NETL Carbon Capture Modeling Overview: CCSI, IDAES

David C. Miller, Senior Fellow

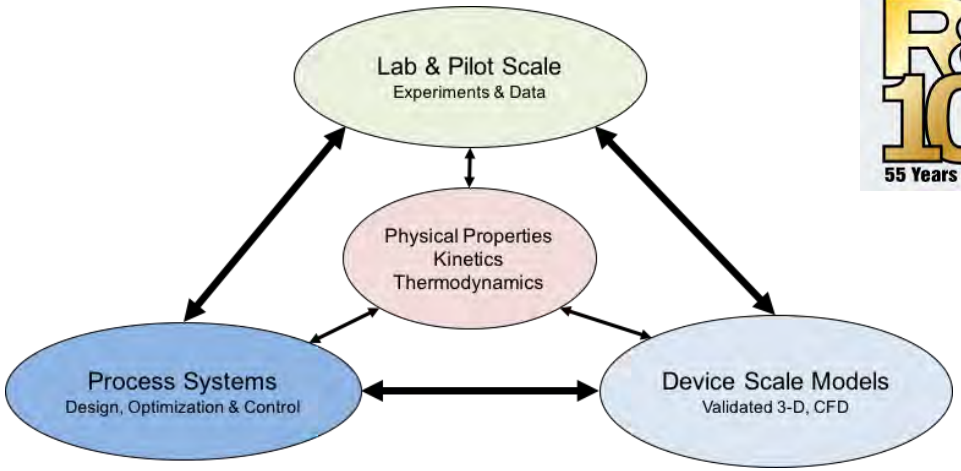
July 31, 2019

CCSI Toolset (2011-2016)

Carbon Capture Simulation Initiative

Maximize the learning at each stage of technology development

- **Early stage R&D**
  - Screening concepts
  - Identify conditions to focus development
  - Prioritize data collection & test conditions
- **Pilot scale**
  - Ensure the right data is collected
  - Support scale-up design
- **Demo scale**
  - Design the right process
  - Support deployment with reduced risk



R&D 100 55 Years of Invention

Industry Collaborators

Available Open Source
https://github.com/CCSI-Toolset/
www.acceleratecarboncapture.org

High Fidelity Process Models for Carbon Capture

Bubbling Fluidized Bed (BFB) Model
- Variable solids inlet and outlet location
- Modular for multiple bed configurations

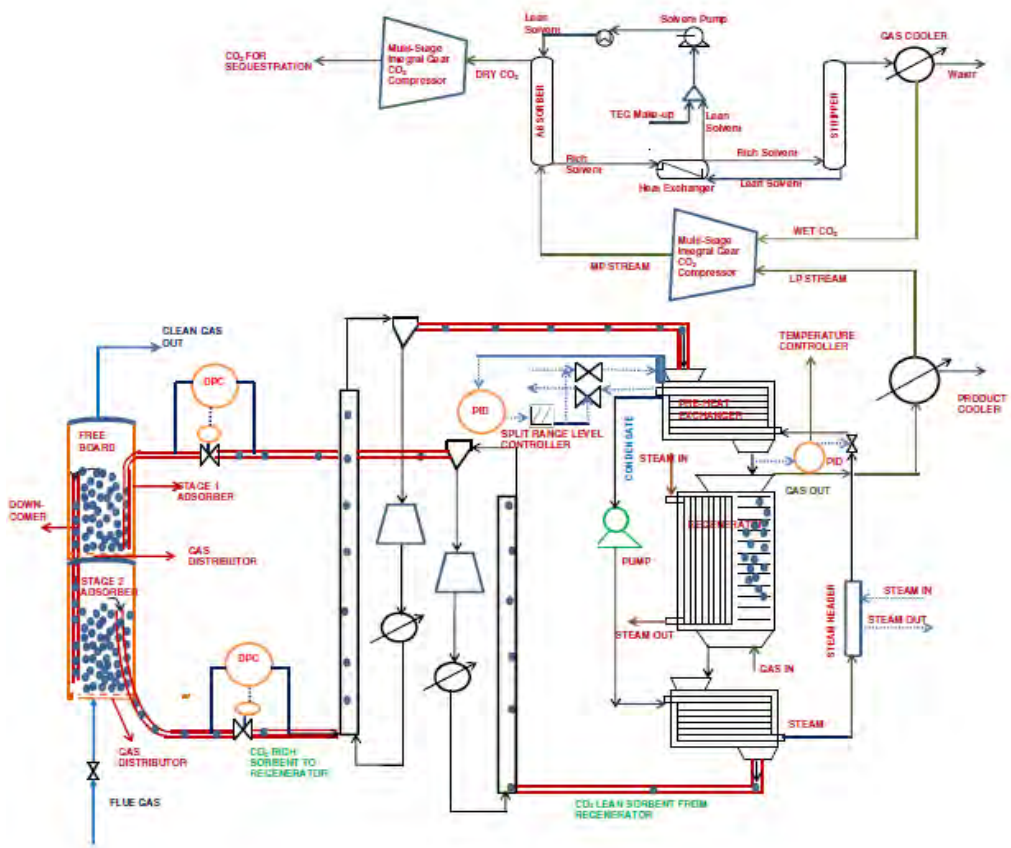
Moving Bed (MB) Model
- Unified steady-state and dynamic
- Heat recovery system

