gPROMS ProcessBuilder for periodic adsorption processes

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Chemicals & Petrochemicals

Overview

- Adsorption technologies
- Modeling of adsorption beds
- Pressure swing adsorption
  - Multi-bed modeling
- Accelerating the convergence of PSA simulations
  - Self-interacting Bed
  - Convergence schemes
- Conclusions

Adsorption technologies

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 vapors from air
  - Ethanol dehydration

- Liquid-phase processes (SMB, chromatography)
  - UOP Sorbex processes
    e.g. separation of mixed aromatic C_8 isomers (Parex™ , Ebex™, MX Sorbex™)

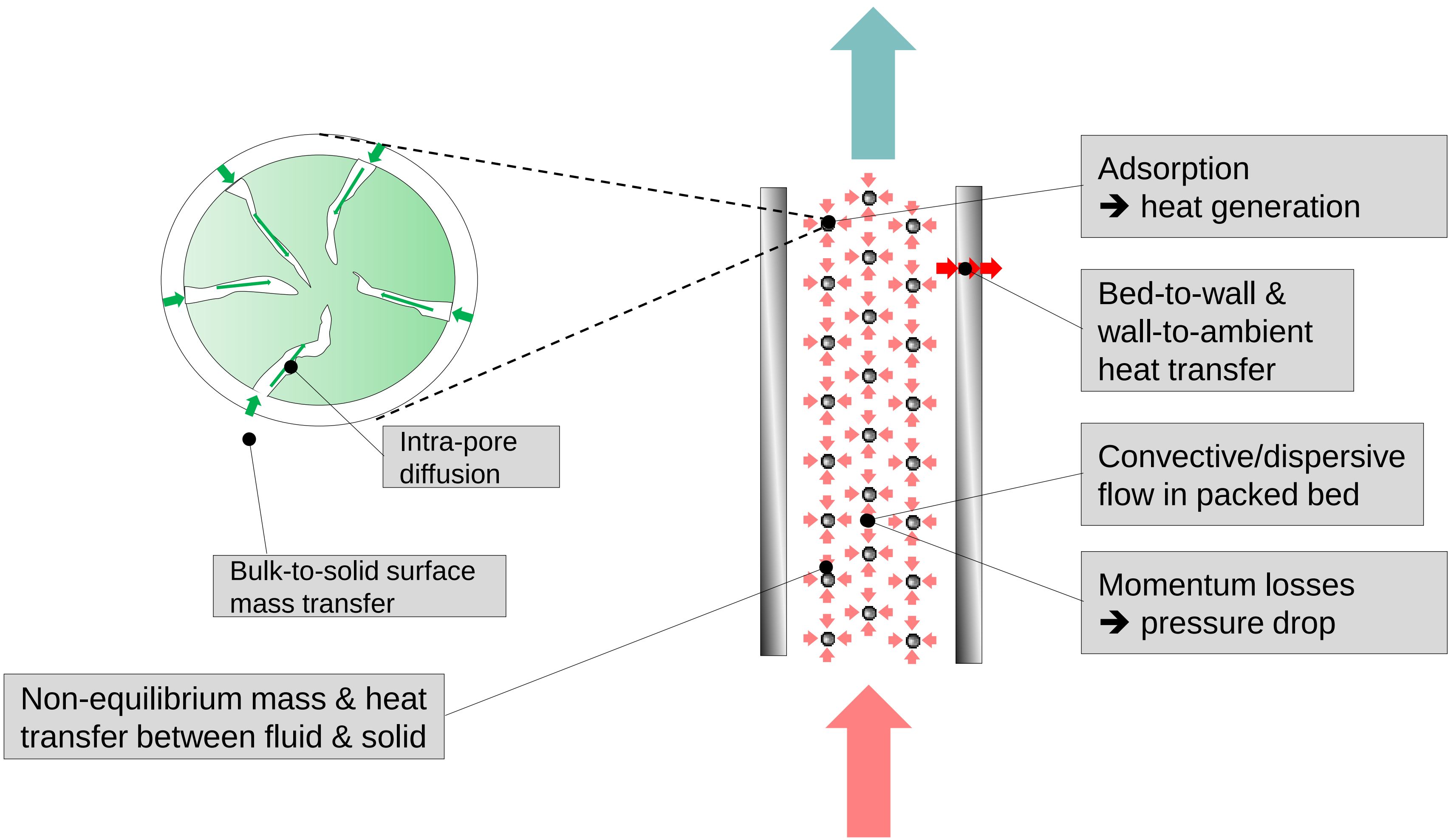
Modeling of adsorption processes
Main considerations/challenges

- Spatially varying properties
  - Axial & radial variations in the adsorbent bed
  - Adsorbed species diffuse through pores in adsorbent
- Inherently dynamic processes
  - Complex operating procedures (“cycle schedules”)
  - Major discontinuities (e.g. flow reversals)
- Process improvement
  - Optimisation of equipment design & operating procedure
  - Usually meaningful only at *cyclic steady state*

