



Setting the Standard for Automation™

Dynamic Modeling and Control of an Integrated Solid Sorbent Based CO₂ Capture Process

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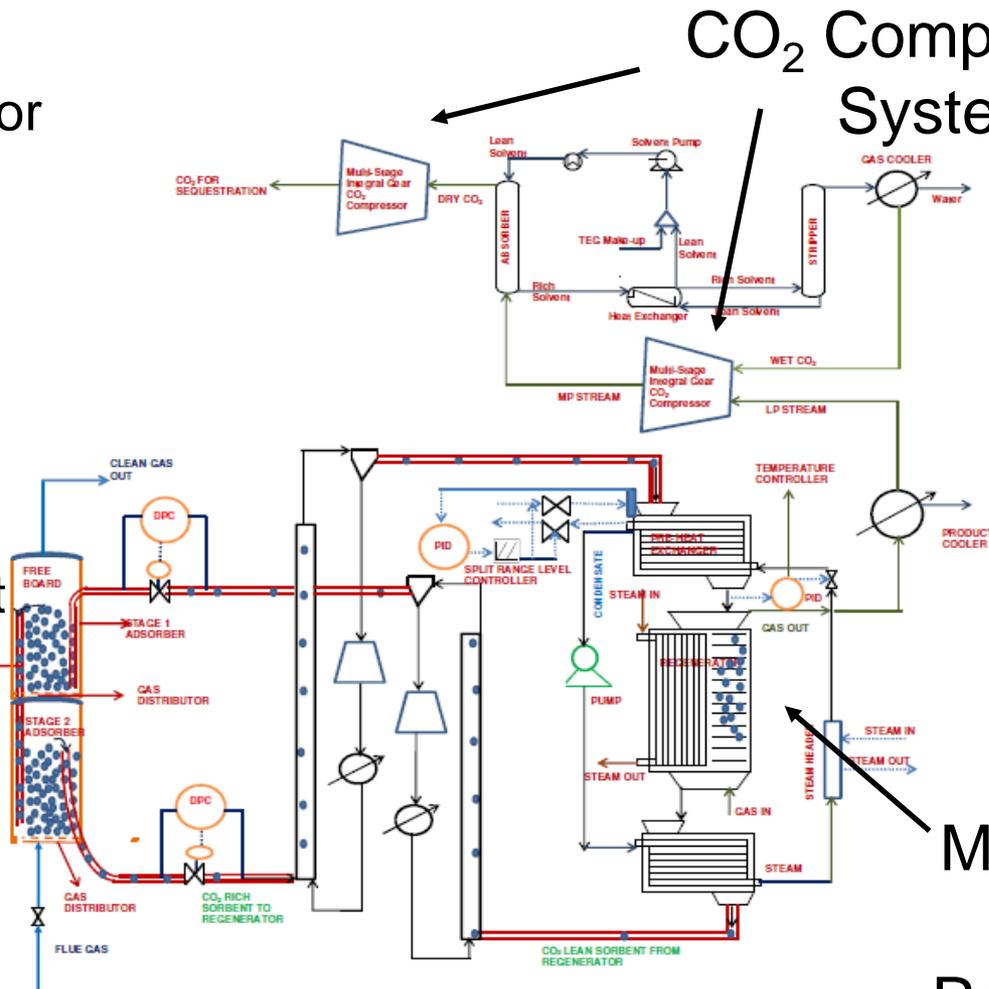
Short Biography of Benjamin Omell

- Post-Doctoral Fellow in the Department of Chemical Engineering at West Virginia University
- PhD from Illinois Institute of Technology, Chicago
- Research interest is in the area of steady-state and dynamic modeling and advanced process control of energy-generating and associated processes
- Member of AIChE
- Hobbies- Biking, hiking

CO₂ Capture & Compression Systems Coupled with the Steam Cycle

- Solid-sorbent systems are energetically superior to typical MEA-based solvent systems
- CCS system requires power and steam
- Dynamics are important during load-following

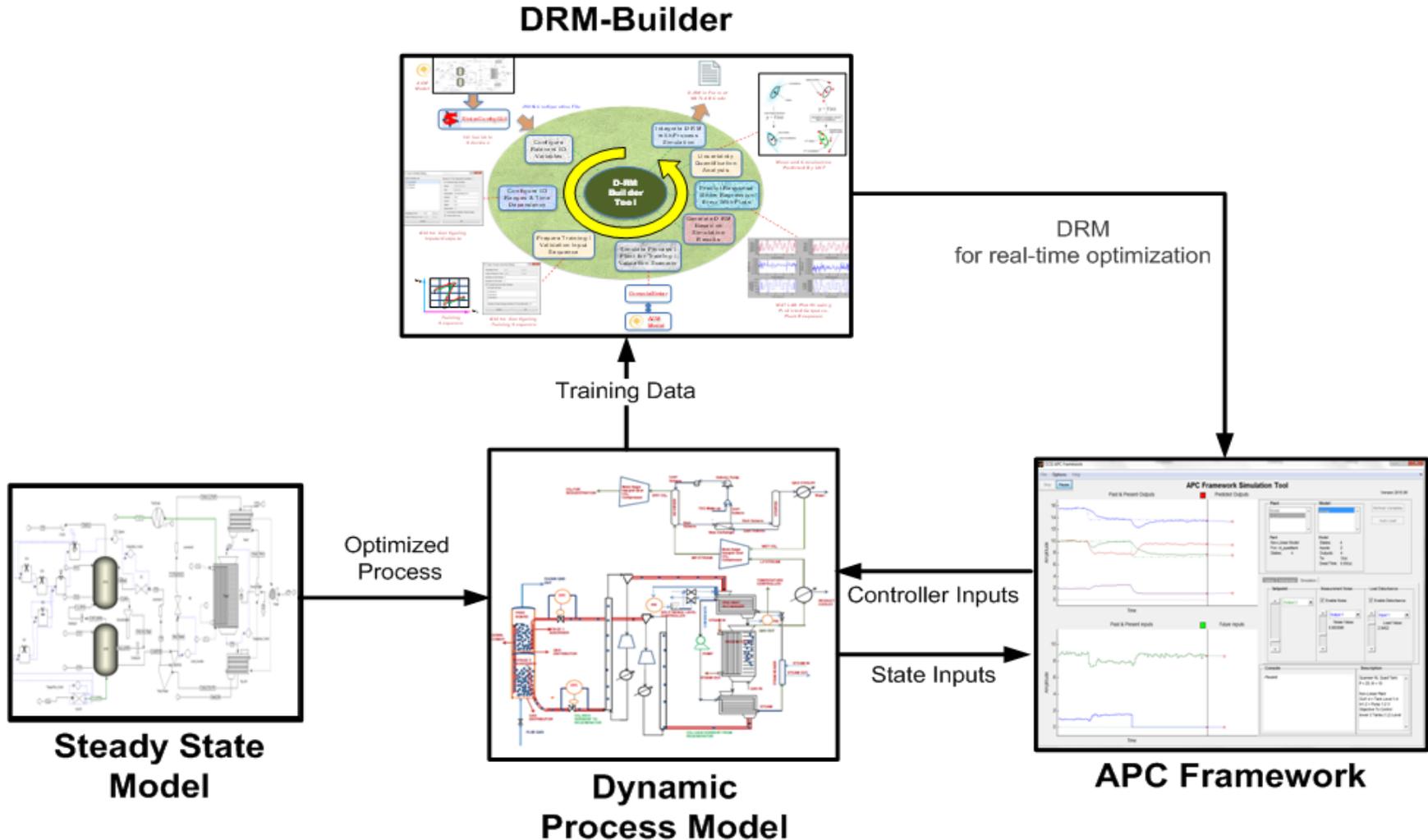
Bubbling Fluidized Bed (BFB) Adsorber



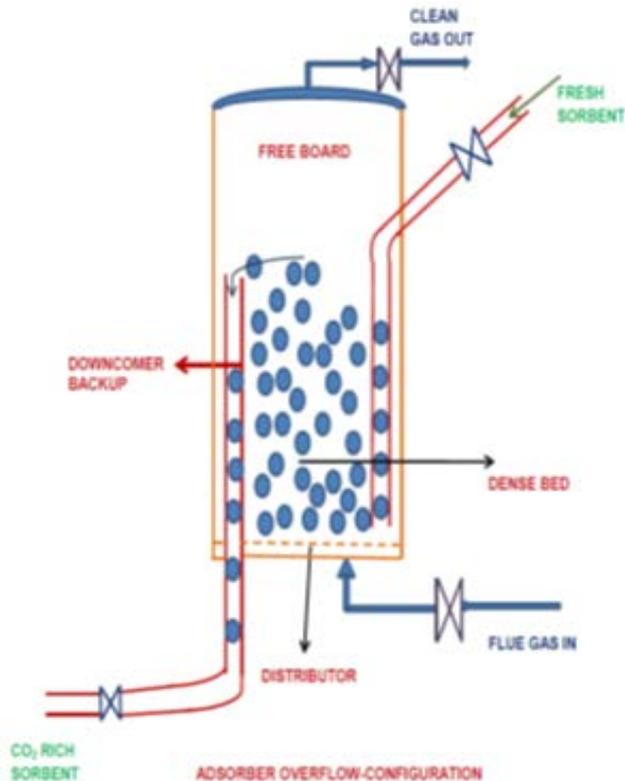
CO₂ Compression System

Moving Bed (MB) Regenerator

- Develop accurate and flexible steady-state and dynamic solid sorbent models for CO₂ capture
 - BFB and MB adsorber/regenerator
 - Solids heat exchangers
 - CO₂ compression
 - Balance of the plant
- Create toolset to simplify implementation of advance control strategies that can perform efficiently in the presence of unmodeled disturbances, noisy measurements, and unmeasured variables
- Use these models and tools for optimization, transient studies, and control system design as part of DOE's Carbon Capture Simulation Initiative (CCSI)



