ADVANCED PROCESS MODELLING FORUM **2014**

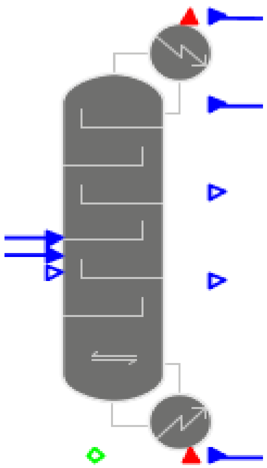
gPROMS ProcessBuilder

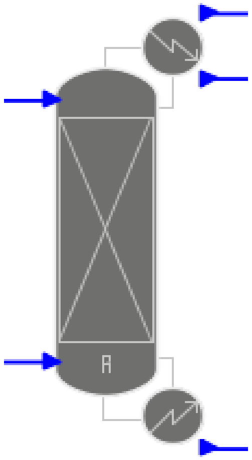
Distillation & absorption

Charles Brand – Consultant

Gas/liquid contacting devices
Models in gPROMS ProcessBuilder

- Representations of phase interactions
  a. Phase equilibrium
  b. Finite rates of mass and heat transfer
     - 1D and 2D models
- Ability to model reactive distillation
  – Including ionic systems
  – 2D rate-based model more appropriate for reactive systems
- Operation modes
  – Steady state
  – Dynamic
    – continuous or batch operation





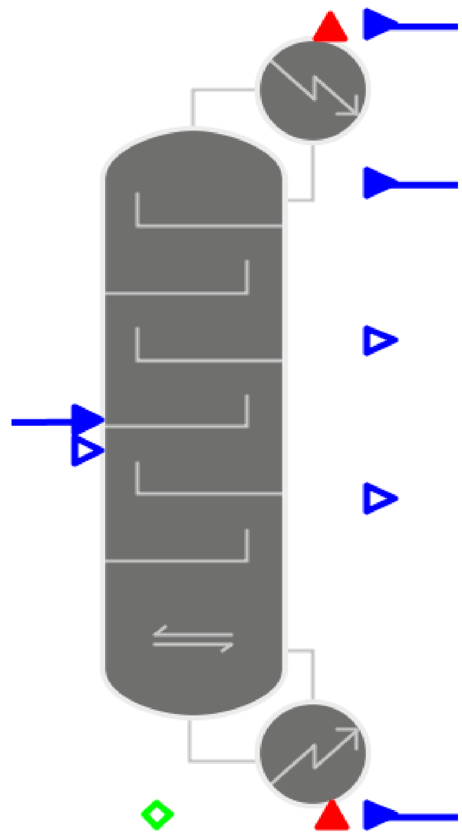
gPROMS ProcessBuilder

Phase equilibrium column moc

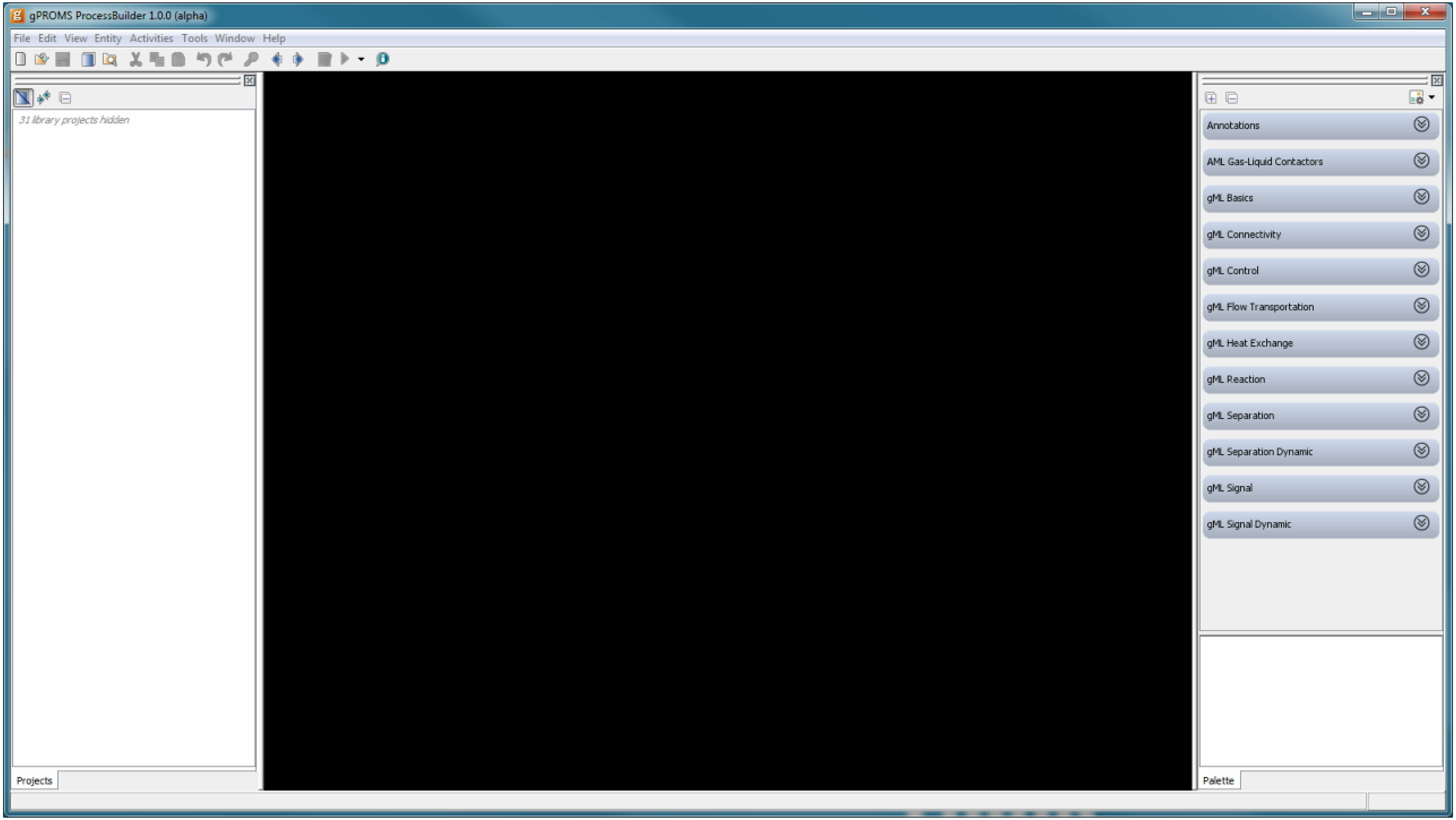
Base product & options	Included	Options
Platform		
gPROMS environment (inc. Case file viewer)	✓	
Flowsheet construction & specification	✓	
Custom modelling		✓
Simulation (steady-state & dynamic)	✓	
Optimisation (steady-state & dynamic)	✓	
Parameter estimation		✓
Experiment design		✓
Export to gPROMS Objects		✓
Packaging & licensing of model libraries		✓
Hybrid Multizonal CFD Inteface		✓
Libraries: ProcessBuilder		
gML:Basics, Connectivity, Signal, Flow Transportation, Heat Exchange	✓	
gML:Compression		✓
gML:Reaction		✓
gML:Separations - Fluid-Fluid		✓
gML:Multipack (Compression, Reaction, Separations - Fluid-Fluid)		✓
gML:Separations - Adsorption		✓
gML:Separations - Membranes		✓
AML:Gas-Liquid Contactors		✓
AML:Fixed-Bed Catalytic Reactors		✓
AML:FBCR - FLUENT interface		✓
AML:FBCR - STAR-CD interface		✓
Physical properties		
gSAFT		✓
gPROMS Properties (MS Windows only)	✓	
gPROMS Properties - DIPPR	✓	

