ADVANCED PROCESS MODELLING FORUM **2014**

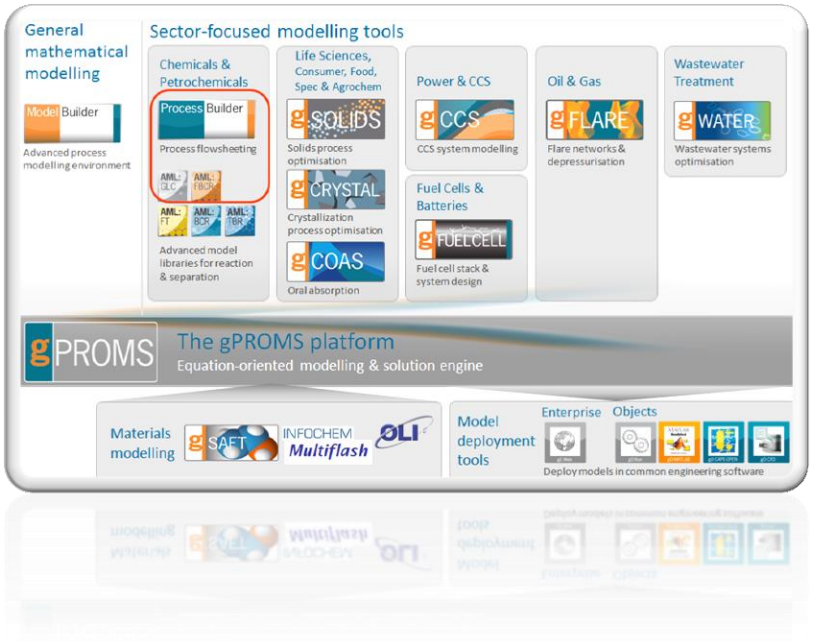
# gPROMS ProcessBuilder

## Advanced Process Simulation for Chemicals & Petrochemicals

Maarten Nauta – Senior Consultant

# gPROMS ProcessBuilder

Process Builder




A **new** product

…based on the gPROMS Platform

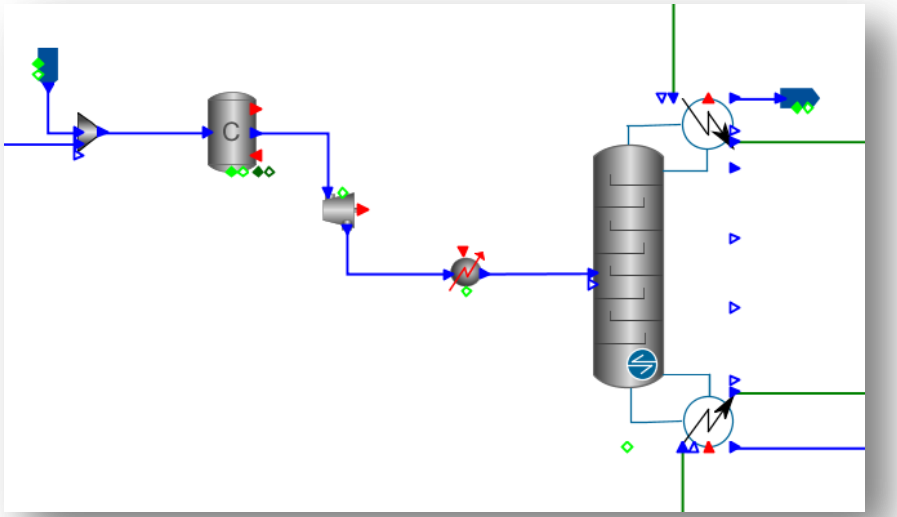
…for the **Chemicals & Petrochemicals** sector

…delivering new levels of functionality, usability & efficiency

# gPROMS ProcessBuilder

## Technical overview

- Drag-and-drop flowsheeting
- Comprehensive library of unit operation models
- Custom modelling
- Advanced thermodynamics
- Steady-state & dynamic simulation
  - ...and transition from one to the other
- Process optimisation



# This morning's presentations

- **Overview**
  - **Dr Maarten Nauta**
- Distillation/absorption
  - Dr Charles Brand
- Pressure Swing Adsorption (PSA)
  - Dr Mayank Patel
- gSAFT physical properties
  - Dr Tom Lafitte
- Conclusion & perspective
  - Prof C.C. Pantelides

# Overview of this presentation

- Content
  - Model libraries
- Workflow
  - Steady-state flowsheeting
  - From steady state to dynamics
- Advanced capabilities for flowsheet simulation

gPROMS ProcessBuilder

# Model libraries

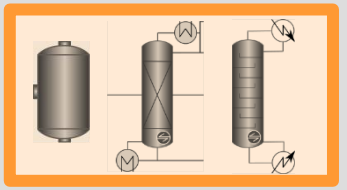
# Model Libraries - I. Separation

| Separations – Fluid-Fluid | Steady-state | Dynamic |
|---|---|---|
| Component splitter | ☑ | |
| Flash drum | ☑ | ☑ |
| Decanter | ☑ | ☑ |
| 3-phase separator | ☑ | ☑ |
| Distillation column (tray, equilibrium) | ☑ | ☑ |
| Distillation column (packed-bed, HETP) | ☑ | ☑ |
| Distillation column (packed-bed, 1D rate-based) | ☑ | ☑ |
| Distillation column (packed-bed, 2D rate-based) | ☑ | ☑ |
| Distillation column (reactive) | ☑ | ☑ |

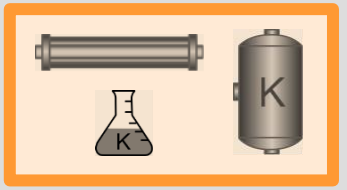
| Separations – Adsorption | Steady-state | Dynamic |
|---|---|---|
| Adsorption bed | | ☑ |
| Schedule for periodic processes (PSA, TSA) | | ☑ |
| Schedule for self-interacting bed approach | | ☑ |

| Separations – Membranes | Steady-state | Dynamic |
|---|---|---|
| Membrane module | ☑ | ☑ |

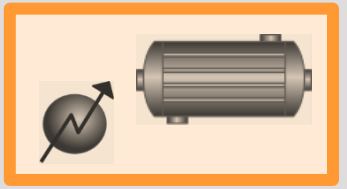
**Separation**



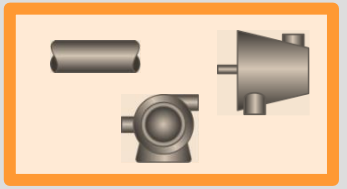
**Reaction**



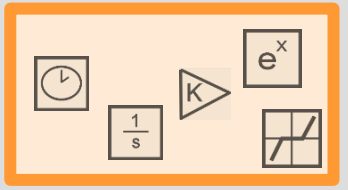

**Heat exchange**



**Flow transportation**



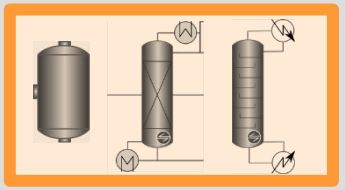
**Instrumentation and control**



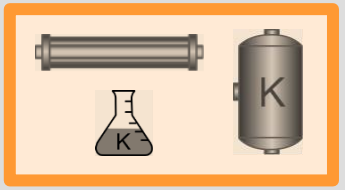
# Model Libraries - II. Reaction

| Reaction | Steady-state | Dynamic |
|---|---|---|
| Conversion reactor | ☑ | |
| Gibbs reactor | ☑ | ☑ |
| CSTR (kinetic & equilibrium reactions) | ☑ | ☑ |
| PFR (kinetic & equilibrium reactions) | ☑ | ☑ |
| Fixed-bed catalytic reactor (1D) | ☑ | ☑ |
| Fixed-bed catalytic reactor (2D) | ☑ | ☑ |
| Fixed-bed catalytic reactor (2D + intra-particle) | ☑ | ☑ |
| | | |
| Reaction mechanisms:<br>▪ Arrhenius<br>▪ Langmuir-Hinshelwood<br>▪ Michaelis-Menten<br>▪ User specified | ☑ | ☑ |

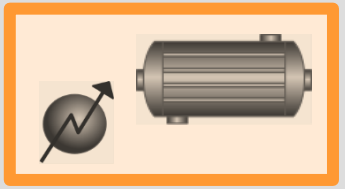
Separation



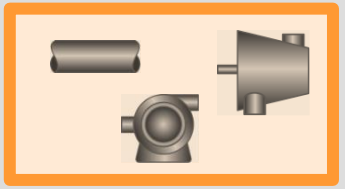
**Reaction**



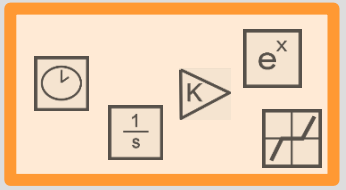

Heat exchange



Flow transportation



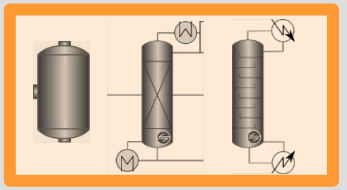
Instrumentation and control



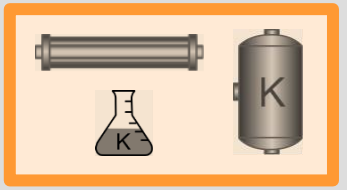
# Model Libraries - III. Heat exchange

| Heat exchange | Steady-state | Dynamic |
|---|---|---|
| Heater | ☑ | ☑ |
| Cooler | ☑ | ☑ |
| Two-stream heat exchanger | ☑ | ☑ |
| Multi-stream heat exchanger | ☑ | ☑ |

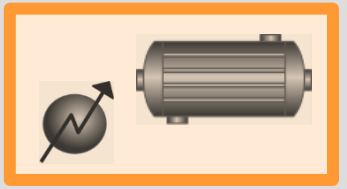
Separation



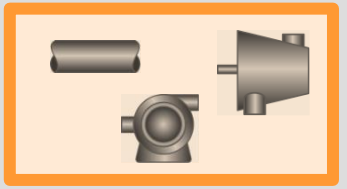
Reaction



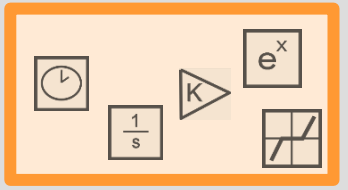

**Heat exchange**



Flow transportation



Instrumentation and control

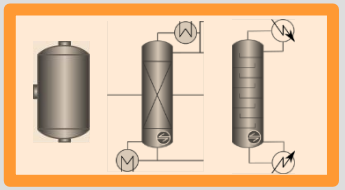


# Model Libraries - IV. Flow transportation

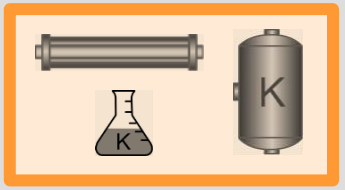
| Flow transportation | Steady-state | Dynamic |
|---|---|---|
| Pipe | ☑ | ☑ |
| Pump | ☑ | ☑ |
| Valve | ☑ | ☑ |

| Compression | Steady-state | Dynamic |
|---|---|---|
| Compressor | ☑ | ☑ |
| Expander | ☑ | ☑ |
| Compressor section | ☑ | ☑ |
| Electric drive | ☑ | ☑ |
| Surge valve | ☑ | ☑ |

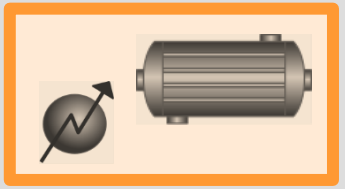
Separation



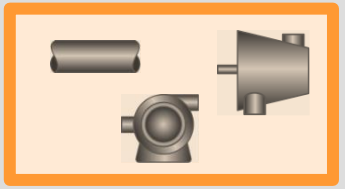
Reaction



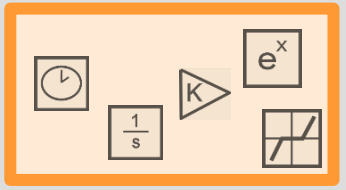

Heat exchange



**Flow transportation**



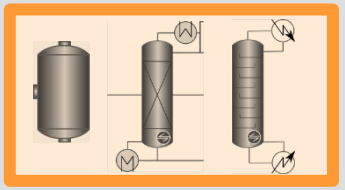
Instrumentation and control



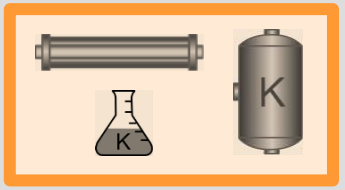
# Model Libraries - V. Instrumentation & control

| Instrumentation and control | Steady-state | Dynamic |
|---|---|---|
| **Controllers**<br>▪ Gain, PID, delays | ☑ | ☑ |
| **Logic**<br>▪ Switches | ☑ | |
| **Linear systems**<br>▪ Transfer function, state-space model | | ☑ |
| **Discrete**<br>▪ Dead zone, hysteresis, saturation | ☑ | ☑ |
| **Mathematics**<br>▪ Functions, basic operations | ☑ | |
| **Signal Sources**<br>▪ Constant, ramp, step signal, function generator, time signal | ☑ | ☑ |
| **Signal Sinks**<br>▪ Display, plot, X-Y plot | ☑ | ☑ |
| **Data**<br>▪ Lookup table, file read, file write | ☑ | ☑ |
| **Functionality**<br>▪ System identification, linearisation,<br>▪ Mixed-integer optimisation | ☑ | ☑ |