Fixed Bed Model
- Rigorous, 1-D, nonisothermal with heat exchange

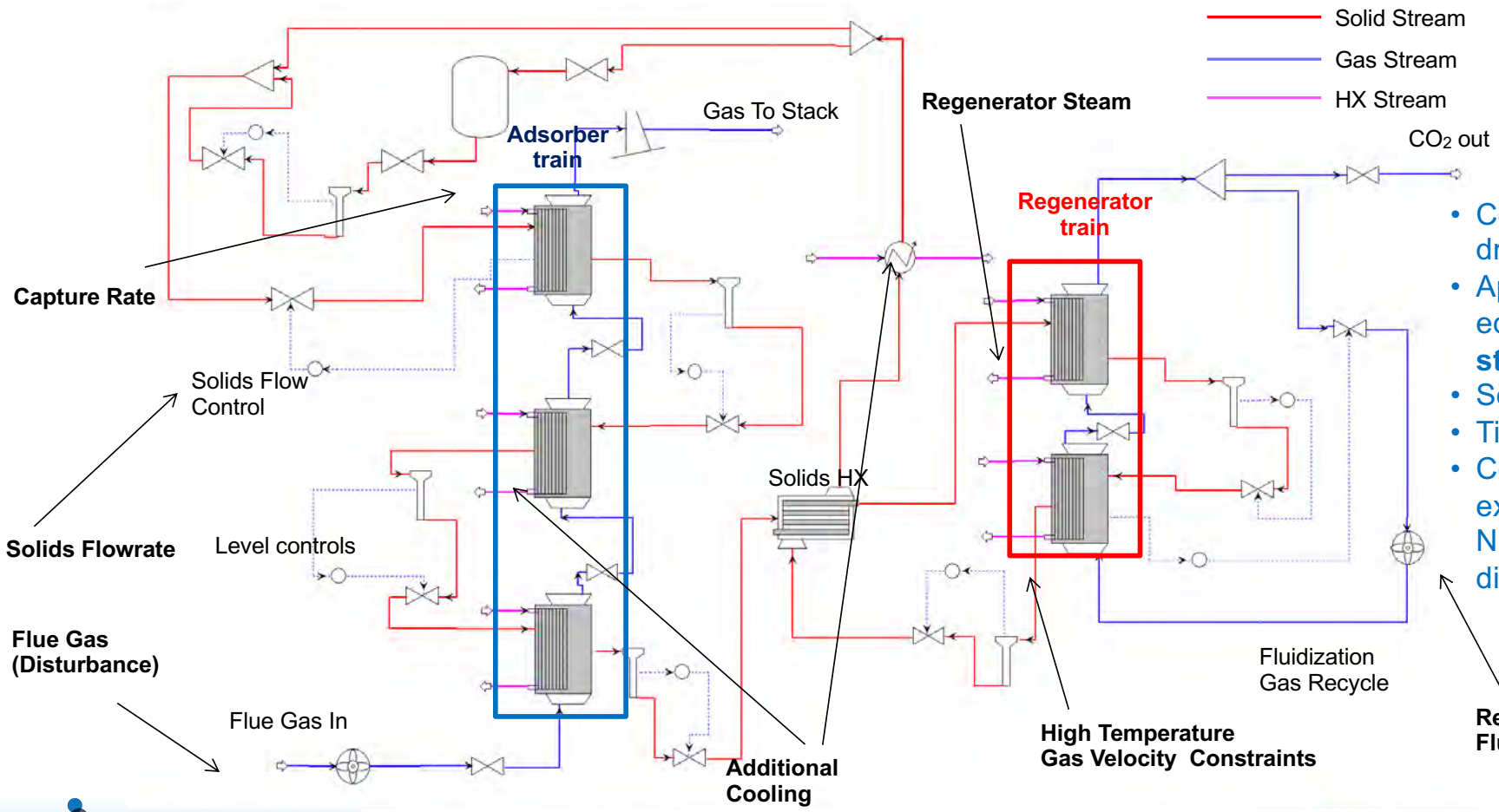
Compression System Model
- Integral-gear and inline compressors
- Determines stage required stages, intercoolers
- Based on impeller speed limitations
- Estimates stage efficiency
- Off-design and surge control

Solvent System Model
- Predictive, rate-based models

Membrane System Model
- Hollow fiber
- Supports multiple configurations



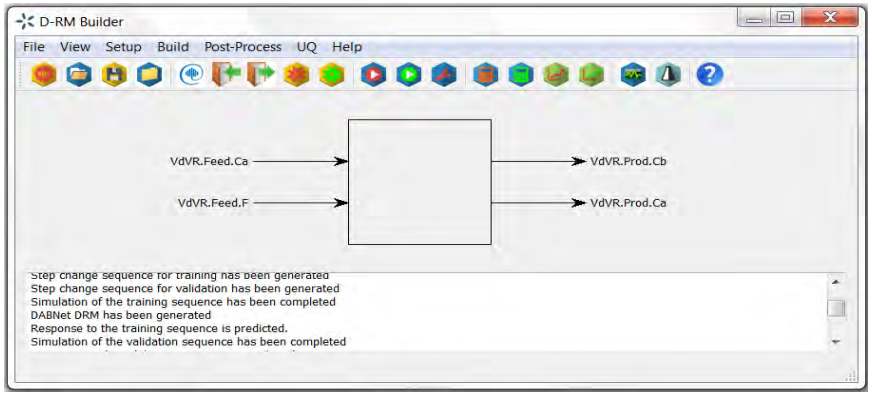
Dynamic Solid Sorbent-Based Carbon Capture System Model