Phase equilibrium column model

- Key assumption: vapour/liquid equilibrium at each stage
  - including reboiler & condenser
  - optional specification of stage efficiencies
- Different calculation modes
  - Rating
  - Design
    - column height
    - column diameter
      - determined from flooding limit
  - Costing
    - standard equipment cost correlations (Seider & Seader, 2010)
- Built-in Model Initialisation Procedures



Acetone-methanol separation



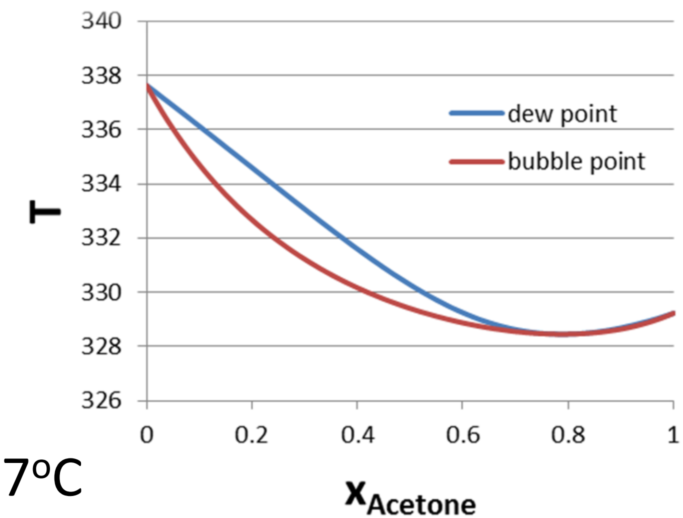
Acetone-methanol separation

Results

	Feedstock	Top product	Bottom product
Temperature (K)	293.1	328.1	328.1
Pressure (bar)	1.0	1.0	1.0
Mass flowrate (kg/s)	1.47	0.732	0.737
Mass fraction			
Acetone	0.88	0.875	0.885
Methanol	0.12	0.125	0.115

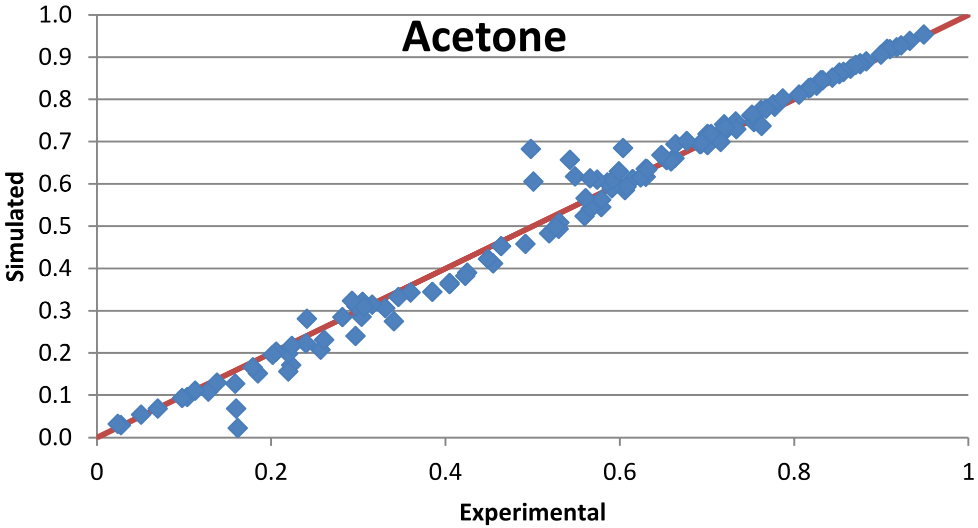
Not much separation is taking place!

