Setting the Standard for Automation™

Modeling and Control of Solid-Sorbent CO_2 Capture Systems

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Hilton Scottsdale Resort

Short Biography of Benjamin Omell

- Post-Doctoral Fellow in the Department of Chemical Engineering at West Virginia University
- Research interest is in the area of steady-state and dynamic modeling and advanced process control for energy-generating and associated processes
- Member of AICHE
- Hobbies- Biking, hiking

OUTLINE

- ❖ Motivation
- ❖ Overview of Carbon Capture Simulation Initiative (CCSI)
- ❖ Dynamic Model Development
- ❖ Dynamic Reduced Model (D-RM) Builder Development
- ❖ Advanced Process Control (APC) Framework Development
- ❖ Results and Discussions
- ❖ Conclusions

MOTIVATION

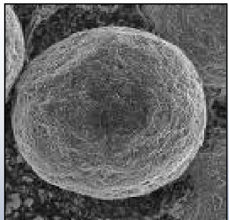
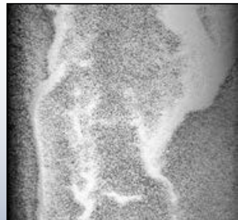
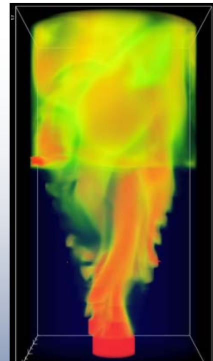
- Under the auspices of US DOE's *Carbon Capture Simulation Initiative (CCSI),* government and university researchers are collaborating to develop computational models and tools for various post-combustion CO_2 capture technologies

- CO_2 capture processes must be designed to operate efficiently in the face of disturbances that are typical of commercial-scale power plants

- Dynamic process models and advanced process control can be used to ensure efficient operation of these CO_2 capture technologies.

CCSI
Carbon Capture Simulation Initiative

ISA


Identify promising concepts → Reduce the time for design & troubleshooting → Quantify the technical risk, to enable reaching larger scales, earlier → Stabilize the cost during commercial deployment

National Labs

- Berkeley Lab
- Pacific Northwest National Laboratory
- NETL
- Los Alamos National Laboratory EST. 1943
- Lawrence Livermore National Laboratory

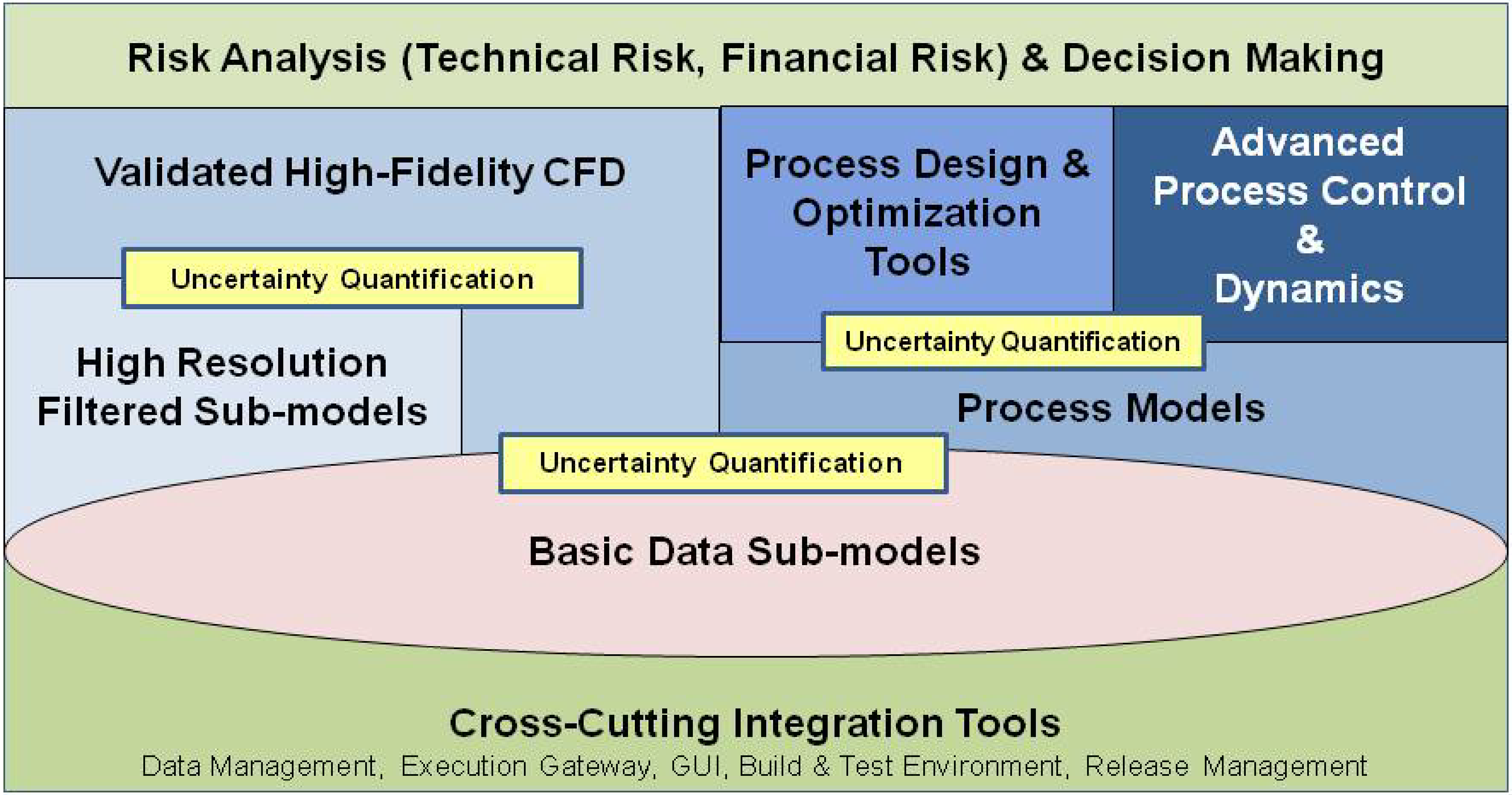
Academia

- Carnegie Mellon
- Princeton University
- West Virginia University
- Boston University
- The University of Texas at Austin
- Institute for Clean and Secure Energy, The University of Utah

Industry

- ADA Environmental Solutions
- ALSTOM
- B&W the babcock & wilcox company
- GE
- EPRI Electric Power Research Institute
- Fluor
- Southern Company
- Phillips 66
- AEP American Electric Power
- Southern California Edison, An Edison International Company, San Onofre Nuclear Generating Station
- Chevron
- URS
- ExxonMobil
- Air Products
- Eastman
- ANSYS
- PSE
- aspentech
- invensys