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

Modeling of adsorption beds

Modeling of adsorption beds



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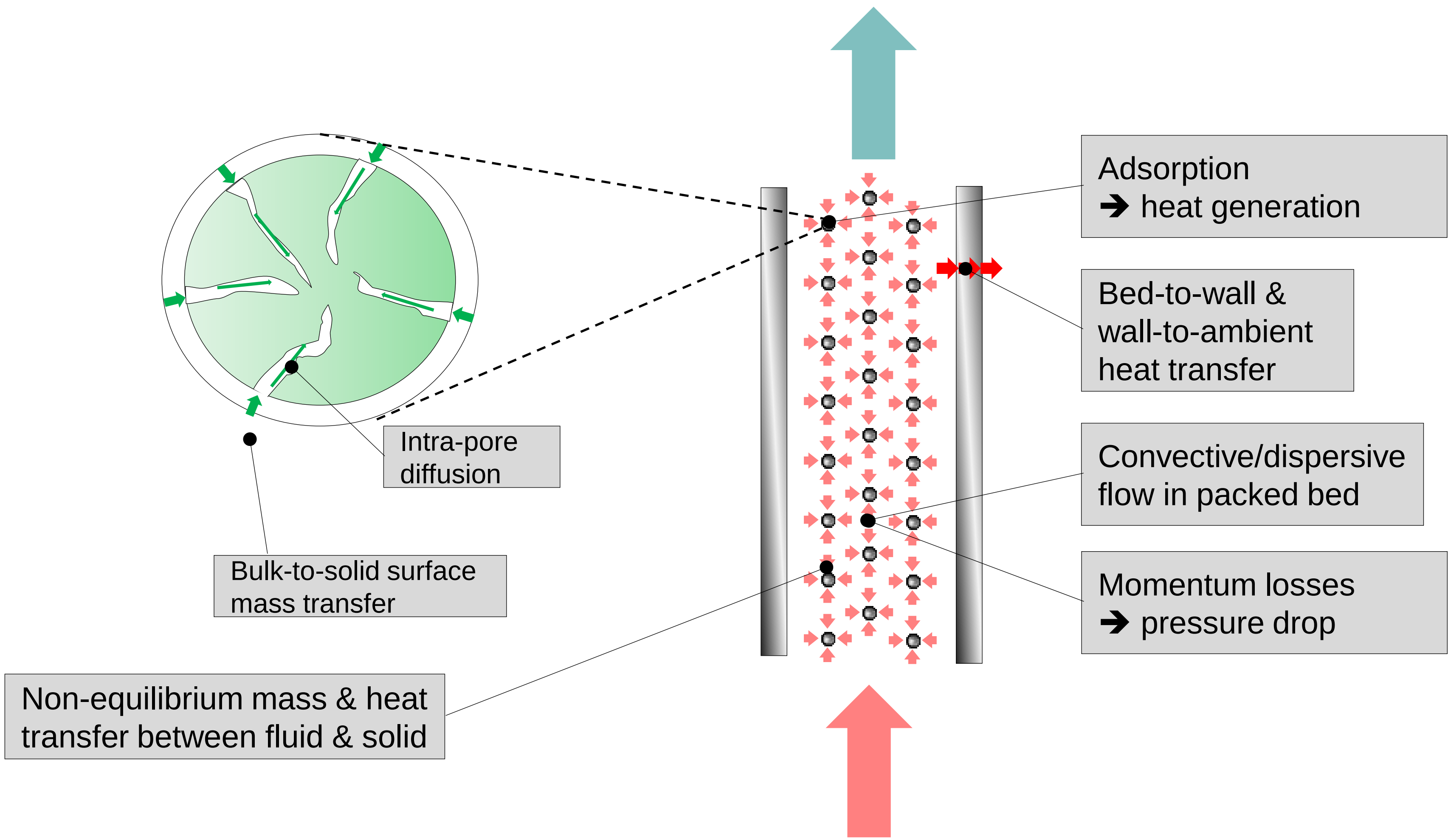
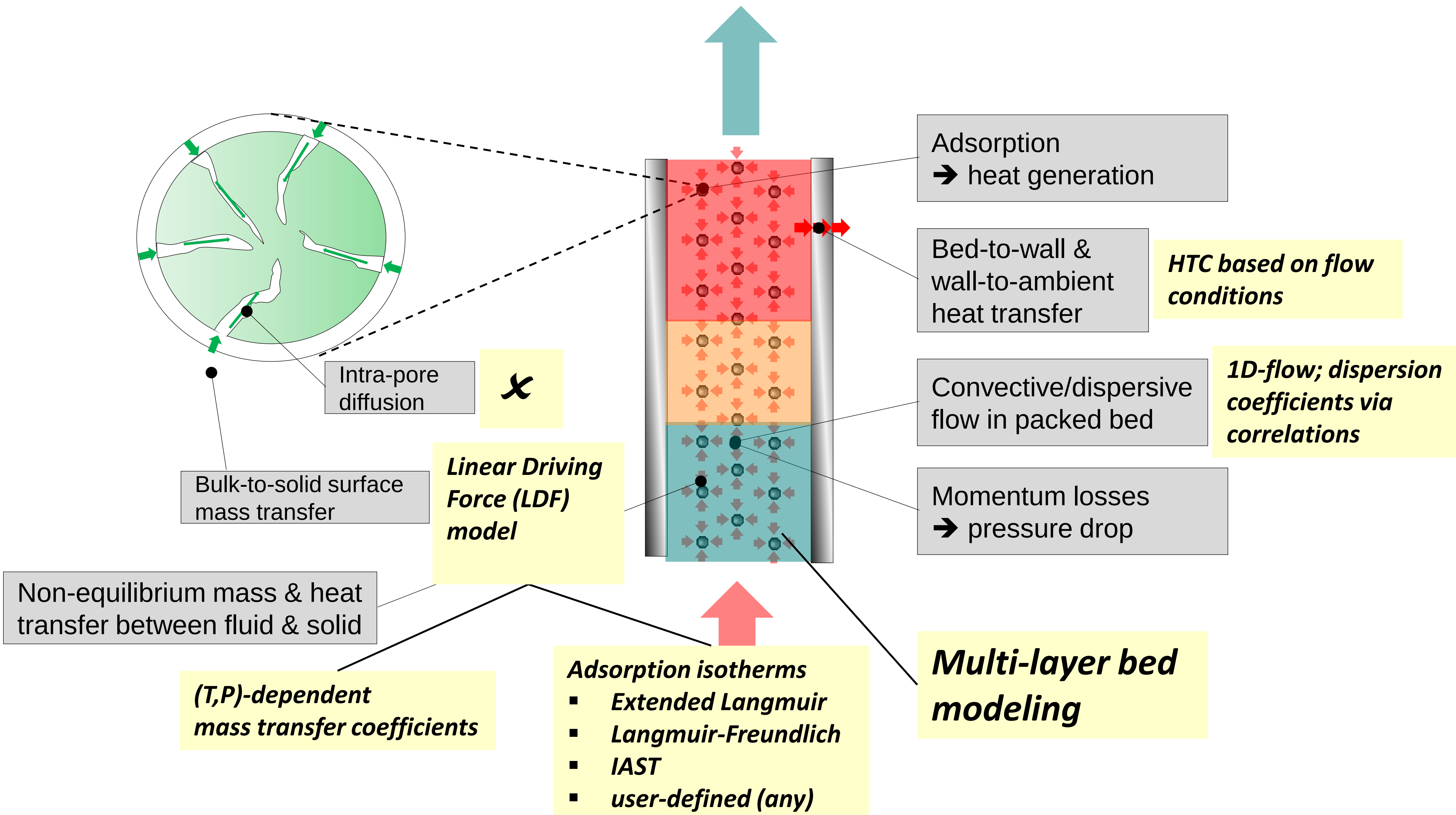
Modeling of adsorption beds in gPROMS ProcessBuilder



Modeling of adsorption beds in gPROMS ProcessBuilder



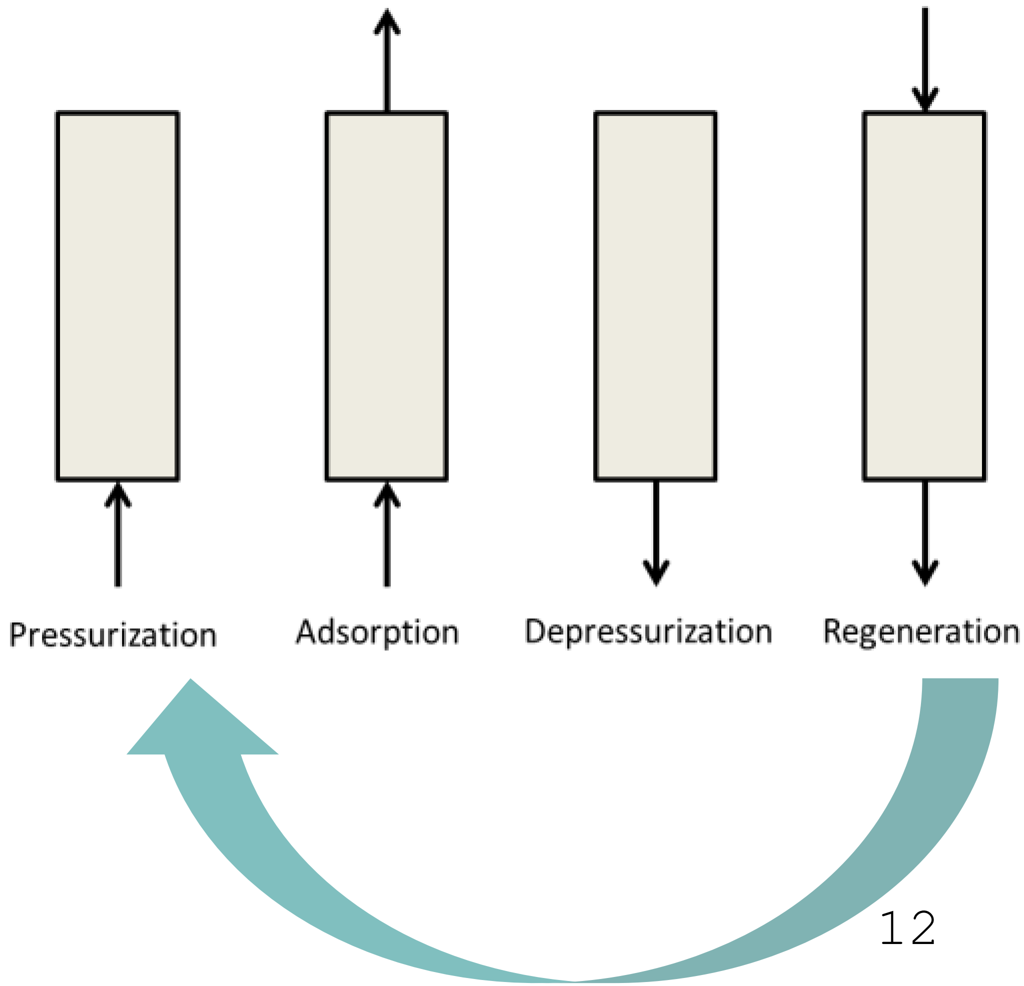
Pressure swing adsorption

Advantages demonstrated:

- New applications – complex dynamic processes
- Comprehensive model libraries
- Complex schedules
- Equation-oriented power

Pressure Swing Adsorption (PSA)

- Process operation **cycles** between adsorption and regeneration steps
- Multibed systems: continuous product delivery
- Example: Skarstrom cycle
  - Pressurisation
  - Adsorption
  - Depressurisation
  - Regeneration