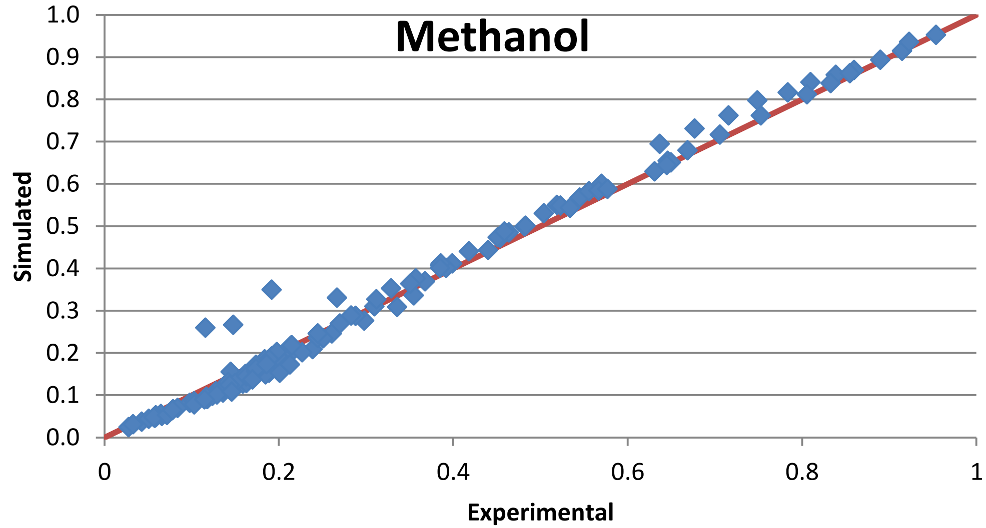
- Acetone-methanol form an azeotropic mixture
  - Acetone bp 56.14°C, Methanol bp 64.53°C
  - Mixture minimum boiling point 55.24°C
    - $x_{Acetone} = 0.862$, $x_{Methanol} = 0.138$
- Add water!
  - acts as entrainer
  - suggested water injection: 200 kmol/hr at 47°C
    Gil *et al.*, *IECR*, 2009, **48**, 4858-4865