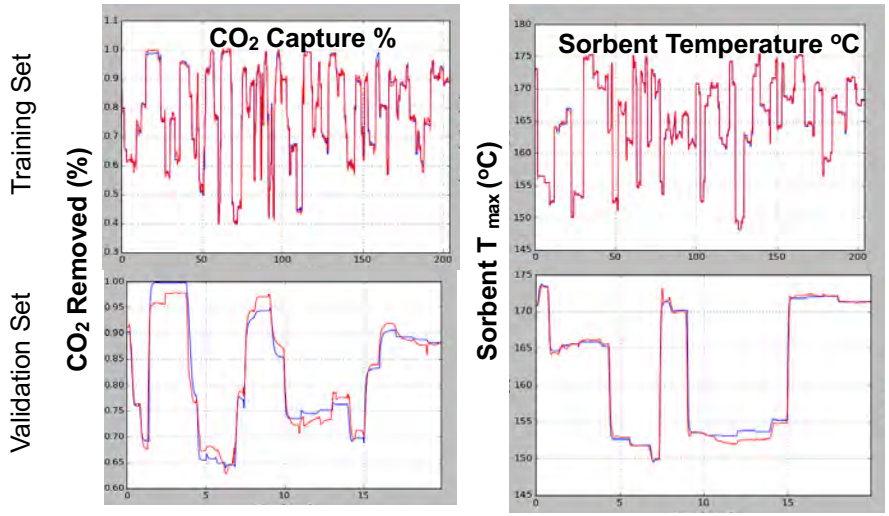


- Complex, pressure driven, dynamic model
- Approximately 126,000 equations **per time step**
- Settling time ~ 1hr
- Time step of 0.02 hrs
- Computationally expensive to apply in NMPC framework directly

Dynamic Reduced Model Builder to Enable Advanced Controls

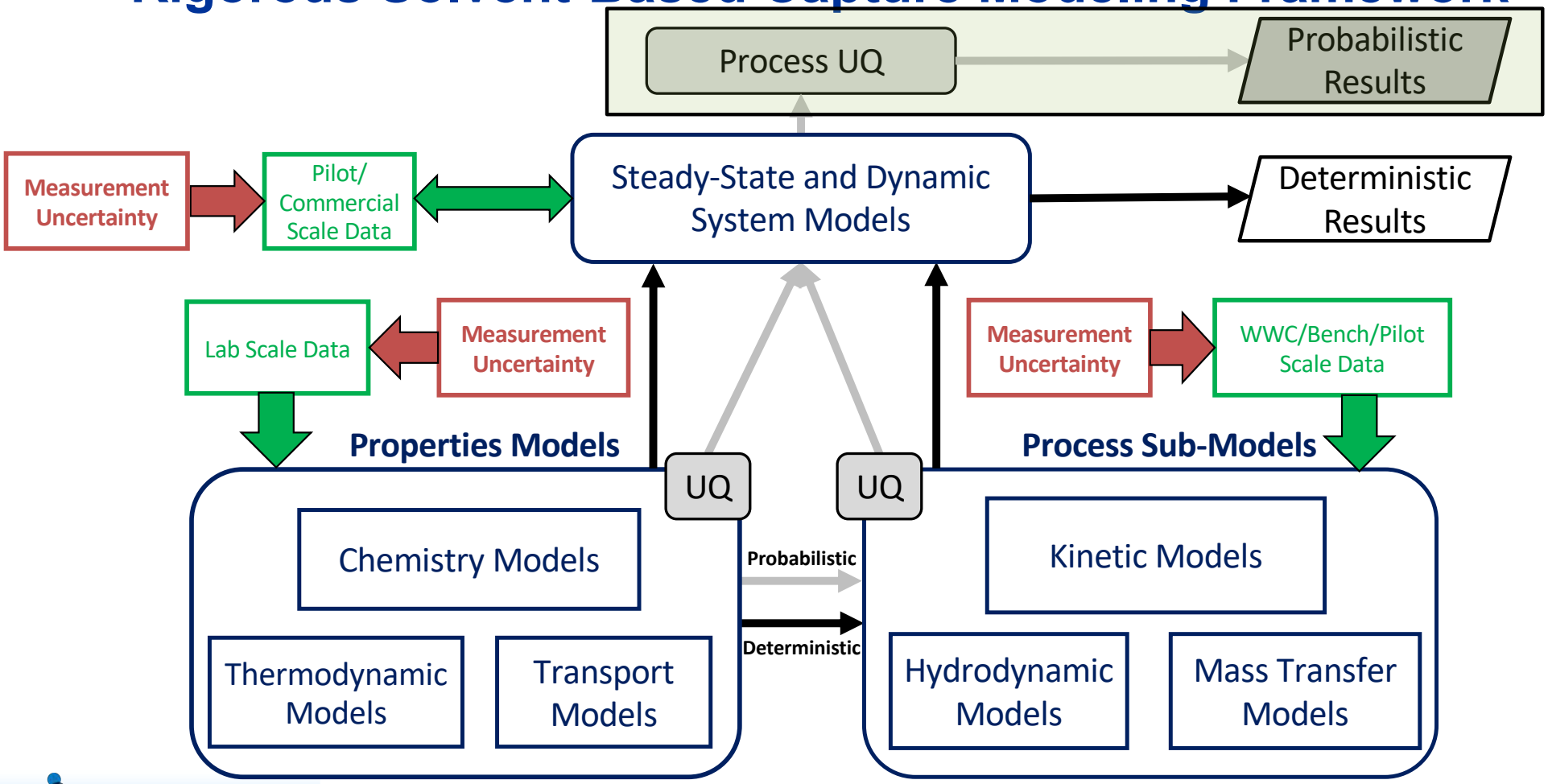
- **Decoupled AB Net (DABNet) model**
  - Data driven model
  - Nonlinear static mapping
    - artificial neural network
- **Multiple-input multiple-output (MIMO)**
- **Options for time delay, linear models, model parameter optimization**
- **Criteria to measure D-RM accuracy for validation**
  - Relative error, R-squared value, UQ analysis with unscented Kalman Filter





*Ma, J., et al. (2016). Computers & Chemical Engineering, 94, 60-74.