Modeling Challenges

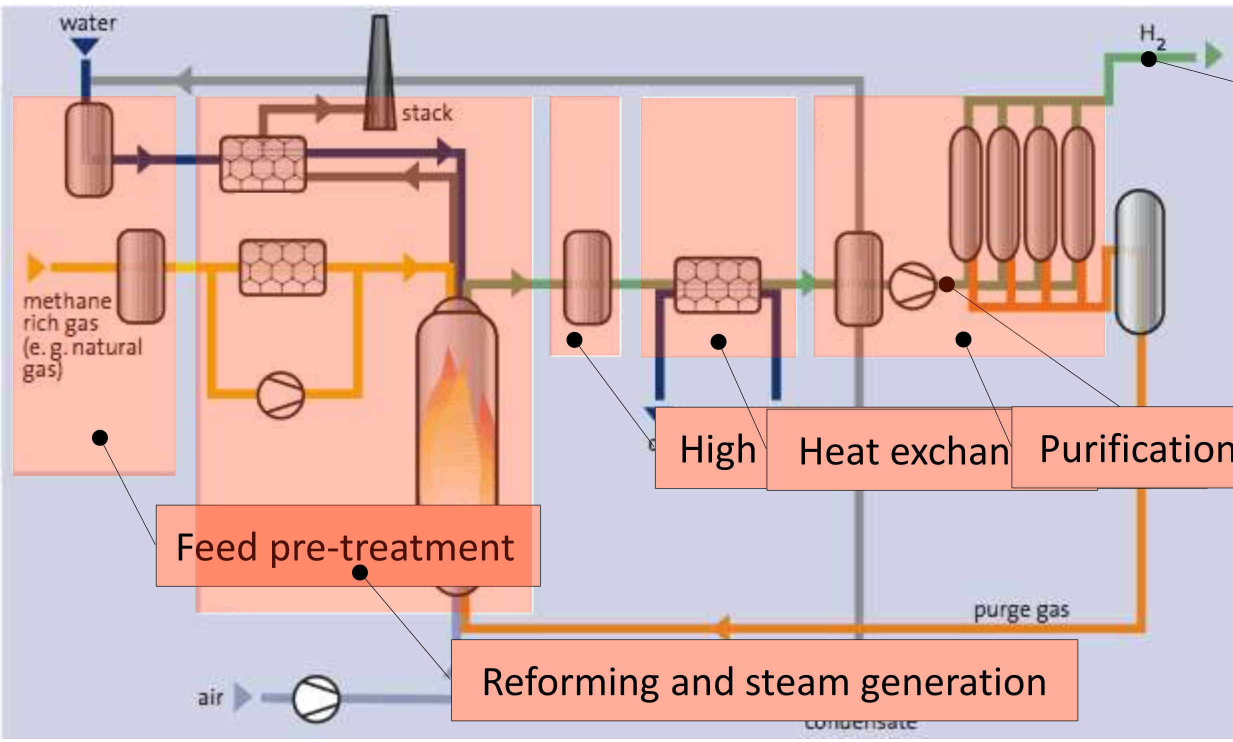
- Described by PDAEs
  - Concentration / temperature profiles vary both spatially and temporally
  - Sometimes multiple spatial dimensions present
    - Axial, radial, intra-particle

- Boundary conditions change throughout each cycle (adsorption, regeneration, etc.)

- Process design and optimisation normally meaningful only at **cyclic steady state (CSS)**

Production of hydrogen from natural gas

- Hydrogen produced from catalytic reforming of natural gas
  - $CH_4 + H_2O \leftrightharpoons 3H_2 + CO$
  - combined with water gas shift reaction: $CO + H_2O \leftrightharpoons H_2 + CO_2$



Source: http://www.global-hydrogen-bus-platform.com/Technology/HydrogenProduction/reforming

High-purity hydrogen obtained via pressure swing adsorption (PSA)

Impurities:
- carbon dioxide
- methane
- carbon monoxide
- nitrogen
- water vapor

PSA process for hydrogen purification

A.M. Ribeiro, C.A. Grande, F.V.S. Lopes, J.M. Loureiro, A.E. Rodrigues *Chem. Eng. Sci.* **63** 5258-5273 (2008)

- Feed molar fractions
  - H_2: 73.3 | CO_2: 16.6 | CH_4: 3.5 | CO: 2.9 | N_2: 3.7
- 2-layer beds
  - 50% activated carbon ➔ $CO_2 + CH_4 + H_2O$
  - 50% zeolite ➔ $CO + N_2$
- Adsorption isotherm: Multisite Langmuir model
- 4-bed, 12-step process

Steps:	1	2	3	4	5	6	7	8	9	10	11	12
Bed 1:	Feed			D1		D2	Bd	Pg	P1	P2		Pres
Bed 2:	P2		Pres	Feed			D1		D2	Bd	Pg	P1
Bed 3:	Bd	Pg	P1	P2		Pres	Feed			D1		D2
Bed 4:	D1		D2	Bd	Pg	P1	P2		Pres	Feed		

$t_{cycle} = 4xt_{feed}$; $t_{D1} = t_{D2} = t_{P1} = t_{P2} = t_{pres} = t_{feed}/2$; $t_{blowd} = t_{purge} = t_{feed}/4$

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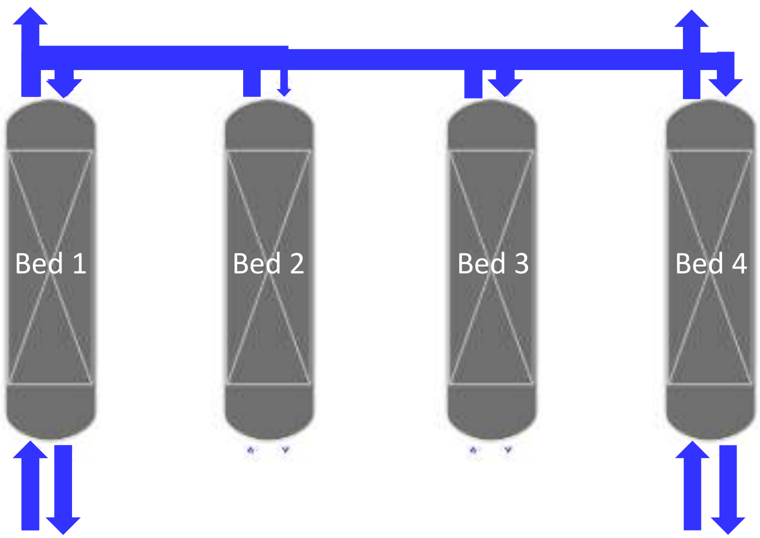

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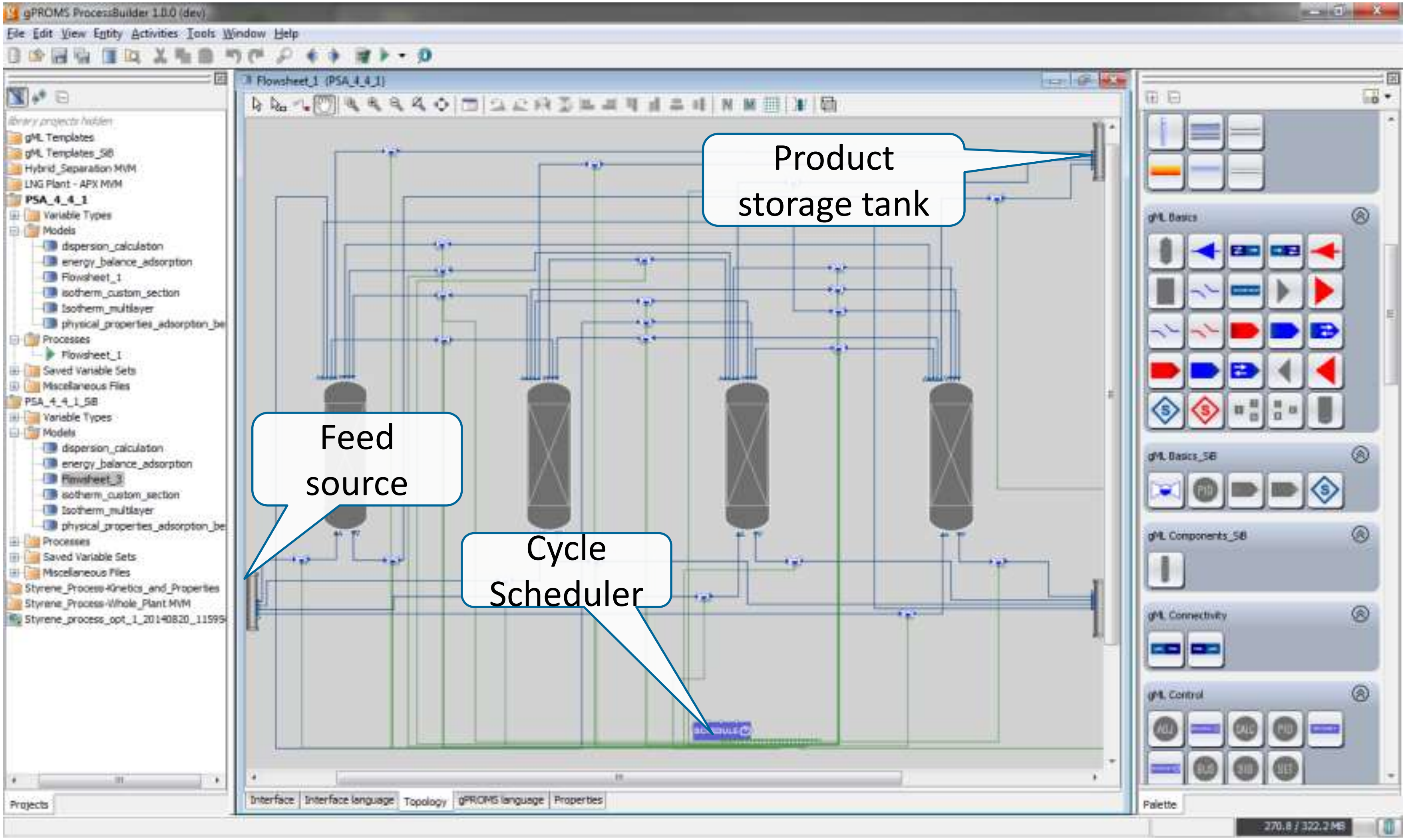
Multi-bed PSA process modeling & simulation