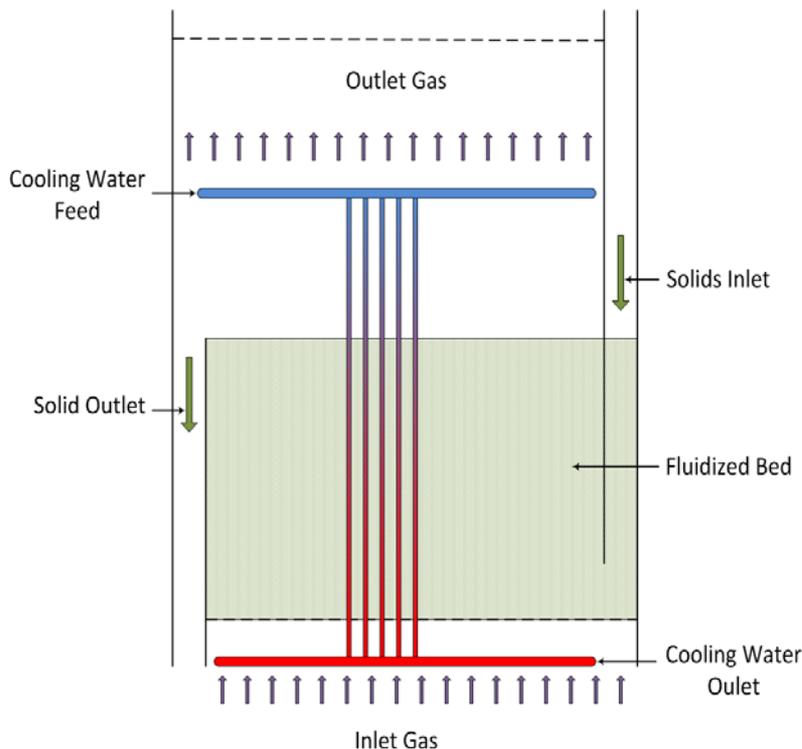
Challenge: Limitations in Previous Bubbling Fluidized Bed Models



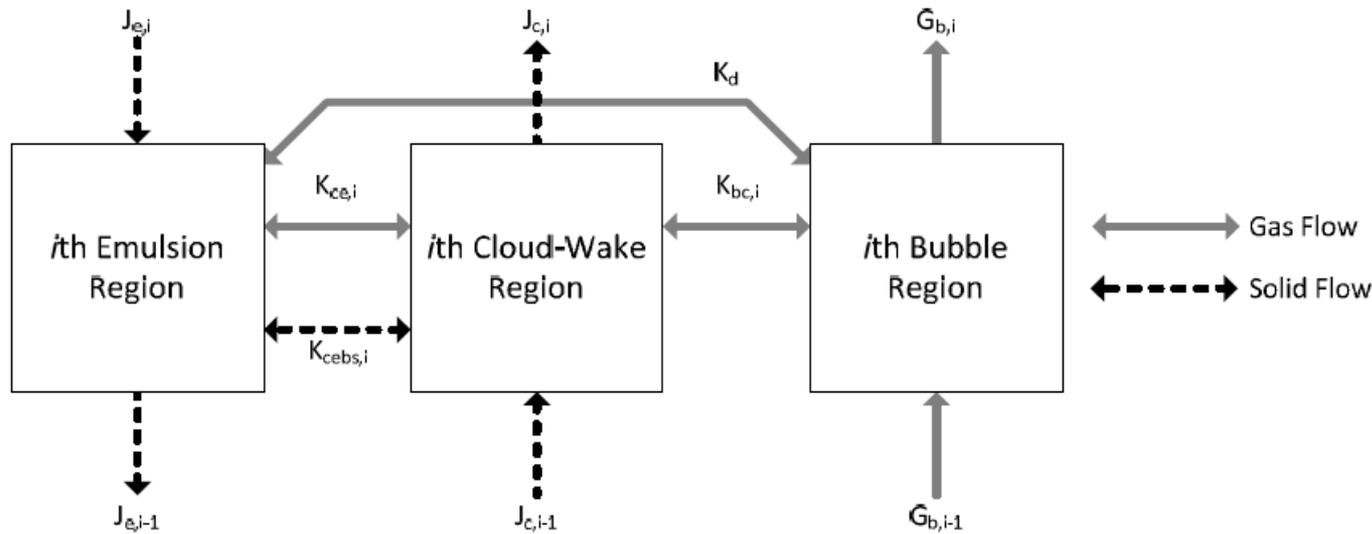
- Typical simplifications to facilitate analytic solutions
 - Isothermal
 - Simplistic reaction kinetics and transport
 - Steady-state
 - Embedded heater/cooler neglected
- Limited support in commercial tools
- Minimal application to CO₂ capture in literature

A Flexible BFB Model

1-D, two-phase, pressure-driven and non-isothermal models developed in both Aspen Custom Modeler (**ACM**) and **gPROMS**



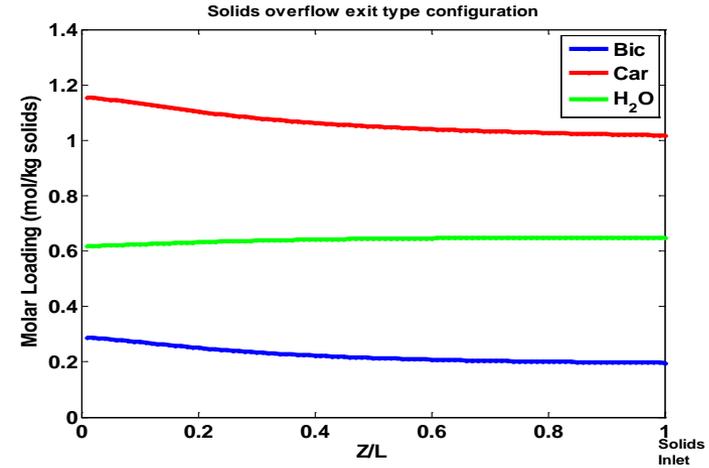
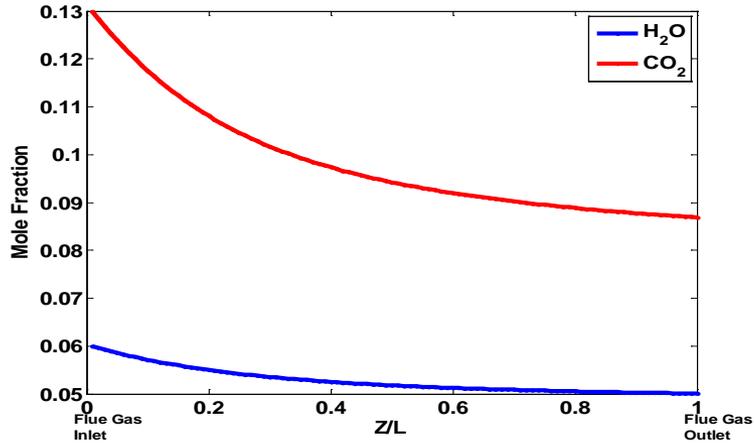
- Flexible configurations
 - Dynamic or steady-state
 - Adsorber or regenerator
 - Under/overflow
 - Integrated heat exchanger for heating or cooling
- Supports complex reaction kinetics
- Compatible with CCSI uncertainty quantification (UQ) tools



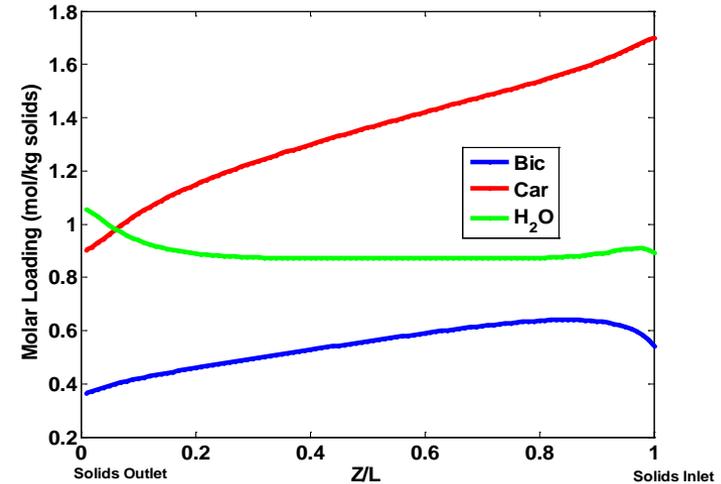
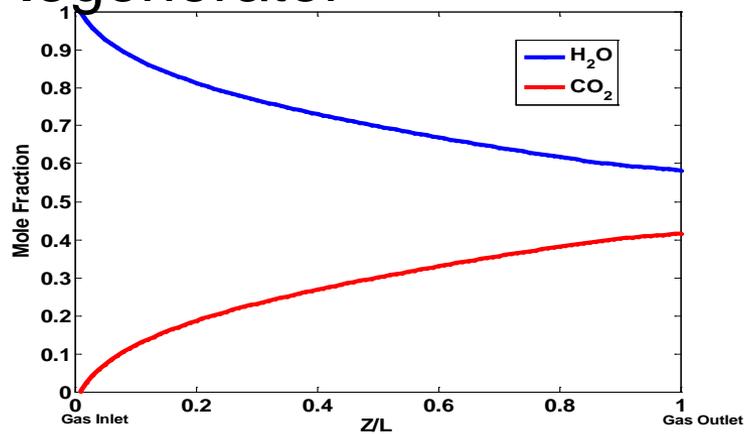
- Gaseous species : CO_2 , N_2 , H_2O
- Solid phase components: bicarbonate, carbamate, and physisorbed water.
- Transient species conservation and energy balance equations for both gas and solid phases in all three regions.

