ADVANCED PROCESS MODELLING FORUM 2014

gPROMS ProcessBuilder

Adsorption

Mayank Patel – Applications Engineer

Adsorption processes – brief overview

Adsorption technologies

Overview

- Gas-phase processes (PSA, VSA, TSA)
  - Hydrogen purification
  - Air separation: O_2 or N_2 enrichment
  - CO_2 capture
  - Recovery of gasoline vapours from air

- Liquid-phase processes (Simulated moving bed/ chromatography)
  - UOP Sorbex processes e.g. separation of mixed aromatic C_8 isomers (Parex™ /Ebex™/MX Sorbex™)

Adsorption technologies

Main considerations

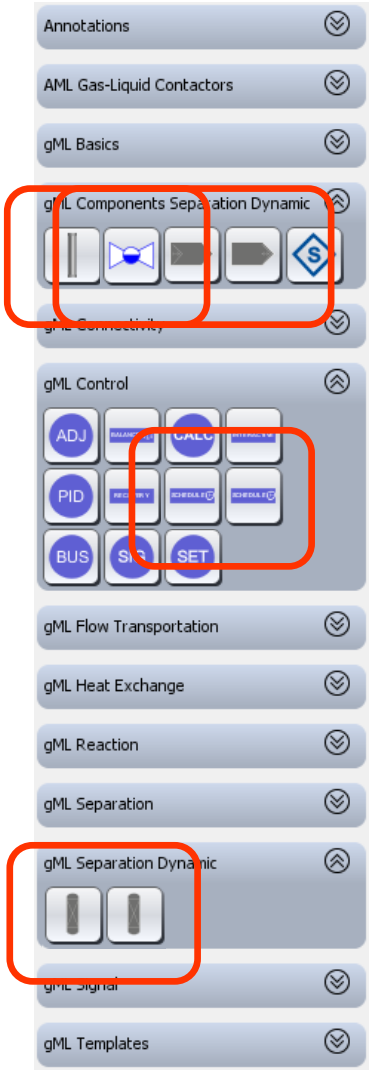
- Inherently dynamic processes
  - Complex cyclic operating procedures
  - Flow reversals, major model discontinuities
- Spatially varying properties
  - Axial & radial variations in the adsorbent bed
  - Adsorbed species diffuse through pores in adsorbent
- Process improvement
  - Usually meaningful only at *cyclic steady state*
  - Optimisation of equipment design & operating procedure

- **gPROMS already a leading modelling tool for adsorption R&D**
  - e.g. Google Scholar search for “swing adsorption gPROMS” ➔ ~**300** hits

Adsorption process modelling in the gPROMS ProcessBuilder

Adsorption-related content in gPROMS ProcessBuilder

- **Models**
  - Adsorption bed (1-D model)
    - Customizable fluid properties model
    - Customizable isotherm model
  - Valve model
    - Static and dynamic valve response
  - Auxiliary models
    - Drum and gas header
      - model material accumulation
    - Sources and sinks
      - track overall production per cycle
- **Tasks**
  - Schedule / operation unit
    - Defines operating schedule for dynamically operated processes



Adsorption-related content in gPROMS ProcessBuilder

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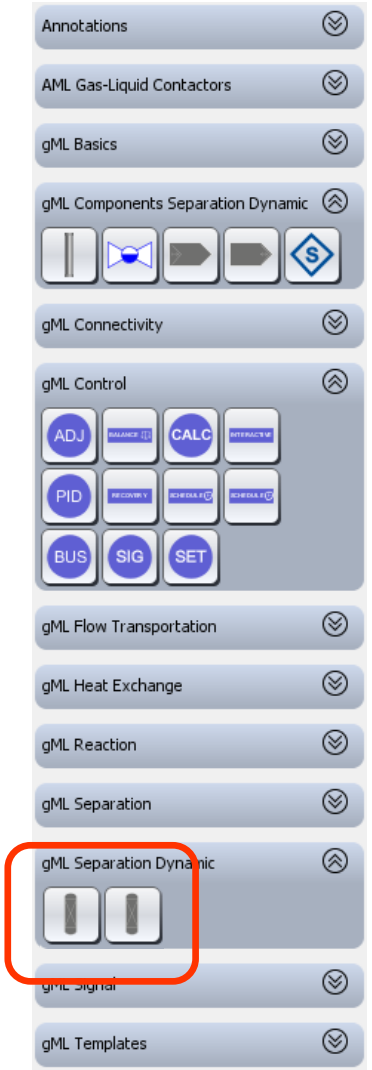
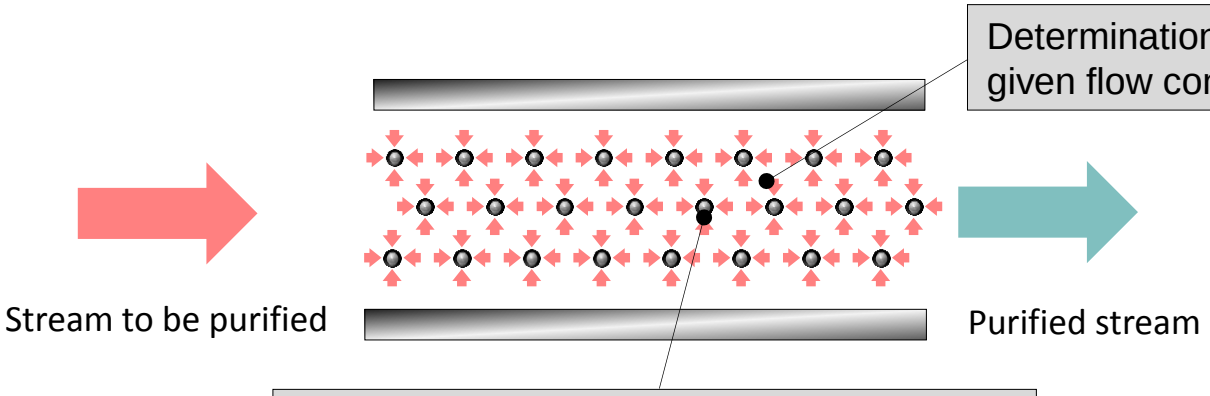


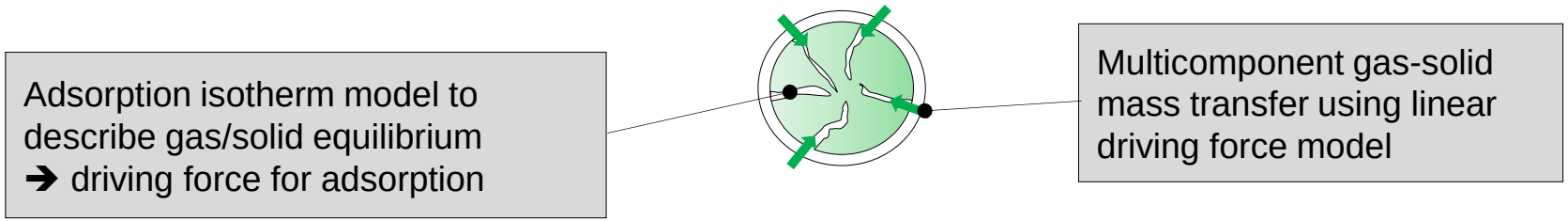
Adsorption bed model

Mass & heat transfer phenomena

- Adsorption bed with pellets



- Single pellet



Adsorption bed model

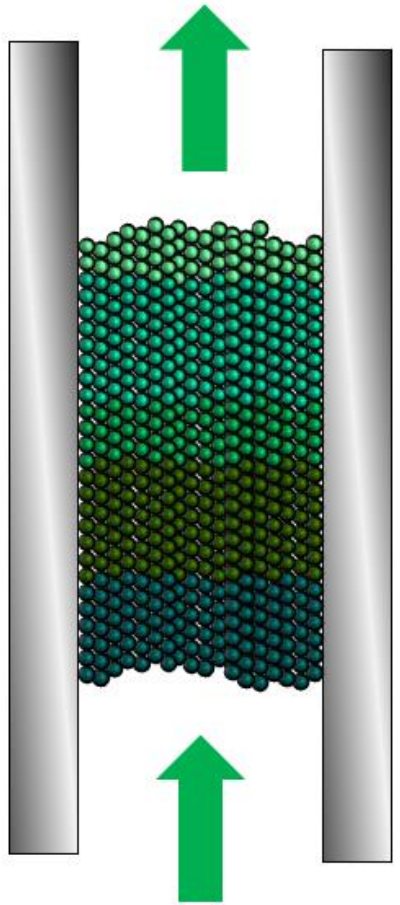
Mass & heat transfer phenomena

- 1D convection/dispersion flow
  - Dispersion coefficients specified by user or calculated via correlations
- Separate mass and heat balances for gas and solid (adsorbed) phase
  - Linear driving force model to predict mass transfer from gas to adsorbed phase
  - Mass transfer coefficient temperature/pressure dependence based on type of limiting mass transfer
    - bulk gas ↔ solid surface vs. intra-pellet
  - Heat of adsorption effects
  - Axial heat conduction in gas and solid phase
- Thermal inertia of bed wall taken into account
  - Heat transfer constant between bed and wall can be estimated based on flow conditions
  - Ambient heat losses