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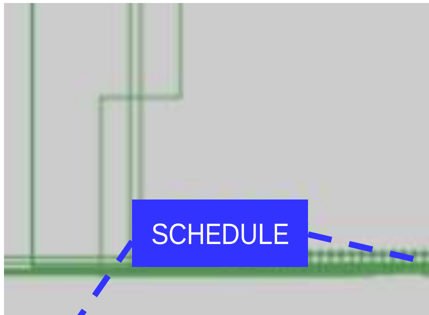

12-step cycle schedule

Steps:	1	2	3	4	5	6	7	8	9	10	11	12
Bed 1:	Feed			D1		D2	Bd	Pg	P1	P2		Pres
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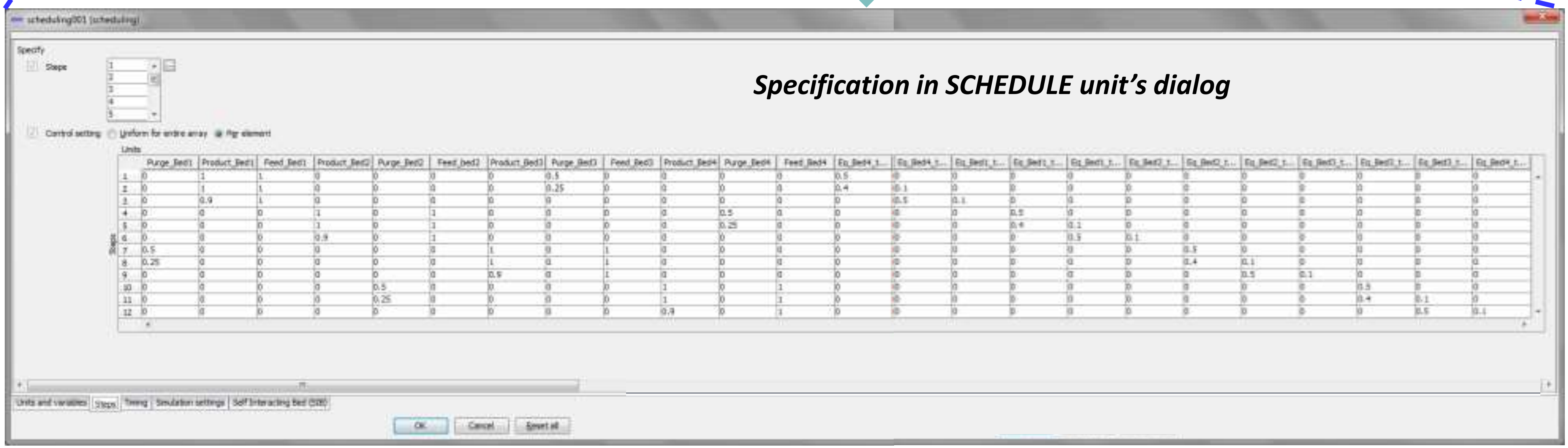
Bed 4:	D1		D2	Bd	Pg	P1	P2		Pres	Feed		

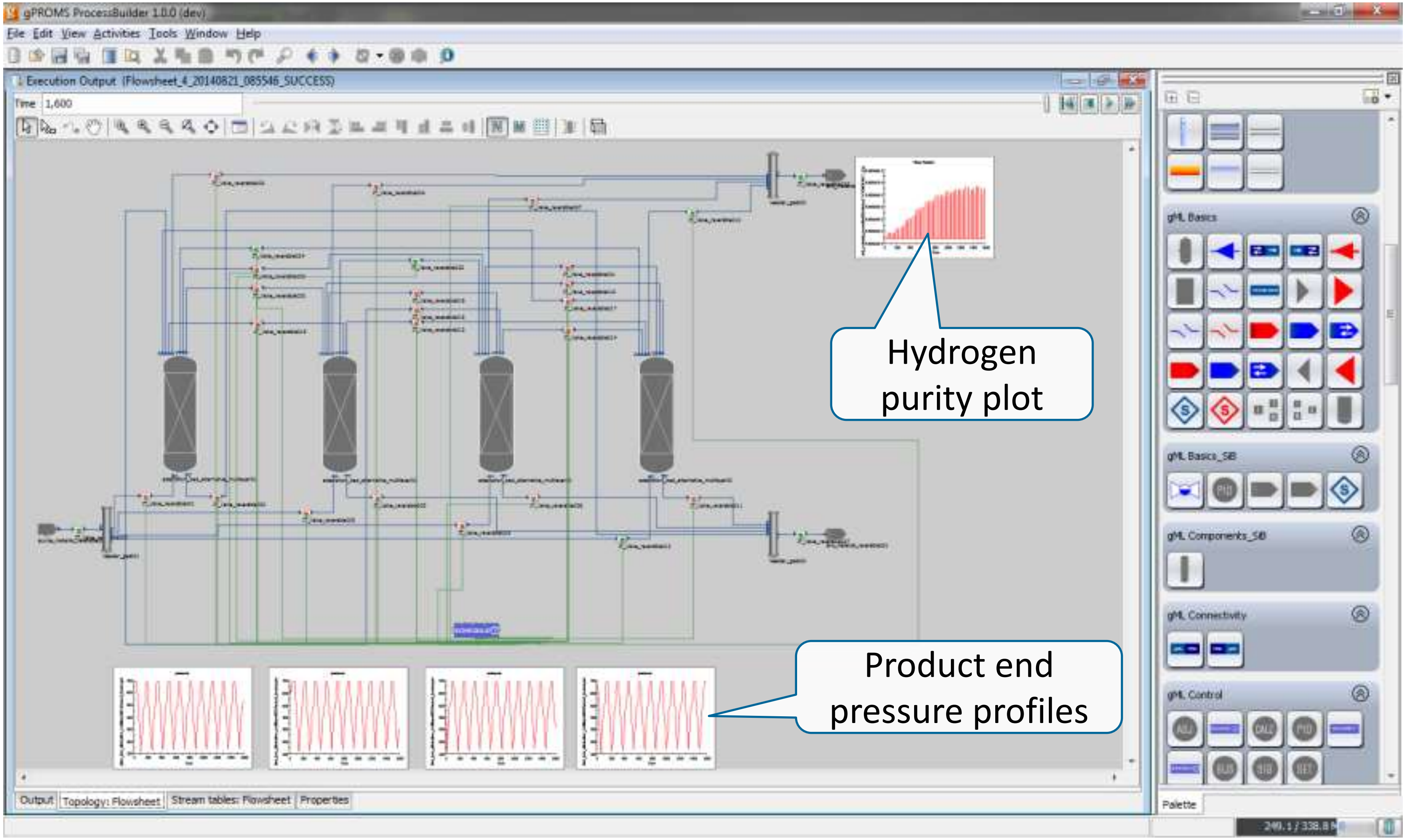
$t_{cycle} = 4xt_{feed}$; $t_{D1} = t_{D2} = t_{P1} = t_{P2} = t_{pres} = t_{feed}/2$; $t_{blowd} = t_{purge} = t_{feed}/4$

