sensitivity
  - Using the graphical TASK language
  - Adding standard perturbations on the flowsheet
- Optimisation

Type of optimisation	Operation	Design	Design + Operation
Cost function	Reboiler duty	Capital cost	Capital cost
Controls	Boilup ratio Reflux ratio	Number of trays Feed location	Number of trays Feed location Boilup ratio Reflux ratio
Constraint	Methanol top purity	Methanol top purity	Methanol top purity

Physical properties

- Select physical properties
  - Multiflash



  - gSAFT
  - CAPE-OPEN Thermo FO compliant

    (e.g. Aspen Properties)