Adsorption bed model

Adsorption isotherms

- Predict equilibrium adsorption for given gas-phase conditions
  - pressure, temperature, composition
- Standard adsorption isotherms supported
  - Langmuir
  - Langmuir-Freundlich
  - IAST
- …or user can implement own adsorption isotherm using gPROMS custom modelling



Modelling a PSA process

Workflow

1. Specifying the adsorption bed model
2. Connecting valves and feed and product streams
3. Defining a schedule
4. Customization
   - isotherms
   - fluid properties
   - mass transfer correlations
5. Saving and restoring states

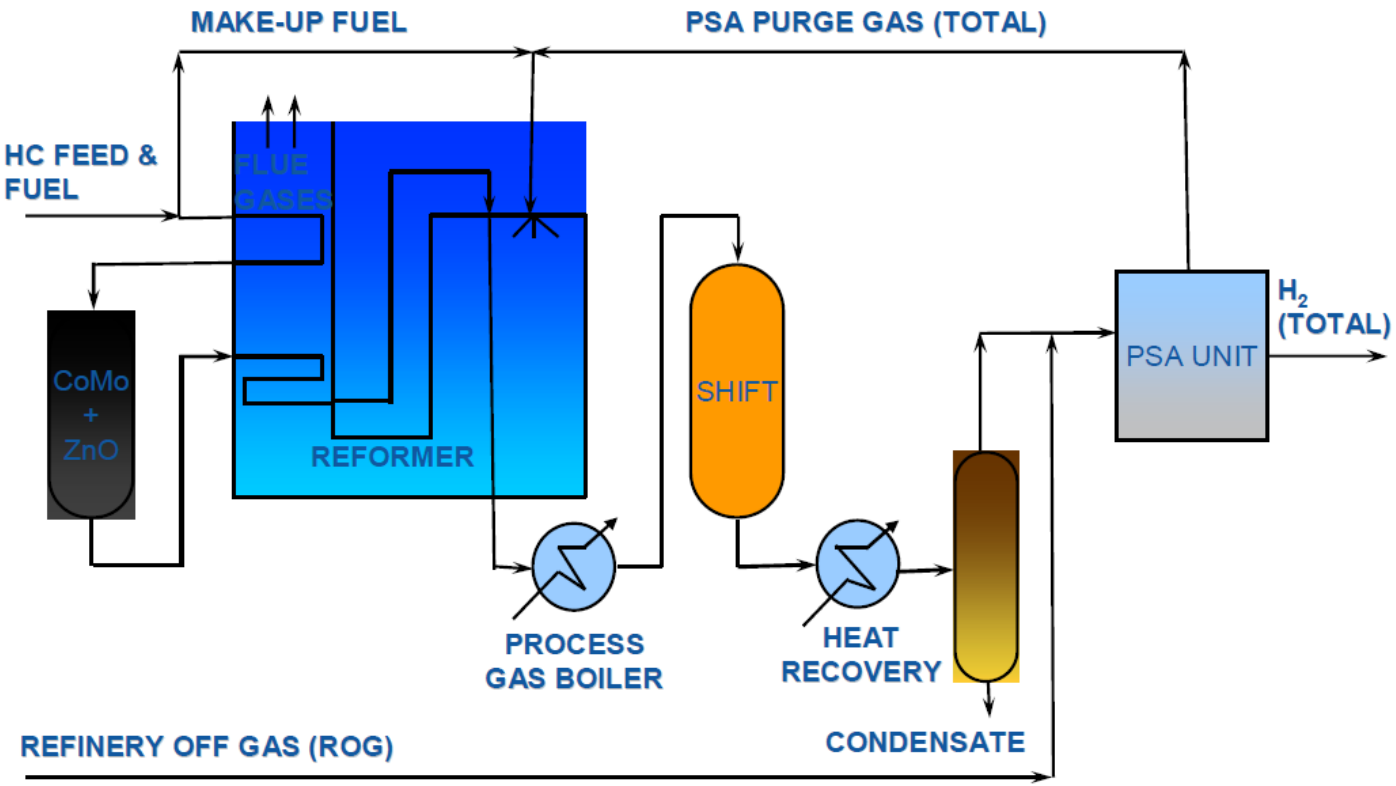
Adsorption modelling in gPROMS ProcessBuilder

Example overview

Example overview

- Separating H_2 from refinery off-gases (ROG)
  - Source Technip

    (http://www.greenbusinesscentre.com/EES2010/Presentations)

