Dynamic Modeling and Control of an Integrated Solid Sorbent Based CO$_2$ Capture Process

Benjamin Omell, Debangsu Bhattacharyya*
Department of Chemical Engineering
West Virginia University, Morgantown, WV

David C. Miller,
National Energy Technology Laboratory
US DOE, Pittsburgh, PA

Jinliang Ma, Priyadarshini Mahapatra, Stephen E. Zitney
National Energy Technology Laboratory
US DOE, Morgantown, WV
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
CO$_2$ 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

CO$_2$ Compression System

Moving Bed (MB) Regenerator

58th Annual ISA POWID Symposium, 7-11 June 2015, Kansas City, Missouri
Goals and Objectives

- 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)
CCSI Toolset Framework

DRM-Building

Training Data

Optimized Process

Controller Inputs

State Inputs

Steady State Model

Dynamic Process Model

APC Framework

DRM for real-time optimization
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

58th Annual ISA POWID Symposium, 7-11 June 2015, Kansas City, Missouri
• Gaseous species: CO₂, N₂, H₂O
• 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.

58th Annual ISA POWID Symposium, 7-11 June 2015, Kansas City, Missouri
Single-Stage BFB Model: Steady-State Results

Adsorber

Regenerator

58th Annual ISA POWID Symposium, 7-11 June 2015, Kansas City, Missouri
Dynamic Results – Increase Inlet Gas Flow by 20.6%
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)

58th Annual ISA POWID Symposium, 7-11 June 2015, Kansas City, Missouri
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-CO$_2$ systems
- For CO$_2$ systems, developed mainly for sCO$_2$ 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 sCO$_2$ cycles
- Typically steady-state
  - Dynamics are essential for load-following in power systems
- Lack of performance curves for CO$_2$ systems
- Surge detection and control algorithms hardly studied for these systems
CCSI CO$_2$ 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

58th Annual ISA POWID Symposium, 7-11 June 2015, Kansas City, Missouri
Integrated Model Enables Investigation of Entire Process Dynamics

Integrated Model in gPROMS (also ACM version)

58th Annual ISA POWID Symposium, 7-11 June 2015, Kansas City, Missouri
Ramp in flue gas
Time=0 : 15.8% increase
Time=20: 28.8% decrease
Dynamics of Integrated Process

- 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
CCSI Toolset Framework

DrM-Builder

Training Data

Optimized Process

Steady State Model

Dynamic Process Model

Controller Inputs

State Inputs

APC Framework

DrM for real-time optimization

58th Annual ISA POWID Symposium, 7-11 June 2015, Kansas City, Missouri
Motivation

- 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

1. **I/O Variable Selection**
   - SinterConfigGUI

2. **Generate D-RM Based on Simulation Results**
   - GUI for Configuring Inputs/Outputs
   - Run Training Sequence

3. **Analyze Reduced Model using UQ Tools, Validation Sets, Plots**
   - D-RM in Form of MATLAB Code

---

58th Annual ISA POWID Symposium, 7-11 June 2015, Kansas City, Missouri
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)

Validation Input Data

- Flue Gas Flow (kmol/hr)
- Sorbent Flow (kg/hr)

Time (sec)
Validation Output Data

Fraction of CO₂ Removed

Time (sec)

Relative Error

Time (sec)
CCSI Toolset Framework

58th Annual ISA POWID Symposium, 7-11 June 2015, Kansas City, Missouri
Utilize proven techniques from control relevant studies in literature and combine them synergistically in an efficient and robust process control framework.

Typical problems with APC applications

- Poor control response for highly nonlinear plants using traditional PID or MPC
- Nonlinear MPC becomes computationally expensive for large-scale plant
- Noisy measurements along with unmodeled disturbance and unmeasured variables provides poor control response
- Controller is too sensitive to user-provided tuning parameters (inexperienced operators)
- Typical APC interface overwhelms the operators (setting up control-model, tuning parameters, etc.)

APC Framework

- DABNet-based Nonlinear System Identification
- Analytical Jacobians and Hessians
- Multiple Model Predictive Control (MMPC)
- Auto Covariance Estimation (ALS Technique)
- IPOPT-based Optimization Technique
- UKF-based State Estimation
- Enhanced User-Friendly GUI
Performance Comparison on 2-Stage BFB Adsorber (ACM)

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

<table>
<thead>
<tr>
<th>Algorithm</th>
<th>Cumulative Residual</th>
<th>Computational Cost</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>Cumulative Control Calculation Time (sec)</td>
</tr>
<tr>
<td>Conventional MPC</td>
<td>0.019</td>
<td>9.54</td>
</tr>
<tr>
<td>DAB-Net NMPC</td>
<td>0.007</td>
<td>19.97</td>
</tr>
</tbody>
</table>

Note: Max. Control Calculation Time << Sample Time (Ts = 20 sec), Real-Time Operation with APC

- Better disturbance rejection
- Active Constraints
- Large changes in flue-gas flowrate (input-disturbance)

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

58th Annual ISA POWID Symposium, 7-11 June 2015, Kansas City, Missouri
Performance Comparison on 2-Stage BFB Adsorber (ACM)

Sensitivity of Control Performance to Tuning Parameter – Comparison with standard MPC controller

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)

58th Annual ISA POWID Symposium, 7-11 June 2015, Kansas City, Missouri
Summary

- Developed high-fidelity steady-state and dynamic solid sorbent models for CO$_2$ 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

DOE’s Carbon Capture Simulation Initiative for funding. Part of this technical effort was performed under the RES contract DE-FE0004000 through National Energy Technology Laboratory’s Regional University Alliance (NETL-RUA).

Disclaimer

This presentation was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.
Thank You
Optimized Process Developed using CCSI Toolset

**Legend**
- Flue Gas
- Clean Gas
- Rich CO$_2$ Gas
- Lean Sorbent
- Rich Sorbent
- LP Steam
- HX Fluid
- Injected Steam
- Cooling Water

**Delta Loading**
- 1.8 mol CO$_2$/kg
- 0.66 mol H$_2$O/kg

<table>
<thead>
<tr>
<th>Solid Sorbent</th>
<th>MEA$^{27}$ (Δ10°C HX)</th>
<th>MEA$^{27}$ (Δ5°C HX)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$Q_{Rxn}$ (GJ/tonne CO$_2$)</td>
<td>1.82</td>
<td>1.48</td>
</tr>
<tr>
<td>$Q_{Vap}$ (GJ/tonne CO$_2$)</td>
<td>0</td>
<td>0.61</td>
</tr>
<tr>
<td>$Q_{Sen}$ (GJ/tonne CO$_2$)</td>
<td>0.97</td>
<td>1.35</td>
</tr>
<tr>
<td>Total Q</td>
<td>2.79</td>
<td>3.44</td>
</tr>
</tbody>
</table>

58th Annual ISA POWID Symposium, 7-11 June 2015, Kansas City, Missouri