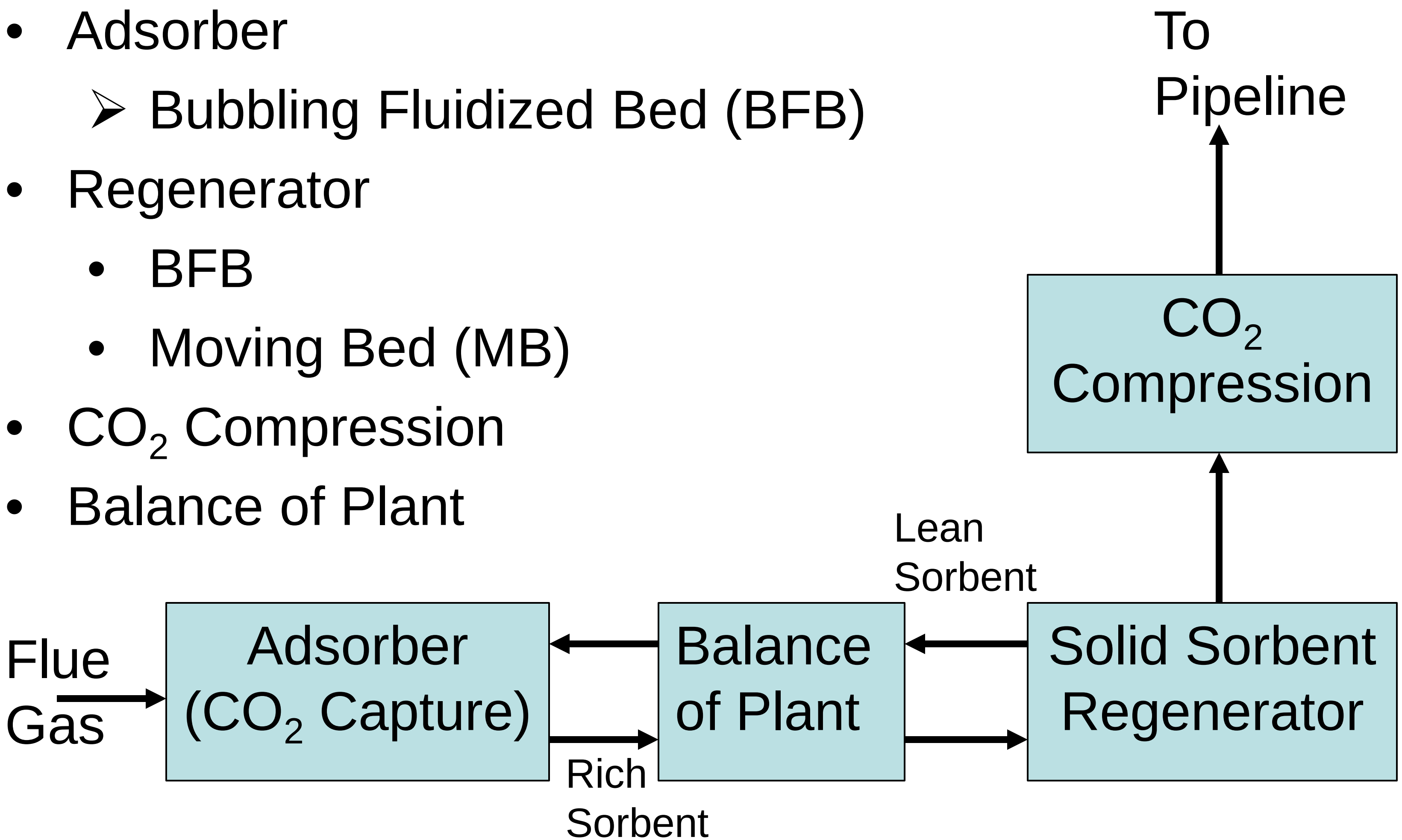
Computational Tools to Accelerate Next-Generation Technology Development



MODEL DEVELOPMENT

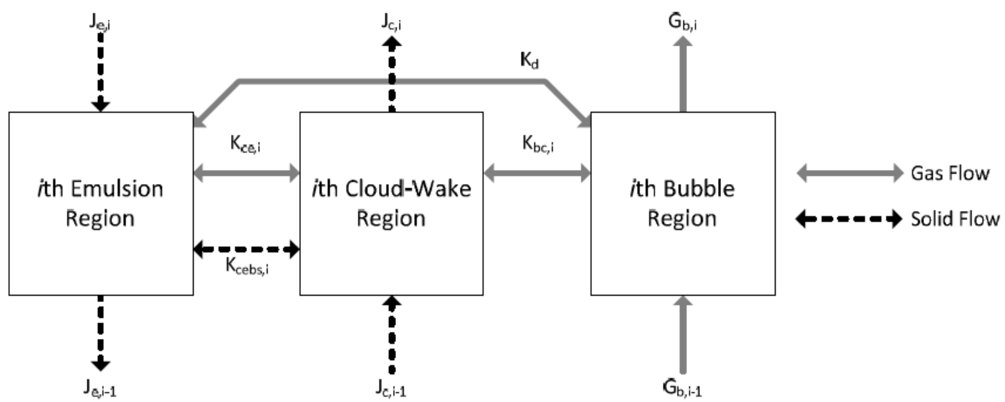
Solid Sorbent-based CO_2 Capture and Compression

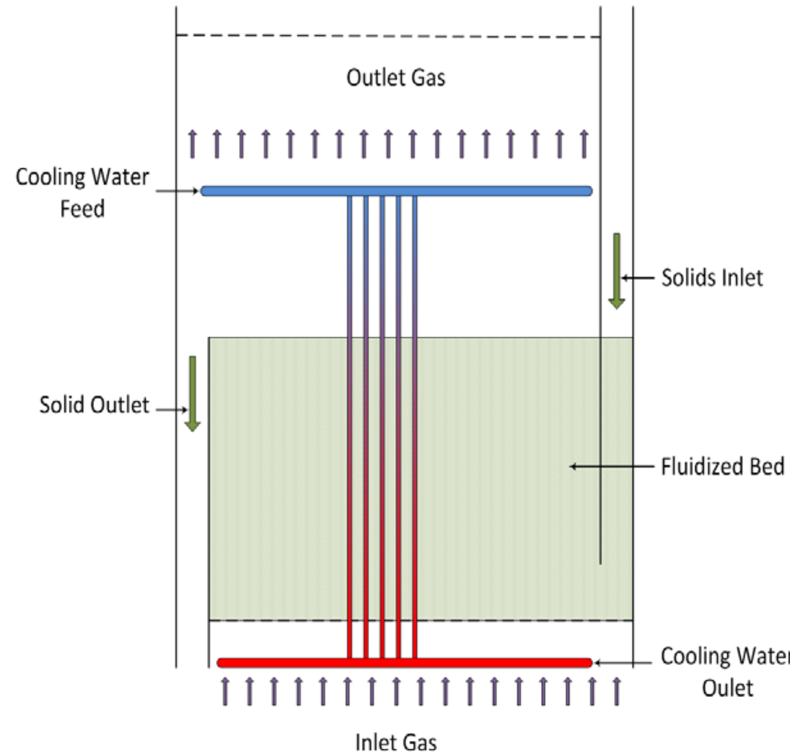
- Adsorber
  - Bubbling Fluidized Bed (BFB)
- Regenerator
  - BFB
  - Moving Bed (MB)
- CO_2 Compression
- Balance of Plant



MODEL DEVELOPMENT
Bubbling Fluidized Bed (BFB)

- 1-D two-phase, pressure-driven, non-isothermal dynamic model
- Model is flexible – adsorber or regenerator, cooler or heater depending on the application

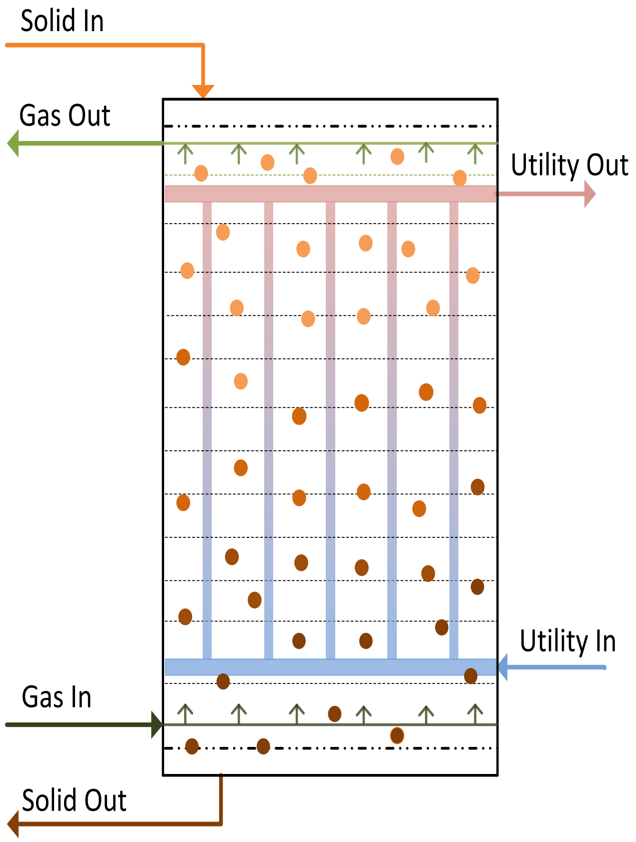




- Transient species conservation and energy balance equations for both gas and solid phases in all three regions
- Rigorous hydrodynamic models

MODEL DEVELOPMENT
Moving Bed Reactor

- 1-D two-phase pressure-driven non-isothermal dynamic model of a moving bed reactor for the regenerator



Model Assumptions

- Vertical shell & tube type reactor
- Gas and solids flows are modeled by plug flow model with axial dispersion.
- Particles are uniformly dispersed through the reactor with constant voidage
- Particle attrition ignored
- Temperature is uniform within the particles