Single-Stage BFB Model: Steady-State Results

Adsorber



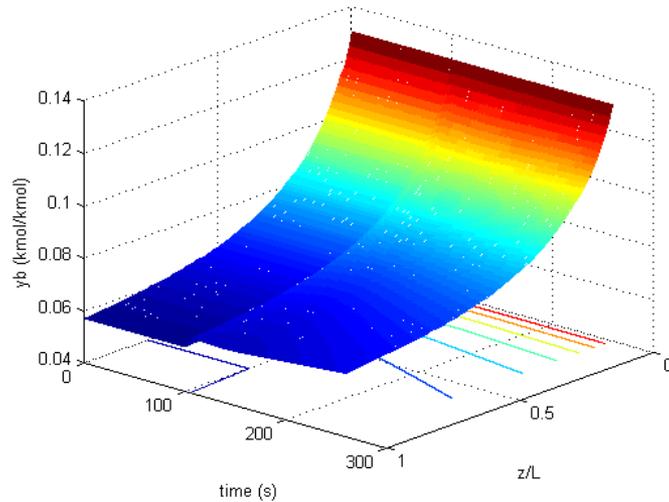
Regenerator



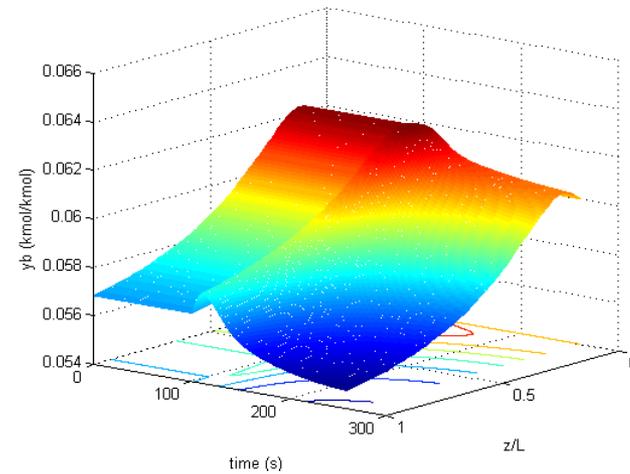
Dynamic Results – Increase Inlet Gas Flow by 20.6%



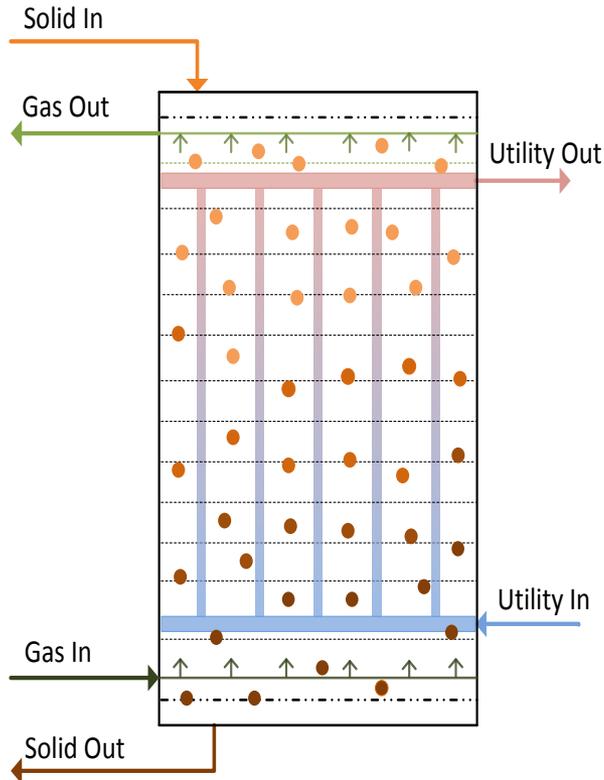
Gas CO₂ Concentration



Gas H₂O Concentration



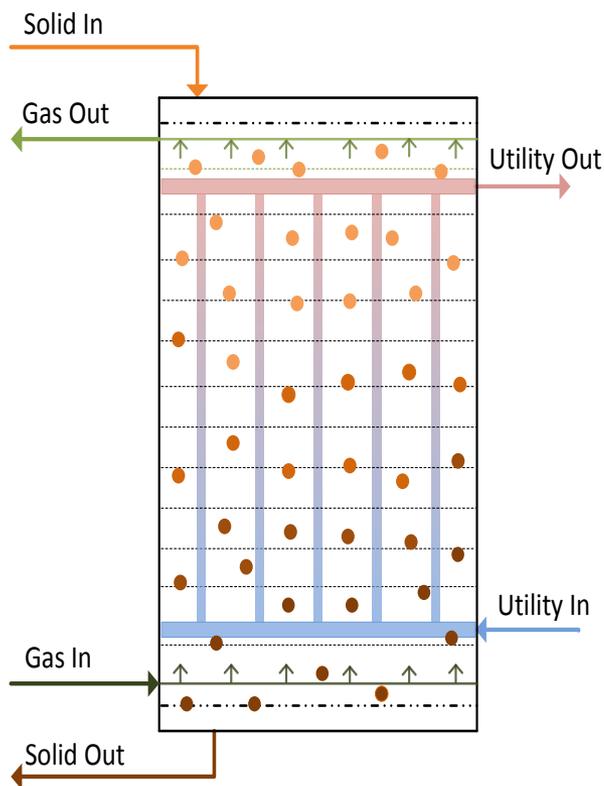
Challenge: Limitations of Existing Moving Bed Models



- Very few references in literature, little application to CO₂ capture
- Previous applications in literature include
 - MB furnaces for iron pellet reduction
 - Dryers
 - Non-catalytic gas-solid reactions
- Lack of mathematical model with large amount of heat transfer for solid sorbent regeneration
- Embedded heater/cooler not modeled
- Mainly steady-state model
- Hardly any model available in the commercial software

CCSI's Moving Bed Models

A1-D, two-phase, pressure-driven and non-isothermal regenerator model developed in both ACM and gPROMS

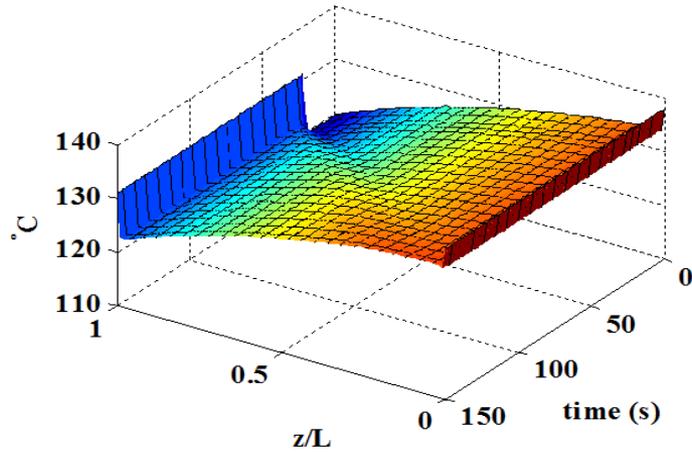


- Flexible dynamic and steady-state models
 - Integrated heat exchanger that can be used interchangeably for heating or cooling
 - Flexible enough for adsorber application

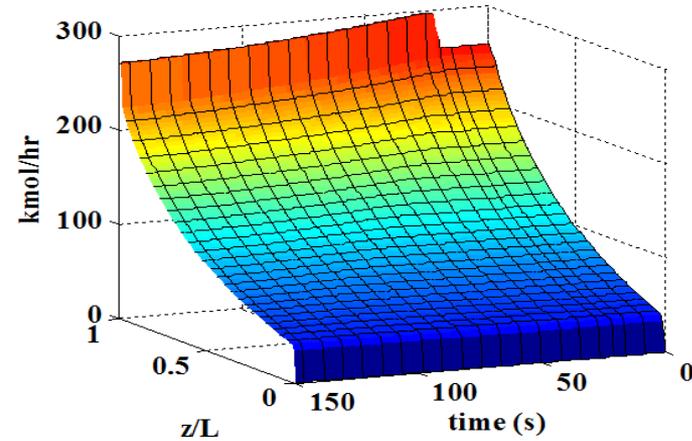
Step Test: Sorbent Temperature



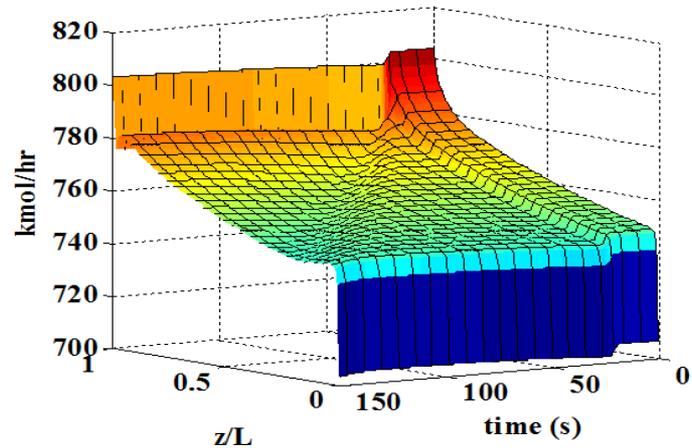
Solid Temperature Profile (gPROMS)



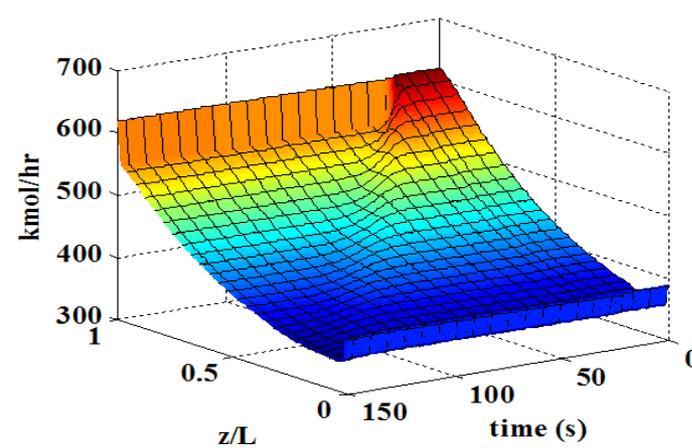
Gas CO₂ Flow (gPROMS)