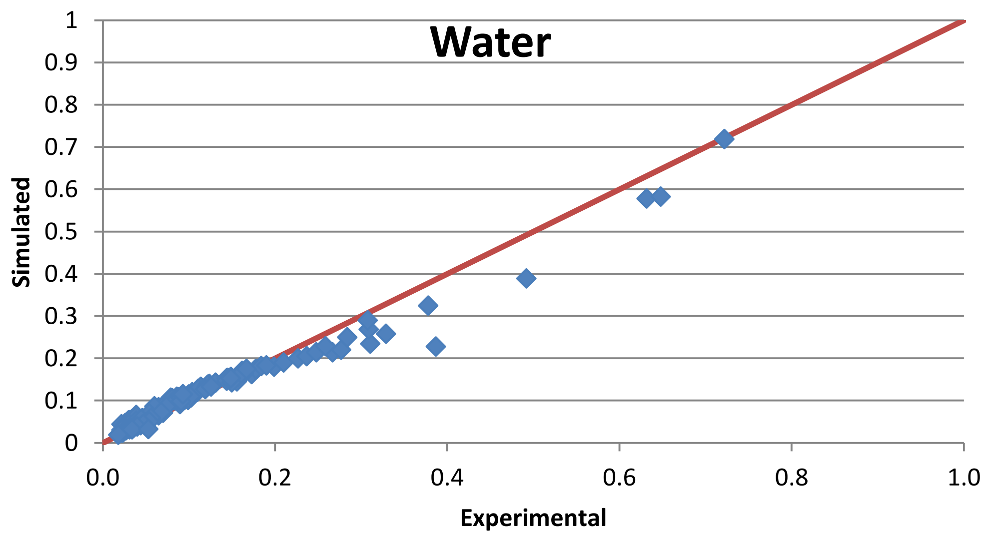


UNIQUAC thermodynamic model – validation

Vapour molar fraction prediction at bubble point



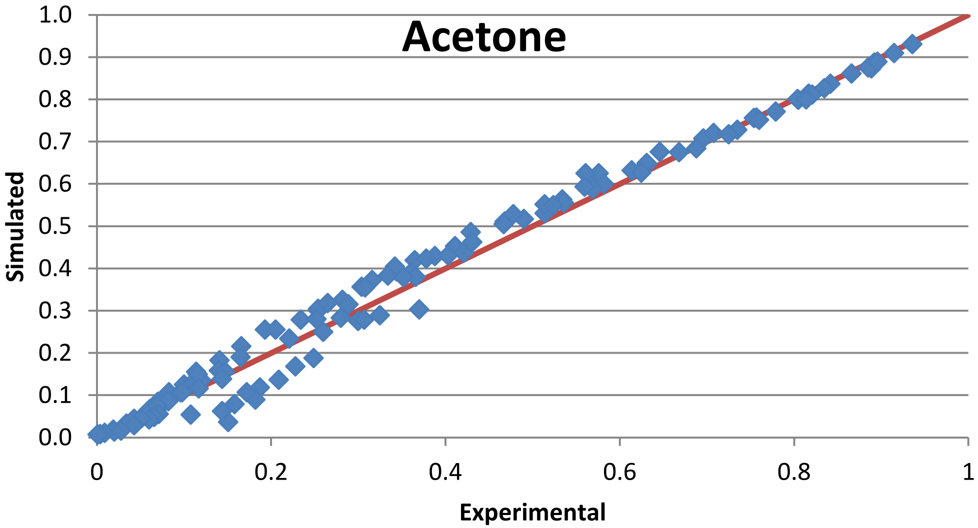


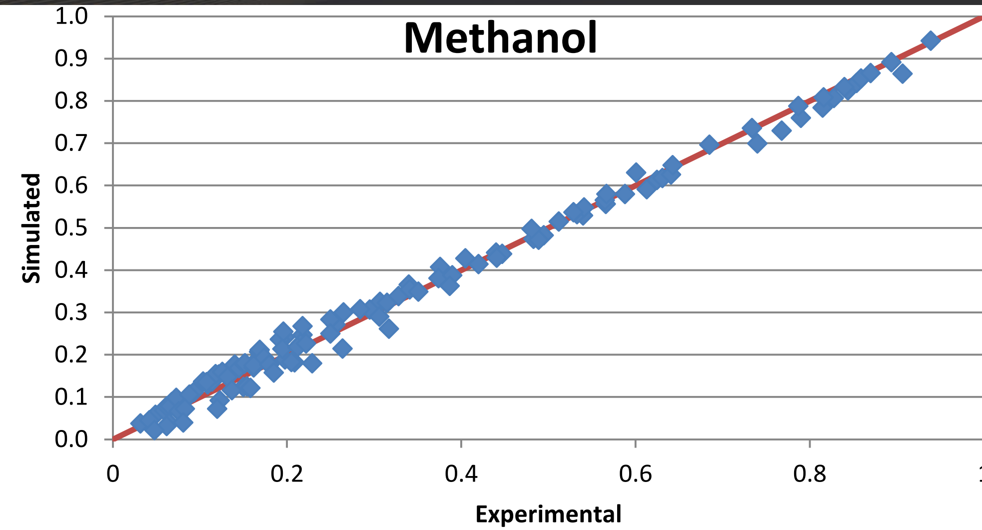


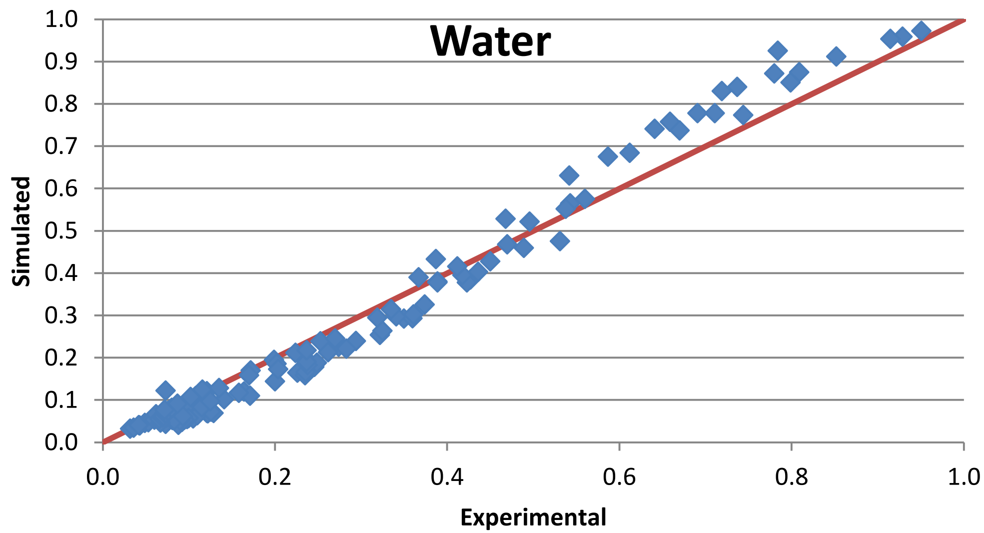
Iglesias *et al.*, *J. Chem. Eng. Data*, 1999, **44**, 661-665