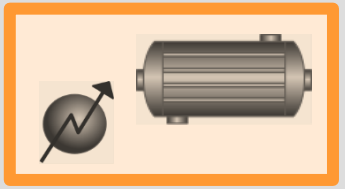
Separation



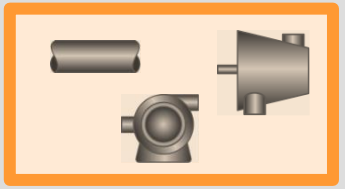
Reaction



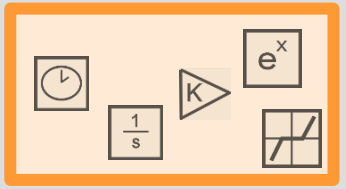

Heat exchange



Flow transportation



**Instrumentation and control**



# Model Libraries

I. Separation
   - fluid/fluid: distillation, absorption
   - fluid/solid: adsorption, membrane

II. Reaction

III. Heat exchange

IV. Flow transportation

V. Instrumentation & control

**VI. Custom models & model libraries**
   - **proprietary, third-party, ….**

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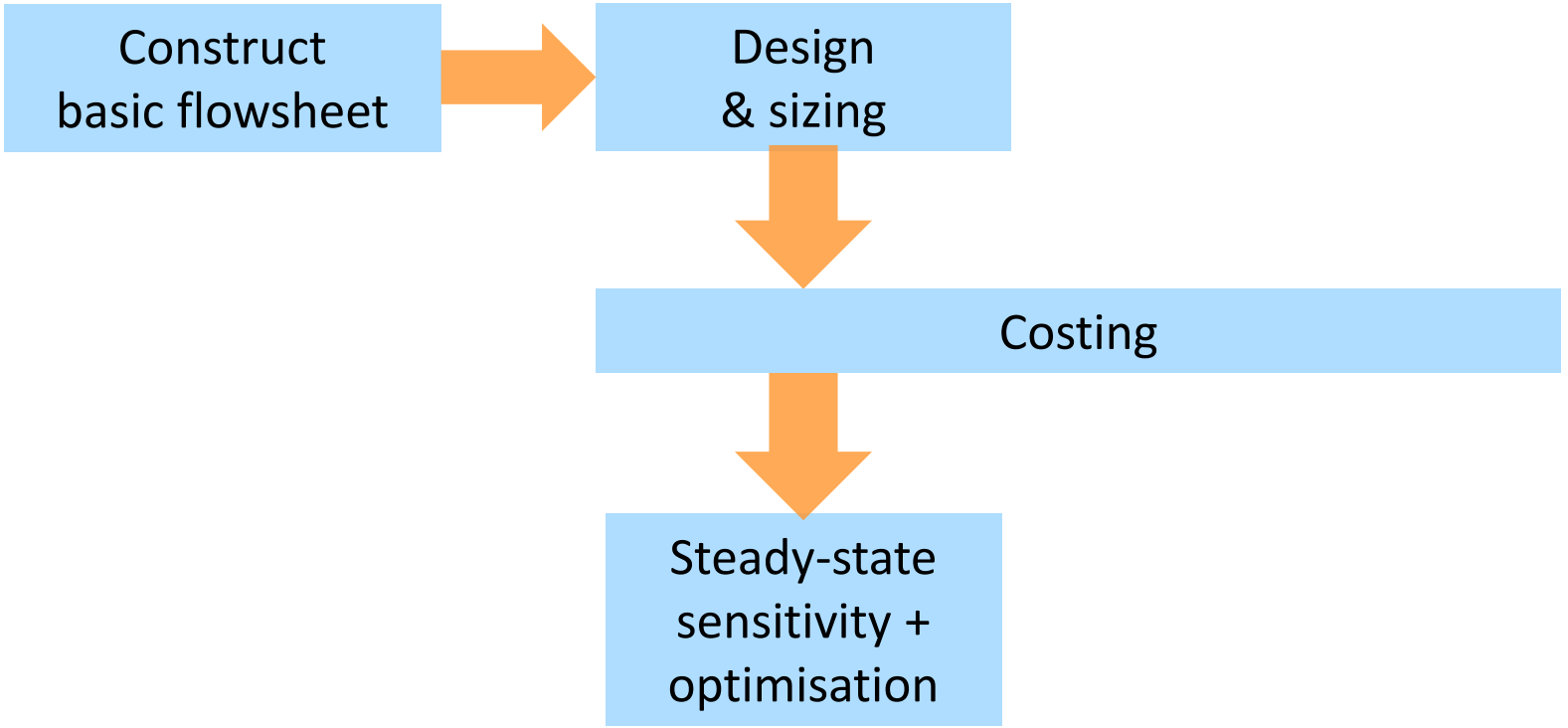
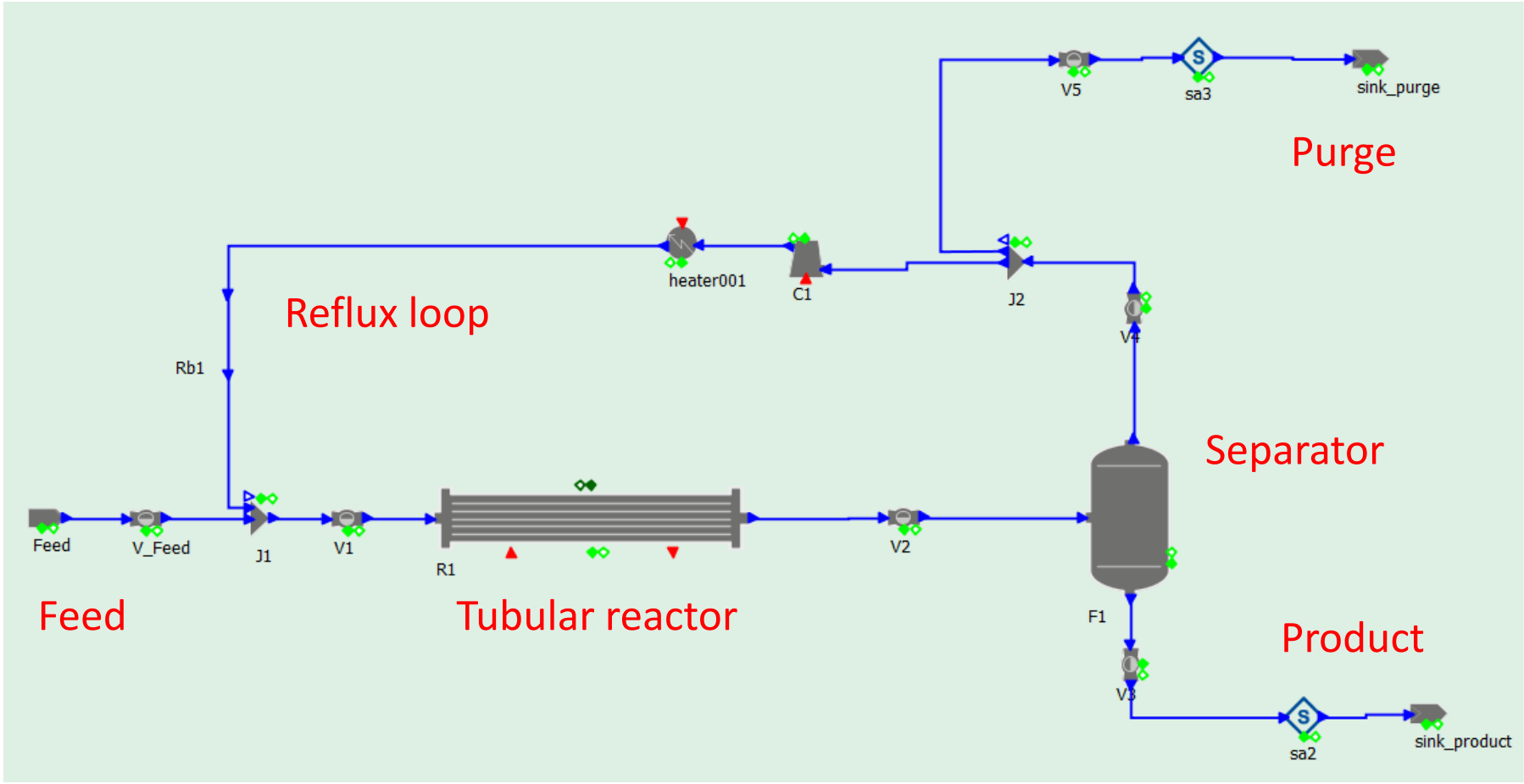
# Steady-state flowsheeting

# Overview of modelling workflow

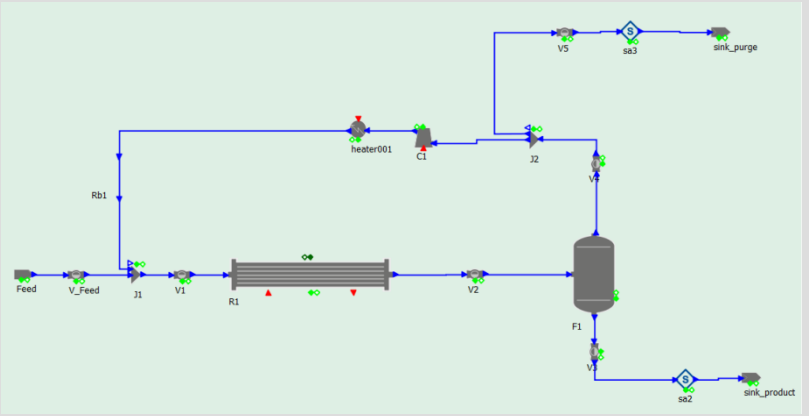


# Example: Methanol production

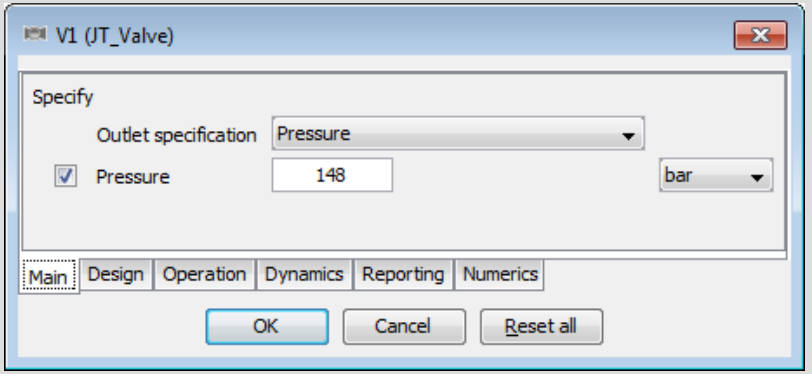


# 1. Basic mass & energy balances

- Drag & drop models on the flowsheet
- Enter output specifications for model in dialogs