Rigorous Solvent-Based Capture Modeling Framework



CCSI Carbon Capture Simulation Initiative

NATIONAL ENERGY TECHNOLOGY LABORATORY

BERKELEY LAB

Lawrence Livermore National Laboratory

Los Alamos NATIONAL LABORATORY

Pacific Northwest NATIONAL LABORATORY

U.S. DEPARTMENT OF ENERGY

CCSI^2

Carbon Capture Simulation for Industry Impact

Technology Centre Mongstad – Summer 2018

www.tcmda.com

Sequential Design of Experiments to Maximize Learning from Carbon Capture Pilot Plant Testing

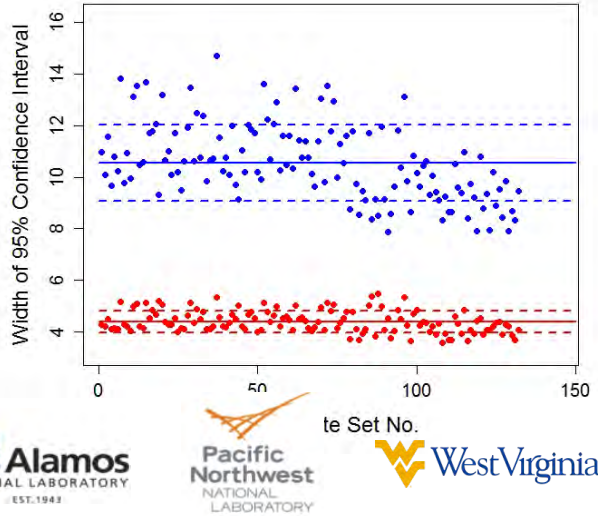
Model + Experiments + Statistics

Ensure right data is collected

Maximize value of data collected

Ultimate Goal

Reduce technical risk associated with scale-up



Prior CI Width: 10.5 ± 1.5

Posterior CI Width: 4.4 ± 0.4

NATIONAL ENERGY TECHNOLOGY LABORATORY

BERKELEY LAB

Lawrence Livermore National Laboratory

Los Alamos NATIONAL LABORATORY EST. 1943

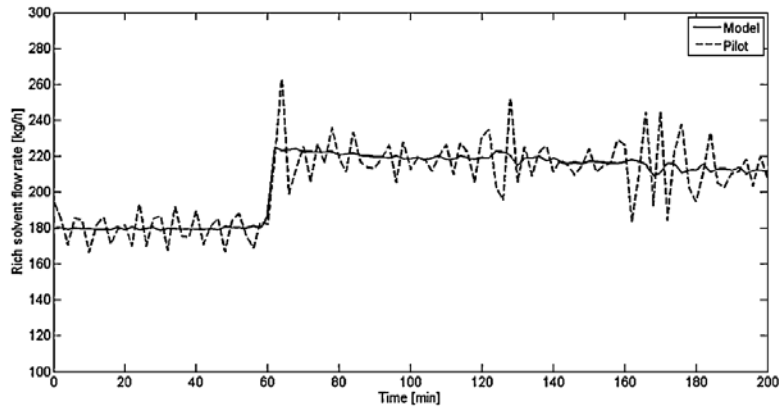
Pacific Northwest NATIONAL LABORATORY

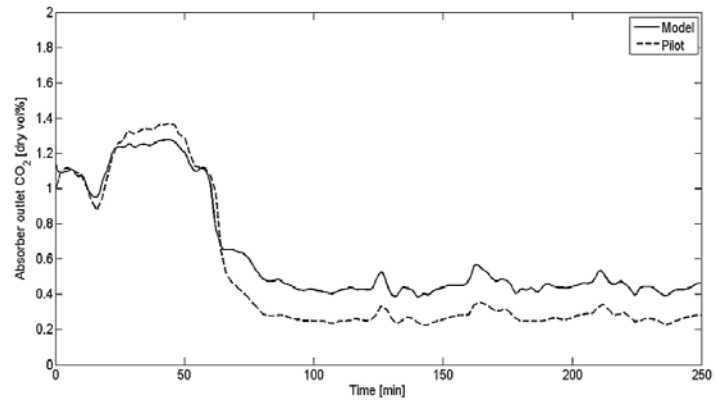
West Virginia University

THE UNIVERSITY OF TEXAS AT AUSTIN

Typical Dynamic Model Validation for Carbon Capture

Dynamic Response due to Step Change in Lean Solvent Flowrate*





- Little work done so far
- Usually single step tests are done mainly for model validation
- Dynamic test runs can provide significantly more information than steady-state test runs in much shorter time thus saving resources and money
- Dynamic tests can be used to estimate parameters corresponding to the accumulation terms, that may not be observable through steady-state tests

Enaasen Flø et al., Dynamic Model Validation of Post-Combustion CO_2 absorption Process, International Journal of Greenhouse Gas Control, 41, 127-141, 2015