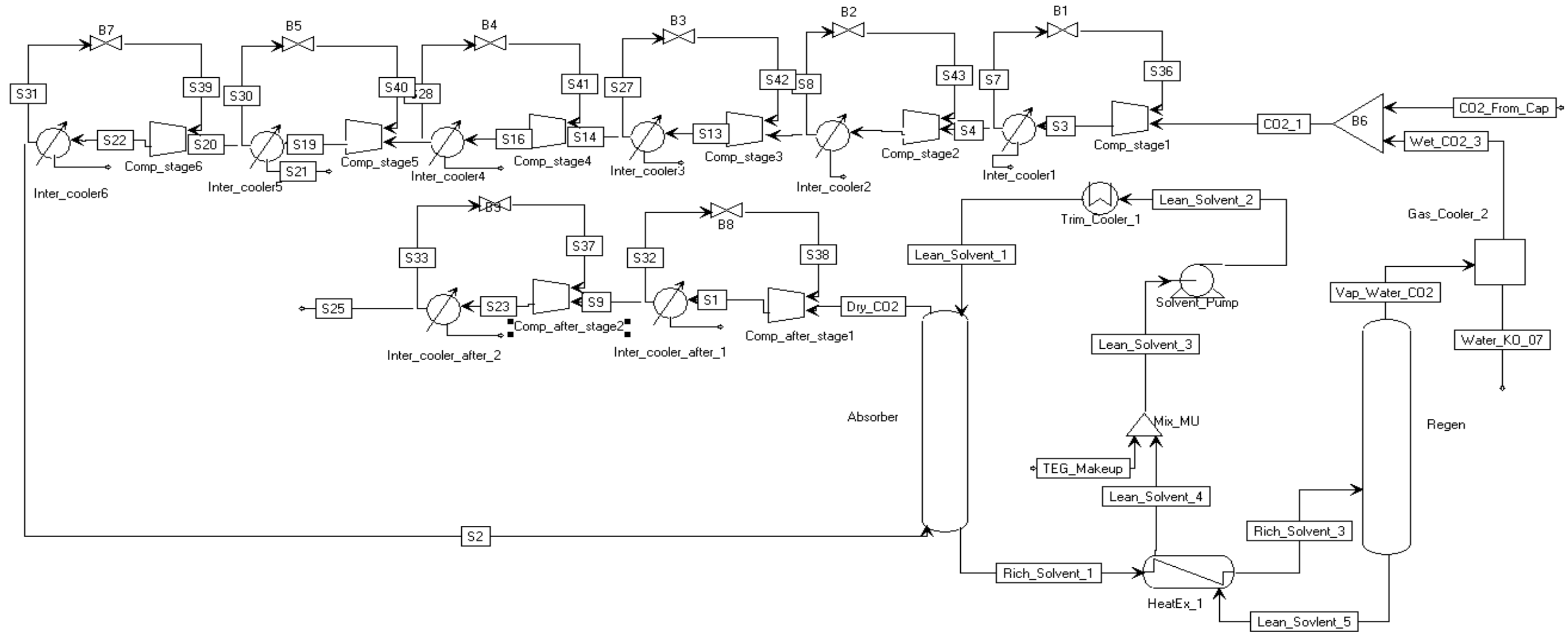
- Gaseous species: CO_2, N_2, H_2O
- Solid phase components: bicarbonate, carbamate, and physisorbed water

MODEL DEVELOPMENT

CO_2 Compression System Model

- Dynamic model of a multi-stage integral gear compressor system with inter-stage coolers, knock-out drums, and TEG absorption system has been developed.

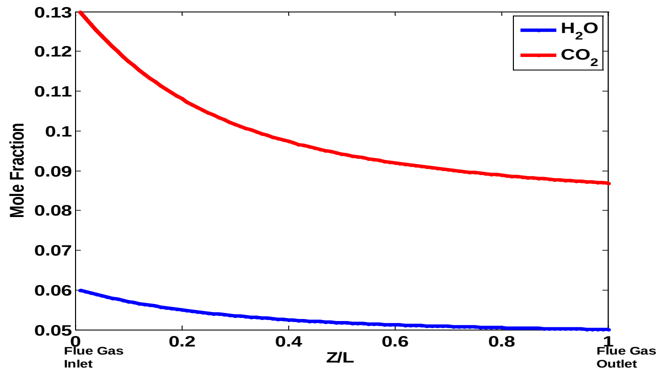
- Performance curves obtained from a commercial vendor have been used for calculating off-design performance.