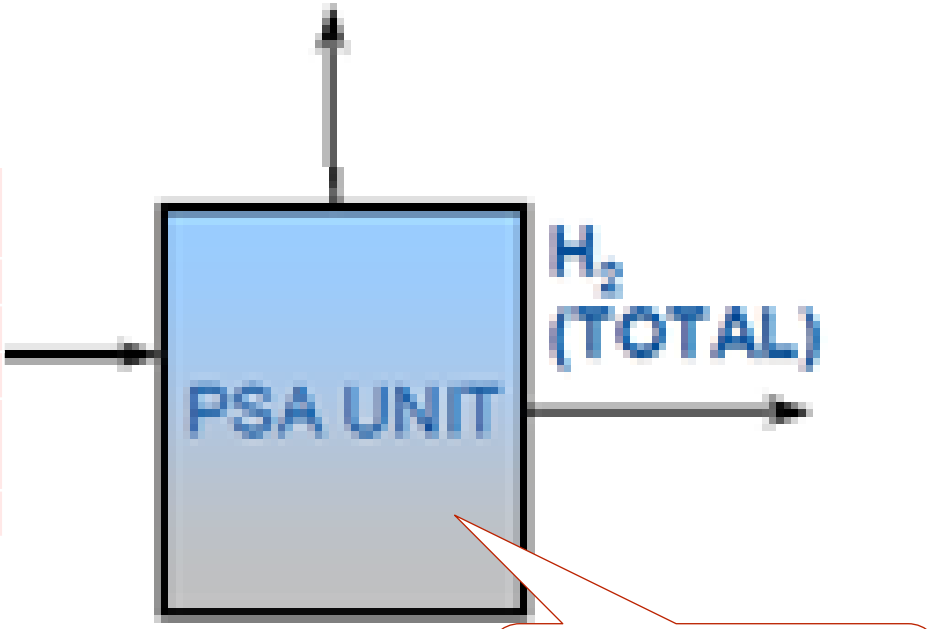


Example overview

- Separating H_2 from refinery off-gases (ROG)
  - Source Technip

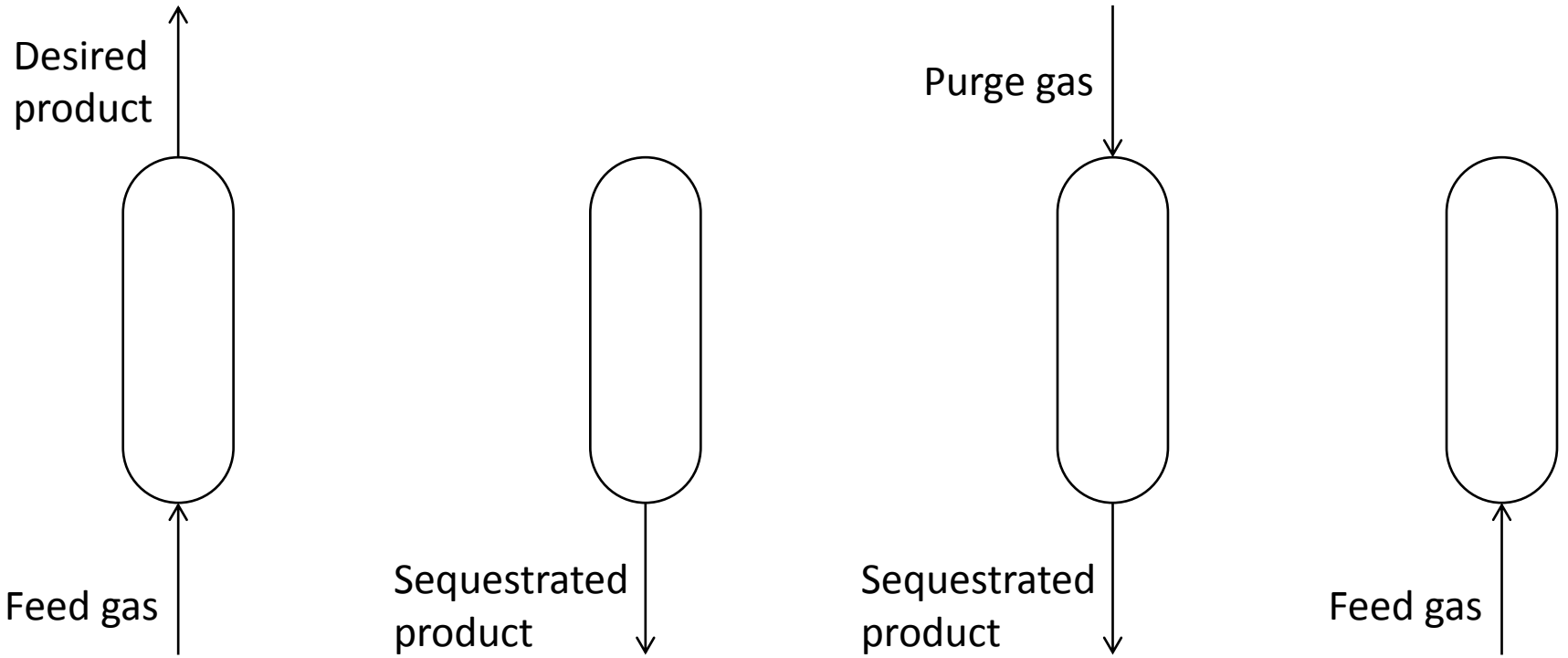
    (http://www.greenbusinesscentre.com/EES2010/Presentations)

Component	Molar fraction
Hydrogen	0.733
Methane	0.035
Carbon Dioxide	0.166
Carbon monoxide	0.029
Nitrogen	0.037