Dynamic Experiments Identify Complex Nonlinear Behavior

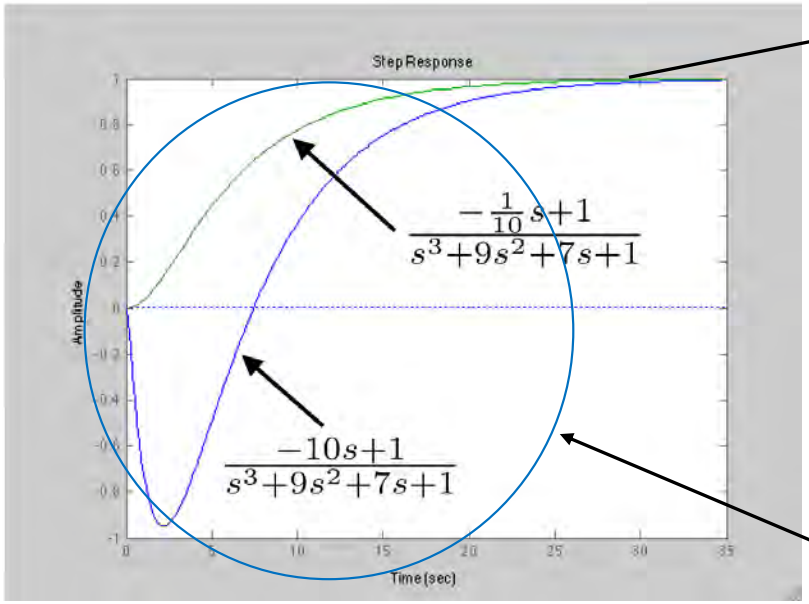
Motivation:

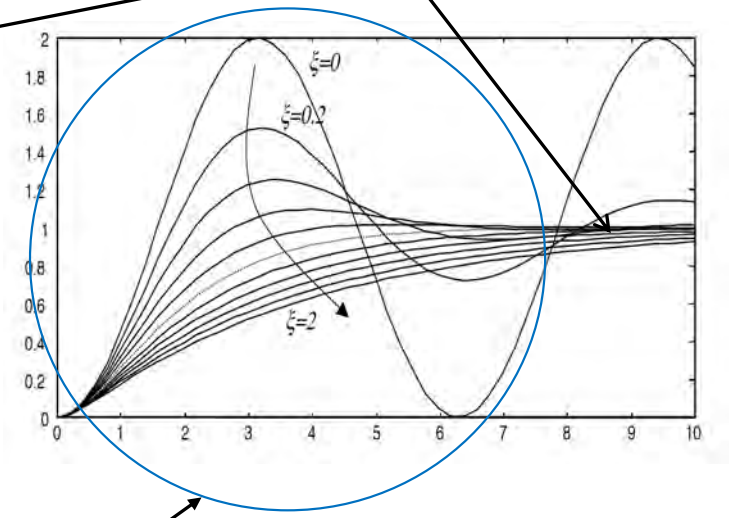
$$\mathbf{H}(\eta, y, u)\dot{\eta} = f(\eta, y, u, \theta)$$
$$\mathbf{g}(\eta, y, u, \theta) \leq 0$$

Normal vs Inverse Response:

Normal vs Oscillatory Response:

Observed in Steady-State Test Runs





Not Observed in Steady-State Test Runs

CCSI Campaigns at the National Carbon Capture Center

- **Steady-State (2014):**
  - Space filling strategy
  - Model Validation
- **Dynamic (2014):**
  - Quasi-PRBS strategy
  - Model Validation
  - Understanding of nonlinear effects
- **Steady-State (2017):**
  - Bayesian DOE strategy
  - Refining of model parameters
- **Dynamic (2017):**
  - PRBS/Multisine DOE strategy
  - Parameter estimation

Dynamic Data Reconciliation and Parameter Estimation

Noisy, inaccurate, and missing measurements

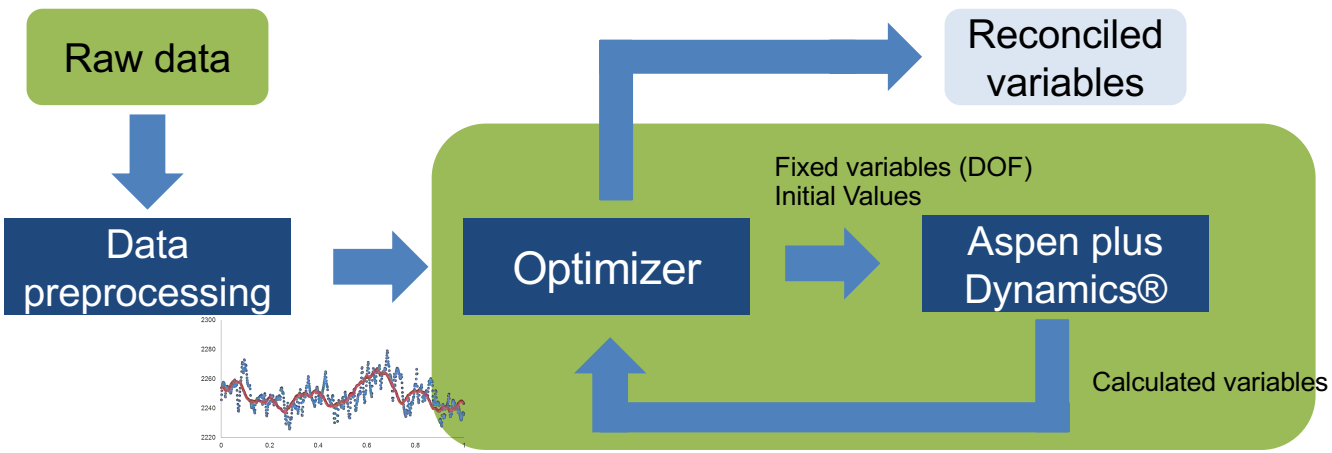
Data reconciliation guarantees mass and energy conservation in the dynamic data