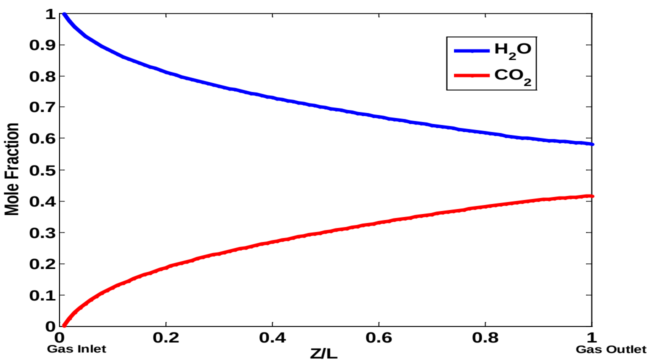
Results

Single-Stage BFB Model

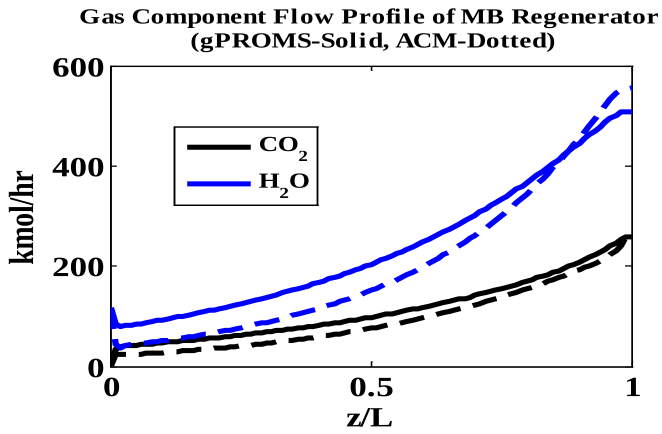
Adsorber

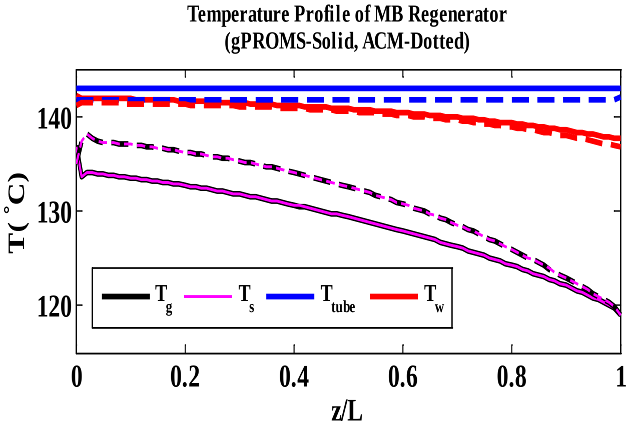


Regenerator



MB Model of Regenerator

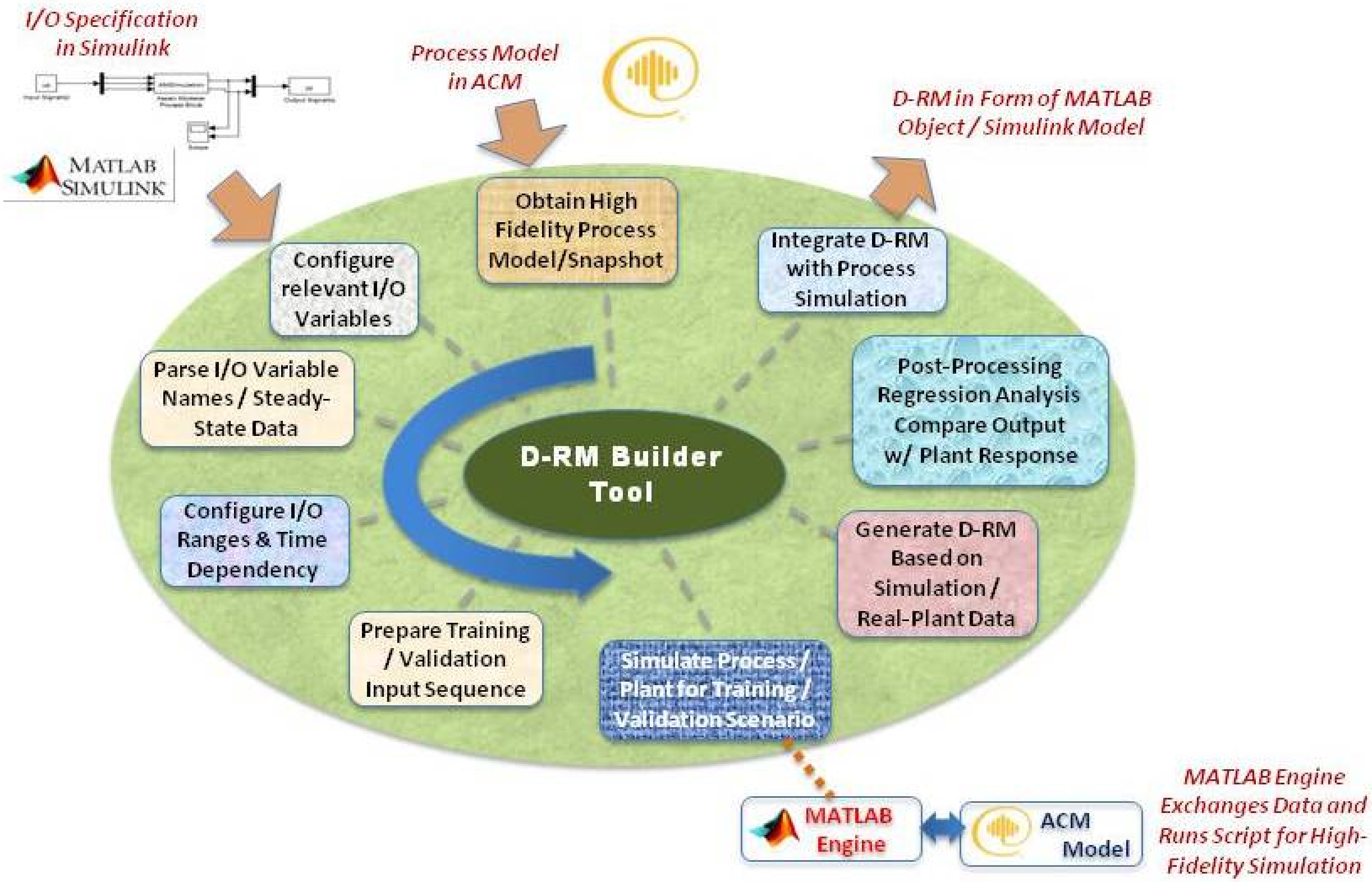




Why Dynamic Reduced Models?

- High-fidelity models are computationally expensive
  - May contains hundreds of thousands of DAEs
  - Require small time steps to handle stiffness
- Dynamic reduced models (D-RMs) could speed up a few orders of magnitude
- Two types of D-RMs
  - Reduced order D-RMs
    - Generated based on equations involved, e.g. POD
    - Generation method is generally model specific
    - On-going CCSI project for BFB reactor
  - Data-driven D-RMs
    - Based on pre-computed results from repeated simulations of a high-fidelity dynamic model over a range of input conditions
- Can be used for off-line operator training systems (OTS) and on-line implementations of advanced process control (APC) and real-time optimization (RTO)