Cycle time = 160 s



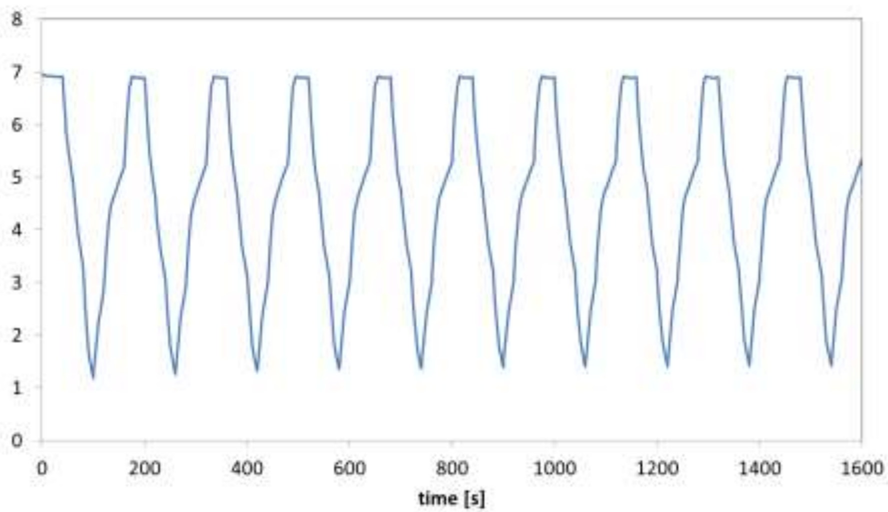
Specification in SCHEDULE unit's dialog

Multi-bed PSA process modeling & simulation

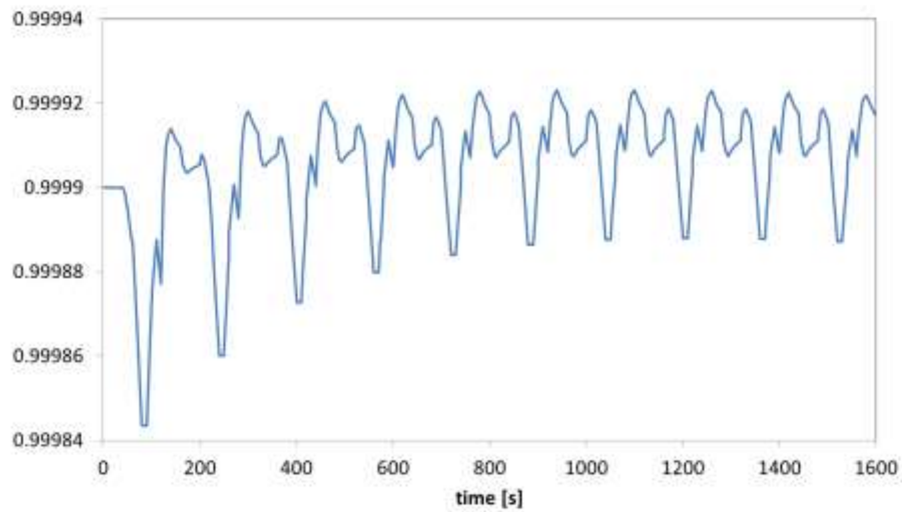


Multi-bed PSA process modeling & simulation

Bed 1 pressure profile at product end



Hydrogen purity at product end



- Simulation of 10 cycles ≈ **1601s** (CPU time)
- Getting to cyclic steady state is computationally expensive

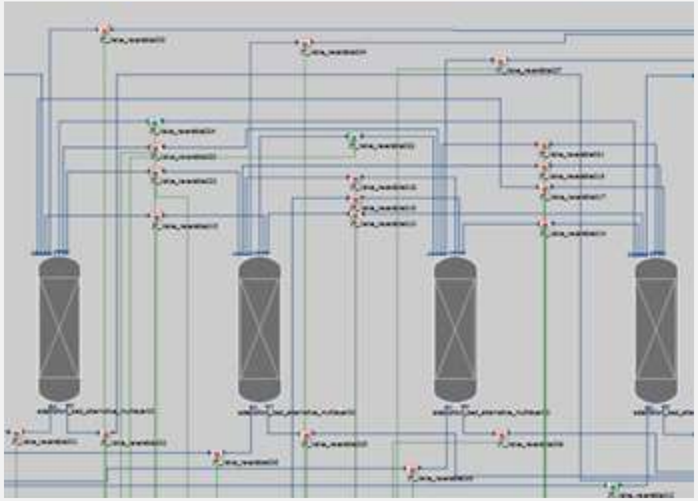
➔ Potential improvements?

Accelerating the convergence of PSA simulations

Self-interacting Bed

Explicit vs. implicit representations of multi-bed process

Multiple beds

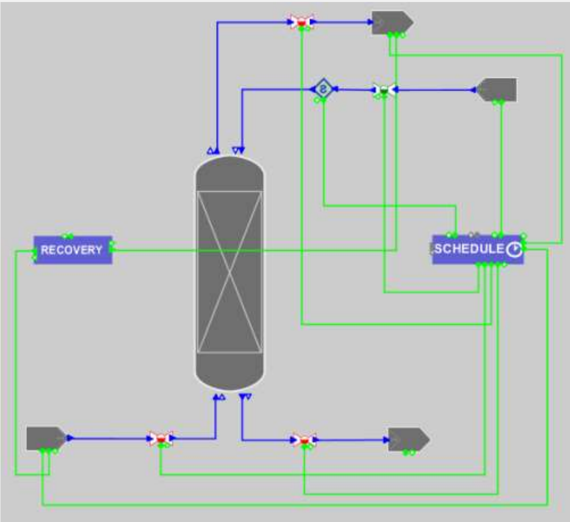


Use for studying detailed PSA process dynamics

- start-up
- effects of disturbances
- control system design & tuning

Identical CSS

Single self-interacting bed



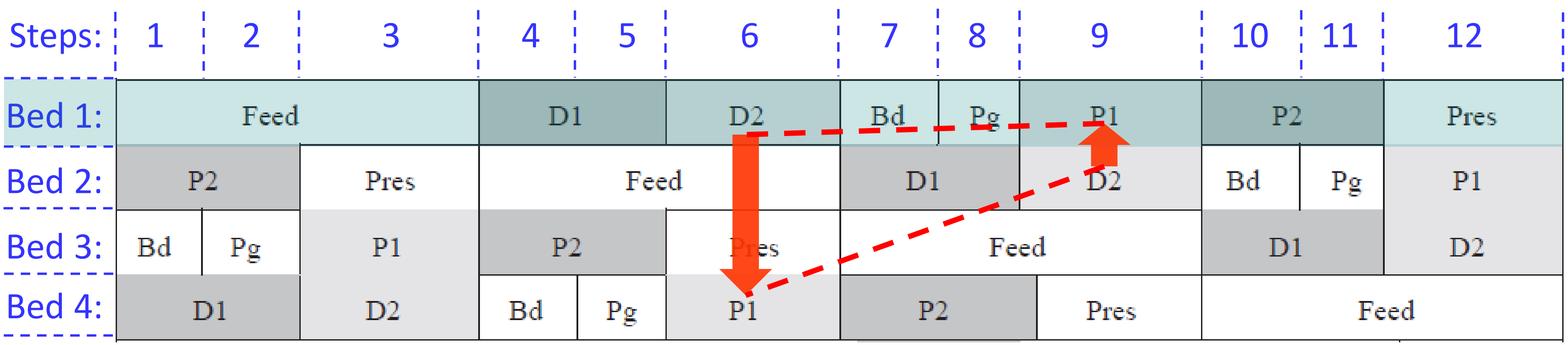
Use for process design & rating

- focus on CSS, not on transient behavior

Self-interacting Bed (SiB) for CSS computation

- All beds reach exactly the same cyclic steady state (CSS)
  ➔ it should be possible to compute the CSS
  by explicitly modeling **only one** of these beds

- **Bed-bed interactions**: At CSS, material entering bed A from bed B during a step in the cycle is identical to material leaving bed A during a different step