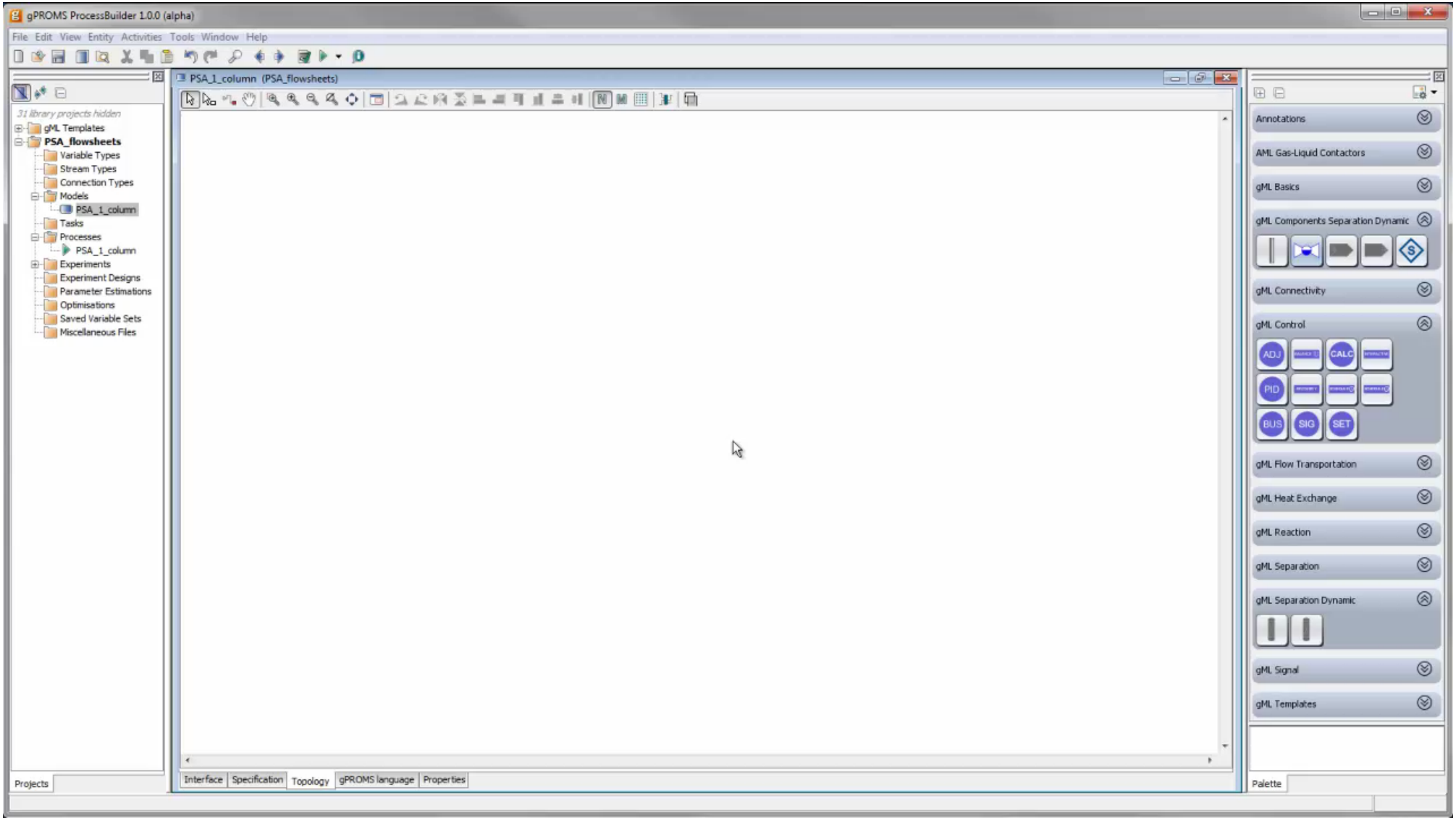
Example overview

- Four-step operation of the PSA process



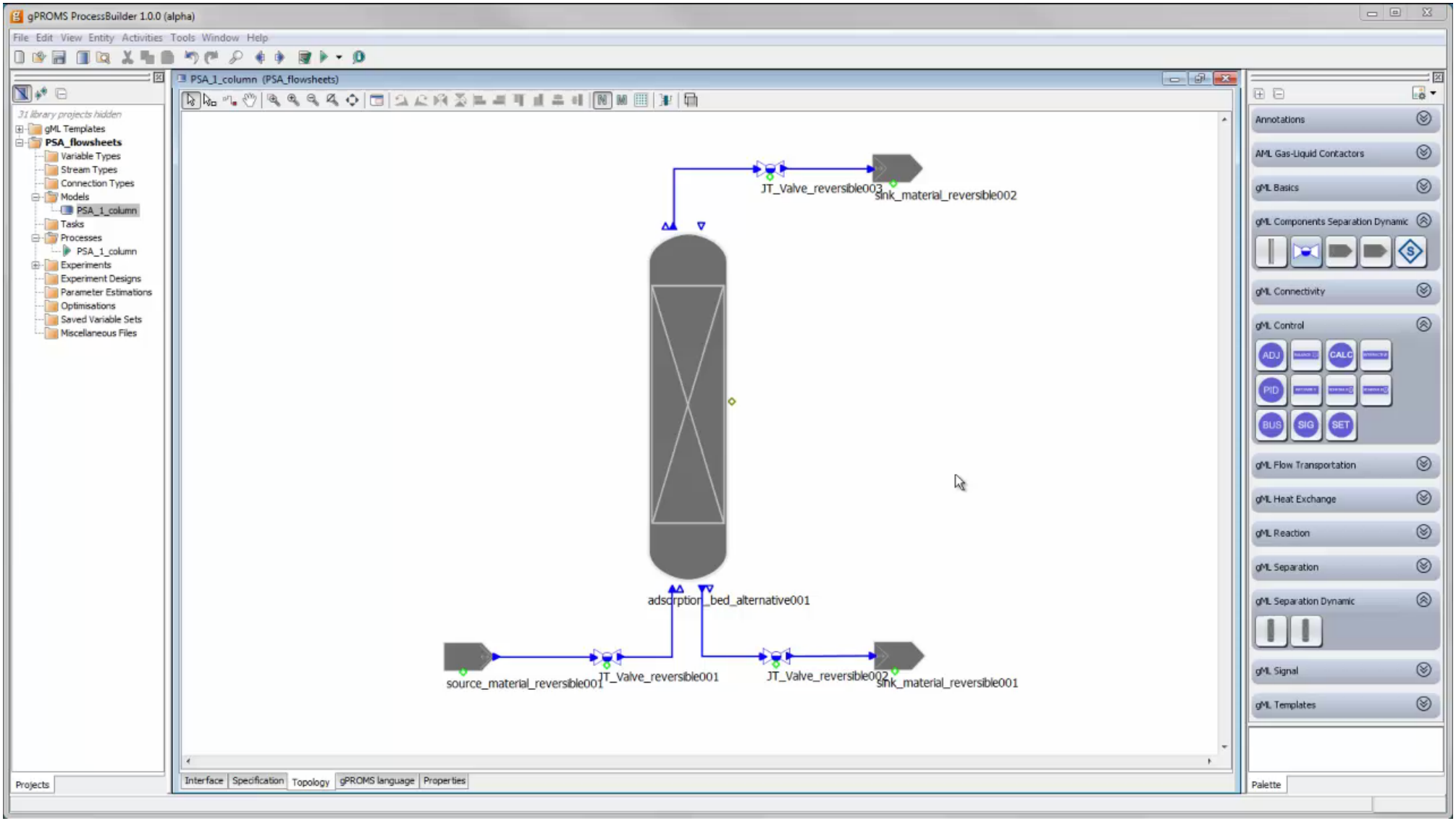
Modelling a PSA process

Single bed flowsheet - construction



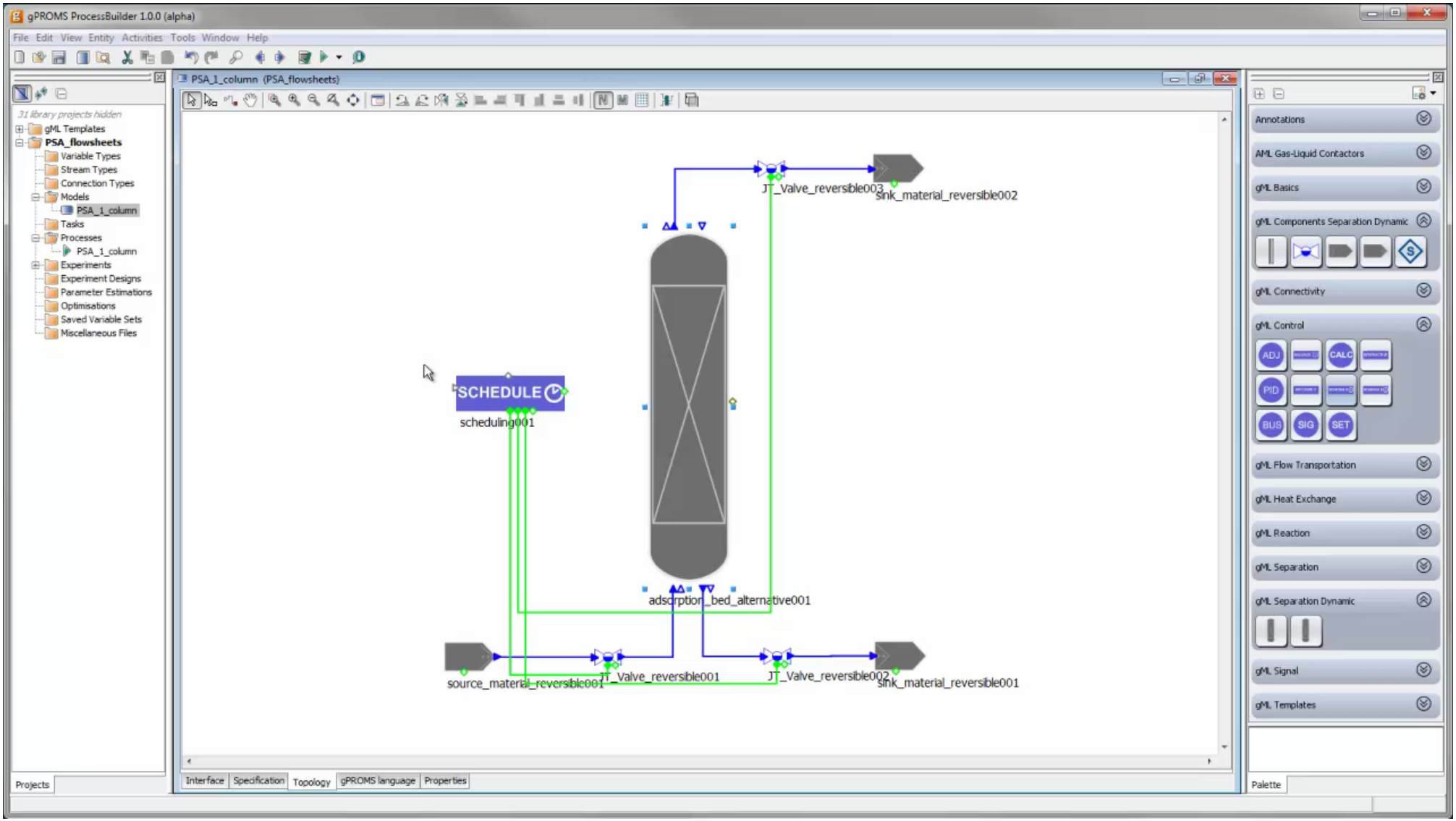
Modelling a PSA process