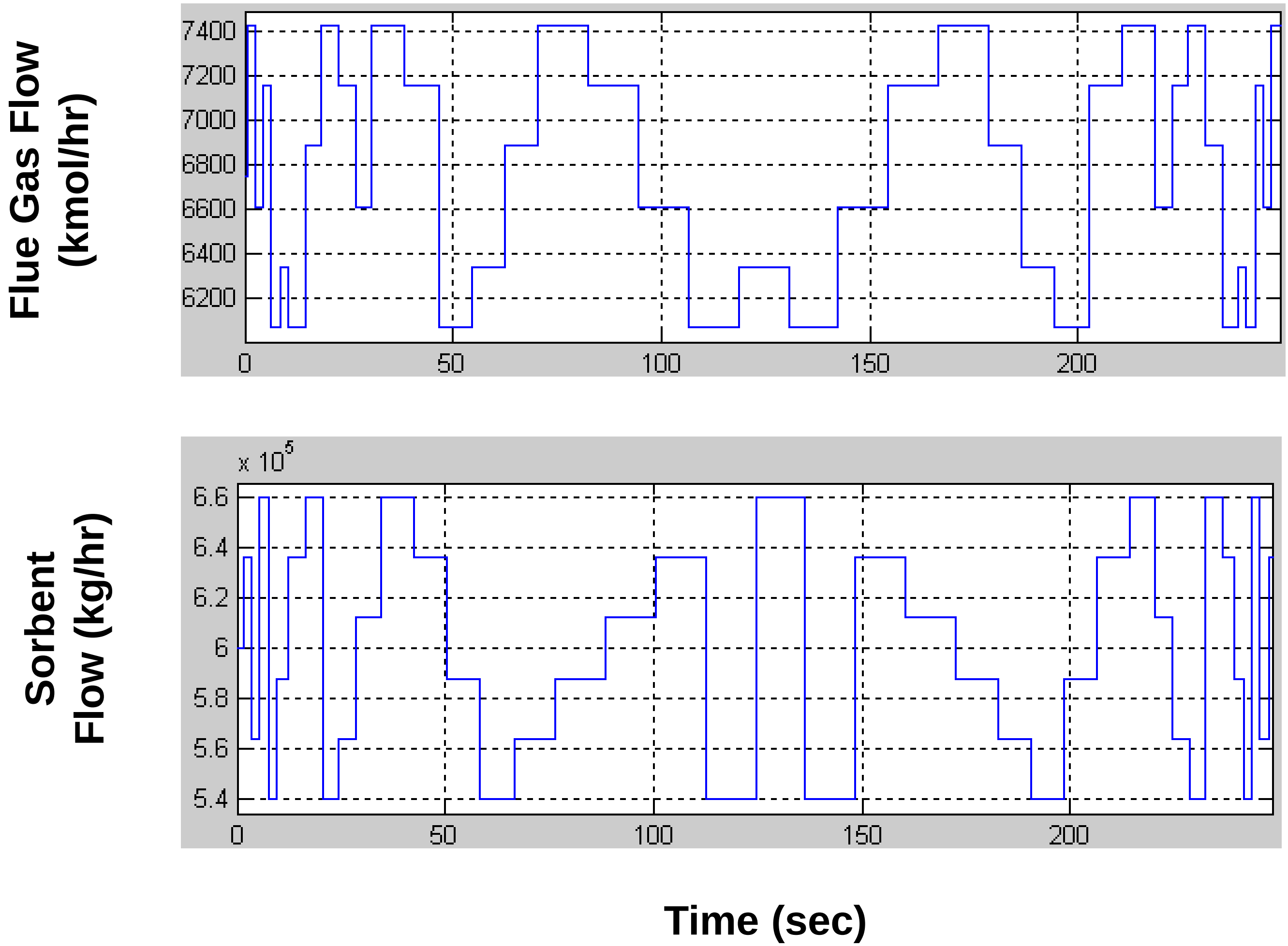
Work Flow of D-RM Builder



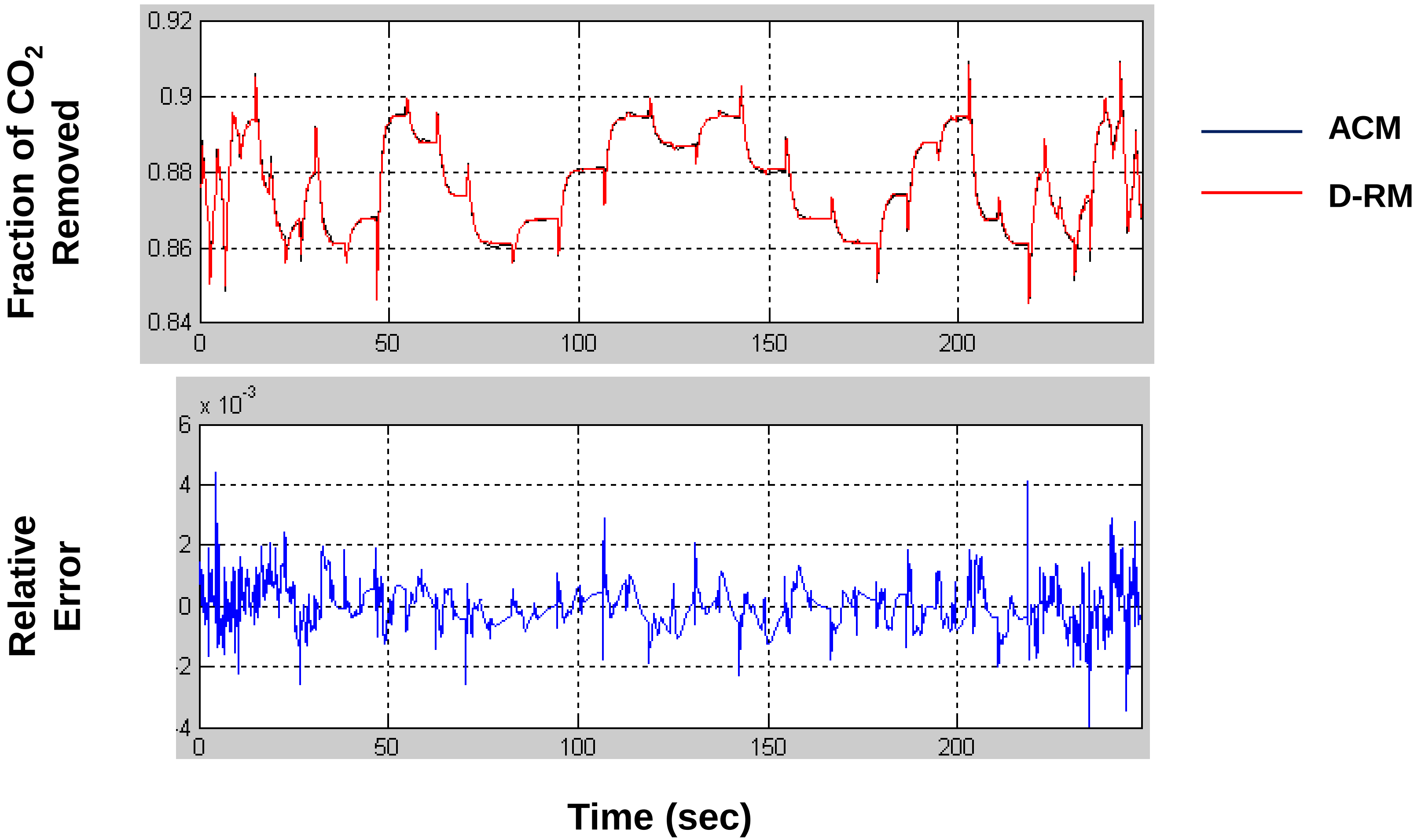
D-RM for the BFB Adsorber

- 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:
  - CO_2 removal (Fraction of CO_2 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)