$$\min \ (y^{exp} - y)' \Sigma^{-1} (y^{exp} - y)$$

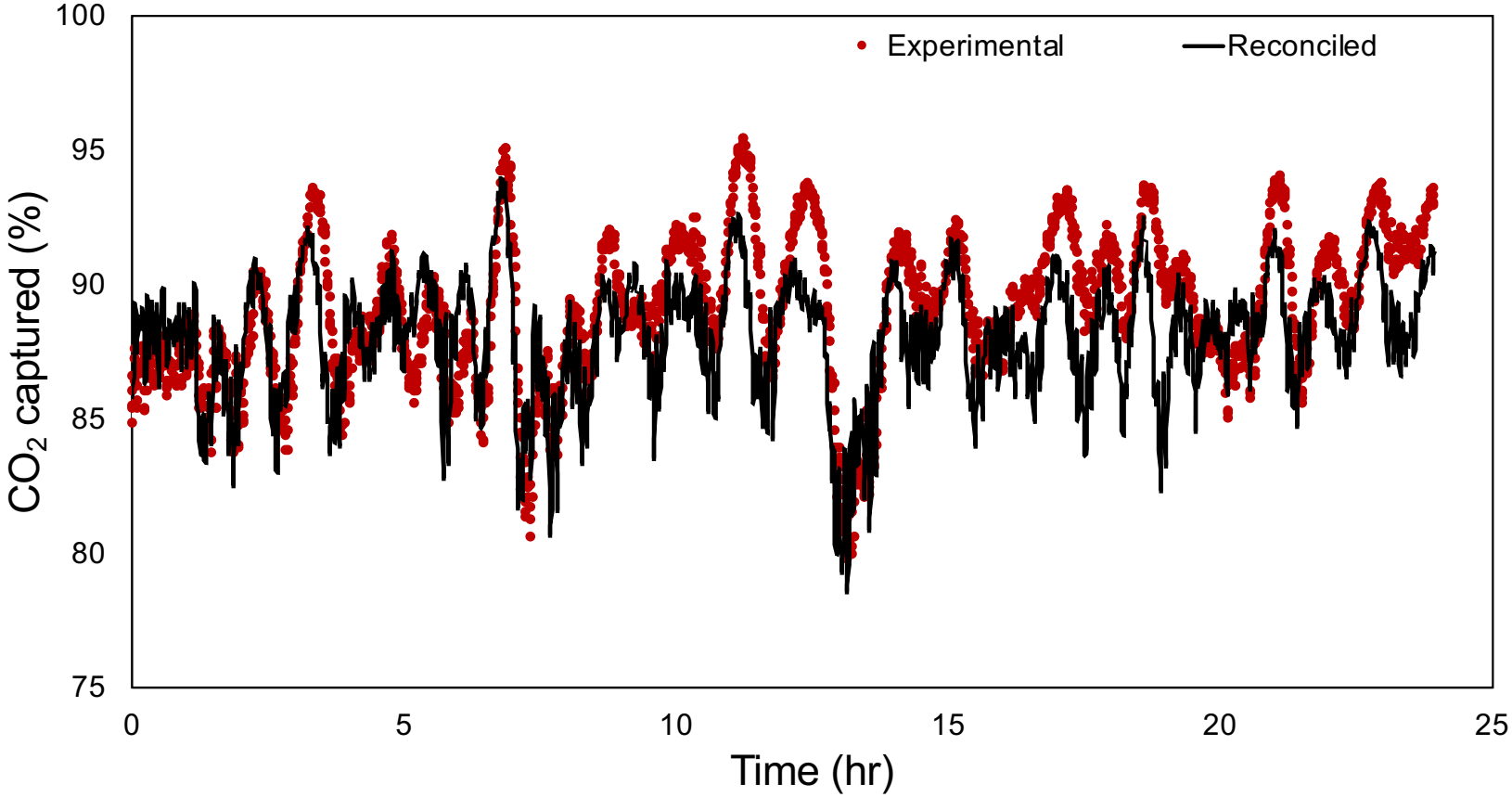
s.t.

$$\mathbf{H}(\eta, y, u, \theta)\dot{\eta} = f(\eta, y, u, \theta)$$

$$\mathbf{g}(\eta, y, u, \theta) \leq 0$$



Model Validation with Dynamic Data Reconciliation



Parameter Estimation via Dynamic Experiments: Holdup Model

Parameter	Original value *	Estimated value
H_{L1}	11.45	11.5
H_{L2}	0.6471	0.39

RMSE analysis (%CO_2 captured)

Dataset	Original holdup parameters	Regressed holdup parameters
Pseudo Random Binary Signal	3.25	3.11
Schroeder-phased input signal	2.15	1.96