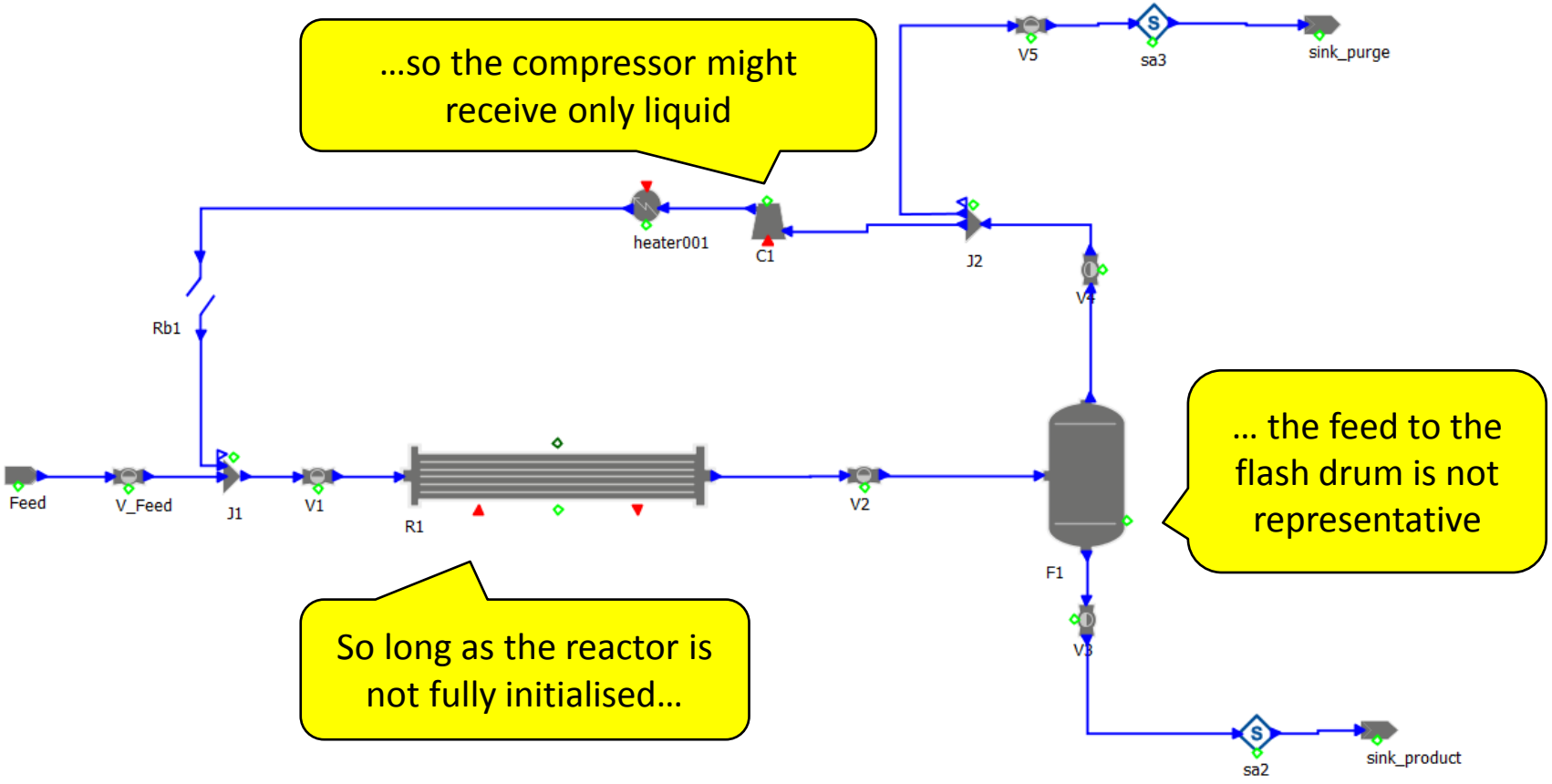

- Determine process mass & energy balances




- Video

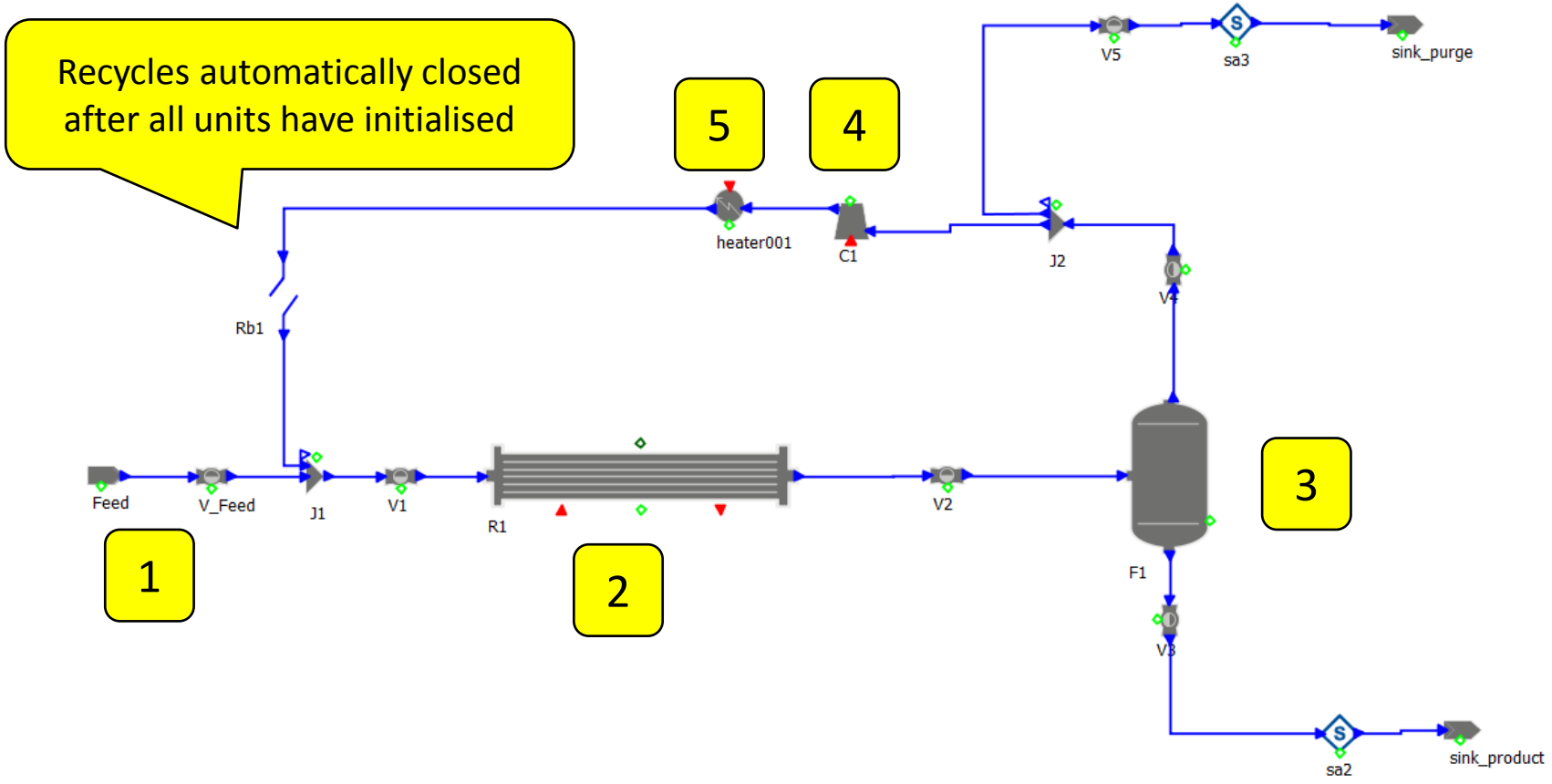
# Sequential flowsheet initialisation

**Problem:** In equation-based flowsheet model initialisation, during the first steps, unit operation models are sometimes "fed" with a non-physical feed



# Sequential flowsheet initialisation

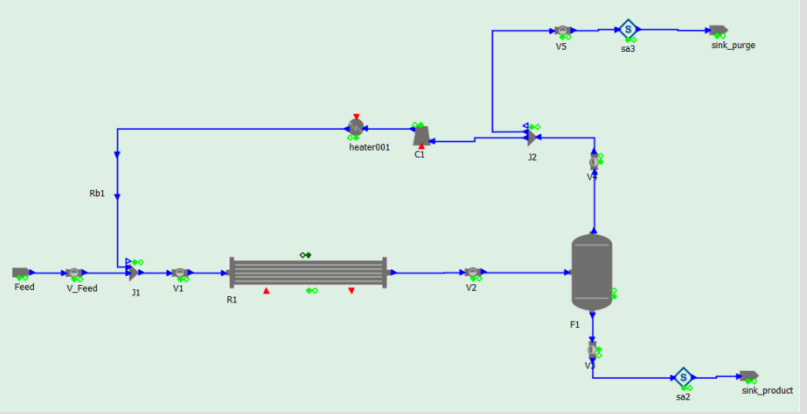
## **Solution:** initialise flowsheet sequentially

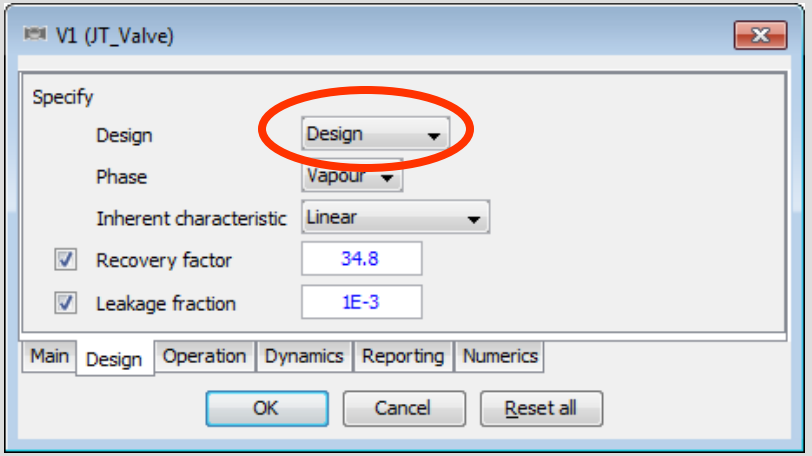


# 2. Sizing

- Switch unit operations to *design* mode
- Refine unit specifications
  - e.g. choose specific type of equipment
- Impose performance specs
  - e.g. separation to be achieved

- Determine
  - sizing
  - operating point
- Video

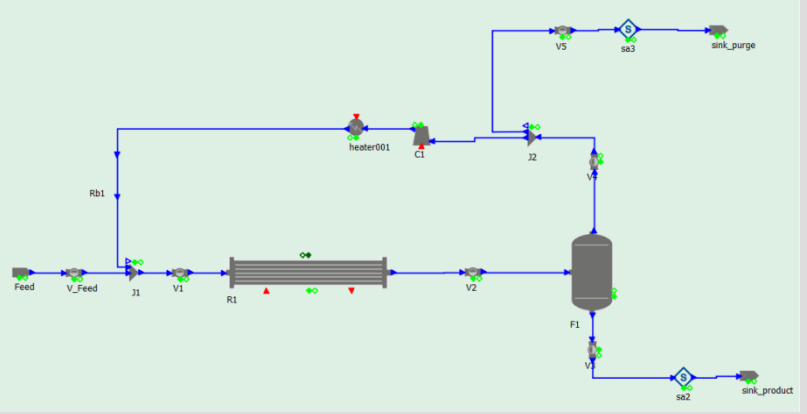


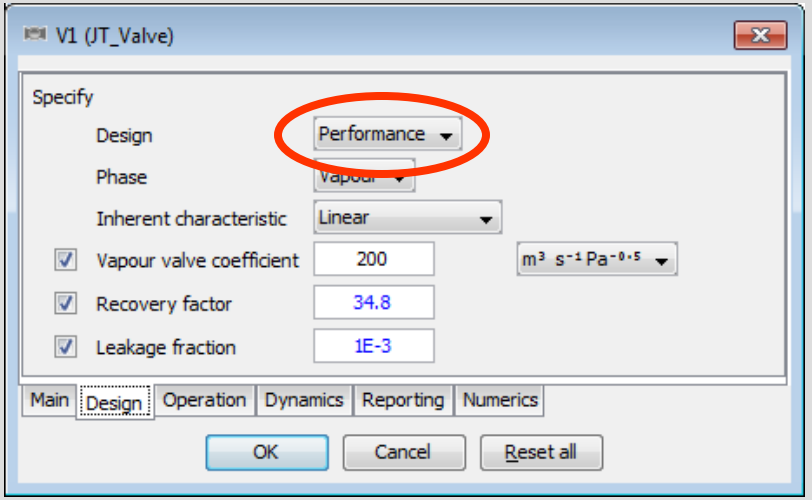



# 3. Performance rating

- Switch unit operations to *performance* mode

- Determine process performance for given input specifications

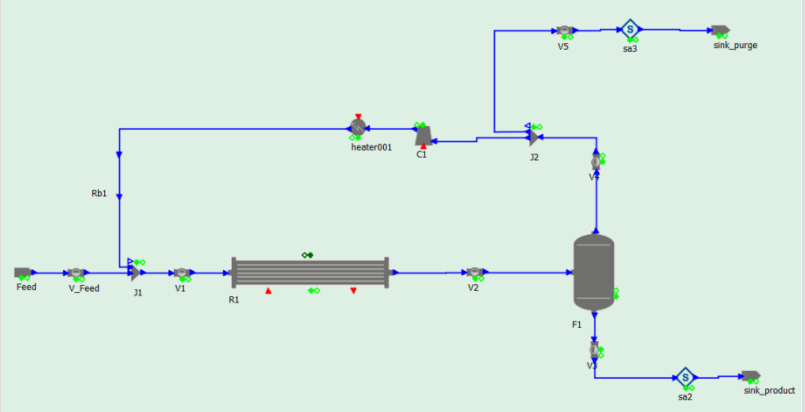


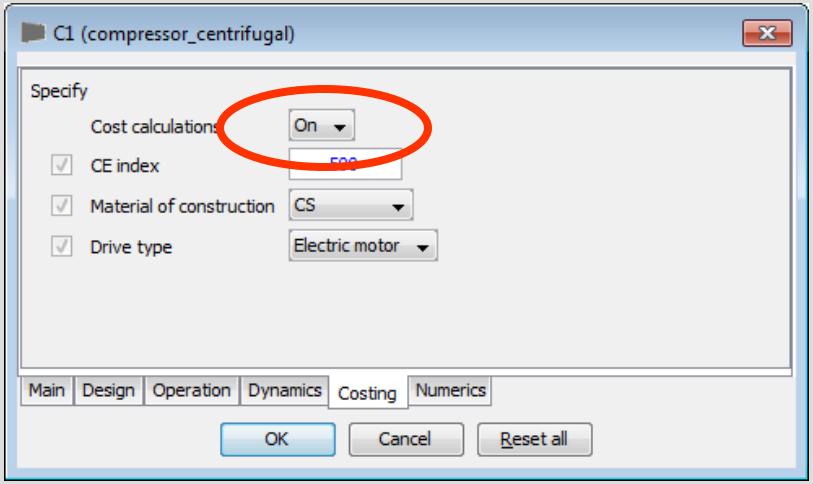



# 4. Costing

- Switch unit operations to *costing* mode
  - models incorporate fixed & variable cost calculations