Single bed flowsheet - scheduling



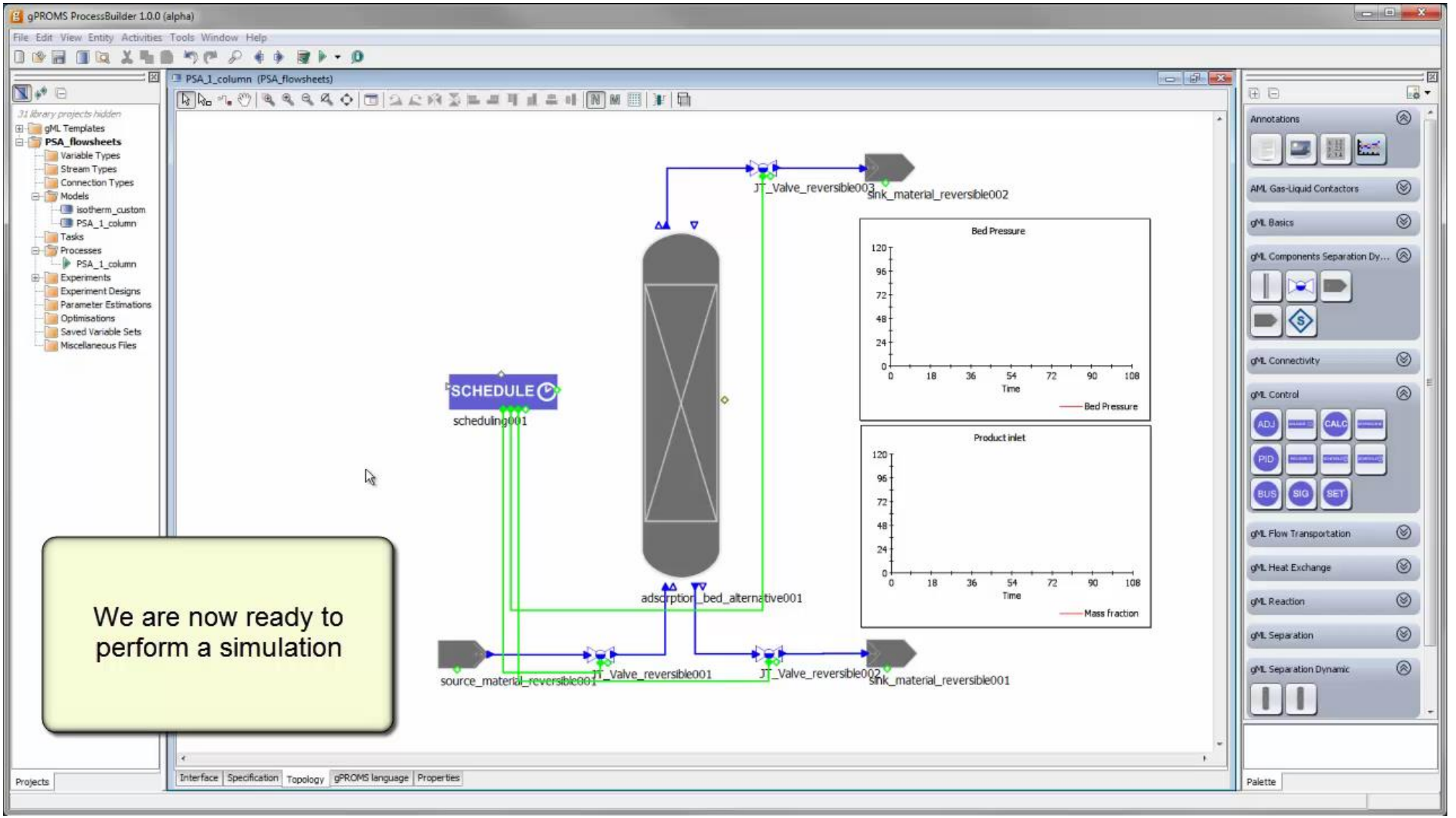
Modelling a PSA process

Single bed flowsheet – isotherm model



Modelling a PSA process

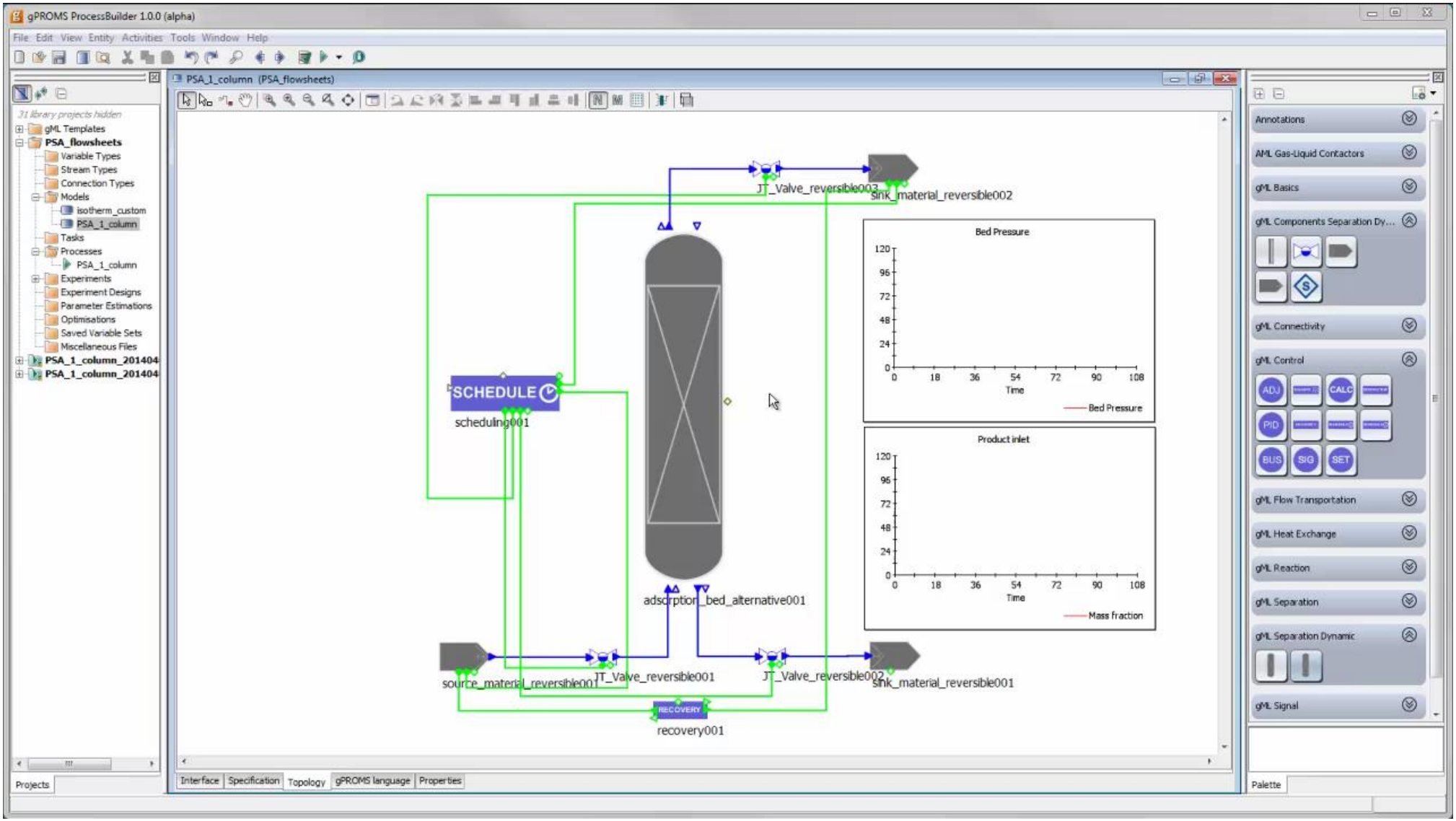
Single bed flowsheet – simulation



We are now ready to perform a simulation