UNIQUAC thermodynamic model – validation

Liquid molar fraction prediction at dew point







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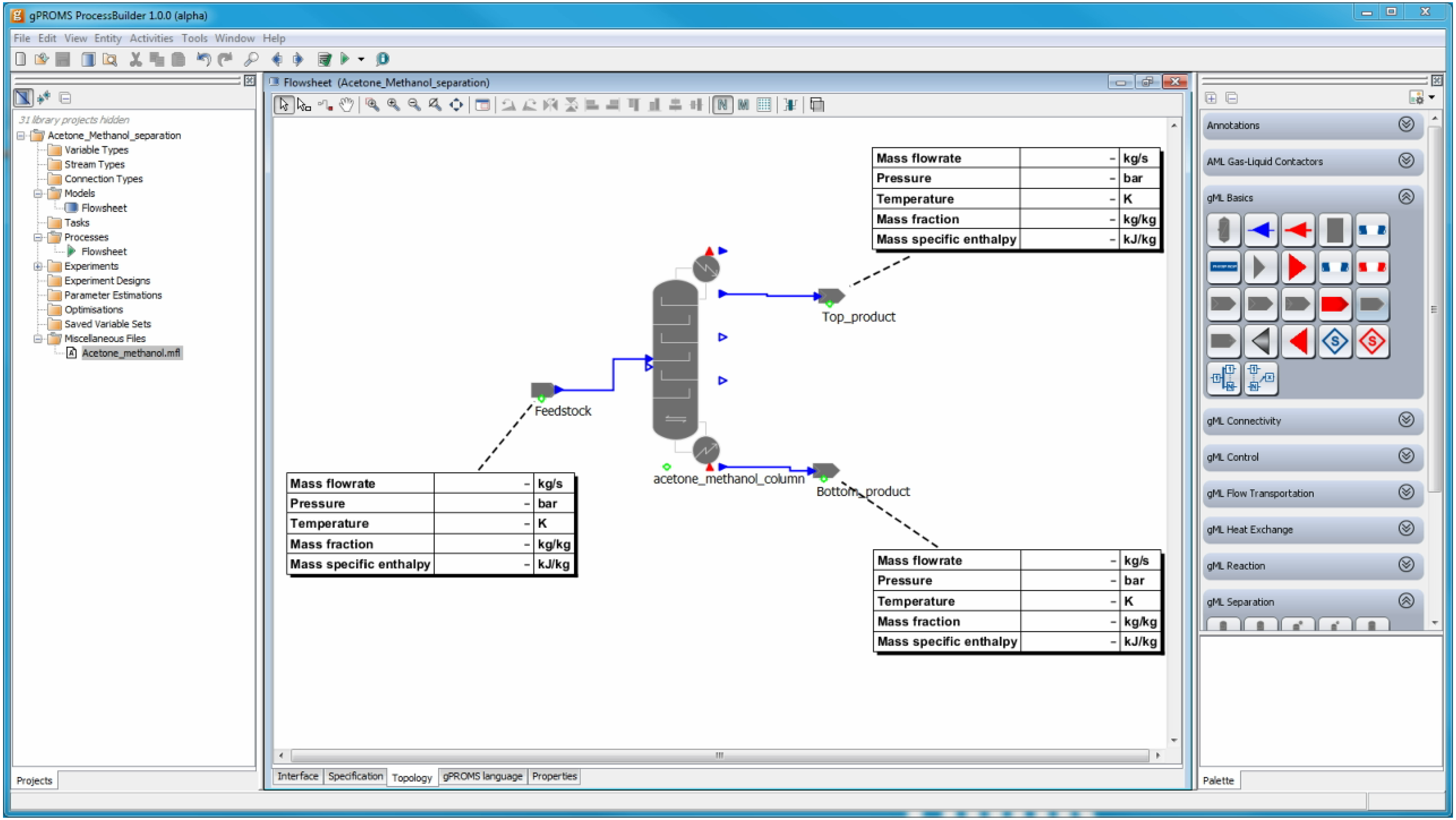
Acetone-methanol separation revisited

Extractive distillation



Acetone-methanol separation revisited

Extractive distillation

	Feedstock	Water Entrainer	Top product	Bottom product
Temperature (K)	293.1	320.1	328.9	354.6
Pressure (bar)	1.0	1.0	1.0	1.0
Mass flowrate (kg/s)	1.47	1.001	1.219	1.252
Mass fraction				
Acetone	0.88	0	0.997	0.062
Methanol	0.12	0	$4.290\ 10^{-7}$	0.141
Water	0	1	$2.657\ 10^{-3}$	0.797

✓

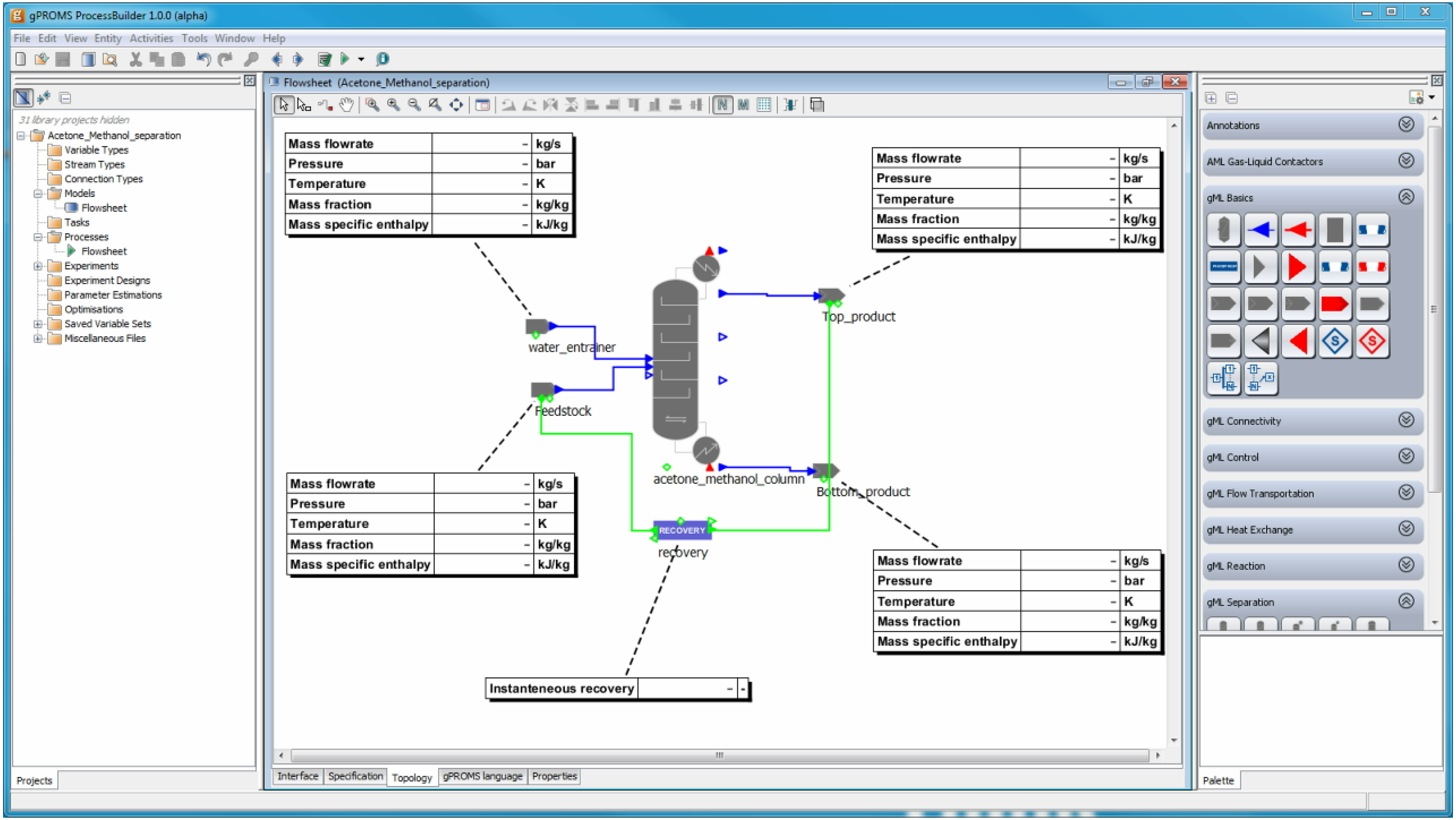
Can we do better?