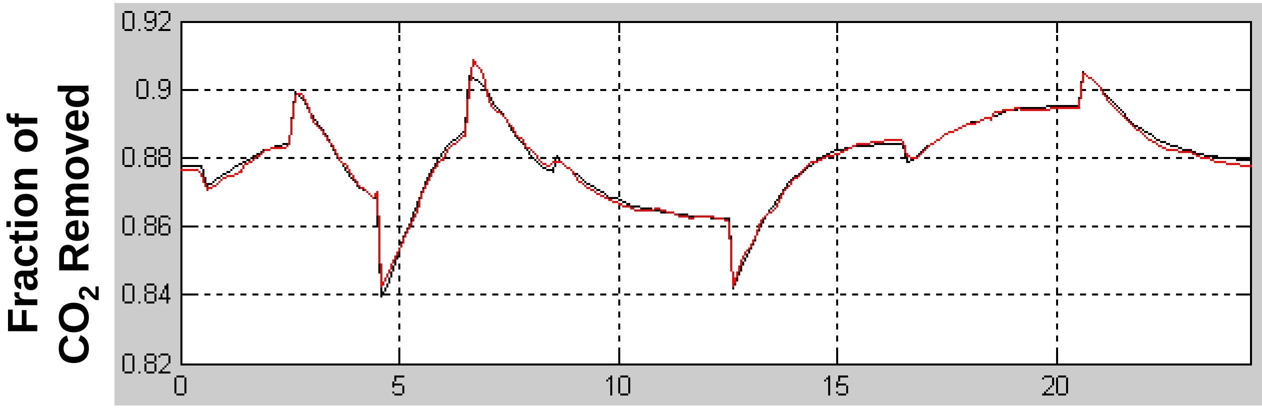
Training Input Data

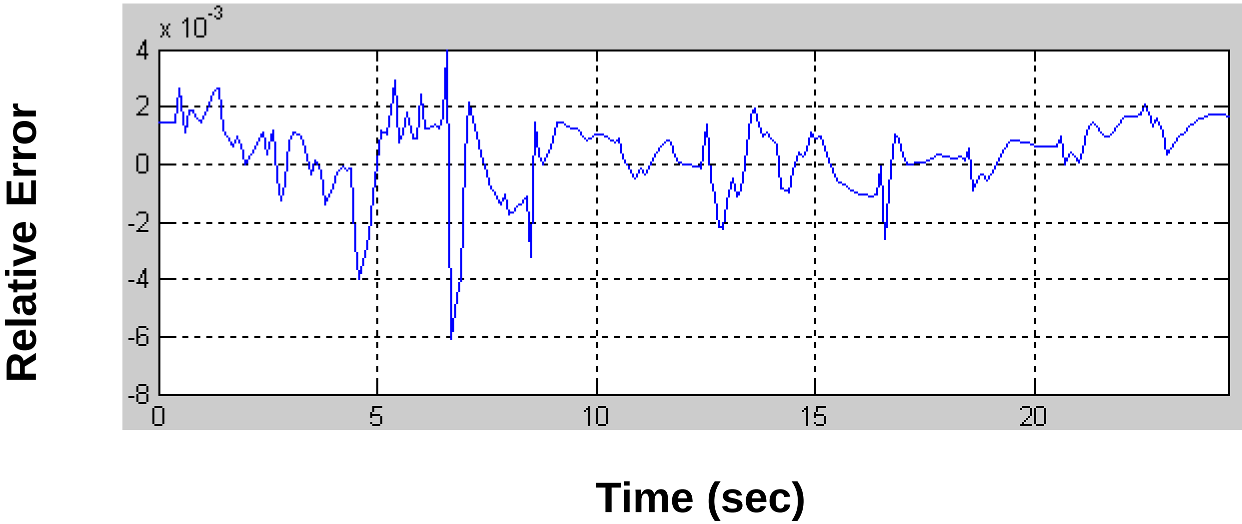


Training Output Data



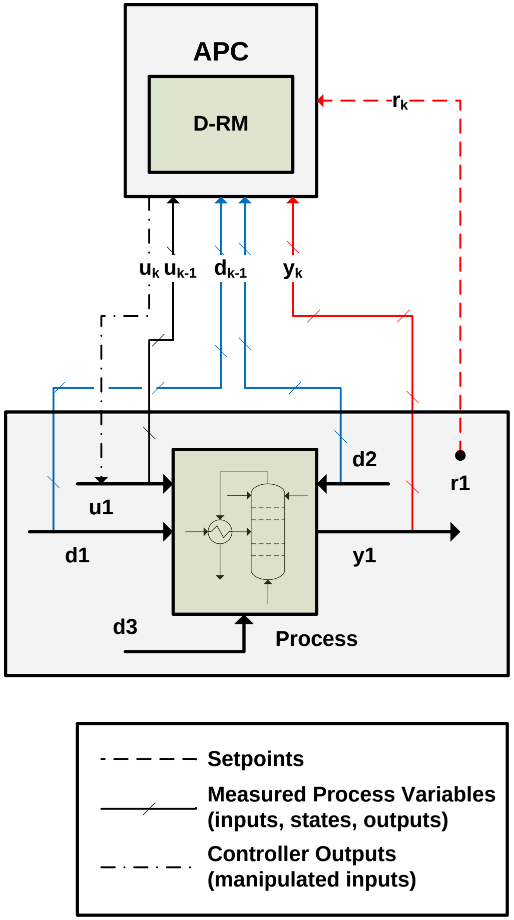
Validation Output Data



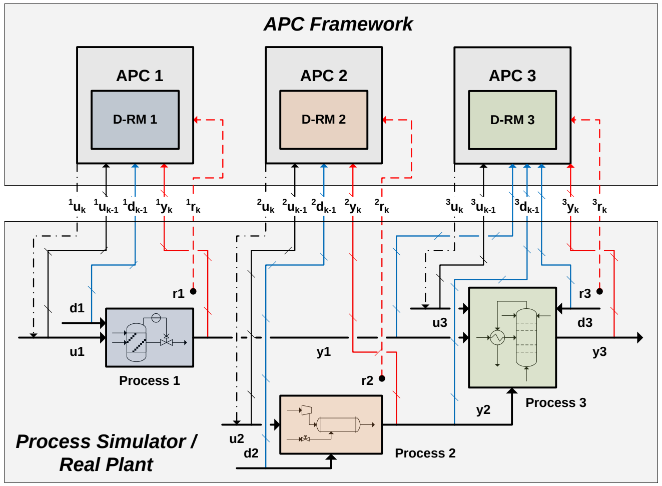


APC FRAMEWORK:
Features

- **Nonlinear Model Predictive Control (NMPC) using DAB-Net DRM model**
- **Unscented Kalman Filter (UKF) feedback and disturbance estimation technique**
  - Accurate capture of true mean and covariance of estimates
- **Extended Kalman Filter (EKF) with Autocovariance Least-Squares (ALS) disturbance-estimation technique**
- **Interior Point Optimizer (IPOPT)**
  - Faster and more effective optimization routine for solving large-scale nonlinear programming (LS-NLP)
- **Advanced Multi-Step NMPC (amsNMPC)**
  - Deals with NLP problems where solution time > sampling period
  - Proven nominal stability
- **Multiple-Model Predictive Control (MMPC) with Multiple Disturbance Models**
  - Capture nonlinearity using model bank across wide operating regimes
  - Prospective alternative to NMPC
  - Significantly low computation cost (compared to NMPC)

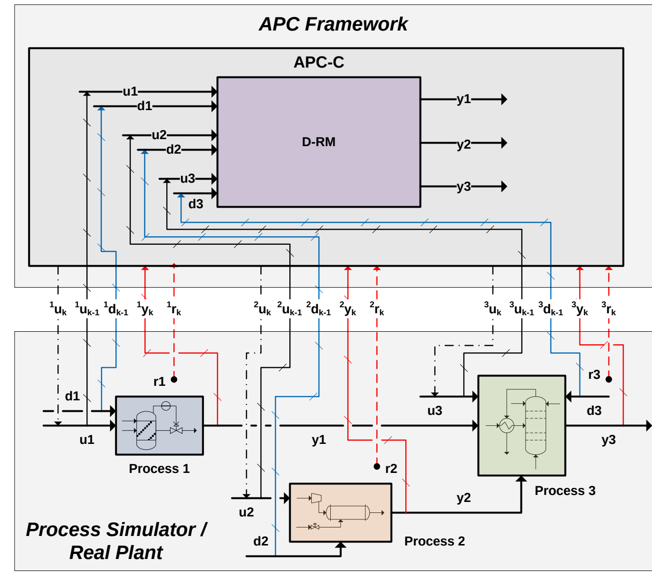


APC FRAMEWORK:
Modes of Operation



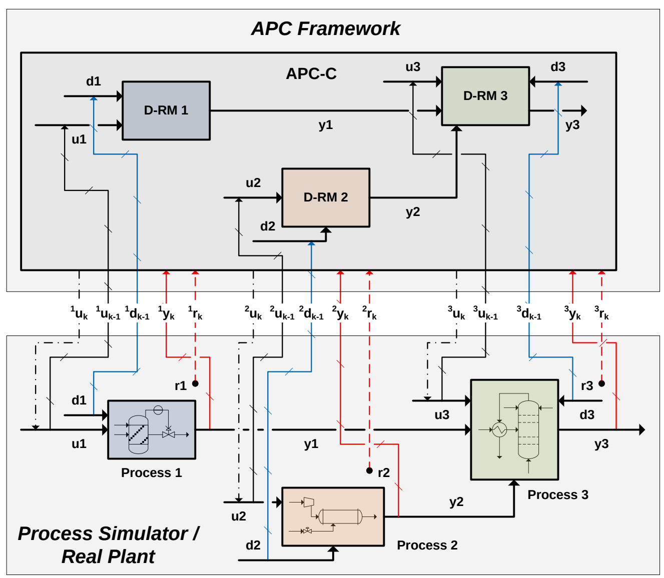
Decentralized APC

Dedicated APC block for each sub-process



Centralized APC using single D-RM

Single APC block using single D-RM for entire flowsheet



Centralized APC

Single APC block using individual D-RM for each sub-process

APC FRAMEWORK:
Formulation (control models & objectives)

Nonlinear

D-AB Net (NSS)

$$\mathbf{x}_{k+1} = \mathbf{A}\mathbf{x}_k + \mathbf{B}_u\mathbf{u}_k + \mathbf{B}_l\mathbf{l}_k + \mathbf{B}_w\mathbf{w}_k$$
$$\mathbf{y}_k = \mathbf{C}\mathbf{x}_k + \mathbf{D}_u\mathbf{u}_k + \mathrm{N}(\mathbf{x}_k, \mathbf{u}_k) + \mathbf{v}_k$$

NARMA

$$\mathbf{y}_{k+1} = \mathrm{N}(\mathbf{y}_k, \mathbf{y}_{k-1}, \mathbf{u}_k, \mathbf{u}_{k-1}, \mathbf{l}_k, \mathbf{l}_{k-1}, \mathbf{w}_k) + \mathbf{v}_k$$

$$\mathbf{x}_{k+1} = \mathrm{f}(\mathbf{x}_k, \mathbf{u}_k, \mathbf{l}_k, \mathbf{w}_k)$$
$$\mathbf{y}_k = \mathrm{g}(\mathbf{x}_k, \mathbf{u}_k) + \mathbf{v}_k$$

Empirical ⟷ **First Principles**

State Space (SS)

$$\mathbf{x}_{k+1} = \mathbf{A}\mathbf{x}_k + \mathbf{B}_u\mathbf{u}_k + \mathbf{B}_l\mathbf{l}_k + \mathbf{B}_w\mathbf{w}_k$$
$$\mathbf{y}_k = \mathbf{C}\mathbf{x}_k + \mathbf{D}_u\mathbf{u}_k + \mathbf{v}_k$$