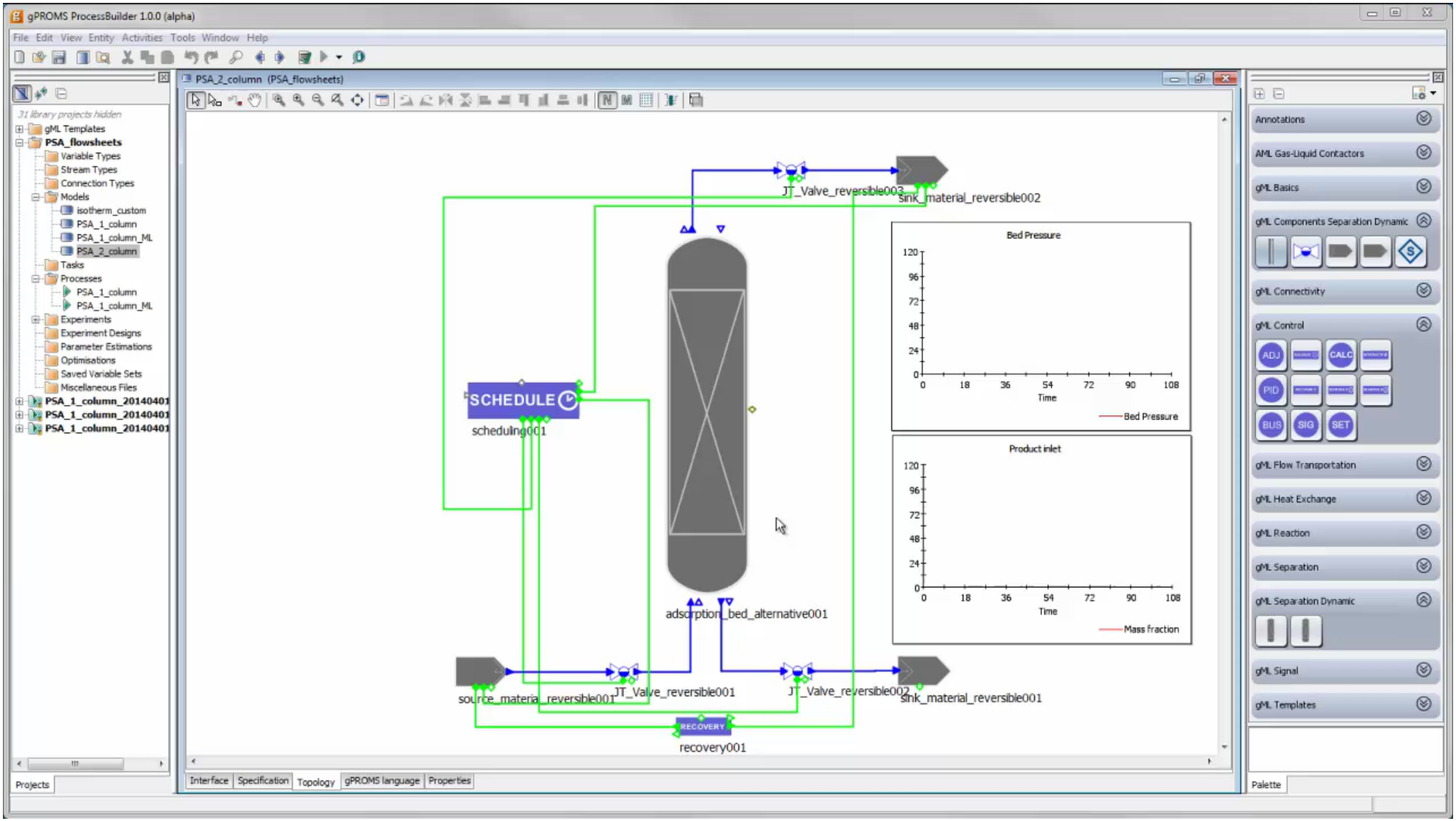
Modelling a PSA process

Single bed flowsheet – multilayer



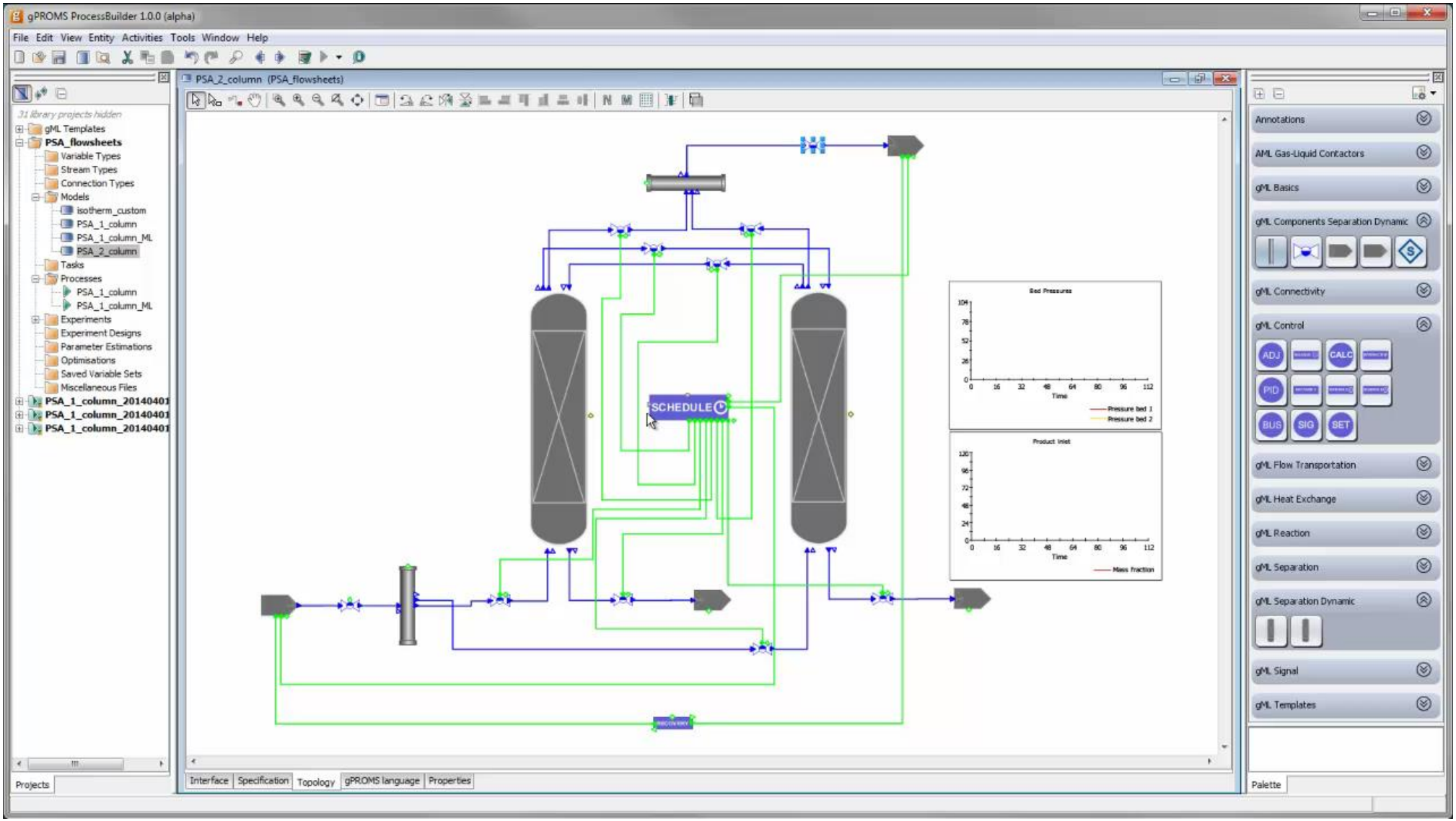
Modelling a PSA process

Multi-bed flowsheet – 2 beds



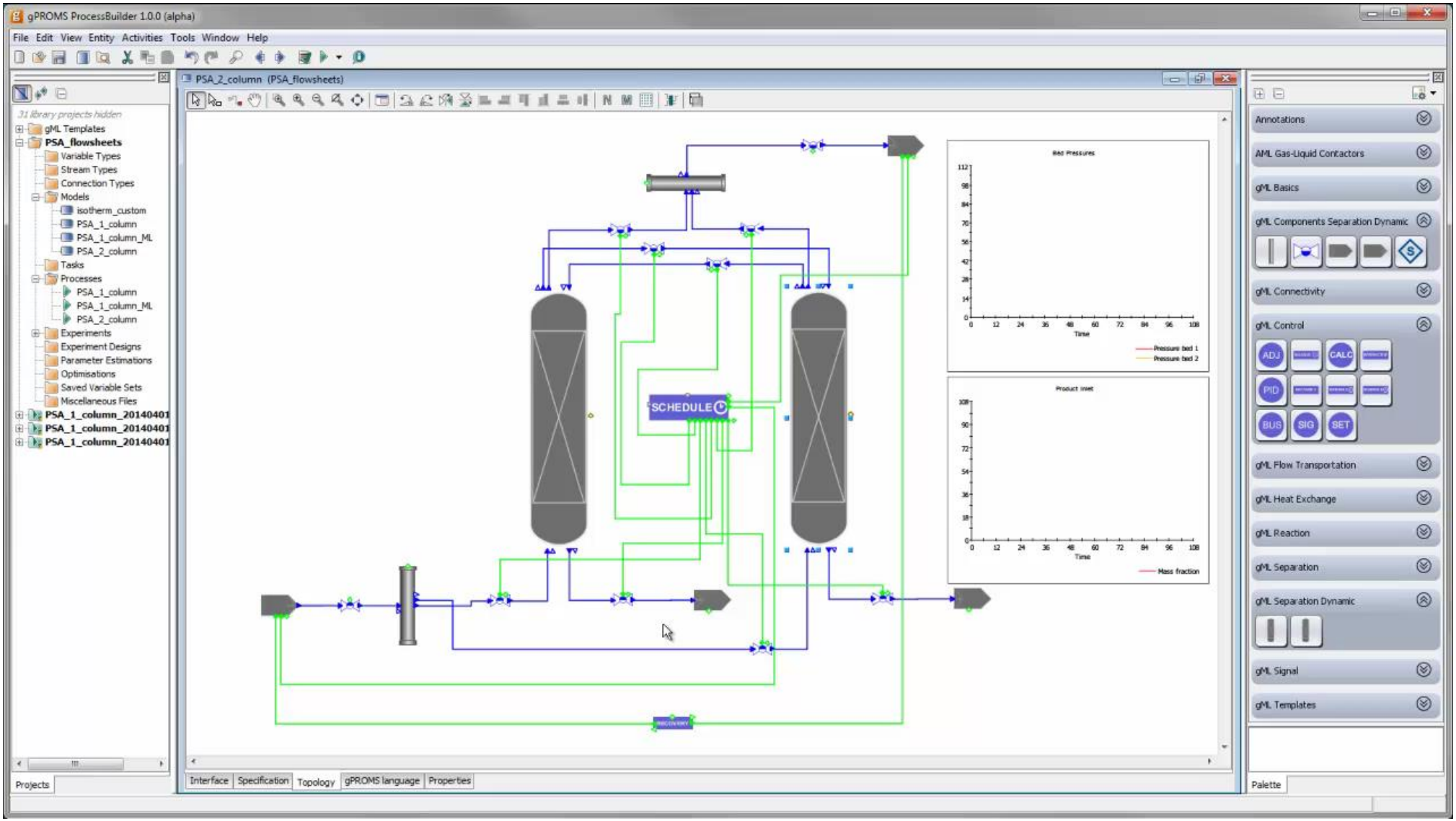
Modelling a PSA process

Multi-bed flowsheet – specifications