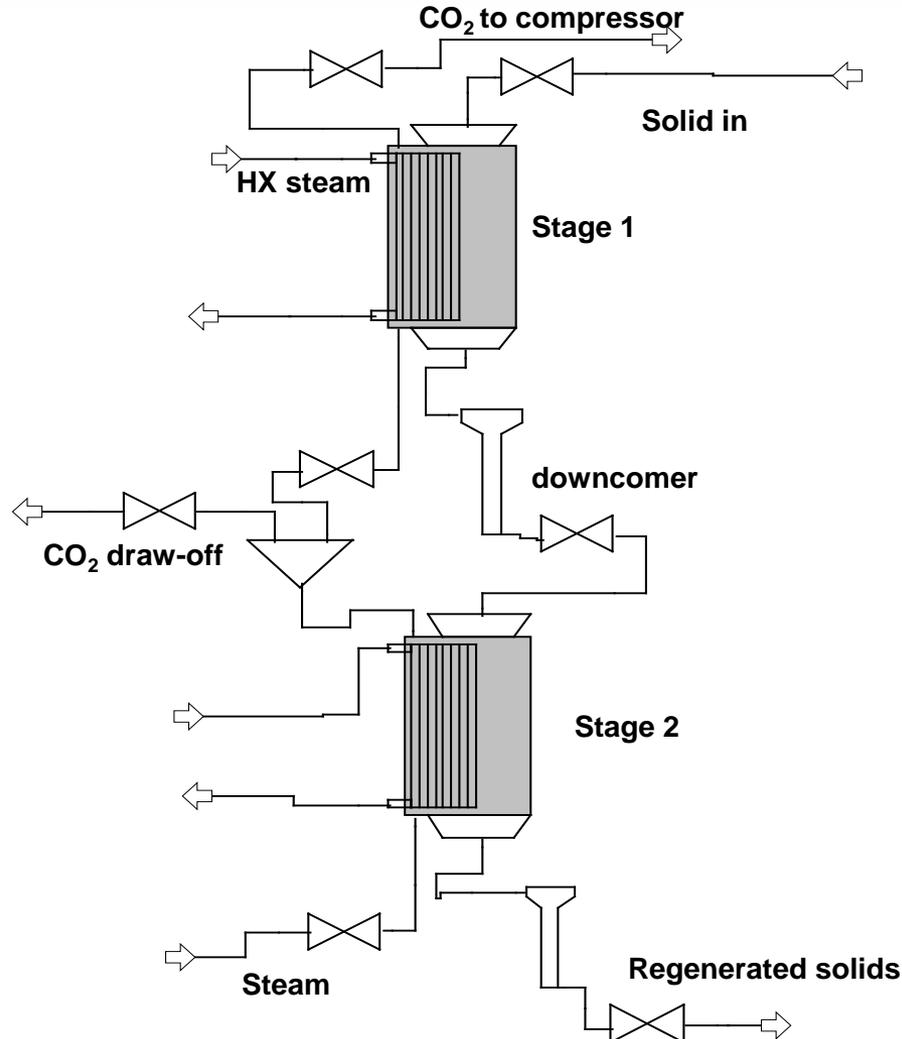
Solid Carbamate Flow (gPROMS)



Physisorbed H₂O Flow (gPROMS)



Multi-Stage Moving Bed Design to Overcome Fluidization Concerns



Concern

Twenty-seven 9 m diameter MB regenerators in parallel required to maintain flow in moving bed regime*

Solution: *Multi-Stage Moving Bed Regenerator*

- Some CO₂ (gas) removed between stages
- Reduced gas flowrate at the top of the MB
- Requires an advanced control strategy

* *Assumptions for preliminary analysis:*
12% CO₂ flue gas @ 2000 mol/s with
90% capture rate

Challenge: Limitations of Existing Compression Systems Models

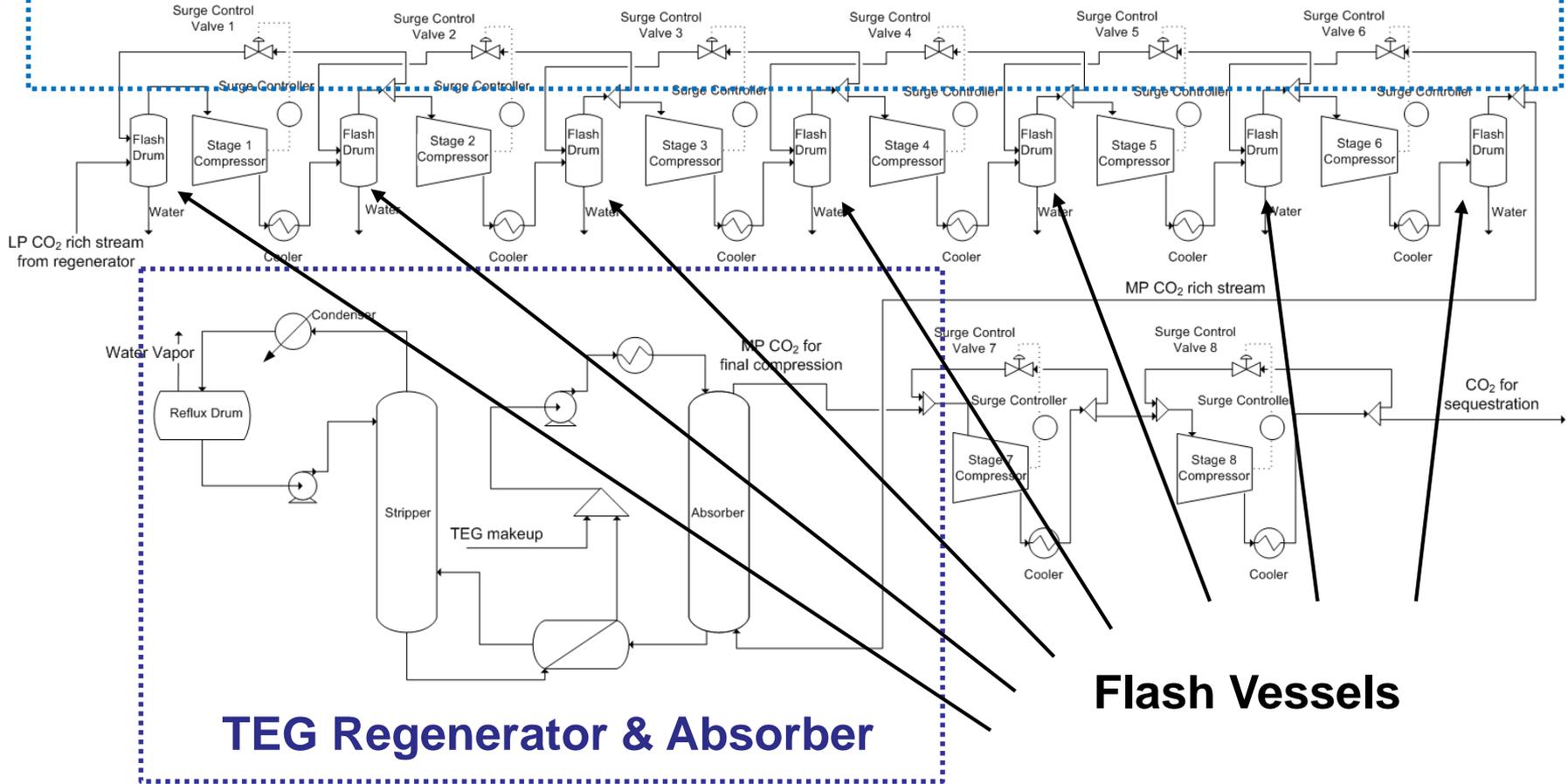
- Has been mostly developed for non-CO₂ systems
- For CO₂ systems, developed mainly for sCO₂ cycles
 - Pressure ratio of 1 to 2.6 (about 150 for CCS)
 - Fixed inventory (variable for CCS)
 - Composition change, especially water content, is not a major concern for sCO₂ cycles
- Typically steady-state
 - Dynamics are essential for load-following in power systems
- Lack of performance curves for CO₂ systems
- Surge detection and control algorithms hardly studied for these systems