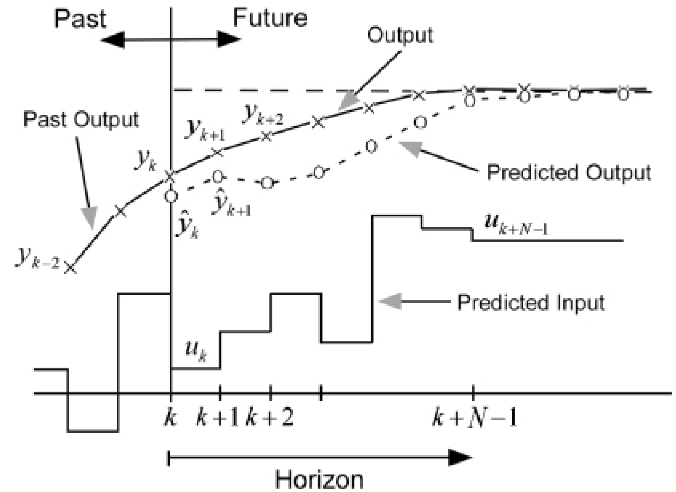
Linear

Dynamic Objective Function

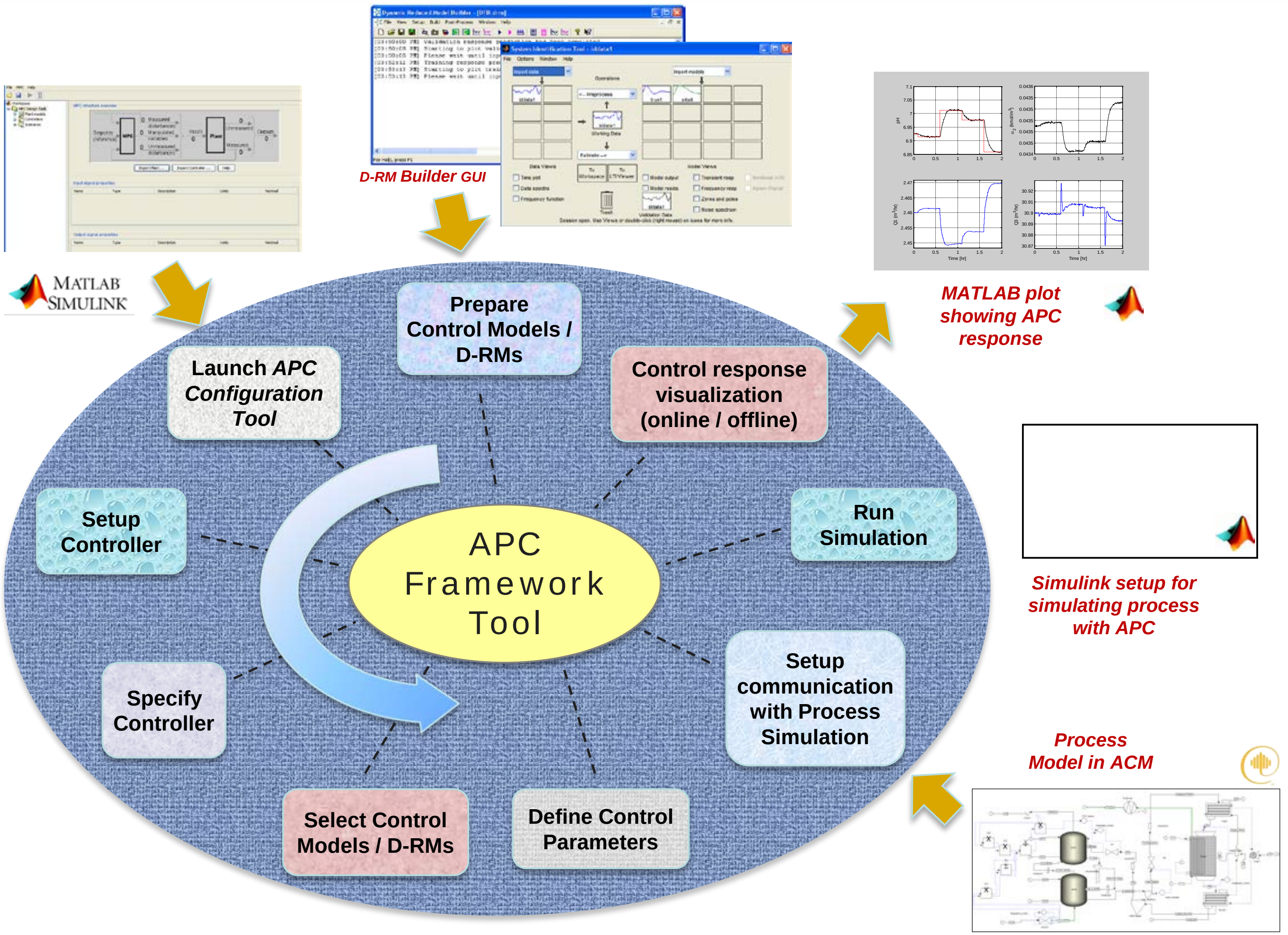
$$\min_{\Delta u} J = \sum_{j=1}^{P}\left(r_k - \hat{y}_{k+j|k}\right)^T W^y \left(r_k - \hat{y}_{k+j|k}\right) + \sum_{j=0}^{M-1} \Delta u_{k+j}^T W^u \Delta u_{k+j}$$

$$u_{\min} \le u_{k+j} \le u_{\max} \qquad \Delta u_{\min} \le \Delta u_{k+j} \le \Delta u_{\max}$$

$$y_{\min} \le \hat{y}_{k+j|k} \le y_{\max}$$

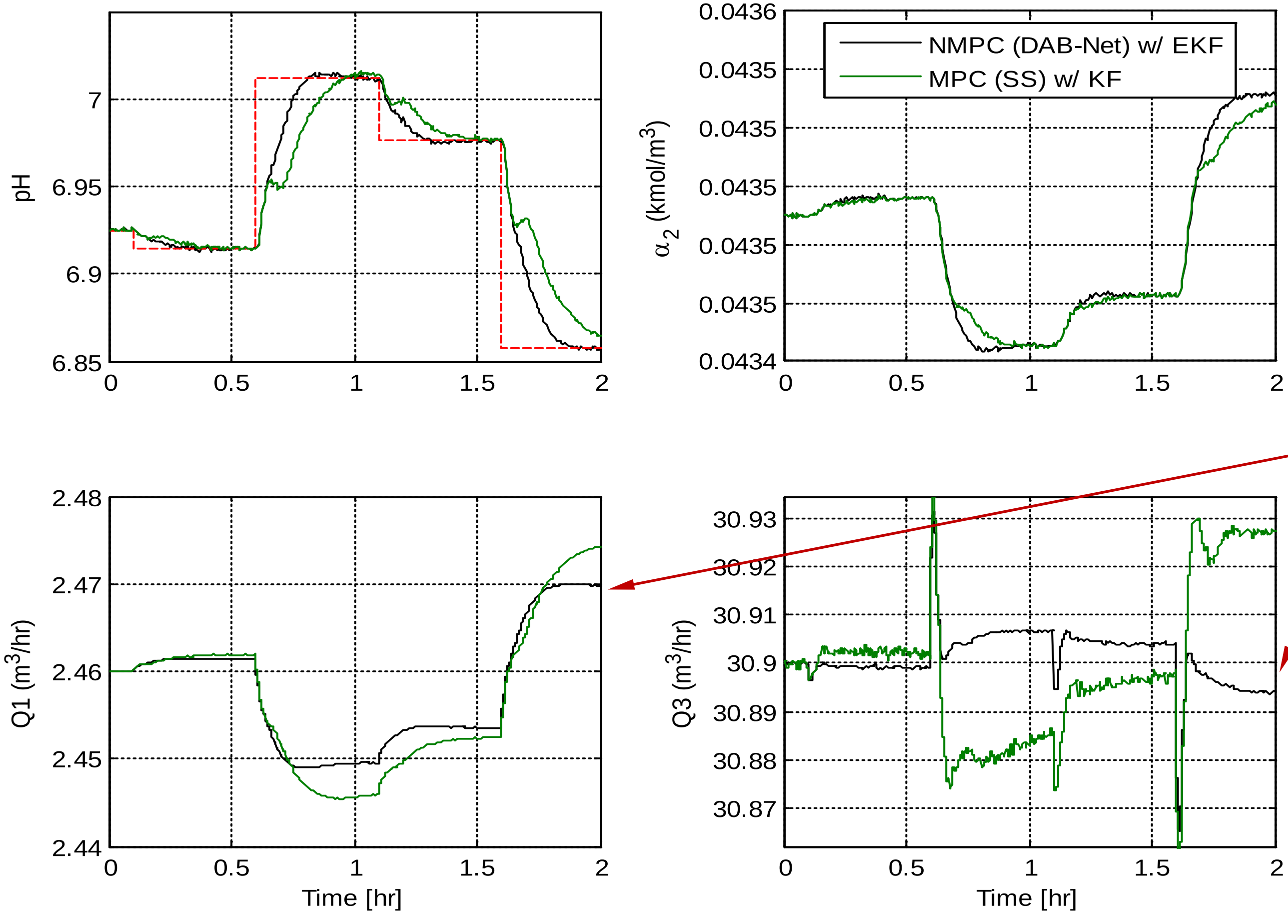


APC FRAMEWORK:
End-User Workflow



APC FRAMEWORK

Results: DAB-Net based NMPC (comparison)