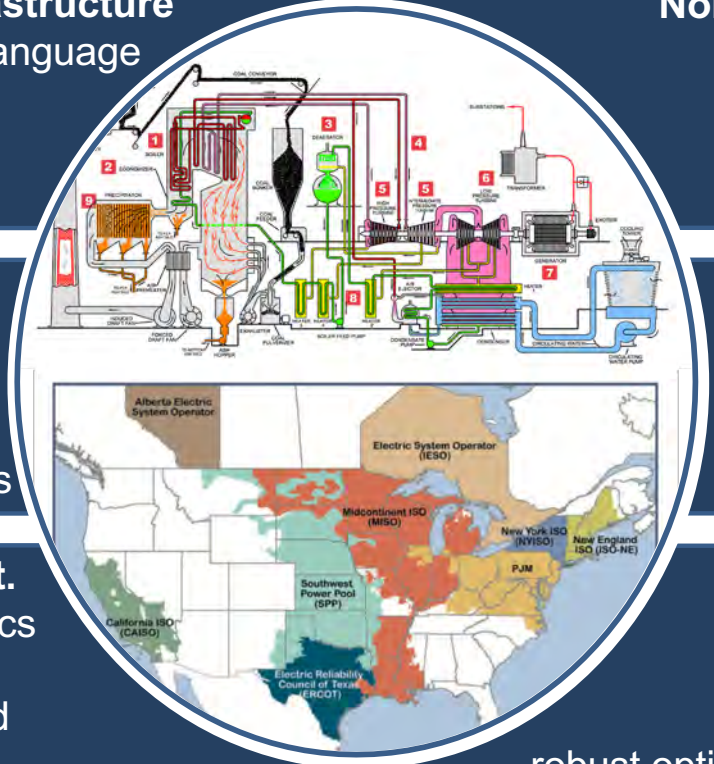
** Soares Chinen, A., et al. "Development of a Rigorous Modeling Framework for Solvent-Based CO_2 Capture. 1. Hydraulic and Mass Transfer Models and Their Uncertainty Quantification." Industrial & Engineering Chemistry Research57.31 (2018): 10448-10463.*

Extending Modeling & Optimization Beyond Commercial Tools

Software and Computational Infrastructure
- open-source, algebraic modeling language with rich programming capabilities
- advanced solvers / architectures
- full data provenance (DMF)

Modeling Framework & Library
- library of process unit operations
- rigorous thermo, properties multiphase physics
- grid operation and planning models

Machine Learning / Parameter Est.
- physical properties, thermodynamics reaction kinetics
- multi-scale surrogate modeling and optimization



Nonlinear Simulation & Optimization
- design, operations, estimation
- optimal control and dynamics, trajectory, state estimation
- rigorous embedded black-box

Discrete Optimization (MILP/NLP)
- design, integration, intensification
- materials optimization
- grid integration, market analysis, grid operations and planning

Uncertainty Quant. / Optimization
- comprehensive, end-to-end UQ
- efficient sensitivity analysis
- two-stage stochastic programming
- robust optimization, adaptive robust optimization

IDAES Institute for the Design of Advanced Energy Systems · NATIONAL ENERGY TECHNOLOGY LABORATORY · BERKELEY LAB · Sandia National Laboratories · Carnegie Mellon · West Virginia University · UNIVERSITY OF NOTRE DAME

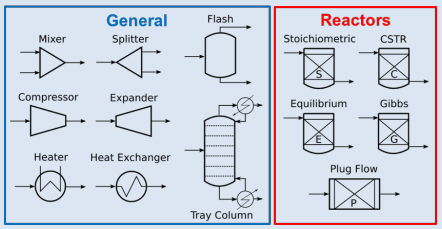
Optimization-Based Machine Learning for Physical Properties Thermodynamics & Reaction Kinetics