CCSI CO₂ Compression System Model



Dynamic model of multi-stage integral-gear compression system

Surge Control Valves



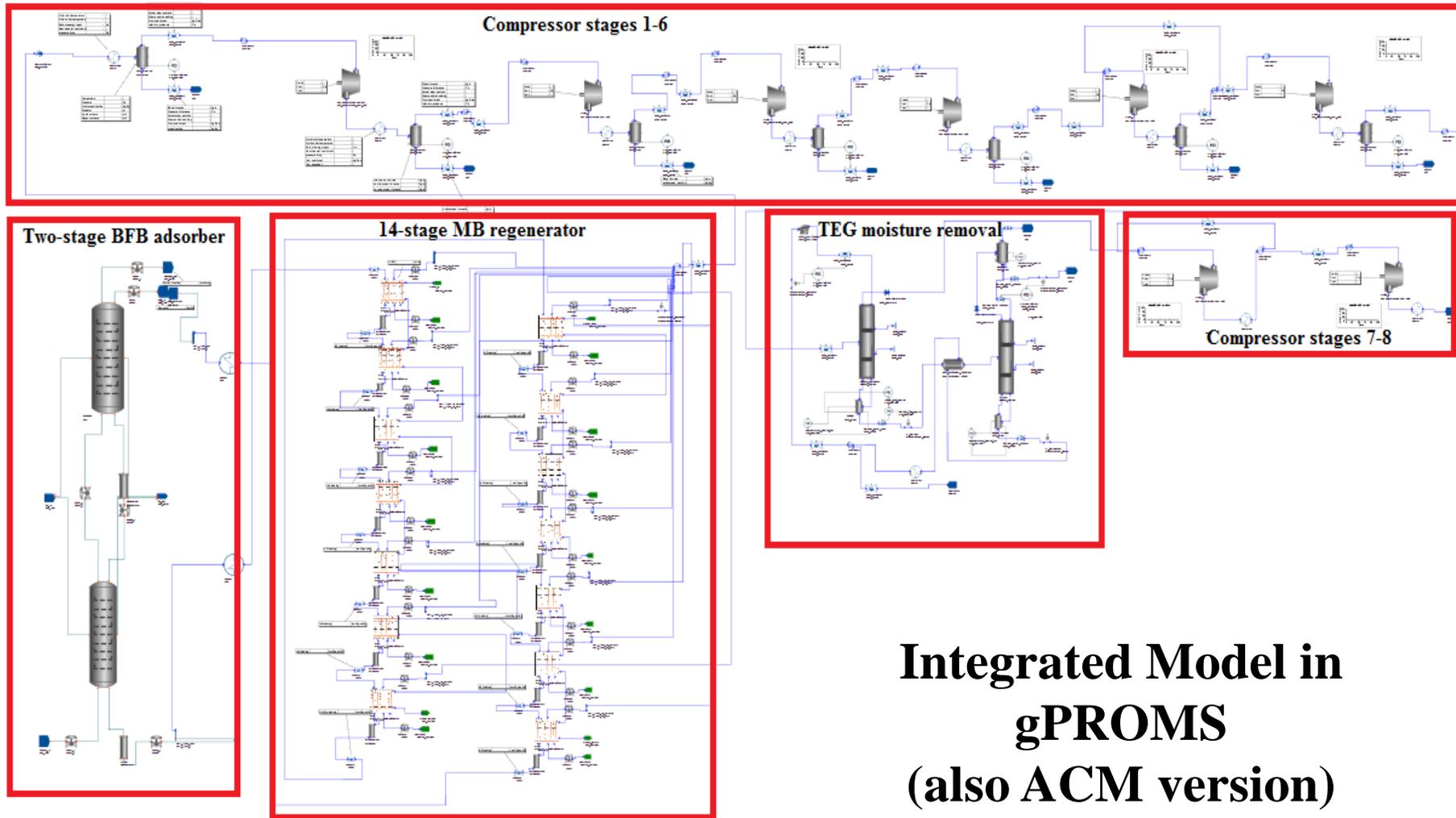
TEG Regenerator & Absorber

Flash Vessels

Surge detection and control algorithm also developed

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Integrated Model Enables Investigation of Entire Process Dynamics



**Integrated Model in
gPROMS
(also ACM version)**

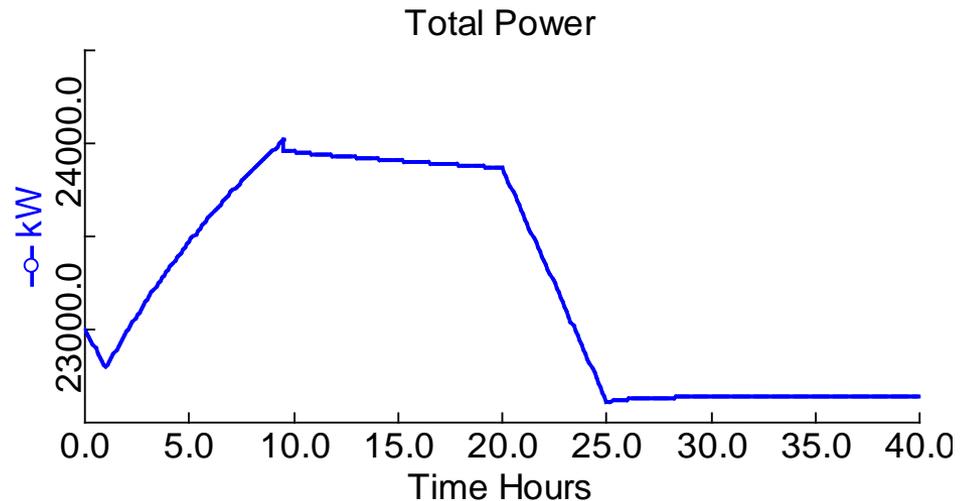
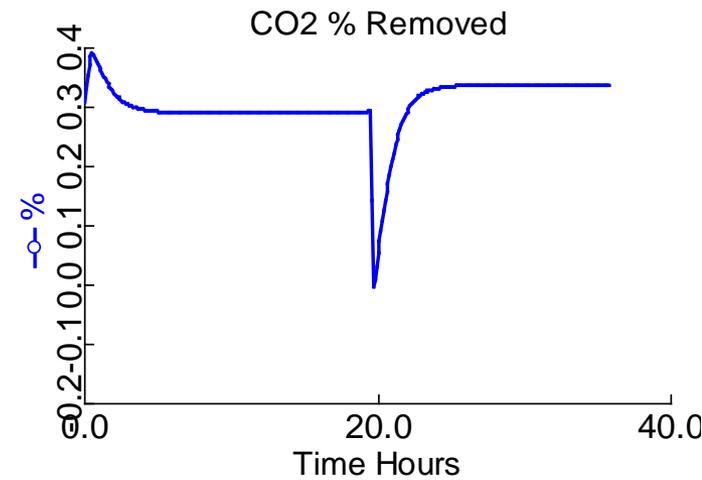
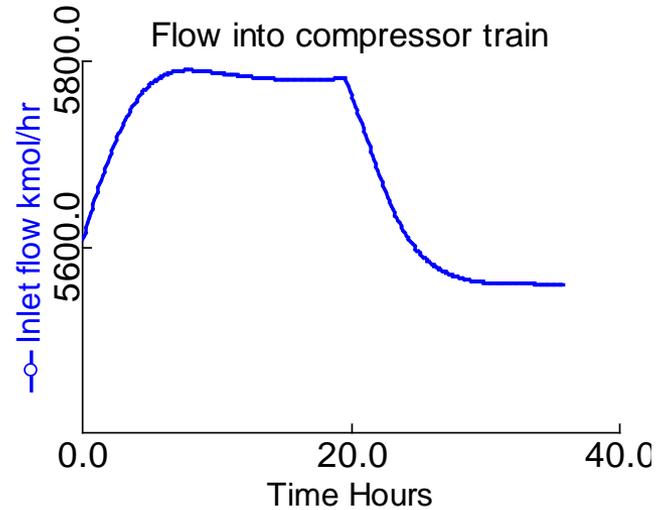
Ramp In Flue Gas