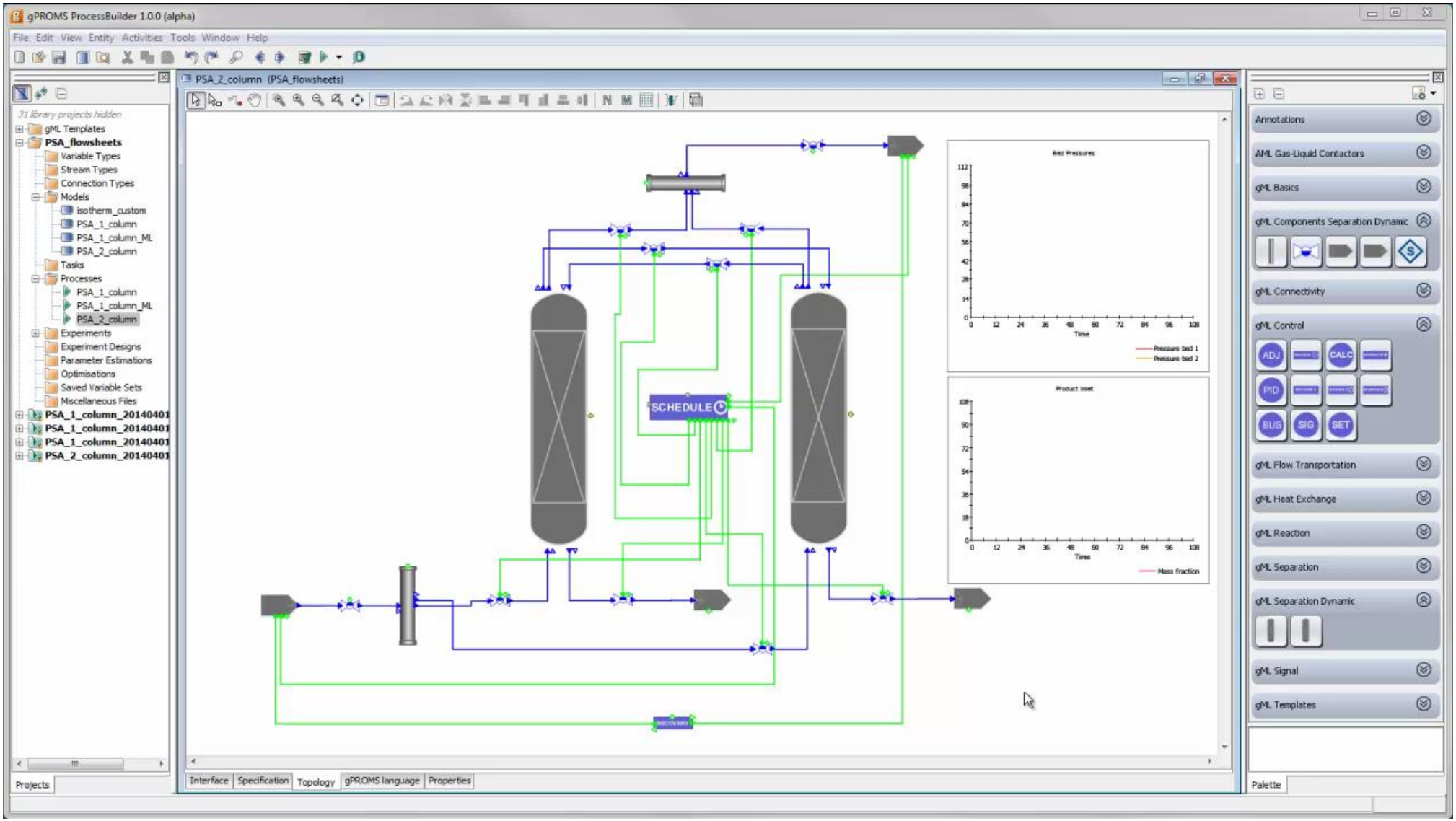
Modelling a PSA process

Multi-bed flowsheet – simulation



Modelling a PSA process

Multi-bed flowsheet – self-interacting bed



Summary

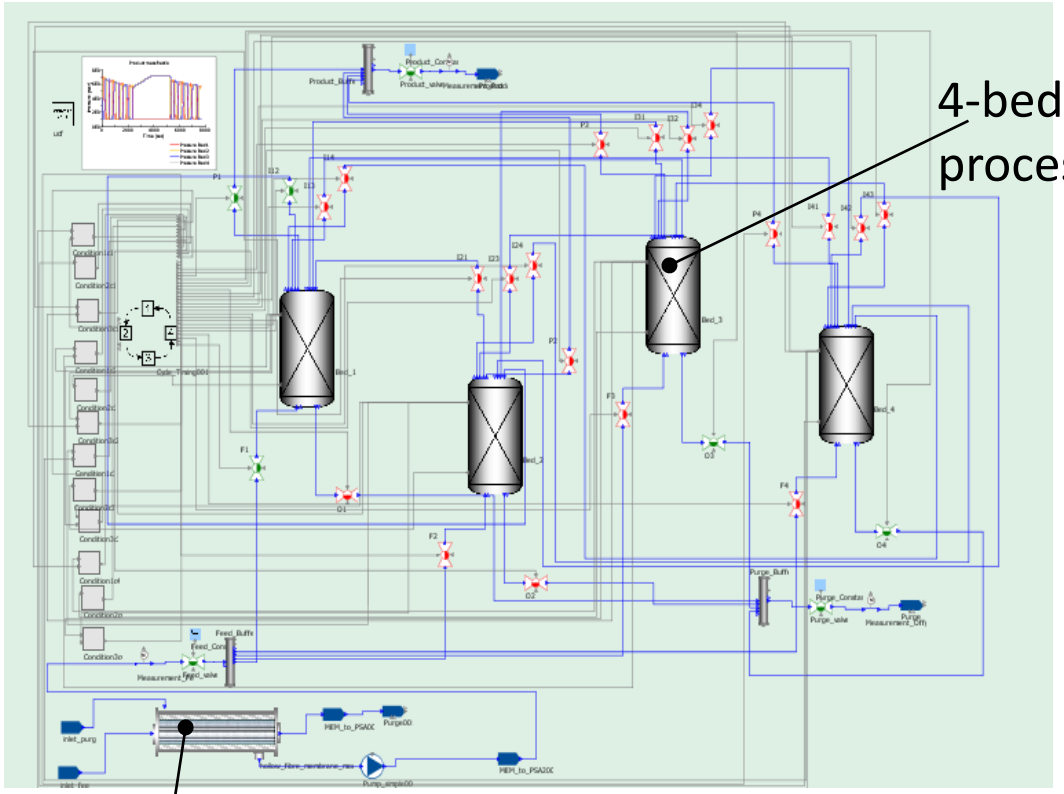
Adsorption modelling in gPROMS ProcessBuilder