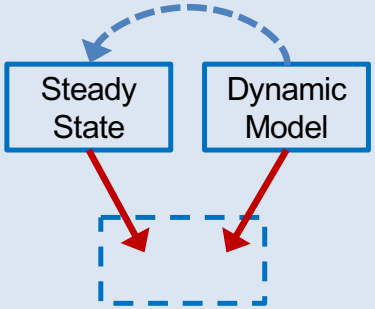
ALAMO
a black-box modeling tool

HELMET

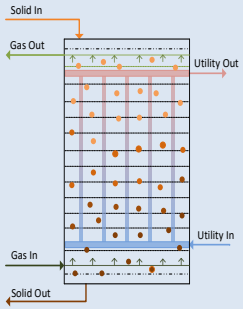
RIPE

Hierarchical Process Model Library





Model Customization

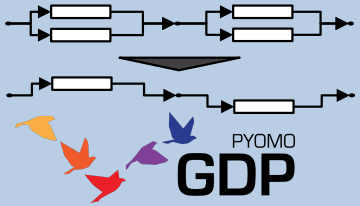


PYOMO

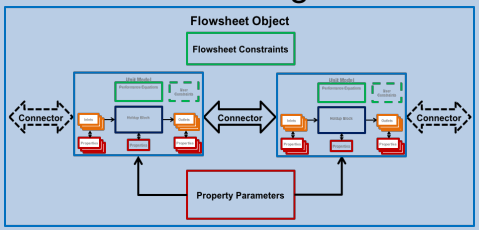
PYOMO DAE

Algebraic Modeling Language

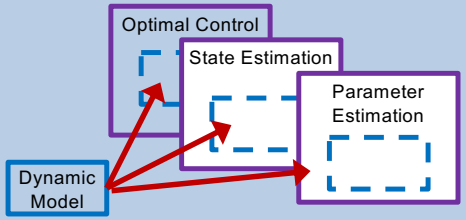
Conceptual Design via Superstructure



Process Design & Optimization Process Integration

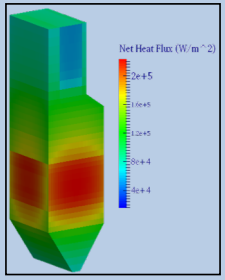


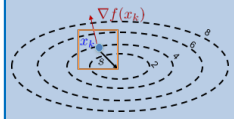
Dynamics & Control

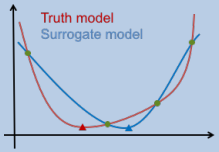


Multi-Scale Surrogate Modeling & Optimization

ALAMO
a black-box modeling tool

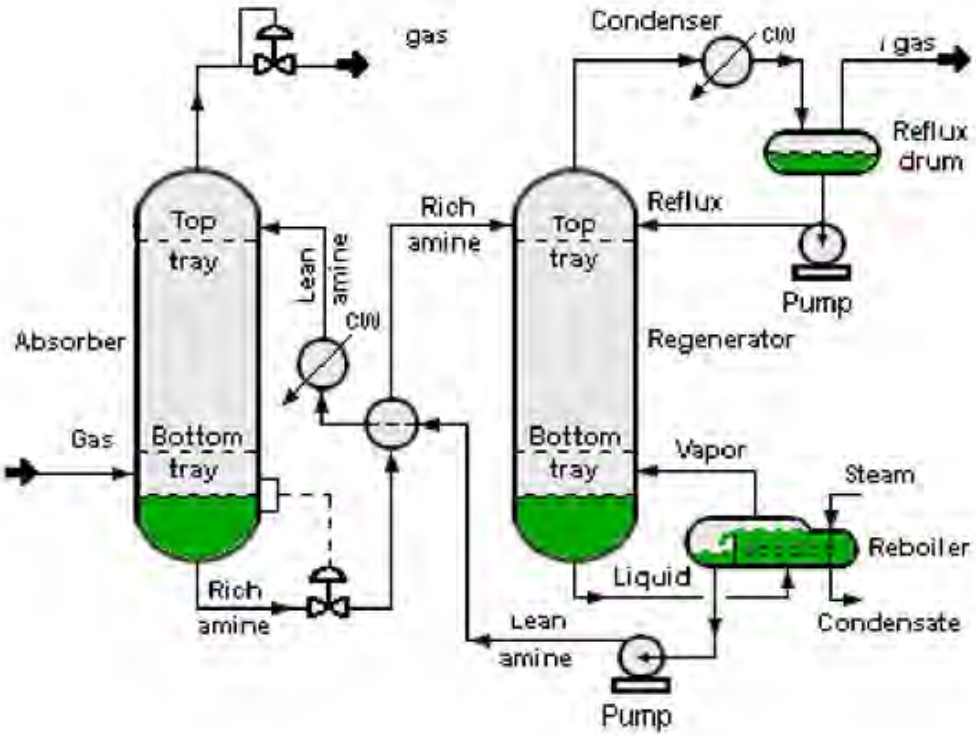


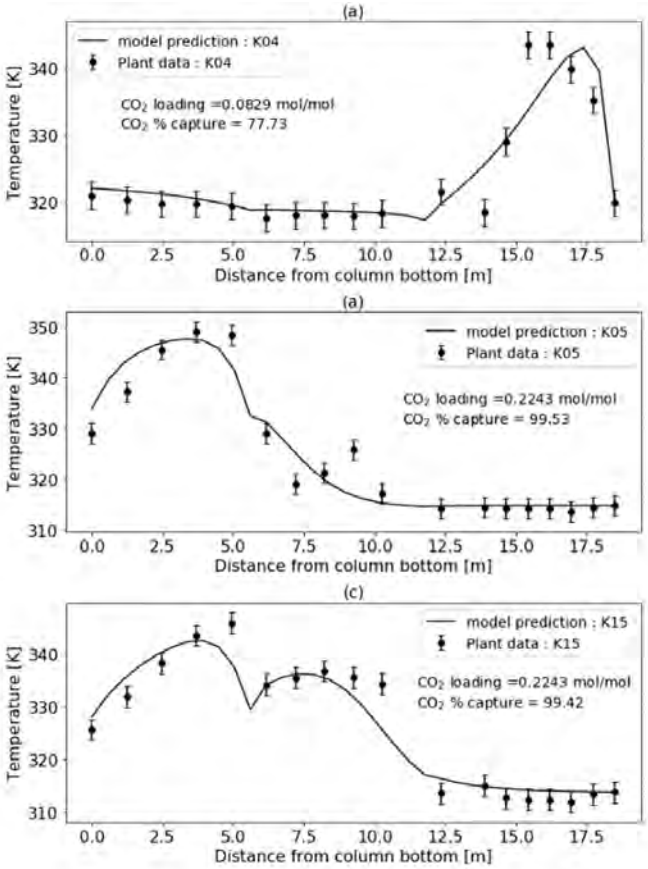




IDAES Institute for the Design of Advanced Energy Systems · NATIONAL ENERGY TECHNOLOGY LABORATORY · BERKELEY LAB · Sandia National Laboratories · Carnegie Mellon · West Virginia University · UNIVERSITY OF NOTRE DAME

Dynamic, Two-Film Tower Model for an Electrolyte System





CCSI^2

Carbon Capture Simulation for Industry Impact

acceleratecarboncapture.org

https://github.com/CCSI-Toolset/

IDAES

Institute for the Design of Advanced Energy Systems

idaes.org

https://github.com/IDAES

David C. Miller, Ph.D.

Senior Fellow

National Energy Technology Laboratory

David.Miller@NETL.DOE.GOV

We graciously acknowledge funding from the U.S. Department of Energy, Office of Fossil Energy, through the Crosscutting Research and Carbon Capture Programs.