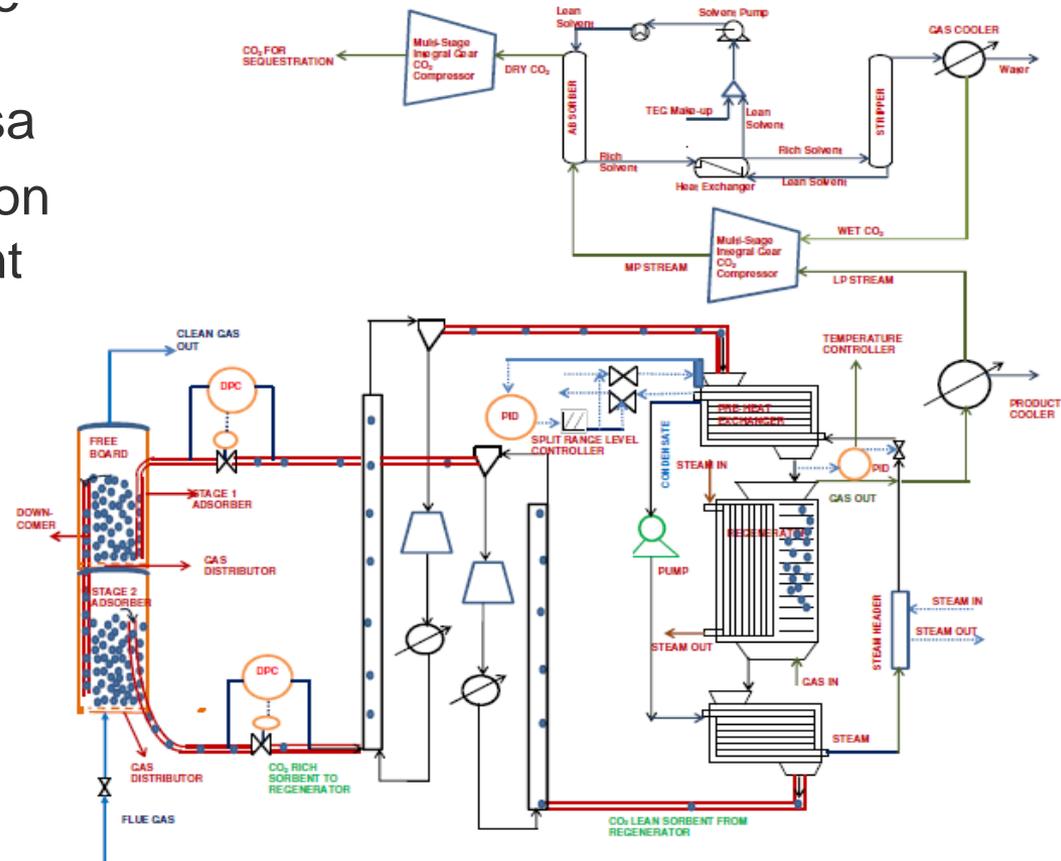
Ramp in flue gas

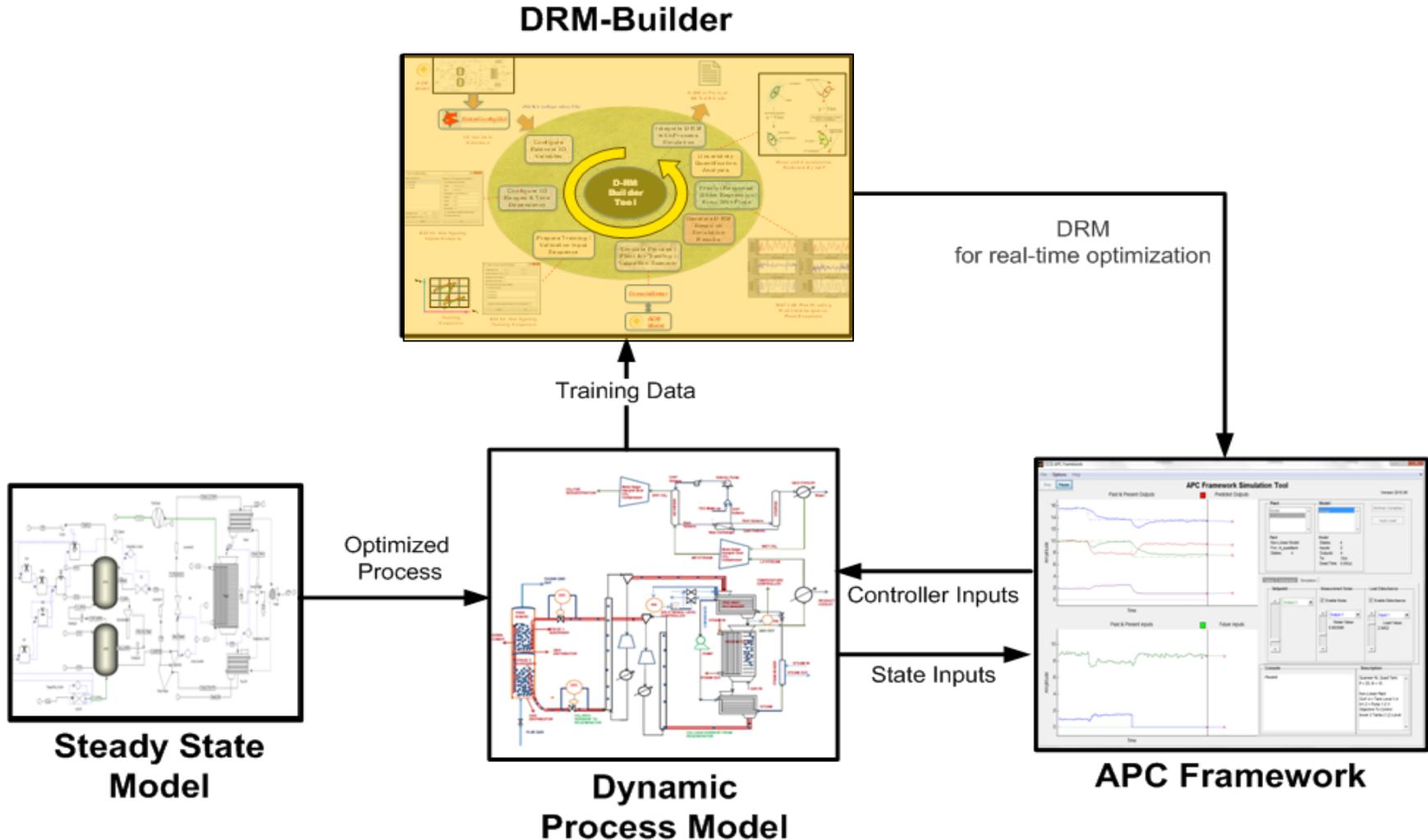
Time=0 : 15.8% increase

Time=20: 28.8% decrease



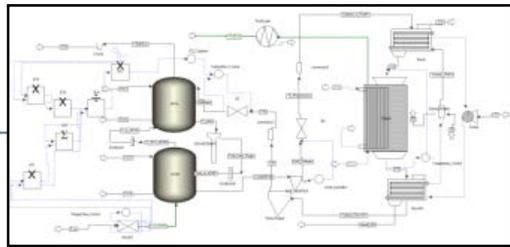
- Transient effect of the capture and compression process on the power plant and vice versa
- Can result in temporal variation in CO₂ capture target-different time constants depending on the type of the bed
- CCSI tools DRM-builder and APC toolset can improve system dynamics





- High-fidelity dynamic models (e.g. ACM dynamic models) are computationally expensive
 - Need to solve many Differential Algebraic Equations (DAEs)
 - May require small time steps due to stiffness of DAEs
 - Not fast enough to catch up with real time
- Dynamic reduced models (D-RMs)
 - Speed up the dynamic simulations
 - Capture dynamic systems with reasonable accuracy
 - Can be used for Advanced Process Control (APC) and Real Time Optimization (RTO)