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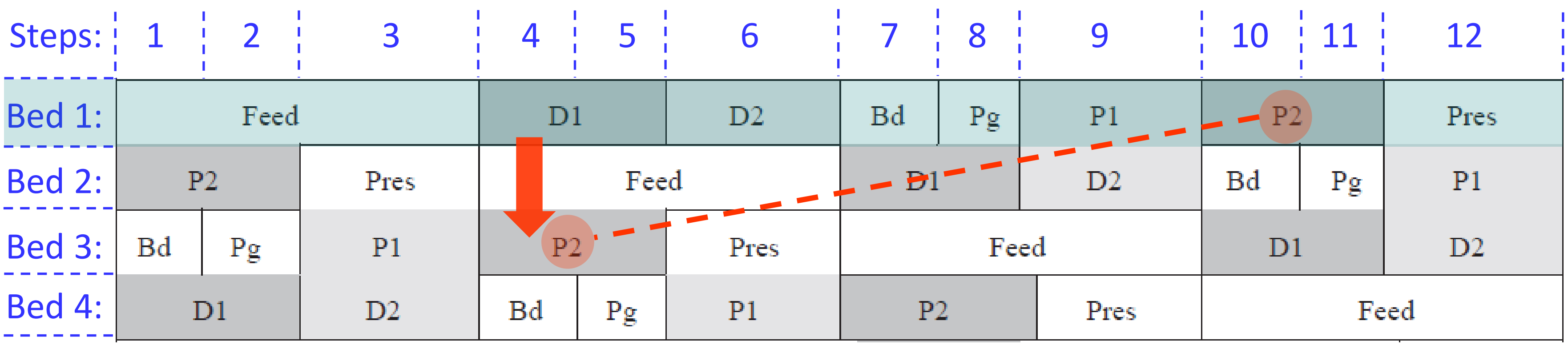
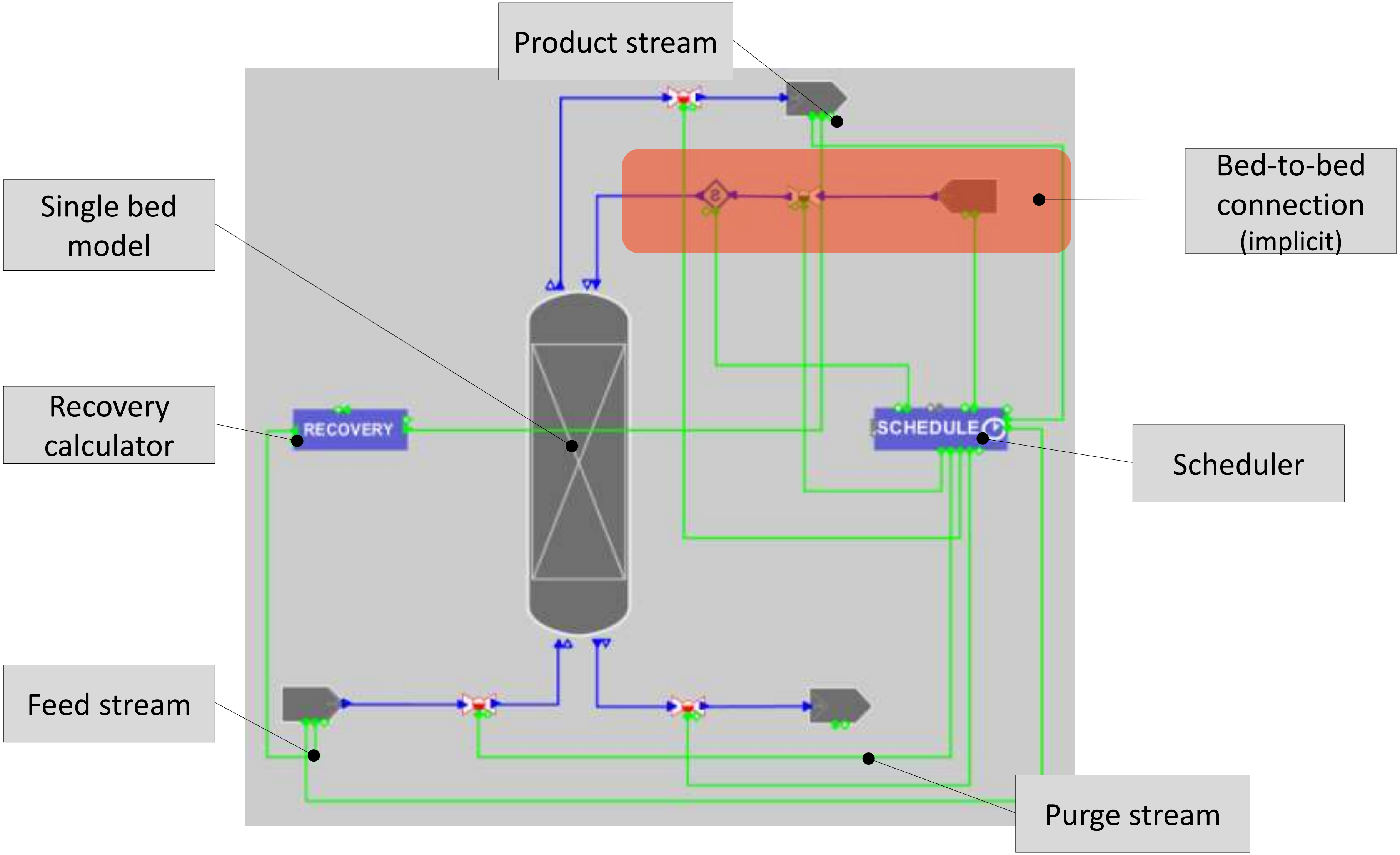


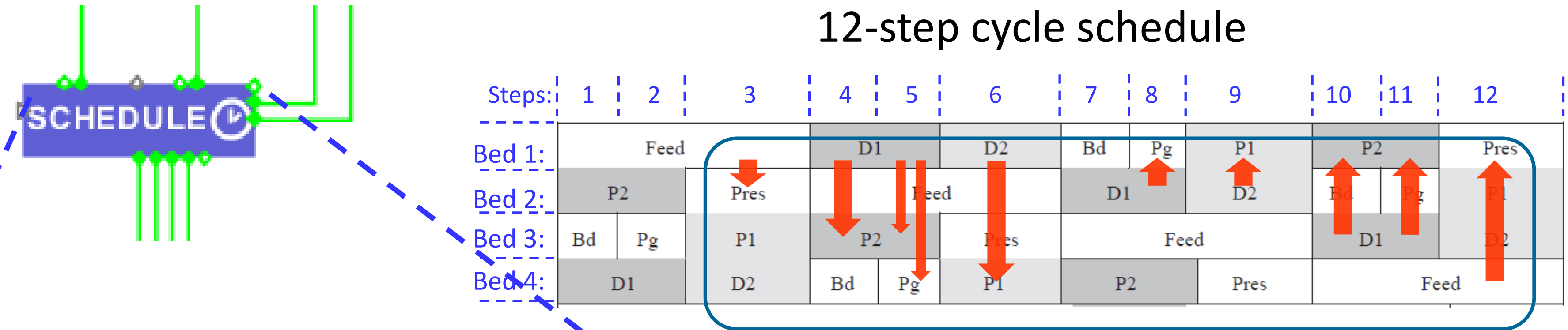
- …similarly for downstream pressure "seen" by any material *leaving* bed A…