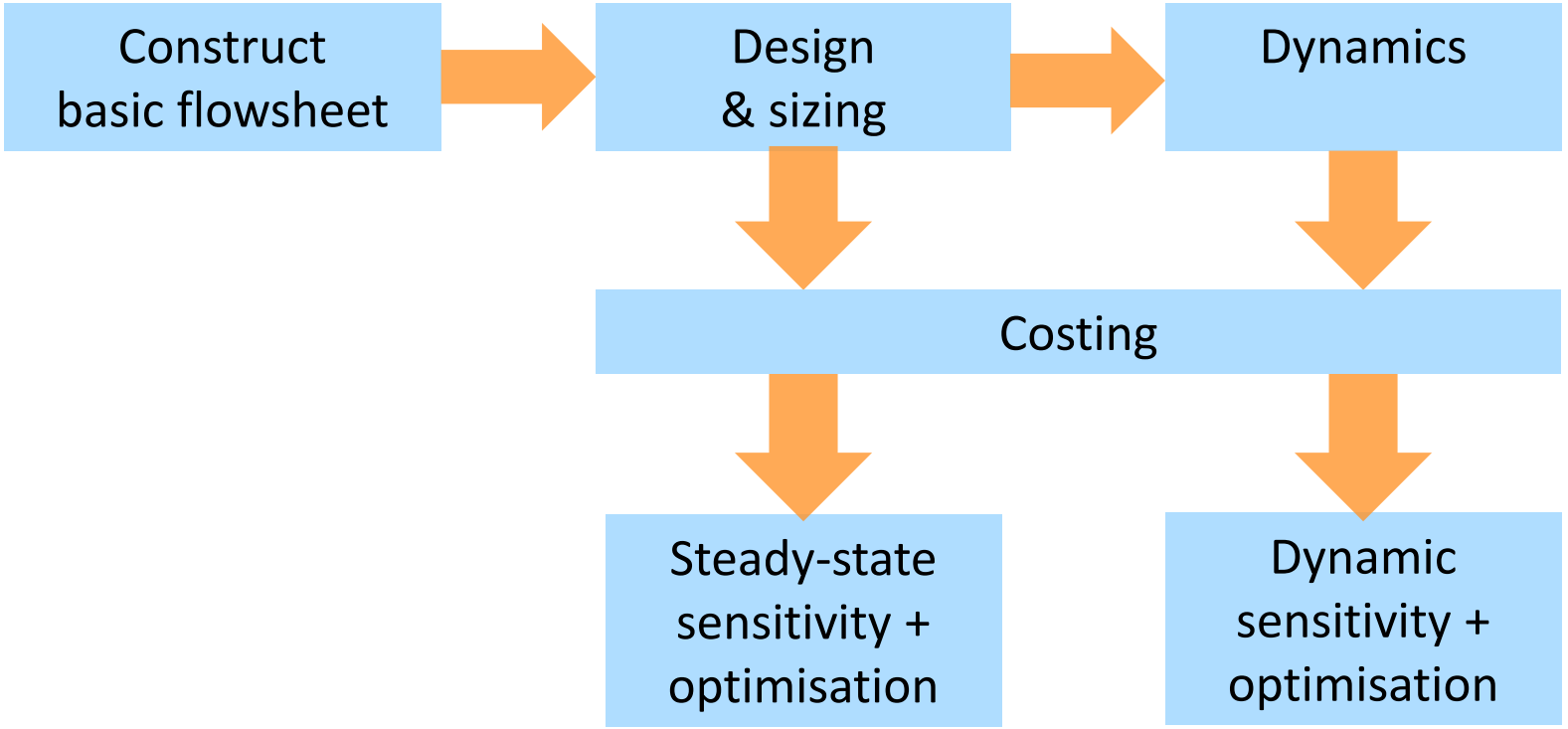
- Simulation: Compute cost for given specifications
- Optimisation: minimise cost by adjusting process design and operation parameters



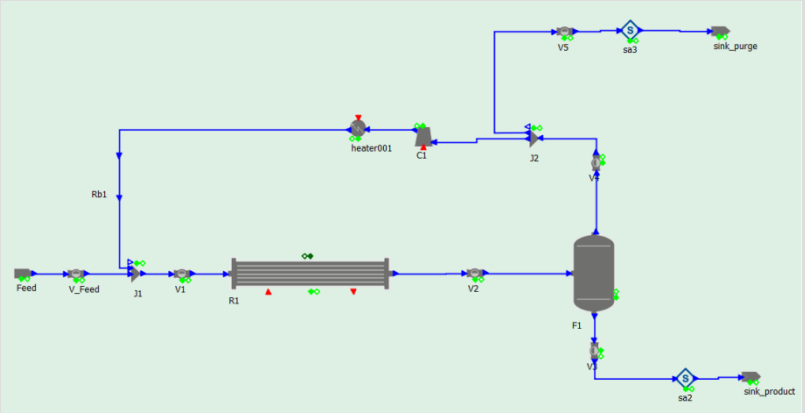
# From steady state to dynamics

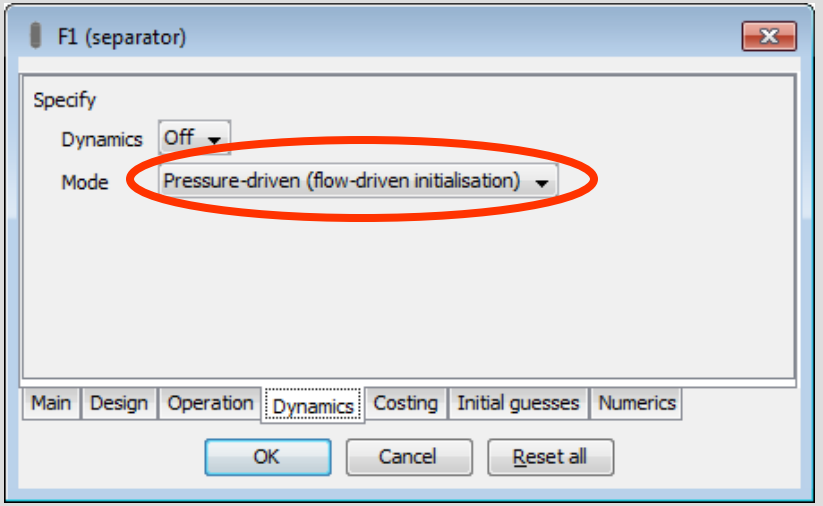
# Overview of modelling workflow



# 5. Pressure-driven mode

- Switch all units to *pressure-driven* mode
- Specify downstream pressures



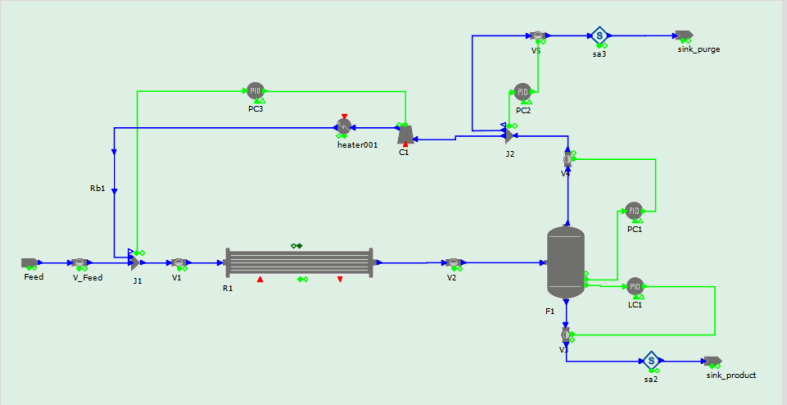



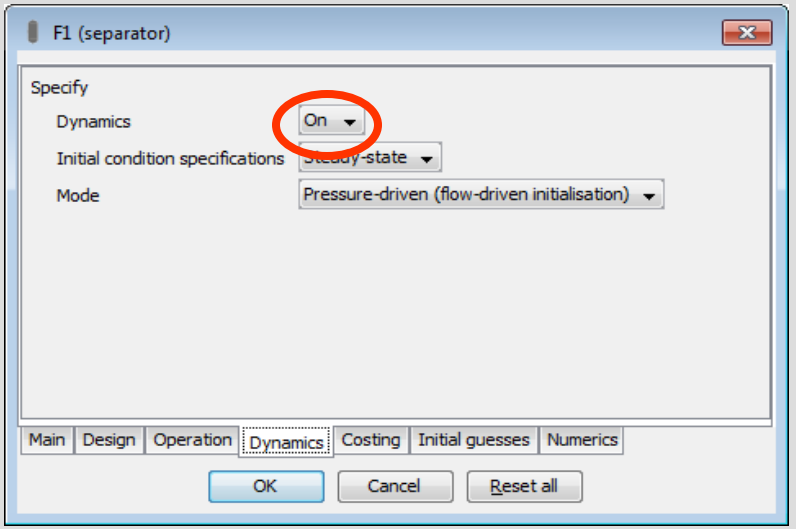

- Determine pressure-driven steady-state operating point
- Video

# 6. Dynamic mode operation

- Switch all units to *dynamic* mode
- Add controllers to enforce unit outlet specifications

- Fully dynamic flowsheet
  - use steady state as default initial condition…
- Video dynamic no control
- Video dynamic control

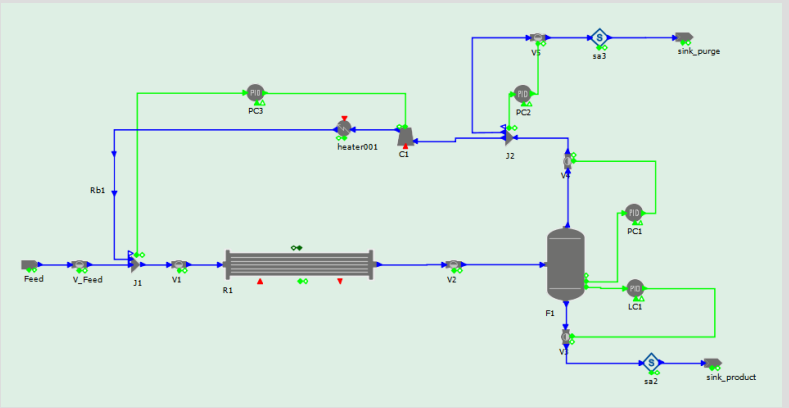


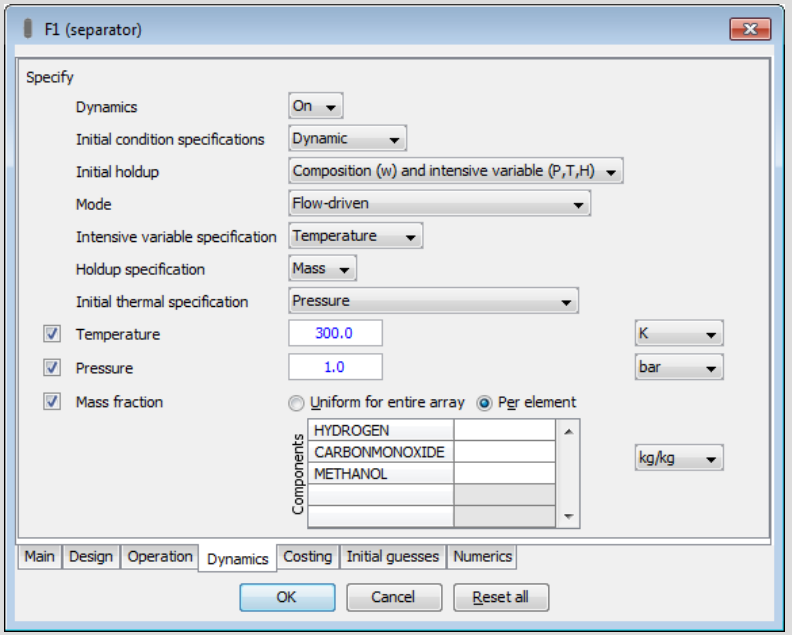



# 6. Dynamic mode operation

- Switch all units to *dynamic* mode
- Add controllers to enforce unit outlet specifications