- Current KPIs
  - acetone purity = 99.7% wt
    - Better than required spec of 99.5%
  - acetone recovery = 94%
    - Should be increased to 95%
  - energy consumption: 2.755MW

Improve via rigorous optimisation

- Eliminate purity give-away
- Improve recovery
- Minimise energy

Column optimisation - demos



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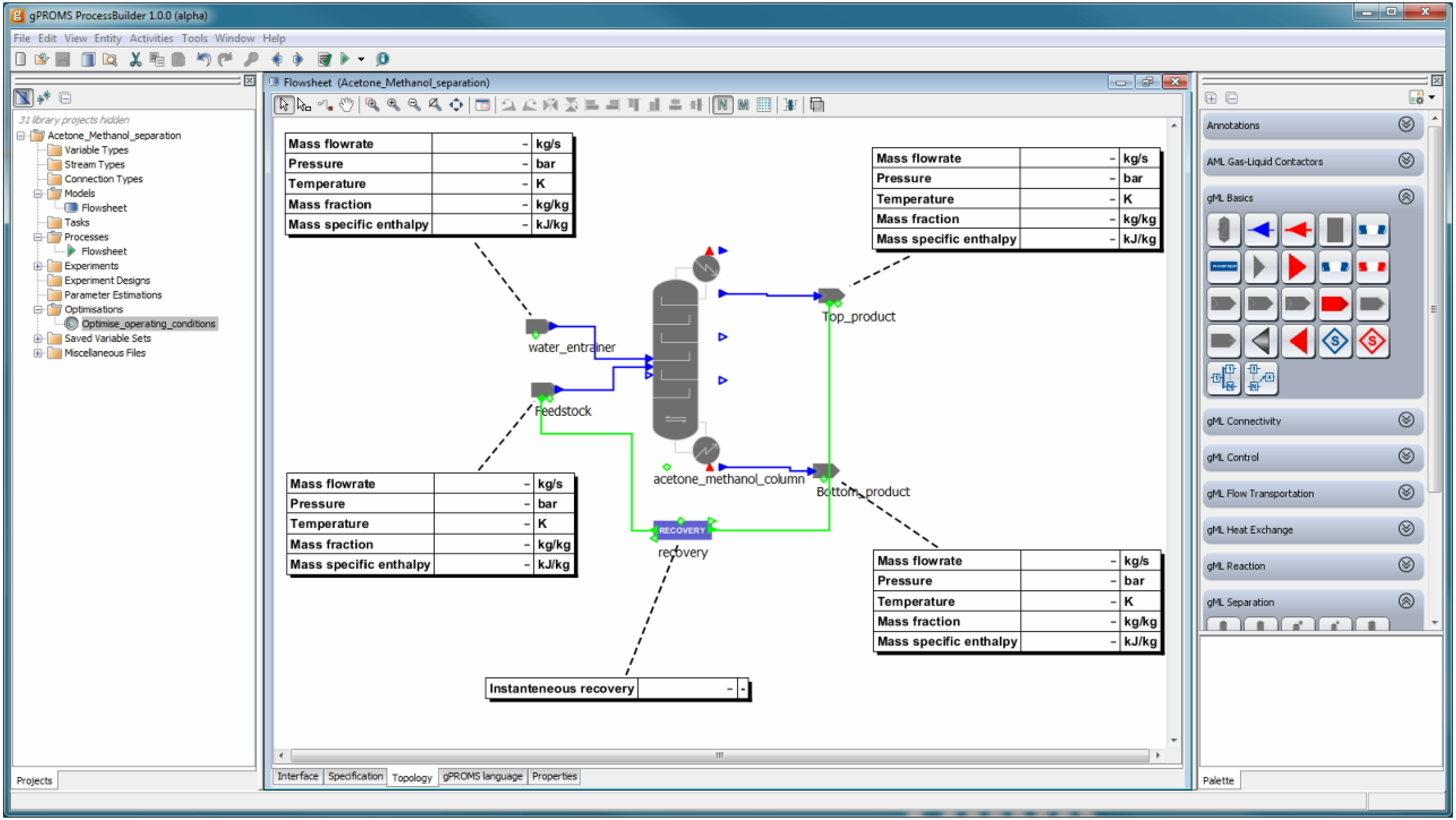

Acetone-methanol separation optimal conditions

Extractive distillation

	Before	After
Water entrainer feed stage	22	29
Water entrainer flowrate (kmol/h)	200	143
Reflux ratio	3.00	1.73
Liquid bottom flowrate (kmol/h)	224	165

- Original KPIs
  - acetone purity = 99.7% wt
  - acetone recovery = 94%
  - energy consumption = 2.755MW
- Optimised KPIs
  - acetone purity = 99.5% wt
  - acetone recovery = 95%
  - energy consumption = 1.971MW