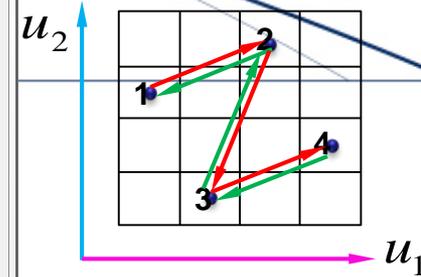
D-RM Builder Workflow



I/O Variable Selection

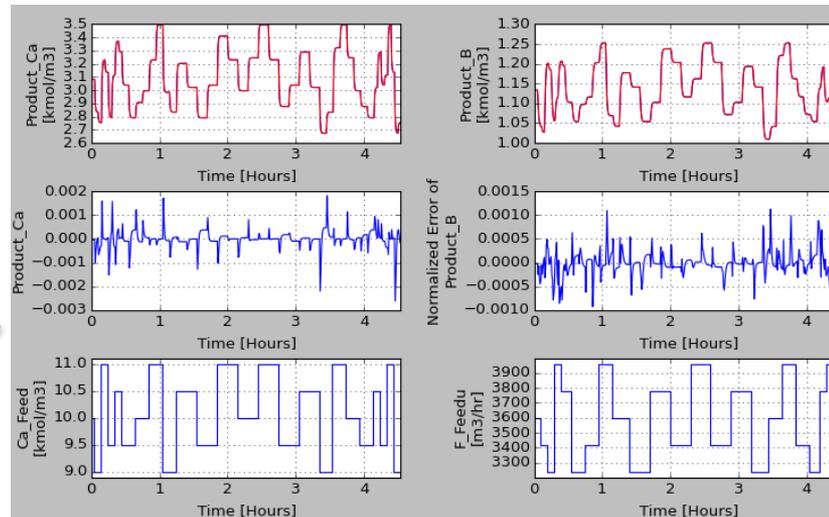
GUI for Configuring Inputs/Outputs

GUI for Configuring Training Sequence



Run Training Sequence

Generate D-RM Based on Simulation Results



Analyze Reduced Model using UQ Tools, Validation Sets, Plots



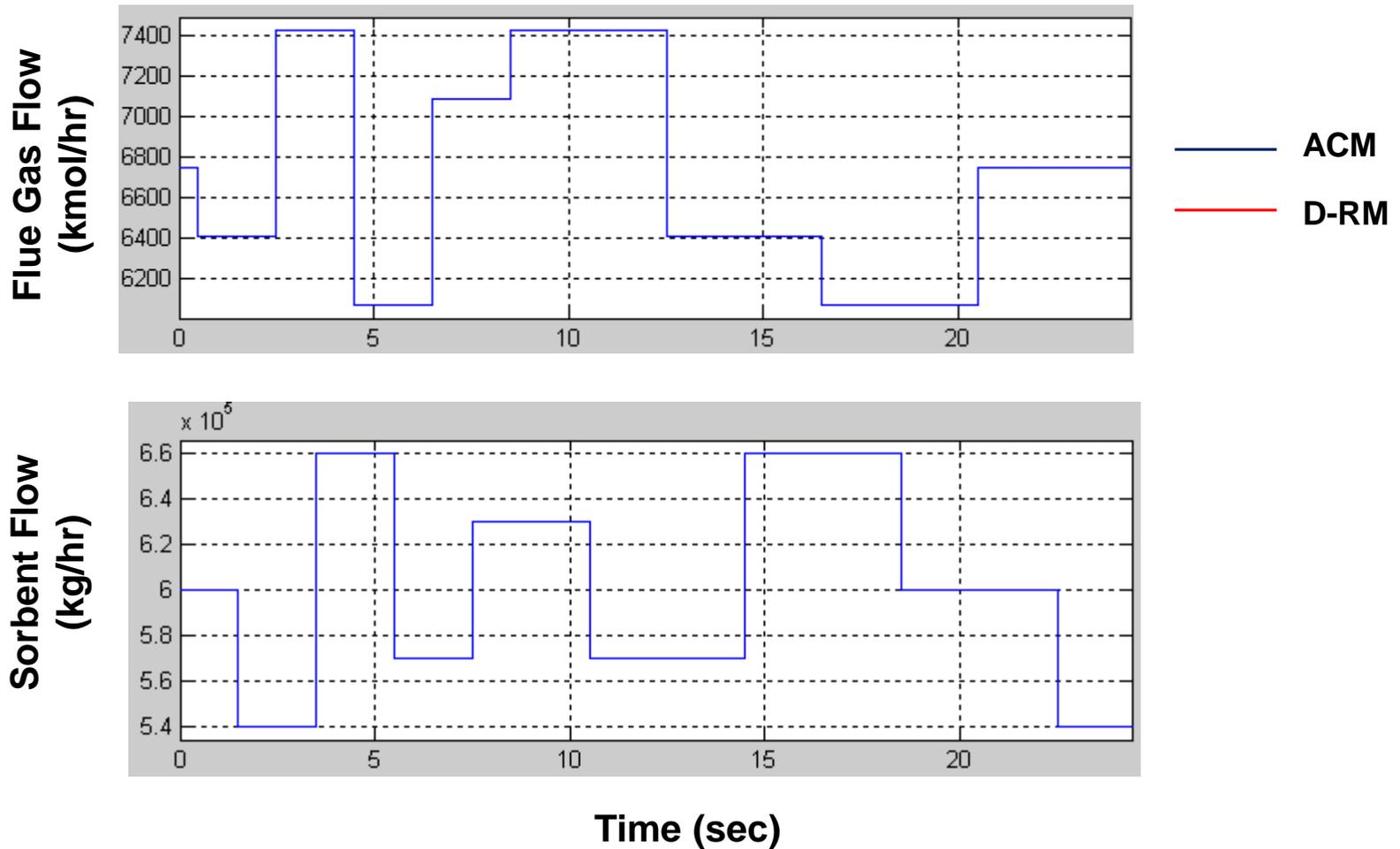
D-RM in Form of MATLAB Code

D-RM for the BFB Adsorber

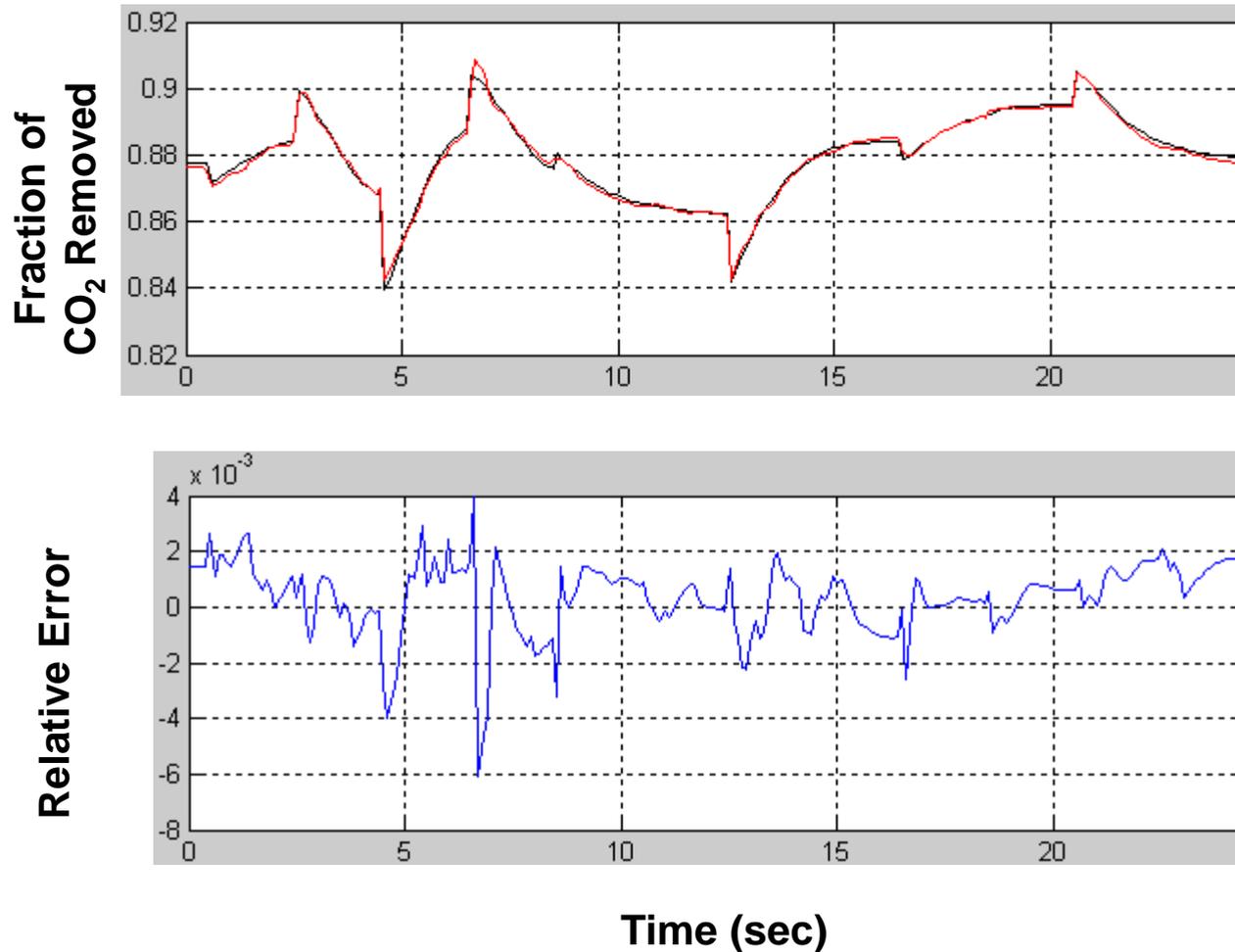
- D-RM generated based on open-loop ACM model
- Inputs:
 - Flue gas flow rate: 6,075 to 7,425 kmol/hr
 - Sorbent flow rate: 540,000 to 660,000 kg/hr
- Output:
 - CO₂ removal (Fraction of CO₂ in flue gas removed)
- DABNet* model with pole values optimized
- CPU time required for ACM simulations
 - Approximately 50 minutes for 2500 sampling steps (Sampling time interval at 0.1 second)

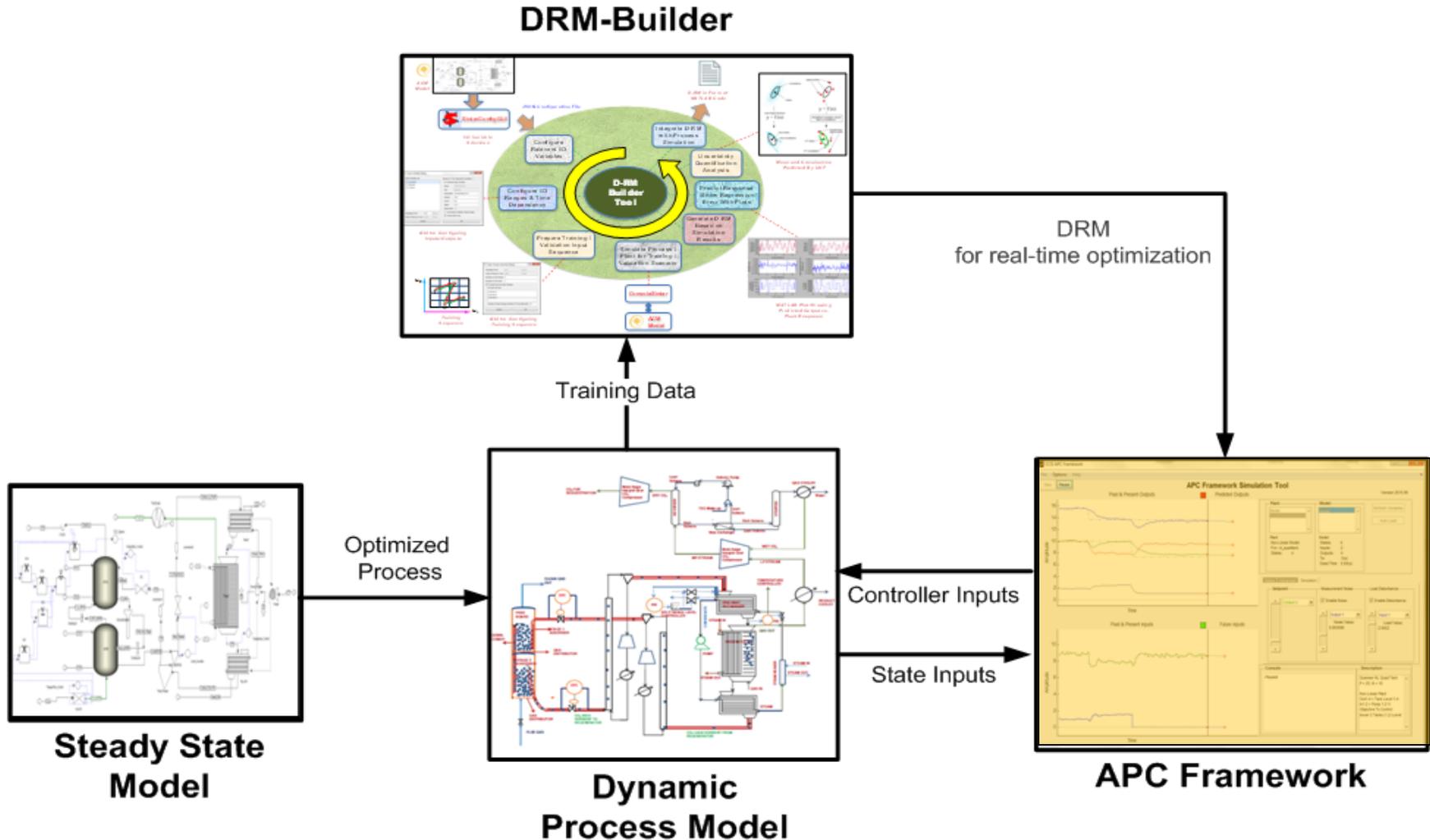
*Sentoni, G.B., L.T. Biegler, J.B. Guiver and H. Zhao, "State-Space Nonlinear Process Modeling: Identification and Universality," AIChE Journal, 44(10), 2229-2239, 1998.