- Fully dynamic flowsheet
  - use steady state as default initial condition…
  - …or specify initial condition via dialog



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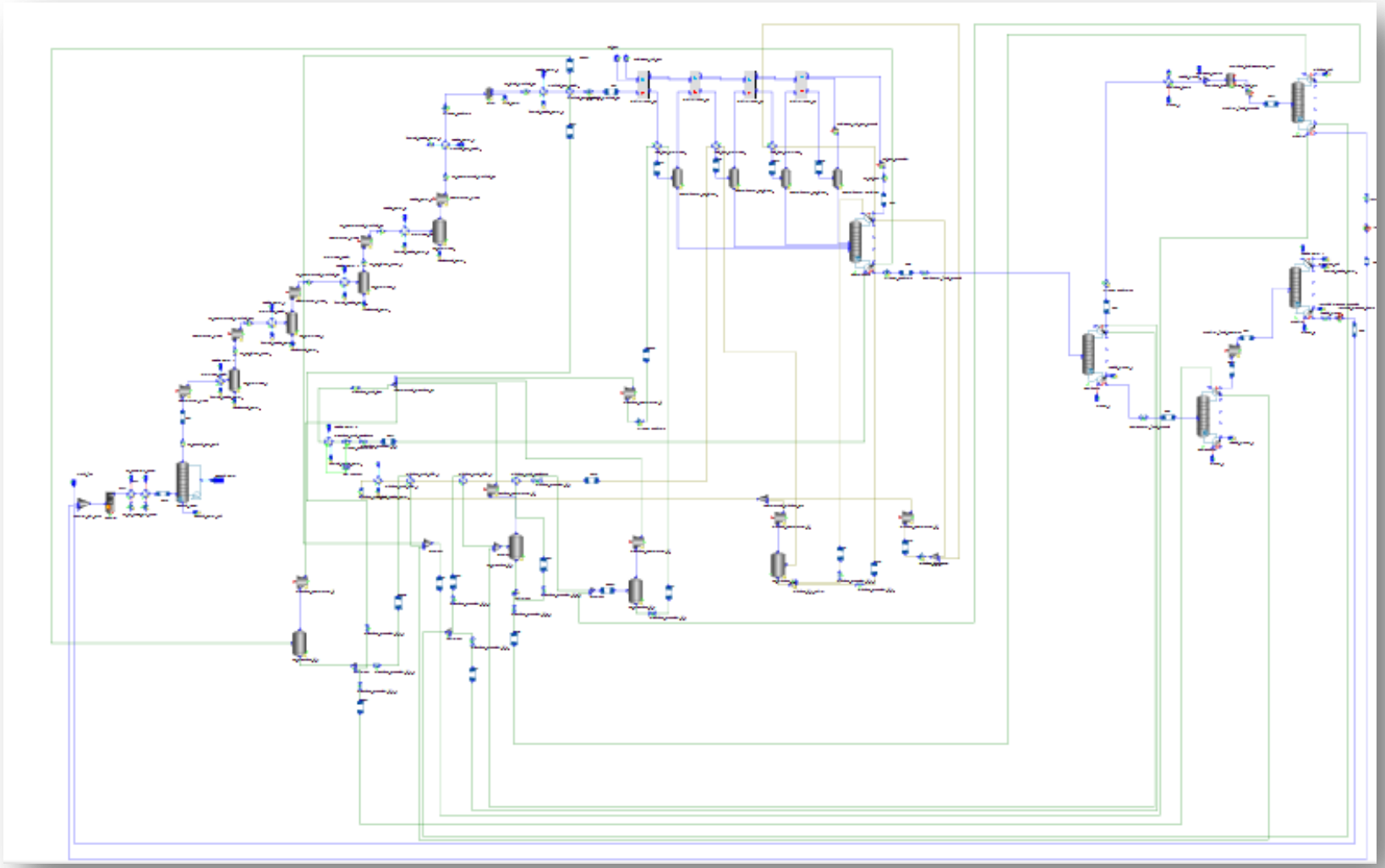
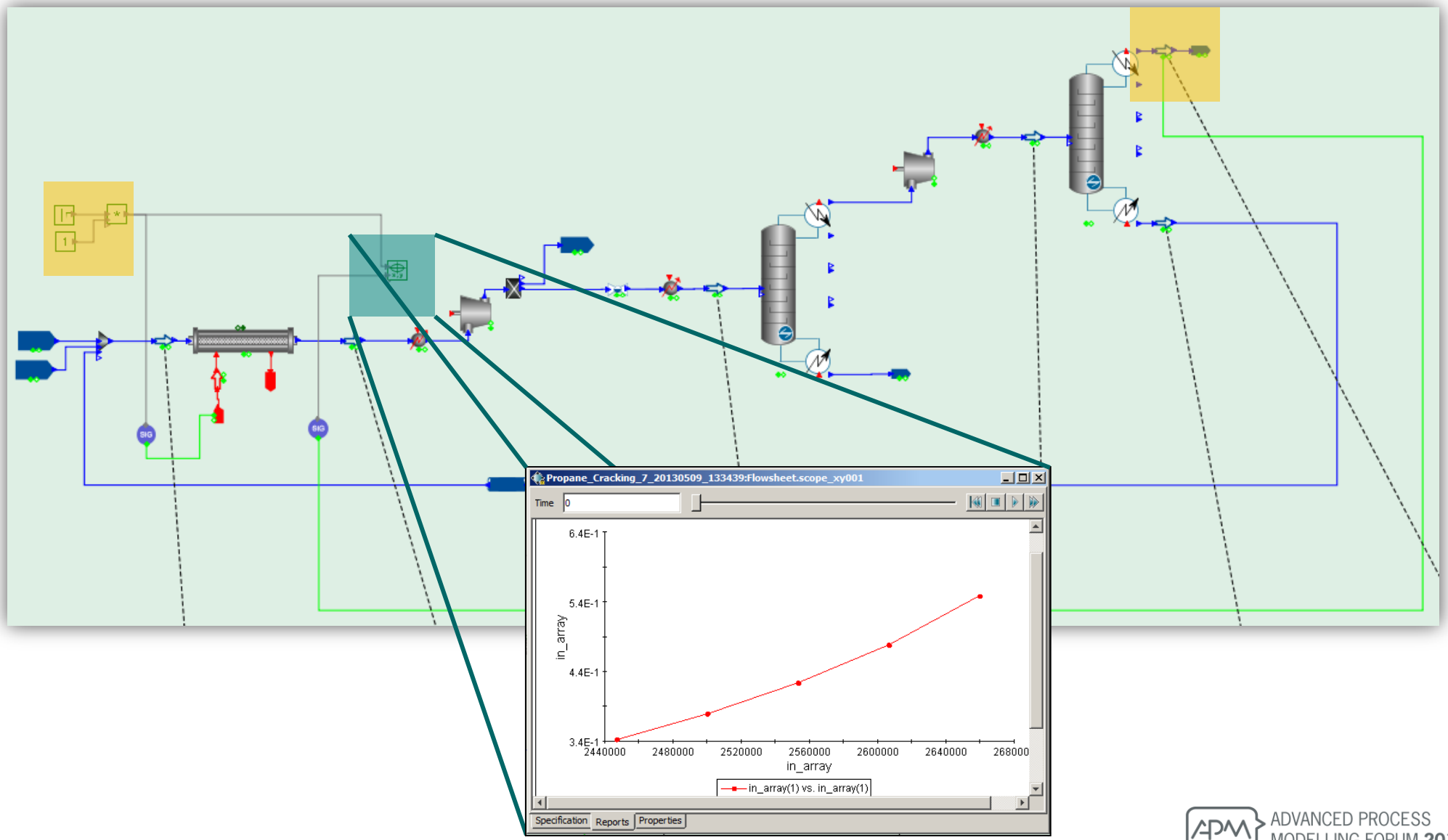
# Advanced capabilities for flowsheet simulation

# Complex flowsheets with multiple recycles

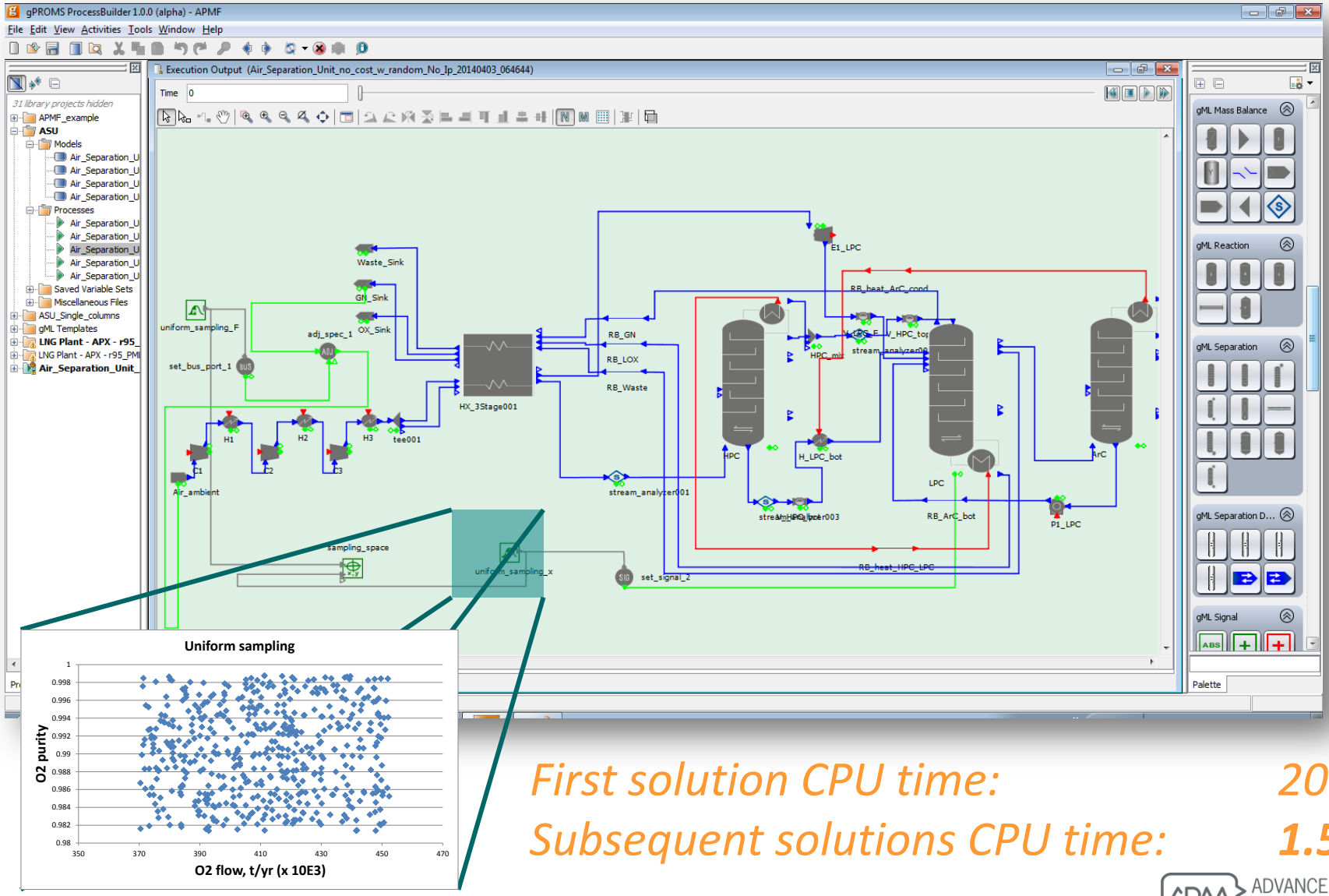
- Ethylene plant model with refrigeration, 70k+ equations