Energy consumption reduction: 28% ✓

gPROMS ProcessBuilder

Rate-based column models

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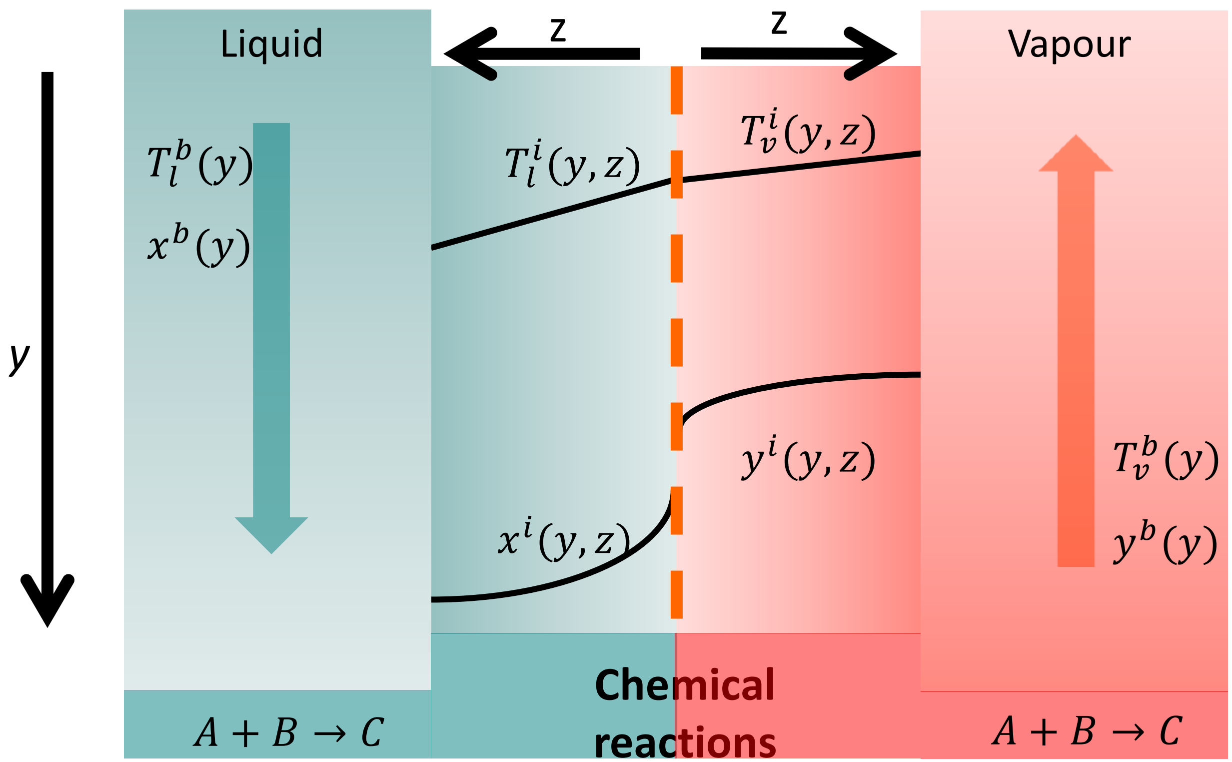
2D rate-based column model



- Dynamic mass and energy balances in fluid **bulks**
- Mass and heat transfer in the **films**
- Energy balance and phase equilibrium at the **interface**
- Chemical reaction in both phases
  - bulk & films

2D rate-based column models

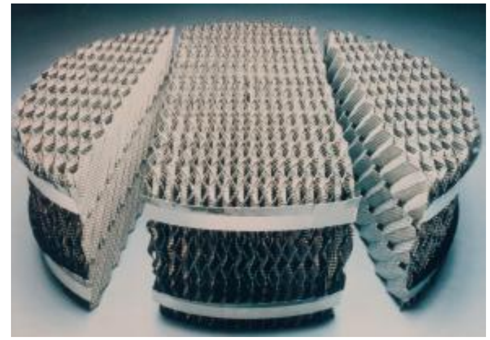
Generality

- **2nd-generation rate-based** approach
  - mass/heat transfer limitations on both sides of gas-liquid interface
  - Maxwell-Stefan formulation used throughout
    - including electrostatic field term
  - full spatial discretisation across films
  - handling of non-condensible & non-volatile species
- Handling of **general reaction systems**
  - irreversible & reversible kinetic reactions
  - equilibrium reactions
- Fully **dynamic** models
  - continuous & batch operations

Rate-based column models

Usability

- **Engineering-oriented** content
  - build-in packing database
  - well-established correlations for hydrodynamics
    and heat and mass transfer
  - standard reaction kinetics



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- **Customisable** via user-defined
  - hydrodynamics correlations
  - heat and mass transfer correlations
  - kinetics reaction schemes