Validation Input Data



Validation Output Data

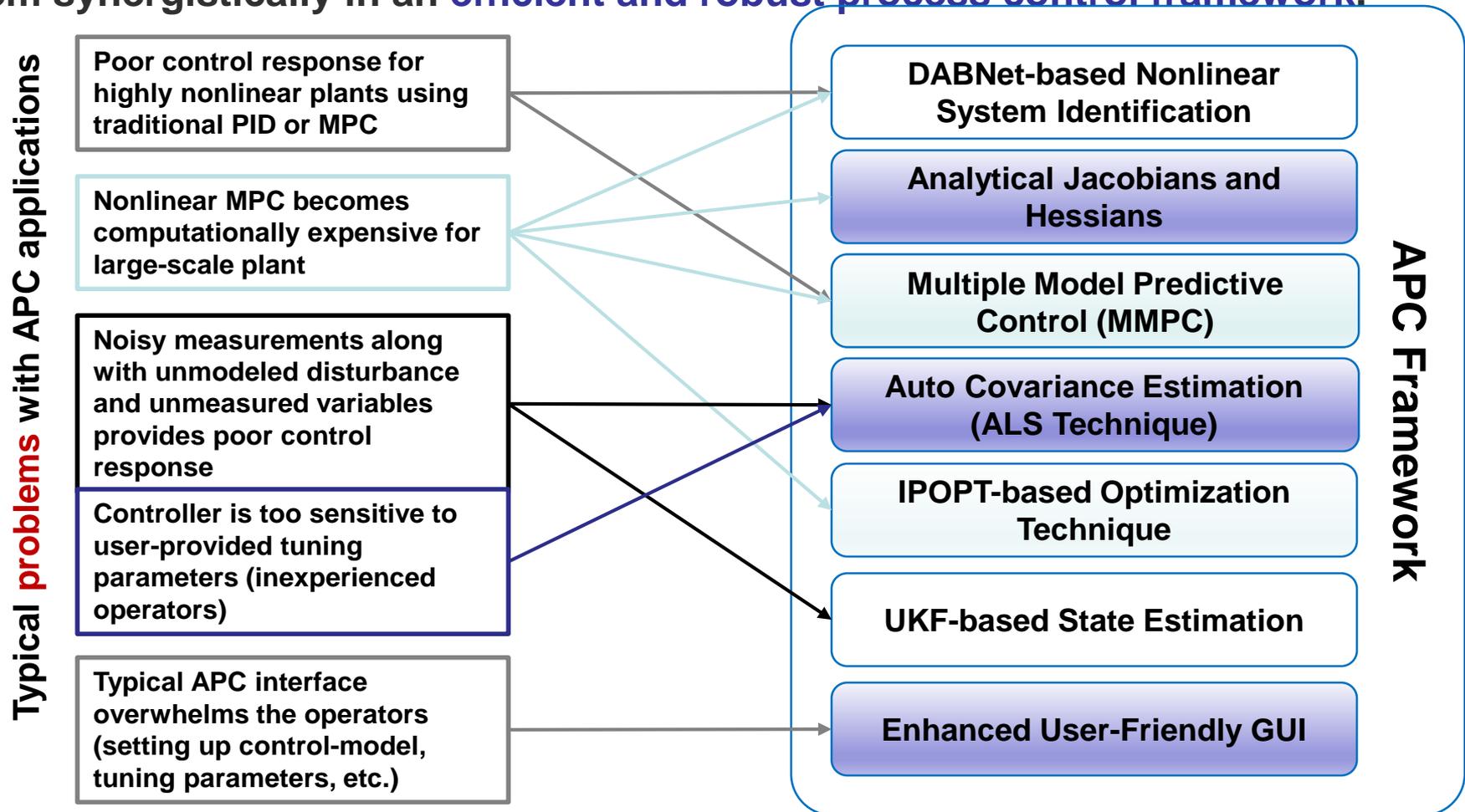




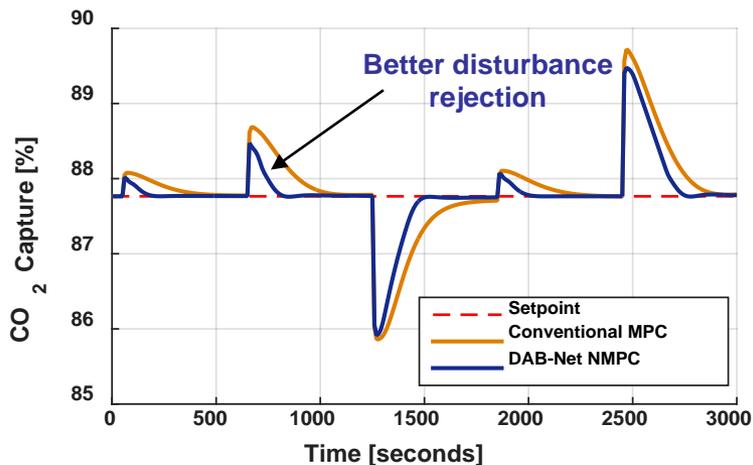
APC Framework's Capabilities



Utilize **proven techniques** from control relevant studies in literature and combine them synergistically in an **efficient and robust process control framework**.



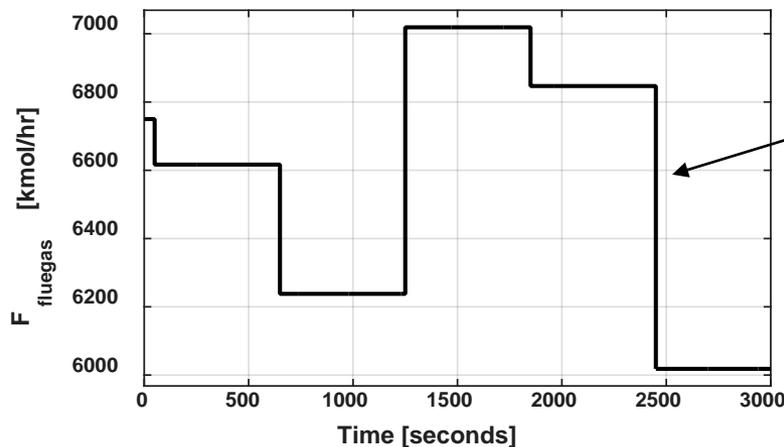
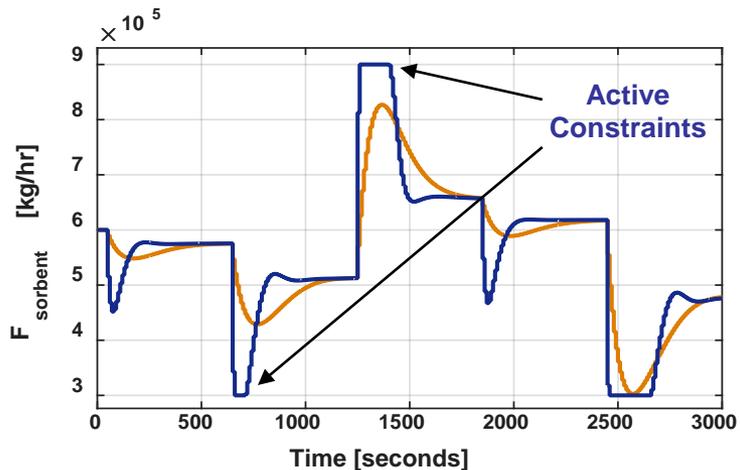
Performance Comparison on 2-Stage BFB Adsorber (ACM)



Controller responses to drastic plant-load changes – Comparison with standard MPC controller

Algorithm	Cumulative Residual	Computational Cost		
		Cumulative Control Calculation Time (sec)	Max Control Calculation Time (sec)	Total Simulation Time (min)
Conventional MPC	0.019	9.54	0.33	18.39
DAB-Net NMPC	0.007	19.97	3.43	18.92

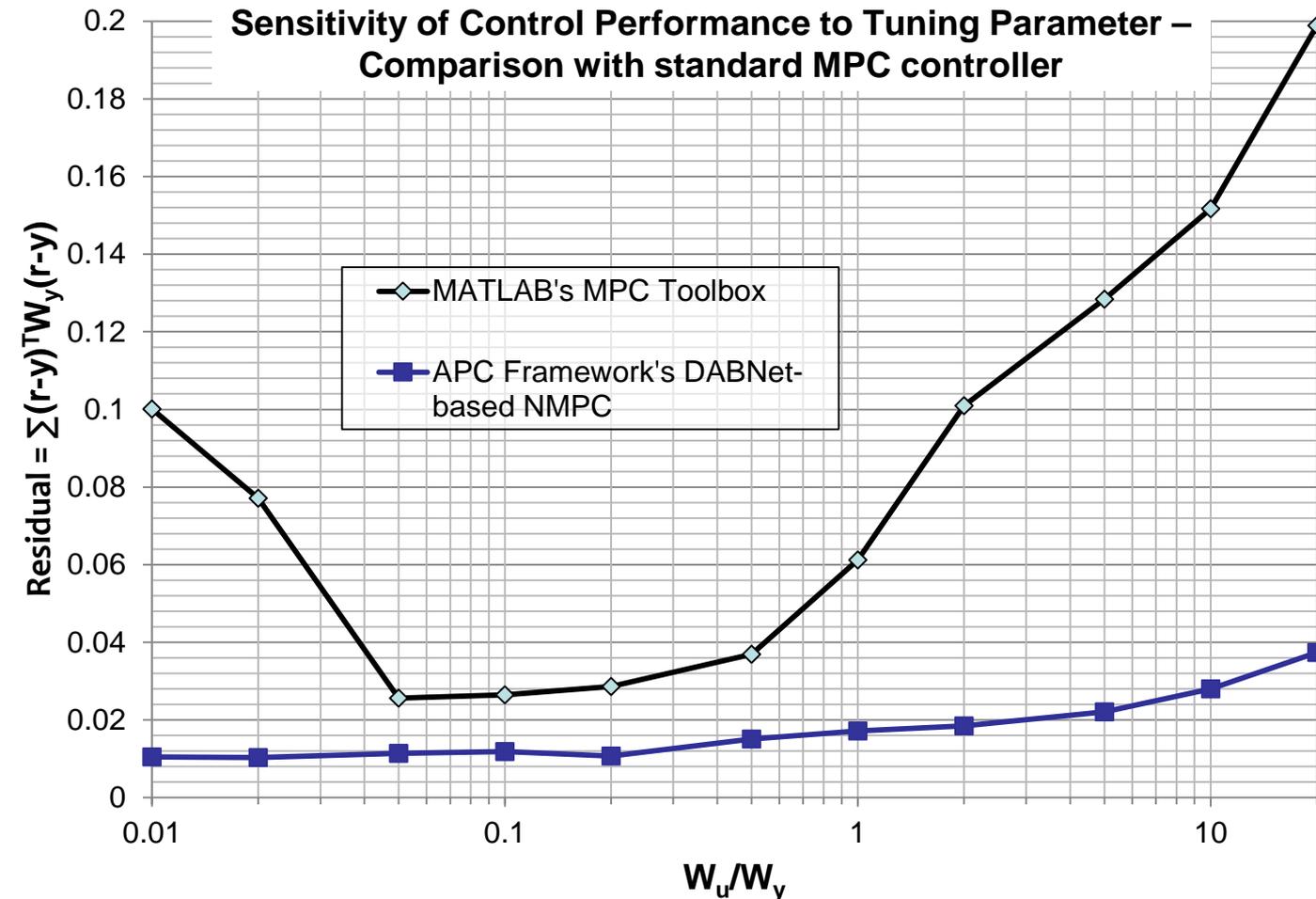
Note: Max. Control Calculation Time \ll Sample Time ($T_s = 20$ sec), Real-Time Operation with APC



Large changes in flue-gas flowrate (input-disturbance)

Controller Parameters
 Prediction Horizon = 50
 Control Horizon = 10
 Wu/Wy = 0.2

Performance Comparison on 2-Stage BFB Adsorber (ACM)



Benefits of APC Framework

1. Low residuals – tracks setpoint better over time
2. Low sensitivity for user-provided tuning parameters (W_u/W_y in this case)

- Developed high-fidelity steady-state and dynamic solid sorbent models for CO₂ capture
- Utilization of DRM-builder tool to generate reduced ordered models
 - Use reduced order model to generate control strategy with APC framework to handle moving boundary problem of multi-stage moving bed regenerator
- APC performance is relatively insensitive to tuning parameters and results in efficient disturbance rejection and load-following characteristics

Acknowledgement

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Thank You

Optimized Process Developed using CCSI Toolset