Self-interacting Bed (SiB) for CSS computation

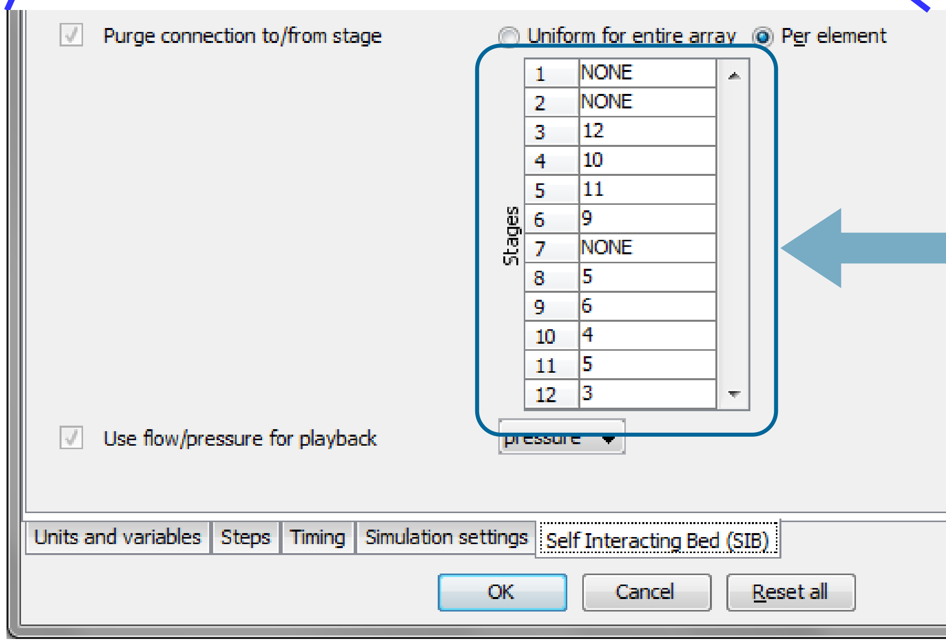


Self-interacting Bed (SiB) for CSS computation

12-step cycle schedule



PSA cycle logic



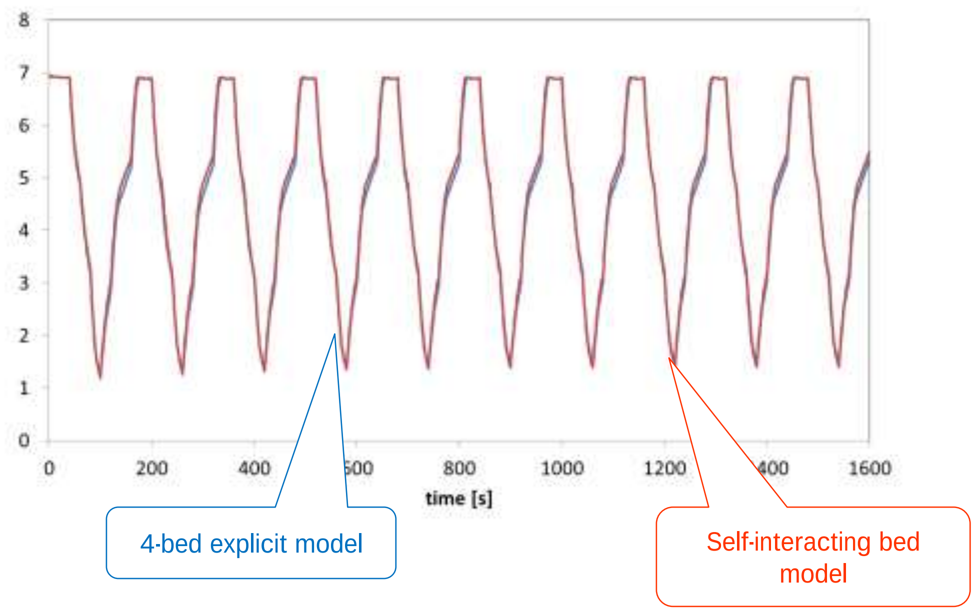
Simulation of 10 cycles ≈ 137s (CPU time)

Efficient mechanism for

- storing key variable trajectories during a cycle
- retrieving necessary variable values during the same or later cycles

Self-interacting bed – Results

Bed 1 pressure profile at product end



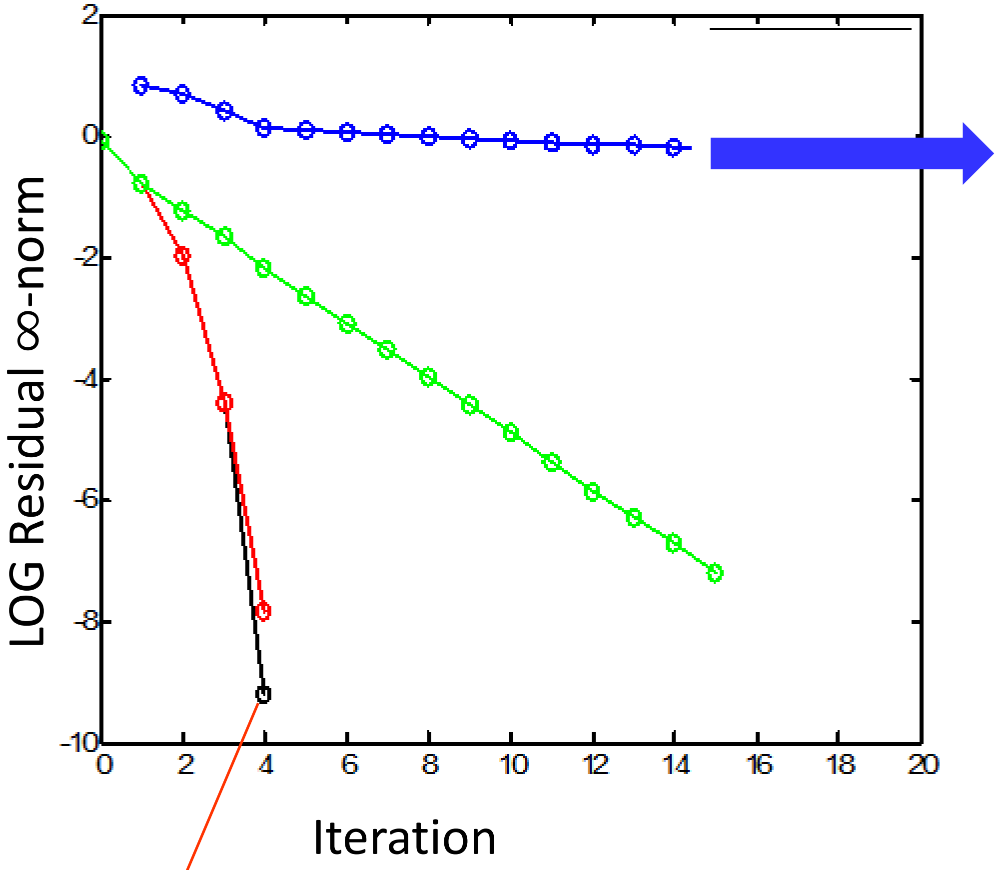
- Simulation of 10 cycles ≈ **137s** (CPU time) [~2 min]
  - much less than the original 1601s [~1/2 hour]

But can we do <u>significantly</u> better than this?

Novel methods for accelerated CSS computation

Ongoing R&D programme

Example #1: 1-bed, 2-step RPSA process

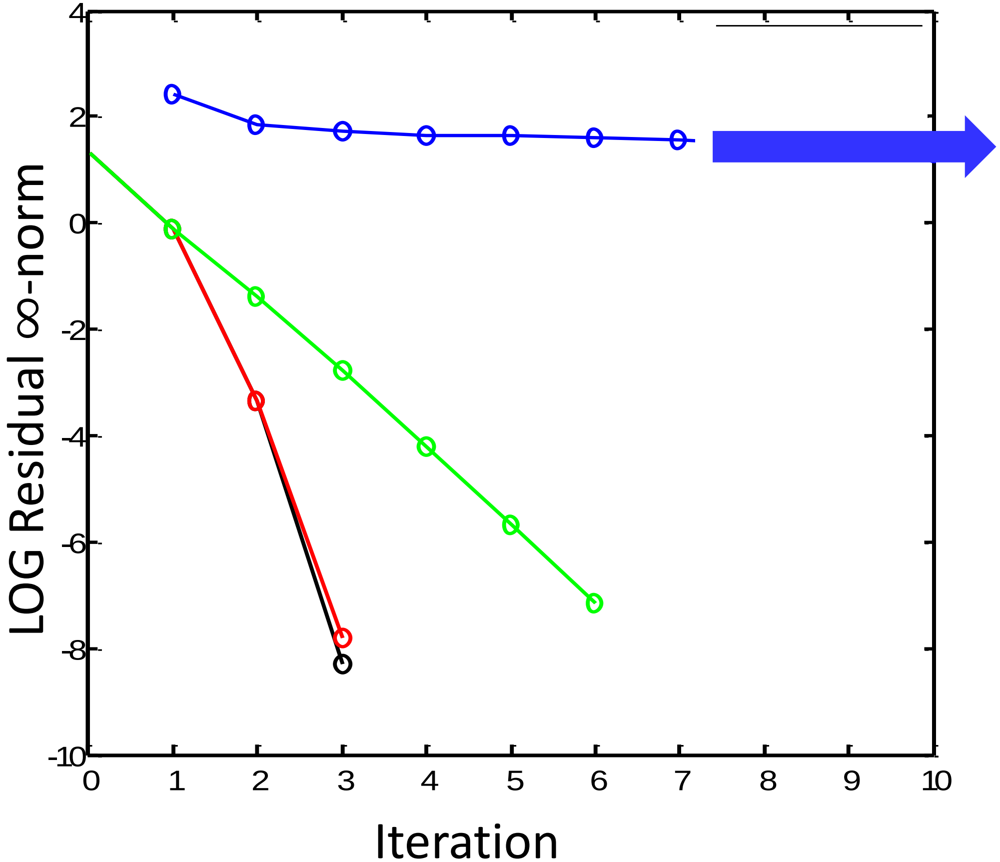


Very tight convergence

	Cycle Simulations	CPU time (sec)
Conventional approach	**> 4000**	**2383**
Method 1	**1456+10***	**867**
Method 2	**379+10***	**198**
Method 3	**98+10***	**57**
Method 4	**47+10***	**28**