# Sensitivity studies – I



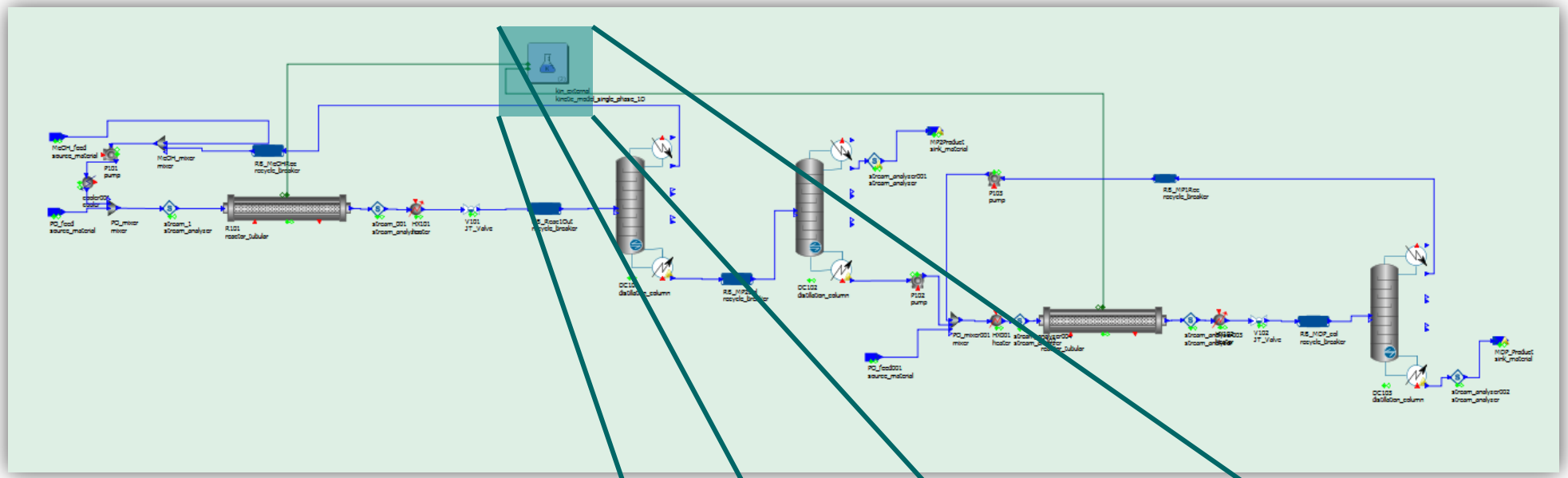
# Sensitivity studies – II




*First solution CPU time:* *200 sec*

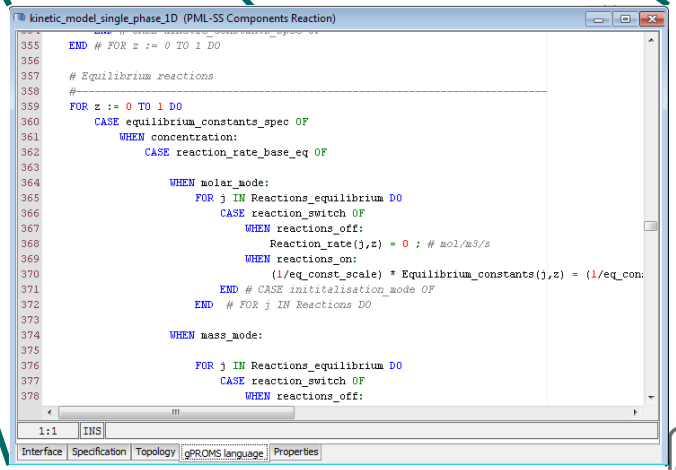
*Subsequent solutions CPU time:* ***1.5 sec***

# Integration with custom models



*Add custom models easily using the gPROMS language*

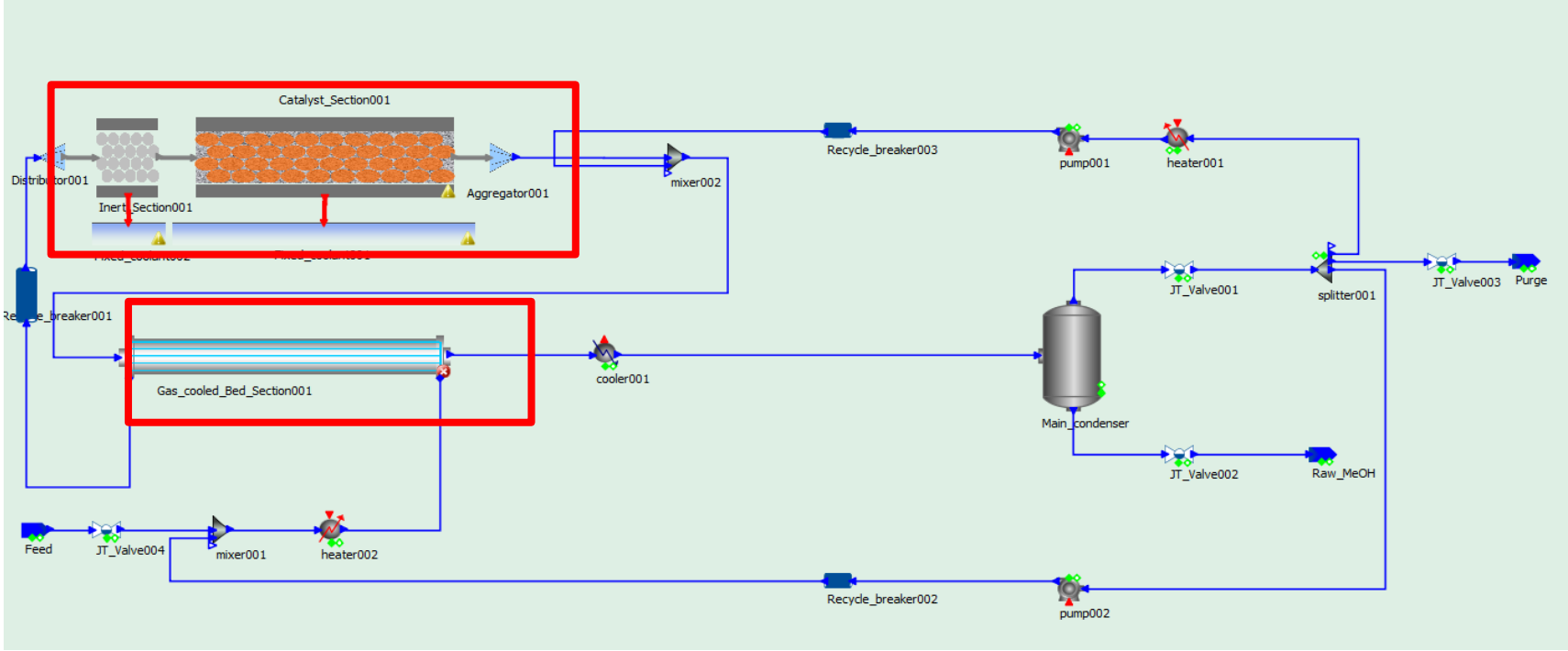
*Templates for constructing* ***ProcessBuilder -compliant*** *custom models provided*



# Flowsheets with high-fidelity unit models

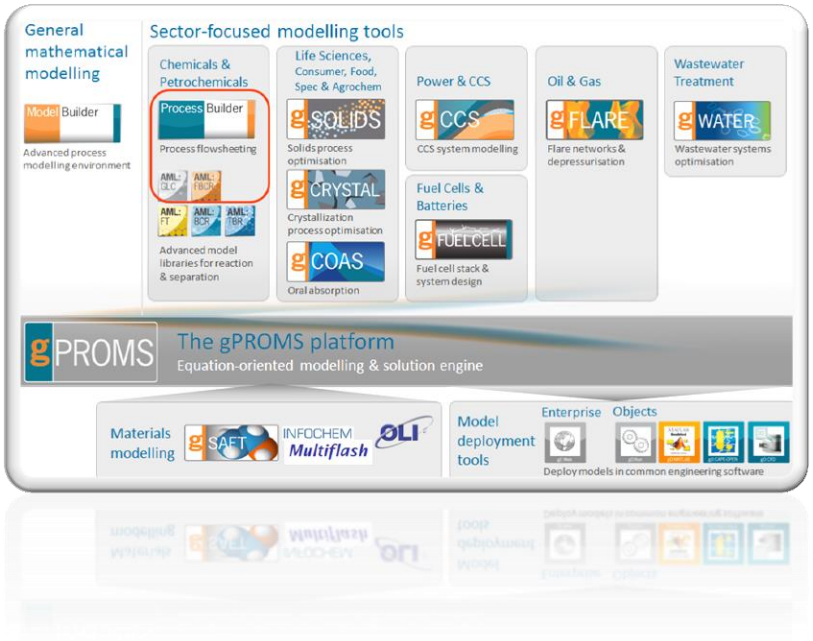
- Auto-thermal reforming process
  - 2 multitubular reactors
  - 2D fixed-bed catalytic reactor models

*Advanced Model Libraries now integrated within ProcessBuilder*
- *AML:FBCR*
- *AML:GLC*



# gPROMS ProcessBuilder

Process Builder




A **new** product

…based on the gPROMS Platform

…for the **Chemicals & Petrochemicals** sector

…delivering new levels of functionality, usability & efficiency

# This morning's presentations

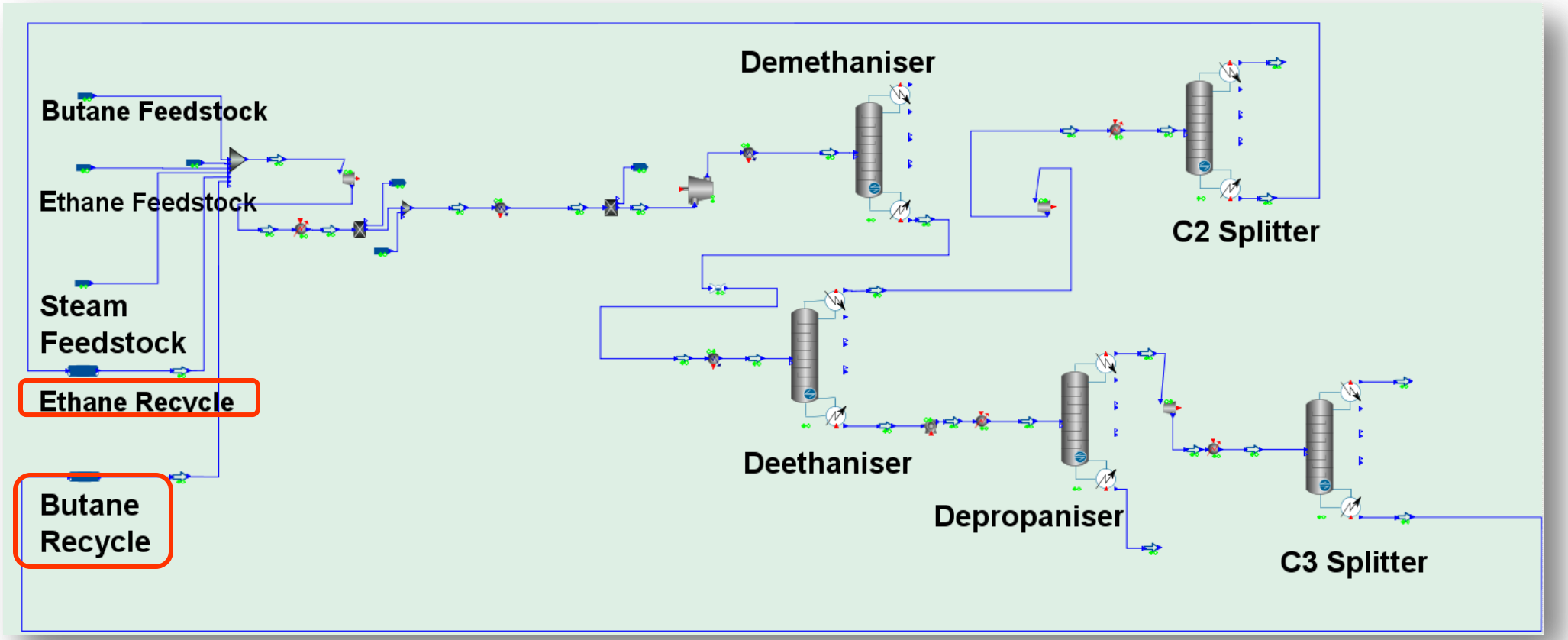
- Overview
  - Dr Maarten Nauta
- **Distillation/absorption**
  - **Dr Charles Brand**
- Pressure Swing Adsorption (PSA)
  - Dr Mayank Patel
- gSAFT physical properties
  - Dr Tom Lafitte
- Conclusion & perspective
  - Prof C.C. Pantelides