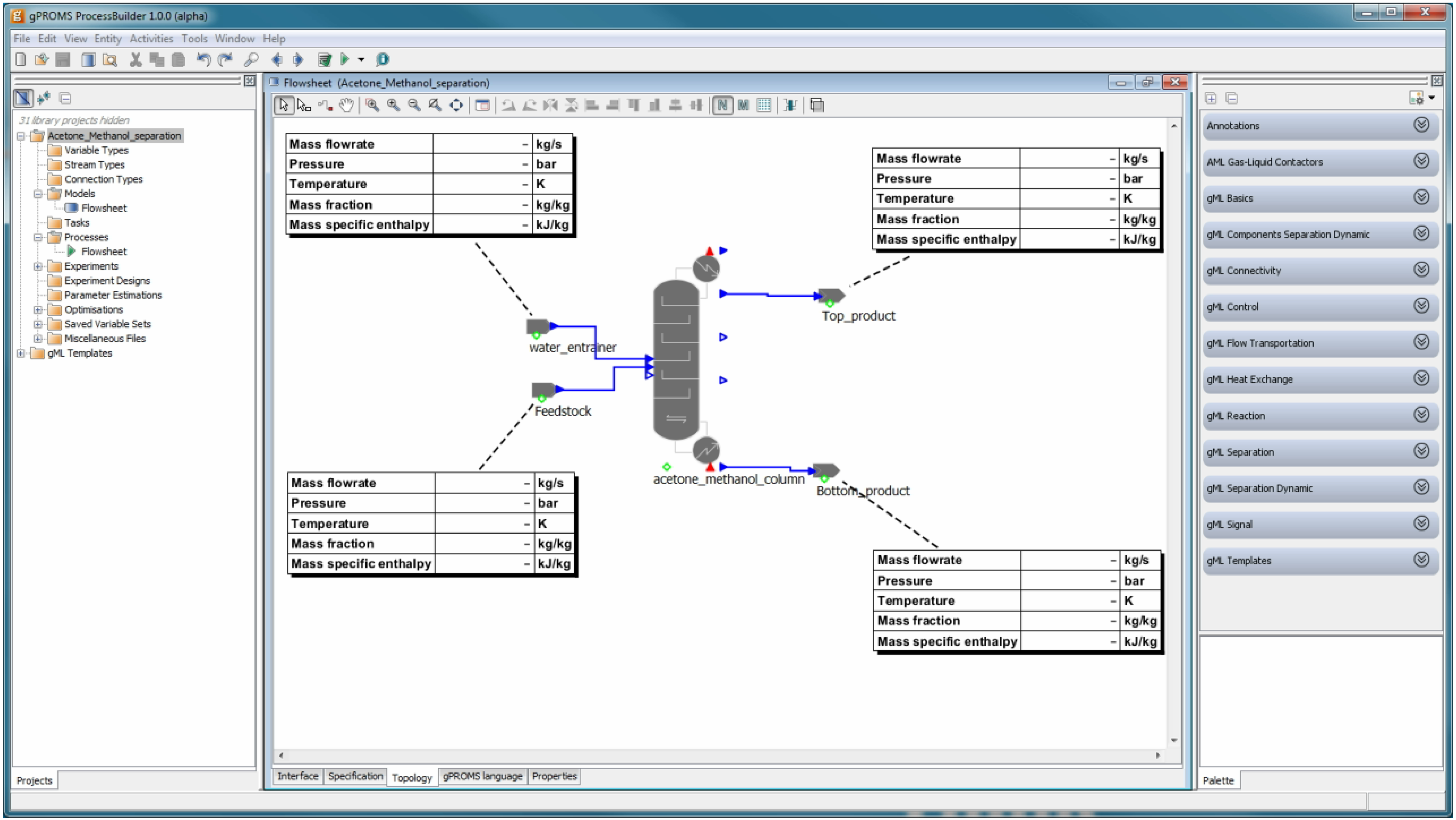
(standard templates provided)

```

EQUATION
    FOR y := 0 to 1 DO
        interfacial_area(y) / surface_area =
            1 - EXP(-1.45 * (Surf_tens_crit/Surface_tension(y))^0
            * (ABS(superficial_liquid_mass_velocity(y) + 0.1) / (:
            * (ABS(superficial_liquid_mass_velocity(y) + 0.1)^2 *
    END
```

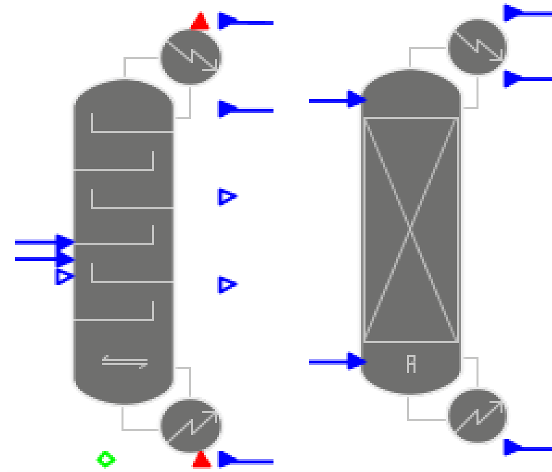
AML: GLC

Rate-based distillation column



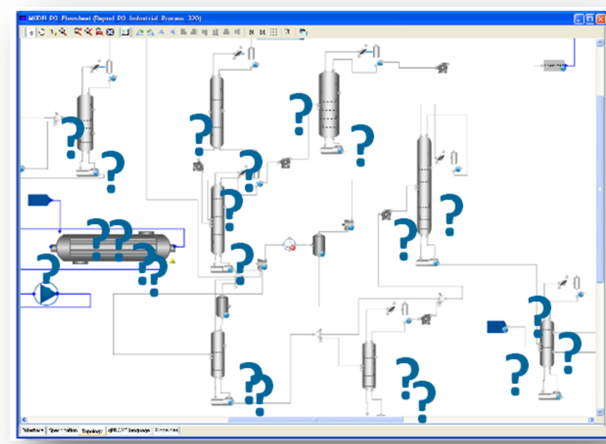
Summary

- A powerful modelling capability for gas/liquid contactors in the gPROMS ProcessBuilder



- Ability to integrate separation section with reaction section
  - capitalise on gPROMS’ well-established modelling capability for complex reactors

  → **<u>whole-plant</u> modelling & optimisation**



- Applications across the process industry
  - chem/petrochem, oil & gas, refining, specialties, pharma, …
  - *batch* distillation case studies ongoing
    - capitalise on gPROMS dynamic optimisation capability

ADVANCED PROCESS
MODELLING FORUM **2014**

Thank you