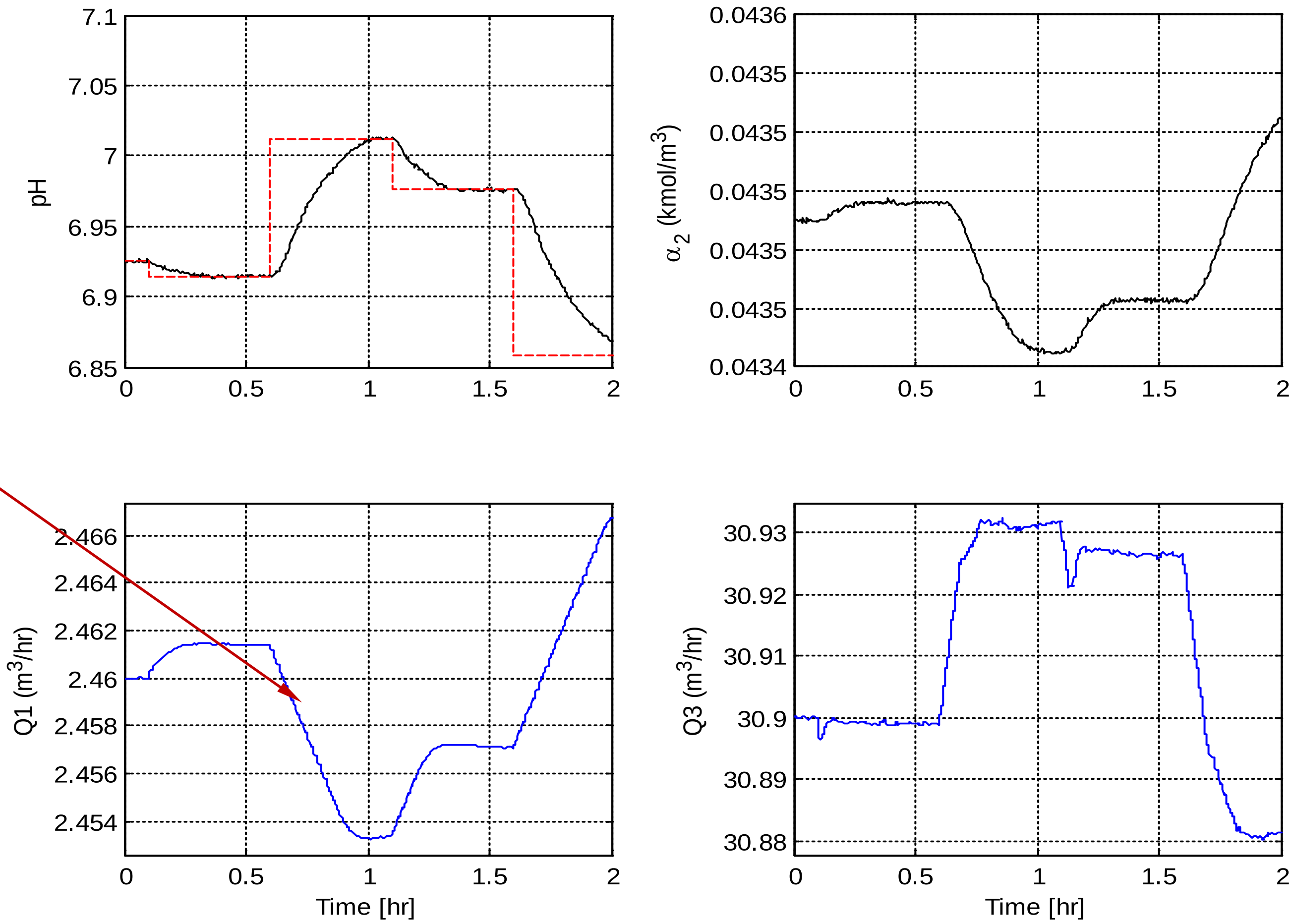


Both controller lead to different final steady-states. NMPC could capture nonlinear behavior during predictions leading to smoother transients

APC FRAMEWORK

Results: DAB-Net based NMPC (input constraints)

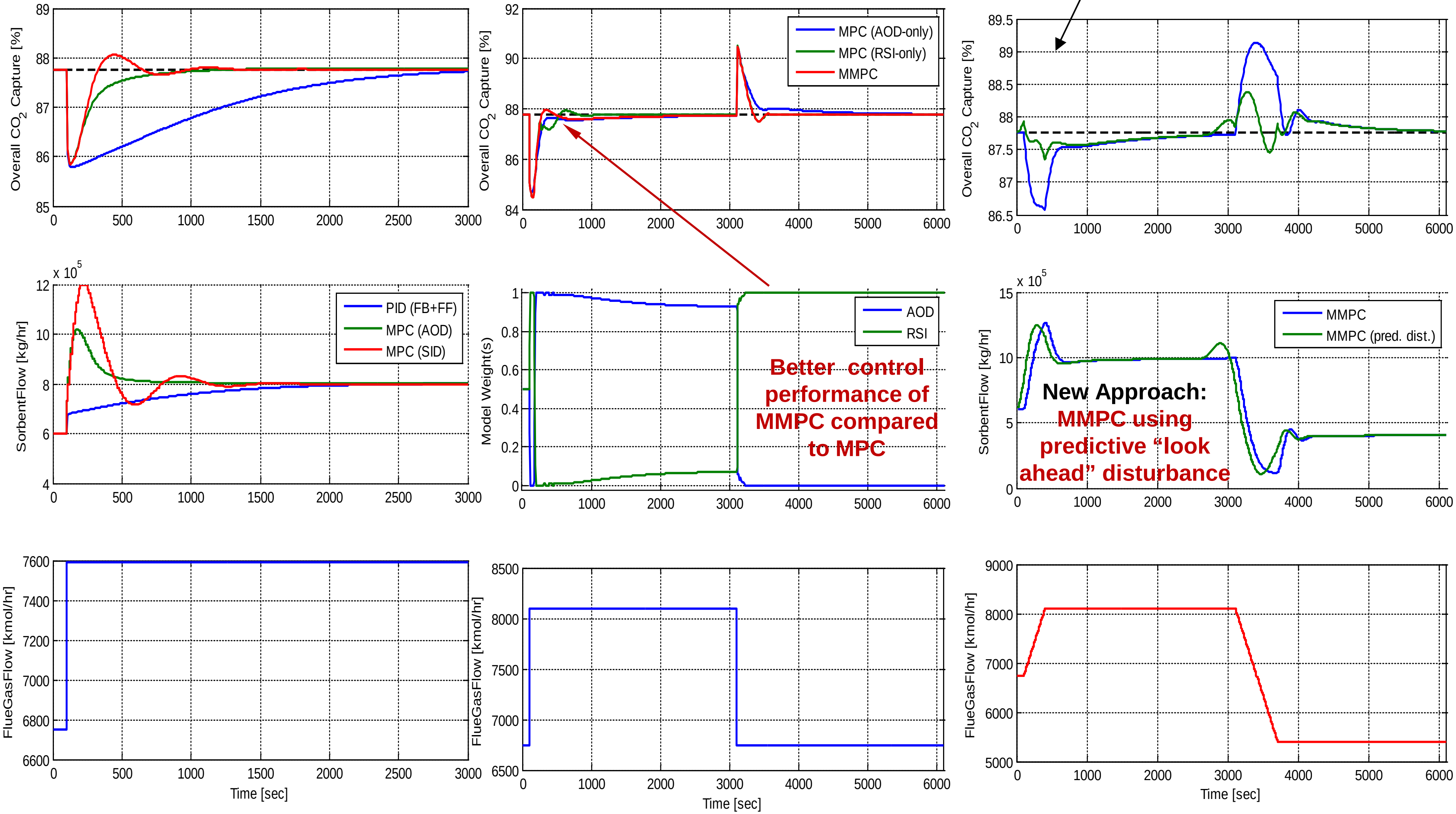
Enforced input rate-constraint of ±1% per time-step



APC FRAMEWORK

Results: MMPC responses

"Look ahead" formulation drastically improves overall CO2 capture during flue-gas ramp-up.



Conclusions

1. 1D non-isothermal, pressure-driven dynamic models of a two-stage BFB adsorber-reactor, a MB regenerator, an integral gear CO_2 compression system along with the balance of the plant have been developed in ACM and gPROMS for solid-sorbent CO_2 capture.

2. The DAB-Net D-RM is found to be satisfactory for the BFB reactor.

3. DAB-Net based NMPC was developed and was shown to provide superior control response for highly nonlinear systems. The MMPC formulation (especially w/ look-ahead disturbance) is found to provide fast and superior load-tracking performance for overall CO_2 capture.

Acknowledgements

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Disclaimer:

Thank you

Questions?