ADVANCED PROCESS
MODELLING FORUM **2014**

# Thank you

# Handling of multiple recycles

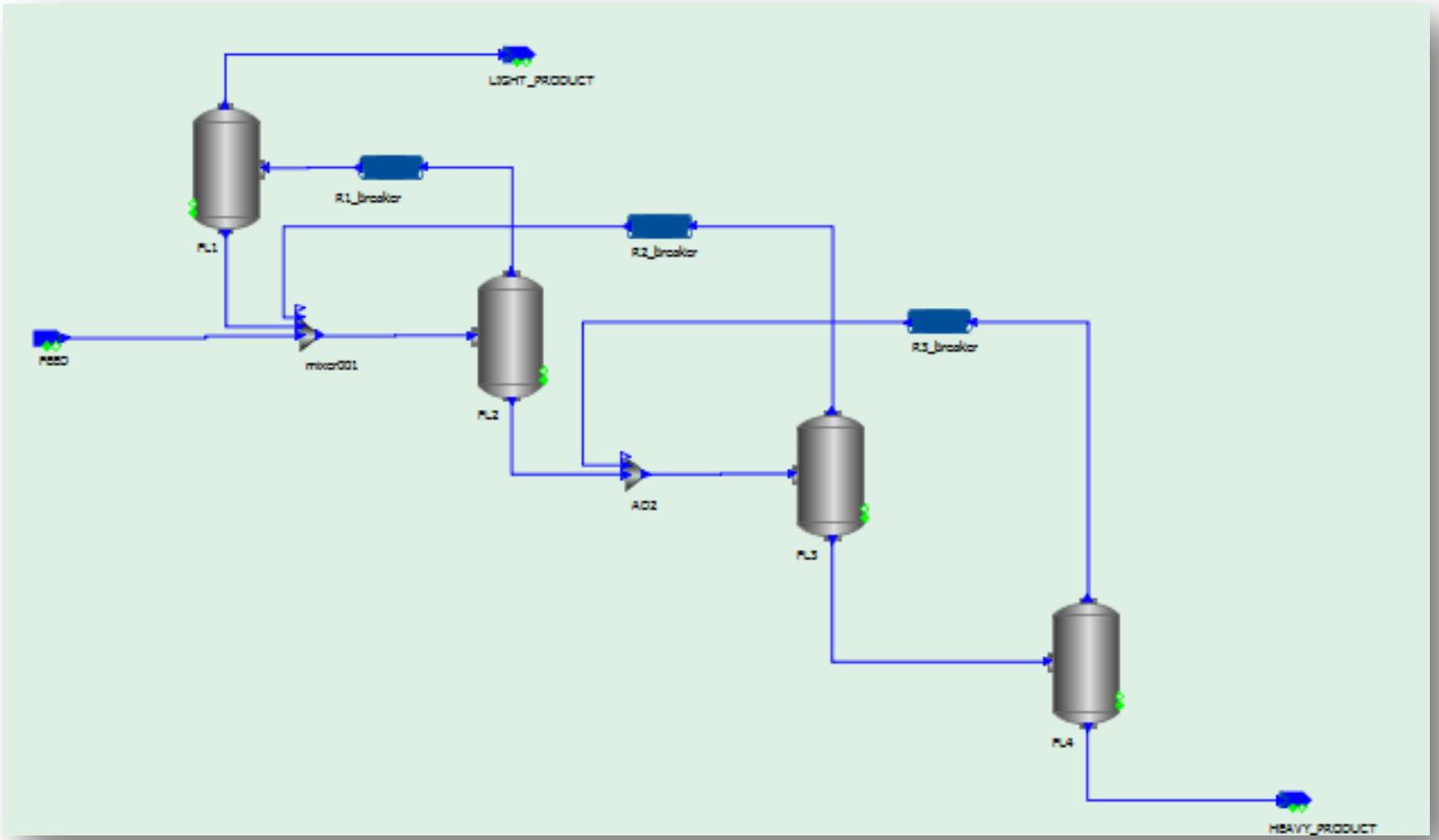
- Solution time with no user-provided initial guesses: 37 CPU s (Intel i7 laptop)




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

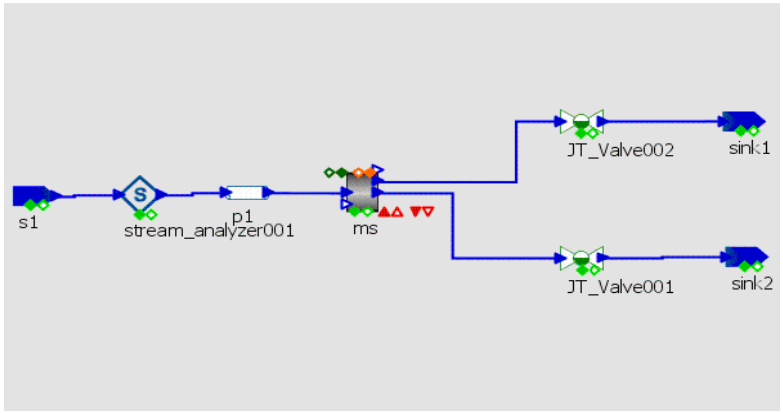
# Basic steady-state flowsheeting

- Cavett problem

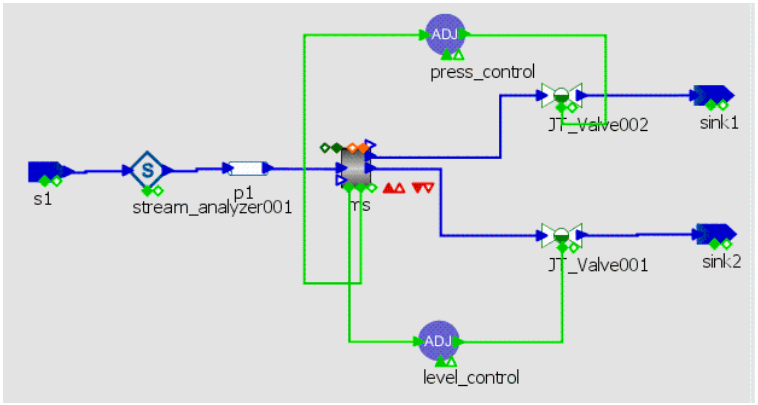


# Dynamics (1)

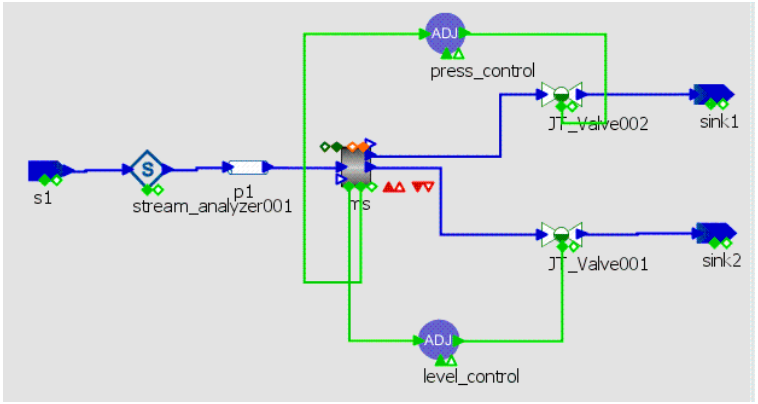
- Transition from steady-state to dynamics



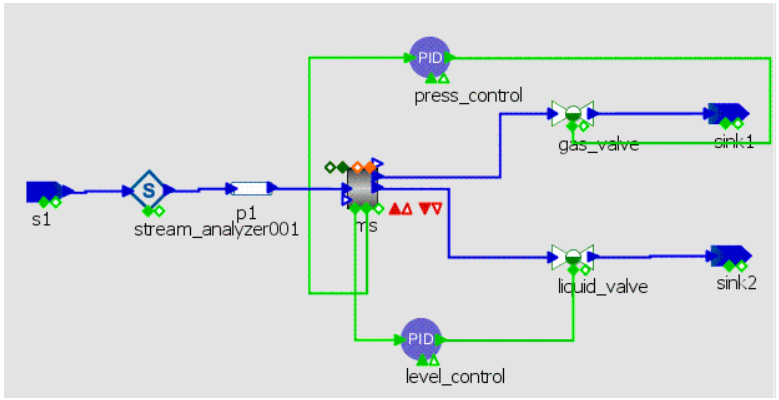

**Flow-driven steady-state flowsheet**




**Flow-driven steady-state flowsheet with design specifications**



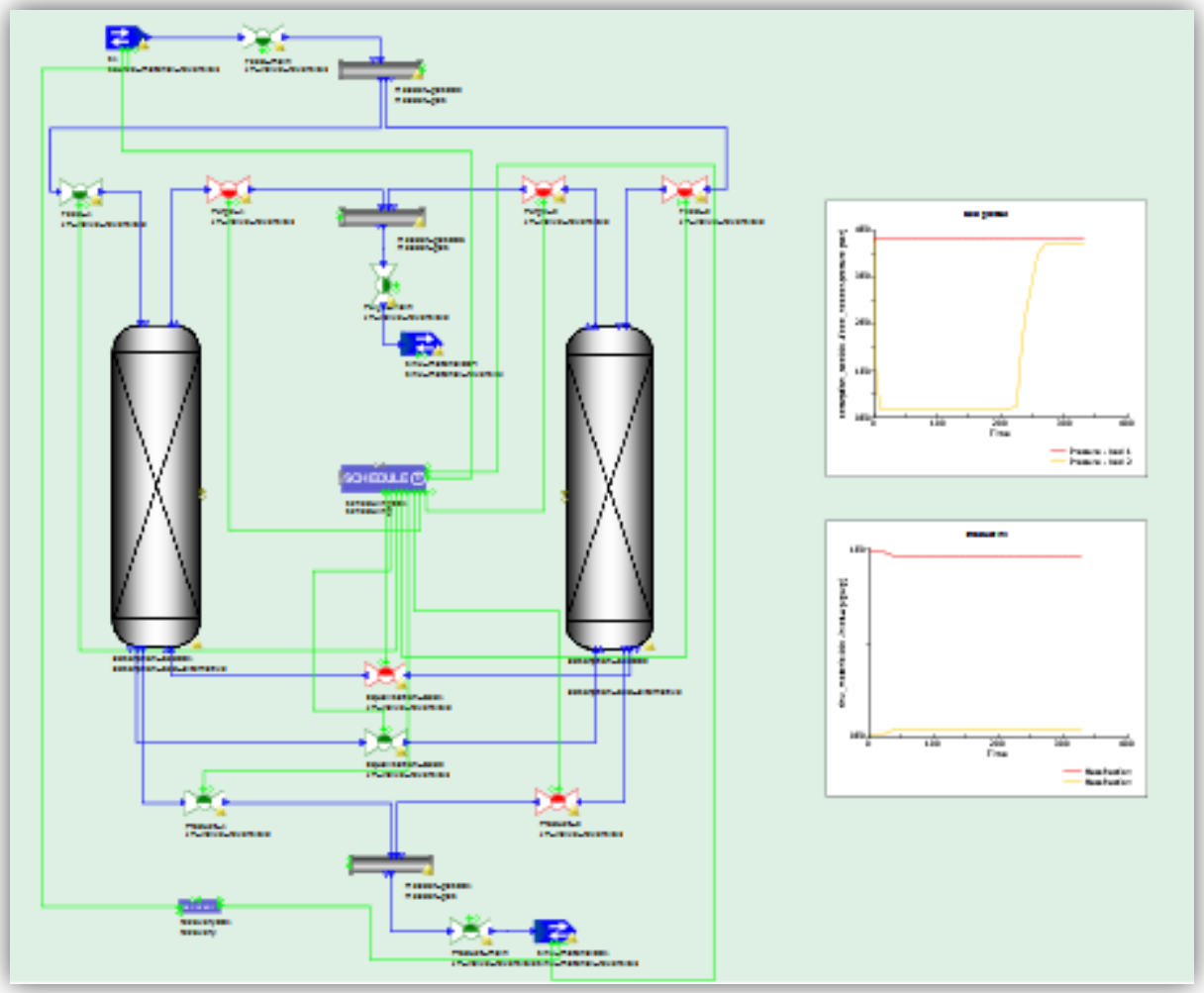

**Pressure-driven steady-state flowsheet with design specifications**




**Pressure-driven dynamic flowsheet at steady-state with control**

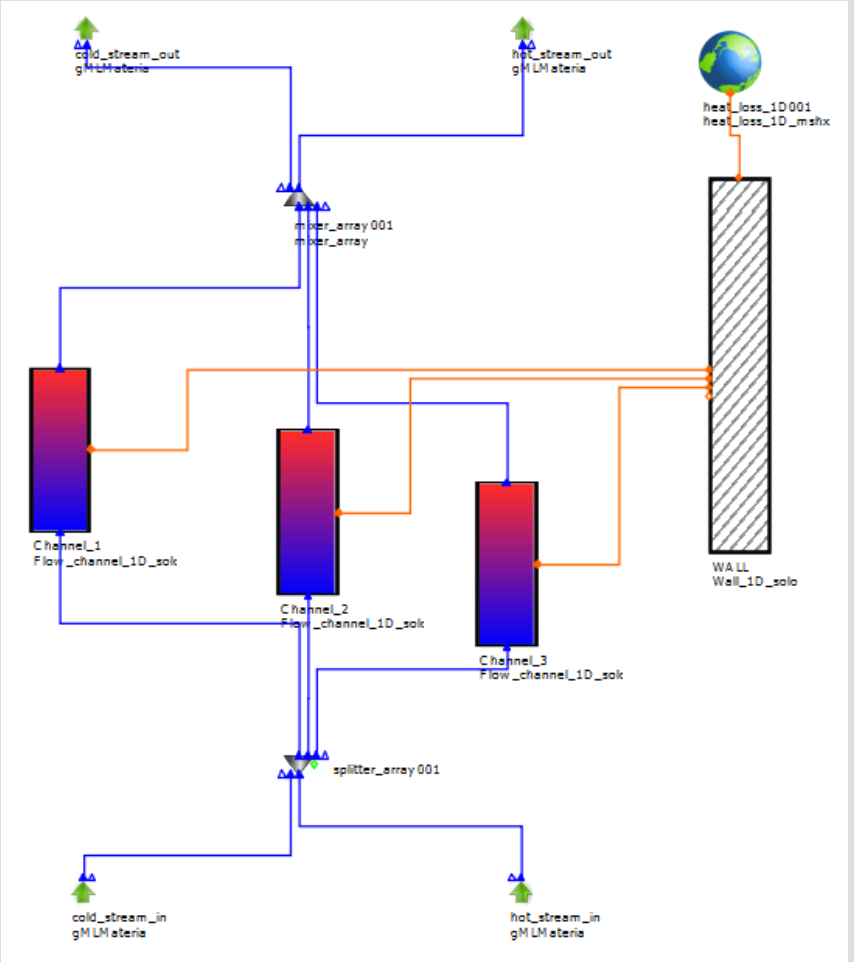
# Dynamics (2)