- Detailed modelling of adsorption processes
  - first-principles models plus engineering content
  - can be extended via user-provided correlations if required
- Graphical/flowsheeting user interface
  - easy construction of multi-bed configurations using drag and drop flowsheeting
  - straightforward specification of complex operation schedules
  - Visual feedback on results
    - e.g. valves indicate open/close status by changing colour during simulation
- Parameter estimation to obtain phase equilibrium & mass transfer parameters
  - e.g. from measured breakthrough curves

Summary

Adsorption modelling in gPROMS ProcessBuilder

- Model adsorption processes (PSA,TSA) within overall plant model



HY2SEPS-2
EU project

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Thank you

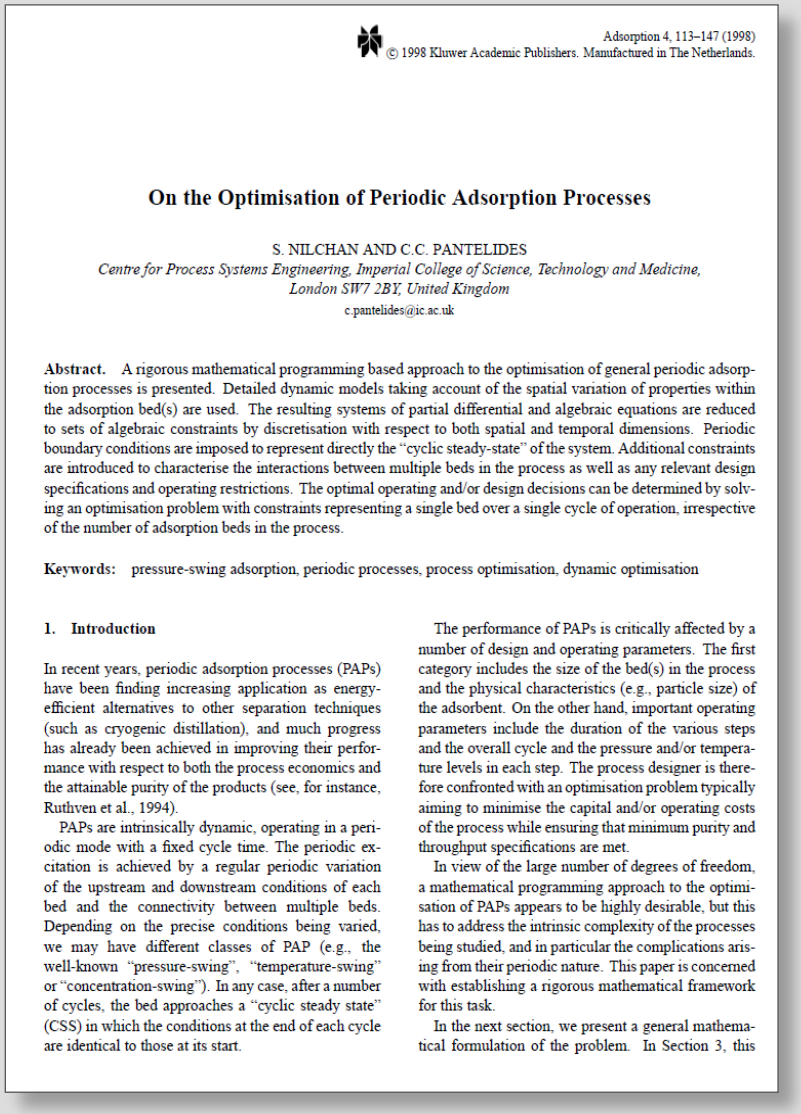
Backup slides

Adsorption: process improvement

Cyclic steady-state: direct calculation/optimization

- Approach: We only need to model one cycle for a single column as all columns behave identically
- Directly impose periodic boundary & initial condition equations that
  - equate values from one period to those from another period in the cycle
    - e.g. The concentration & temperature profiles in the bed at the initial time are equal to the equivalent profiles at the end of the cycle

Solved in gPROMS by discrertising both time and spatial domains: leading to a fully algebraic model



Adsorption 4, 113–147 (1998)

On the Optimisation of Periodic Adsorption Processes

S. NILCHAN AND C.C. PANTELIDES
Centre for Process Systems Engineering, Imperial College of Science, Technology and Medicine, London SW7 2BY, United Kingdom
c.pantelides@ic.ac.uk

Abstract. A rigorous mathematical programming based approach to the optimisation of general periodic adsorption processes is presented. Detailed dynamic models taking account of the spatial variation of properties within the adsorption bed(s) are used. The resulting systems of partial differential and algebraic equations are reduced to sets of algebraic constraints by discretisation with respect to both spatial and temporal dimensions. Periodic boundary conditions are imposed to represent directly the "cyclic steady-state" of the system. Additional constraints are introduced to characterise the interactions between multiple beds in the process as well as any relevant design specifications and operating restrictions. The optimal operating and/or design decisions can be determined by solving an optimisation problem with constraints representing a single bed over a single cycle of operation, irrespective of the number of adsorption beds in the process.

Keywords: pressure-swing adsorption, periodic processes, process optimisation, dynamic optimisation

1. Introduction

In recent years, periodic adsorption processes (PAPs) have been finding increasing application as energy-efficient alternatives to other separation techniques (such as cryogenic distillation), and much progress has already been achieved in improving their performance with respect to both the process economics and the attainable purity of the products (see, for instance, Ruthven et al., 1994).

PAPs are intrinsically dynamic, operating in a periodic mode with a fixed cycle time. The periodic excitation is achieved by a regular periodic variation of the upstream and downstream conditions of each bed and the connectivity between multiple beds. Depending on the precise conditions being varied, we may have different classes of PAP (e.g., the well-known "pressure-swing", "temperature-swing" or "concentration-swing"). In any case, after a number of cycles, the bed approaches a "cyclic steady state" (CSS) in which the conditions at the end of each cycle are identical to those at its start.

The performance of PAPs is critically affected by a number of design and operating parameters. The first category includes the size of the bed(s) in the process and the physical characteristics (e.g., particle size) of the adsorbent. On the other hand, important operating parameters include the duration of the various steps and the overall cycle and the pressure and/or temperature levels in each step. The process designer is therefore confronted with an optimisation problem typically aiming to minimise the capital and/or operating costs of the process while ensuring that minimum purity and throughput specifications are met.

In view of the large number of degrees of freedom, a mathematical programming approach to the optimisation of PAPs appears to be highly desirable, but this has to address the intrinsic complexity of the processes being studied, and in particular the complications arising from their periodic nature. This paper is concerned with establishing a rigorous mathematical framework for this task.

In the next section, we present a general mathematical formulation of the problem. In Section 3, this

Nilchan & Pantelides, Adsorption. 1998, 4, 113-147