*10 successive cycles used to provide a good initial guess

Example #2: 2-bed, 6-step Skarstrom cycle process

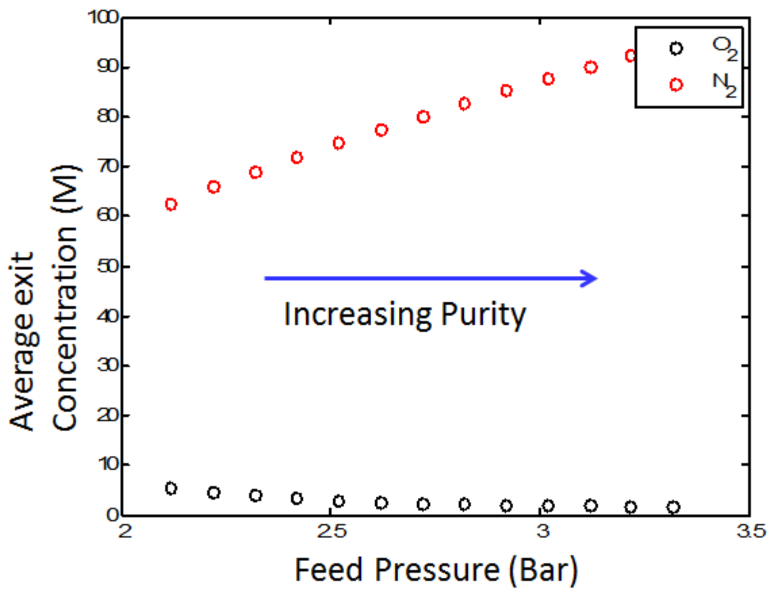


	Cycle Simulations	CPU time (sec)
Conventional approach	90	306
Method 1	1824+10*	6202
Method 2	614+10*	2088
Method 3	33+10*	110
Method 4	31+10*	106

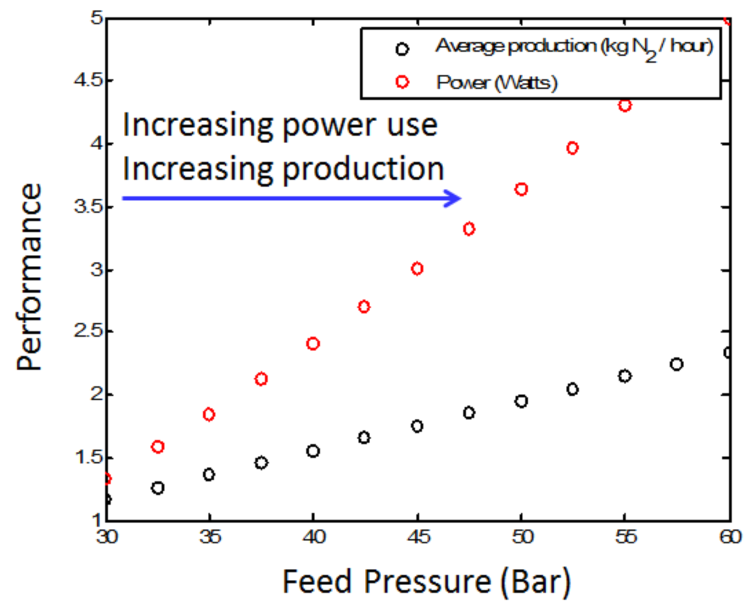
*10 successive cycles used to provide a good initial guess

Parametric sensitivity analysis for PSA processes

- Example: adjust feed pressure, analyze resulting changes in KPIs (average exit composition, power use, production rate)



1-bed, 2-step RPSA process



2-bed, 6-step Skarstrom cycle process

Repeated determination of CSS

13 parametric points for each example

Numerical solution performance

1-bed, 2-step RPSA process	Cycle simulations per parameter point (median across all 13 points)
Method 3	80
Method 4a	52
Method 4b	38
Method 4c	12

2-bed, 6-step Skarstrom cycle process	Cycle simulations per parameter point (median across all 13 points)
Method 3	29
Method 4a	28
Method 4b	19
Method 4c	10

- Technique generally applicable to all periodic processes
  - PSA, TSA, SMB, …
- **Work in progress!**

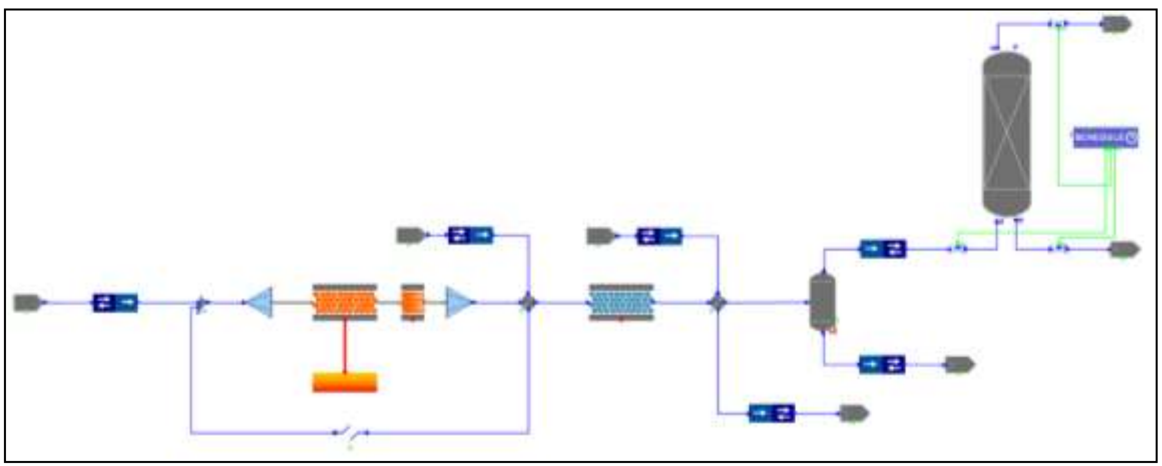
cf. 57 cycles for one-off simulation (>4000 cycles with conventional method)

cf. 41 cycles for one-off simulation (90 cycles with conventional method)

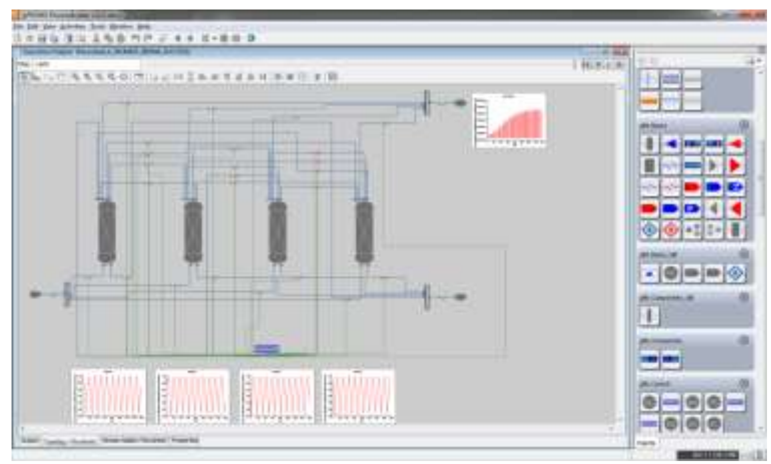
Conclusions

Conclusions – I

- Detailed modeling of
  - physics of adsorption bed
  - cycle schedules of periodic adsorption process
- gPROMS ProcessBuilder advantages
  - easy setup and initial solution
  - rapid solution of CSS
  - allows direct integration of adsorption units with other units



Catalytic reforming of methane + water gas shift + PSA-based hydrogen purification



Hybrid membrane/PSA process for hydrogen purification

Conclusions – II

- ProcessBuilder brings power of gPROMS® platform to adsorption processes
  - Custom modeling
    - customisation of adsorption isotherms,
      mass & heat transfer coefficient correlations, etc.
  - Parameter estimation
    - estimation of mass transfer characteristics from breakthrough experiments
  - Optimisation of bed design parameters, operating conditions, cycle schedule
    - dynamic optimization problem
    - efficient handling of cyclic steady state poses special problems
- Ongoing R&D aiming at significant breakthroughs in periodic process simulations

Thank you