- Dynamic applications, Pressure Swing Adsorption (PSA)

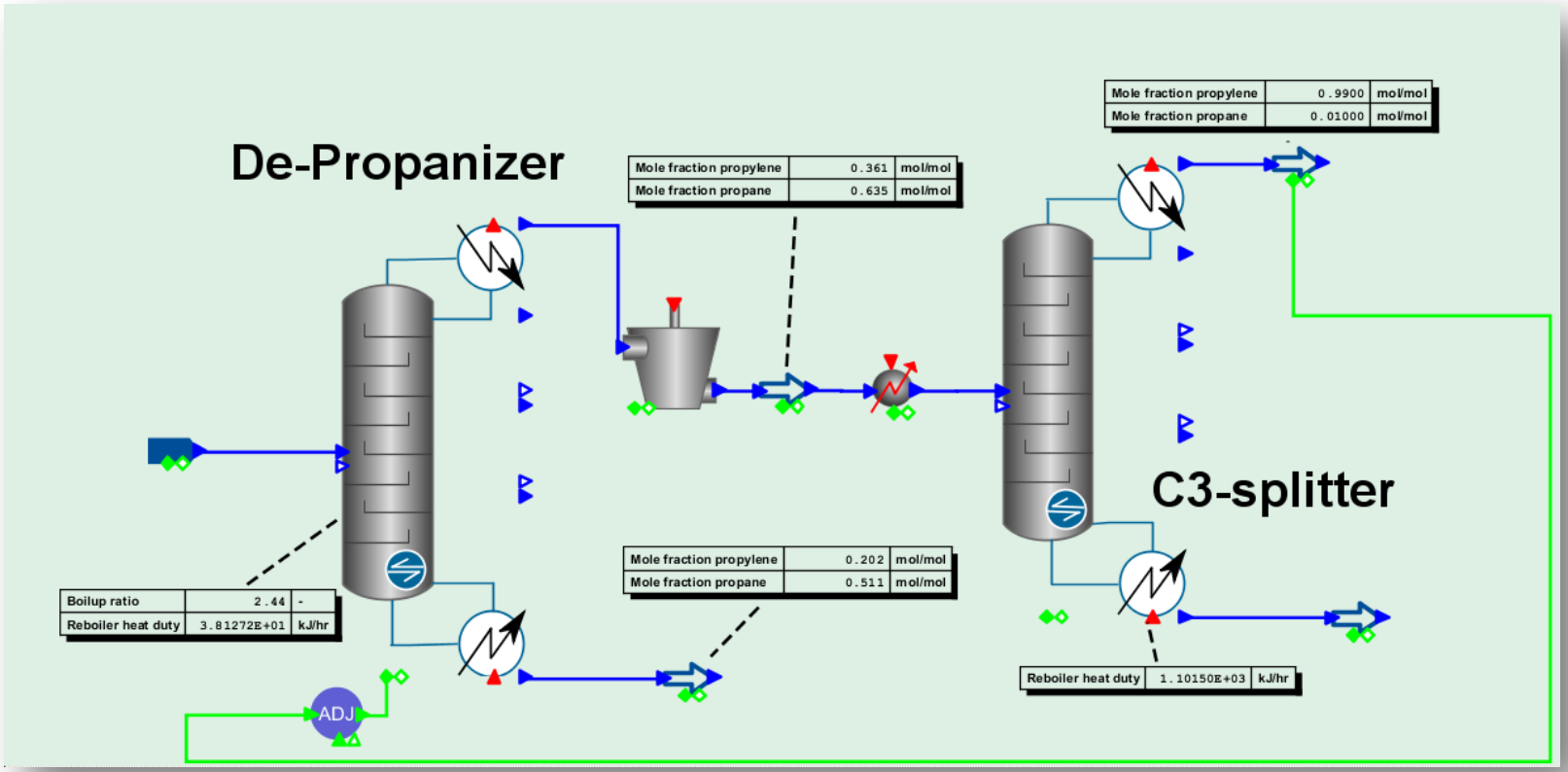


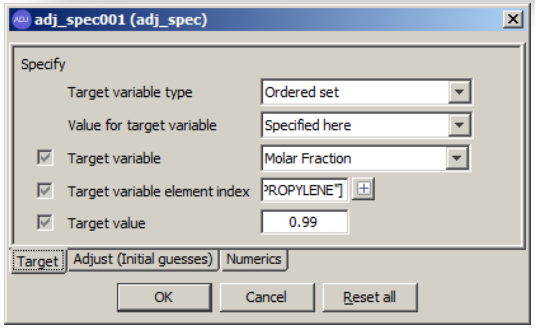
# Detailed design of individual units

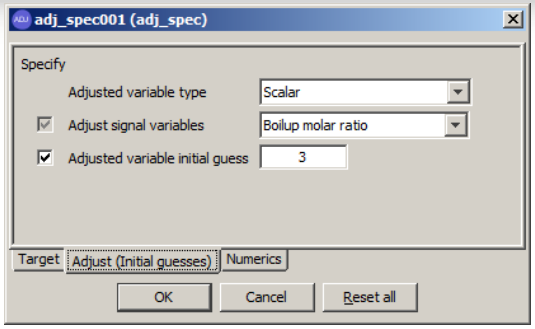
- Detailed design of individual unit operations using flowsheeting
  - Multistream heat exchanger
  - Multilayer adsorption bed
  - Fixed bed-catalytic reactor configurations
  - Custom distillation column configurations

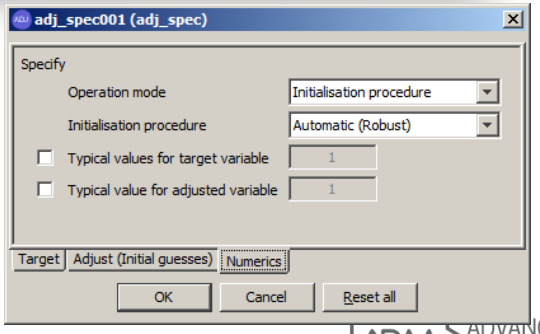


# Specification trade-offs across units

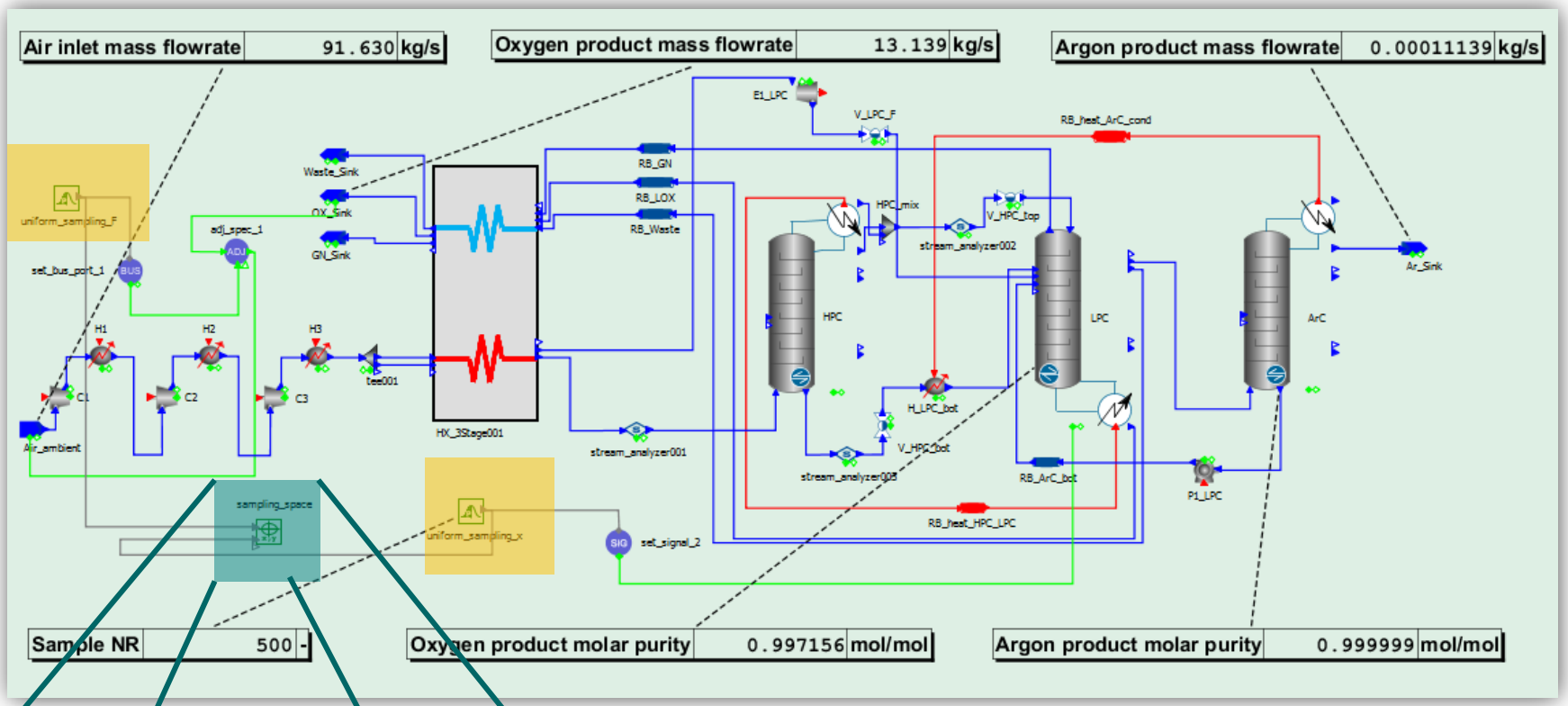


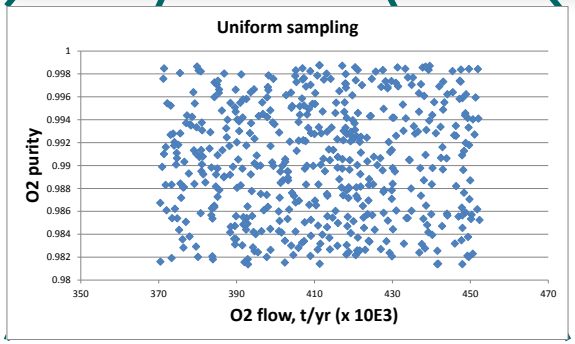



# Sensitivity studies – II




*First solution CPU time:* *200 sec*

*Subsequent solutions CPU time:* ***1.5 sec***

# ProcessBuilder key benefits

# Key benefits

- Rapidly construct flowsheet models of a wide array of chemical processes
  - Drag-and-drop construction of flowsheets
  - Easy configuration of unit models
- Built-in optimisation capability
- Seamless integration with custom modelling
  - Processes with custom unit operations
  - Detailed characterisation of kinetics, mass transfer, isotherms….
  - Custom cost calculations
- Steady-state and dynamic simulation using a single library
- Only “true equation oriented” flowsheeting tool
  - Rapid convergence of process flowsheets, even with multiple recycles
  - Full exploitation of recent developments on Model Initialisation Procedures
    - Ensure robustness of solution with little/no user intervention

# ProcessBuilder Roadmap

# ProcessBuilder Roadmap

- Flowsheet diagnostics
- Batch processes and plant start-up
- Extend number of distillation column initialisation algorithms
- Documentation, testing and quality control