CCSI

Carbon Capture Simulation Initiative

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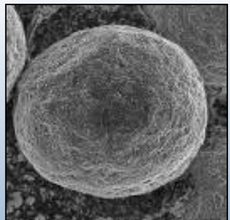
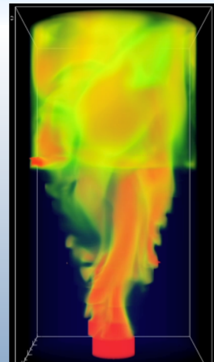
CCSI For Accelerating Technology Development

Carbon Capture Simulation Initiative






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**

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GE
EPRI Electric Power Research Institute
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Phillips 66
AEP American Electric Power
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invensys
PSE

Motivation and Timeline

- 2009: Carbon Regulations Imminent
- How can development & commercialization be accelerated while minimizing cost and risk?
- Role of advanced simulation & modeling in accelerating development, scale up and commercialization
  - Build on existing modeling & simulation tools used by industry
- 2010: Multi-lab - industry working group
- HQ organized Scientific Peer Review: Jan 25, 2011
- Preliminary Release of CCSI Toolset: September 2012
  - Five companies sign Test & Evaluation License
- 2013 Toolset Release: October 31, 2013

Goals

- **Develop** new computational tools and models to enable industry to more rapidly develop and deploy new advanced energy technologies

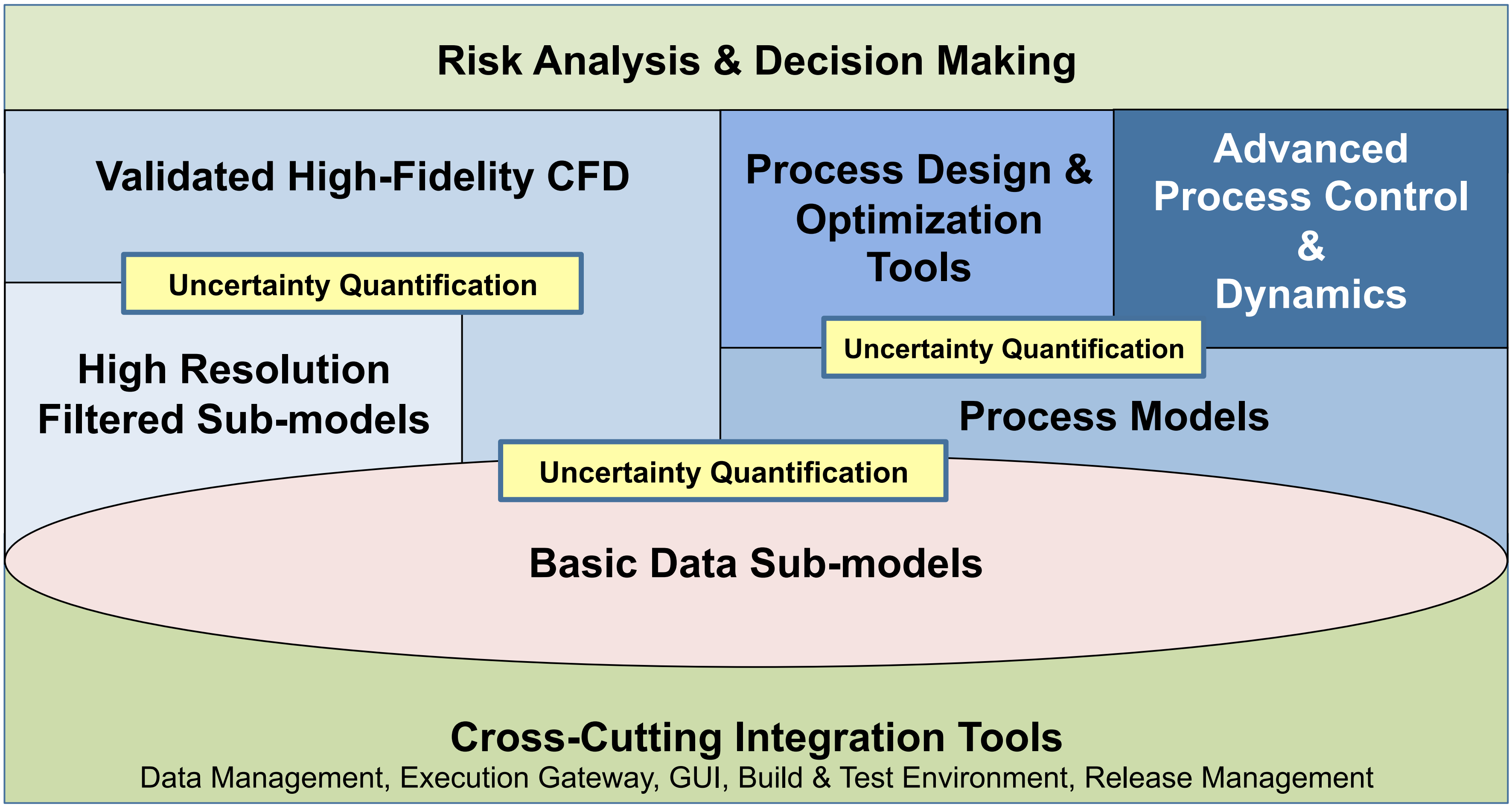
- **Demonstrate** the capabilities of the CCSI Toolset on non-proprietary case studies
  - Solid sorbent
  - Solvent system

- **Deploy** the CCSI Toolset to industry
  - Support initial industry users
  - Feedback on features and capabilities

Challenges of Simulating Carbon Capture (and other) Processes

- **Multiple Scales**
  - **Particle**: individual adsorbent behavior, kinetics and transport
  - **Device**: fluid and heat flows within a sorbent bed
  - **Process**: integration of devices for a design of a complete sorbent system
- **Integration across scales**
  - Effective simplifications
    - Detailed models too complex to integrate/optimize
- **Verification/Validation/Uncertainty**
  - Create confidence in predictions of models
- **Decision support**
  - Evaluate key process performance issues affecting choices of technology deployment/investment

Advanced Computational Tools to Accelerate Carbon Capture Technology Development



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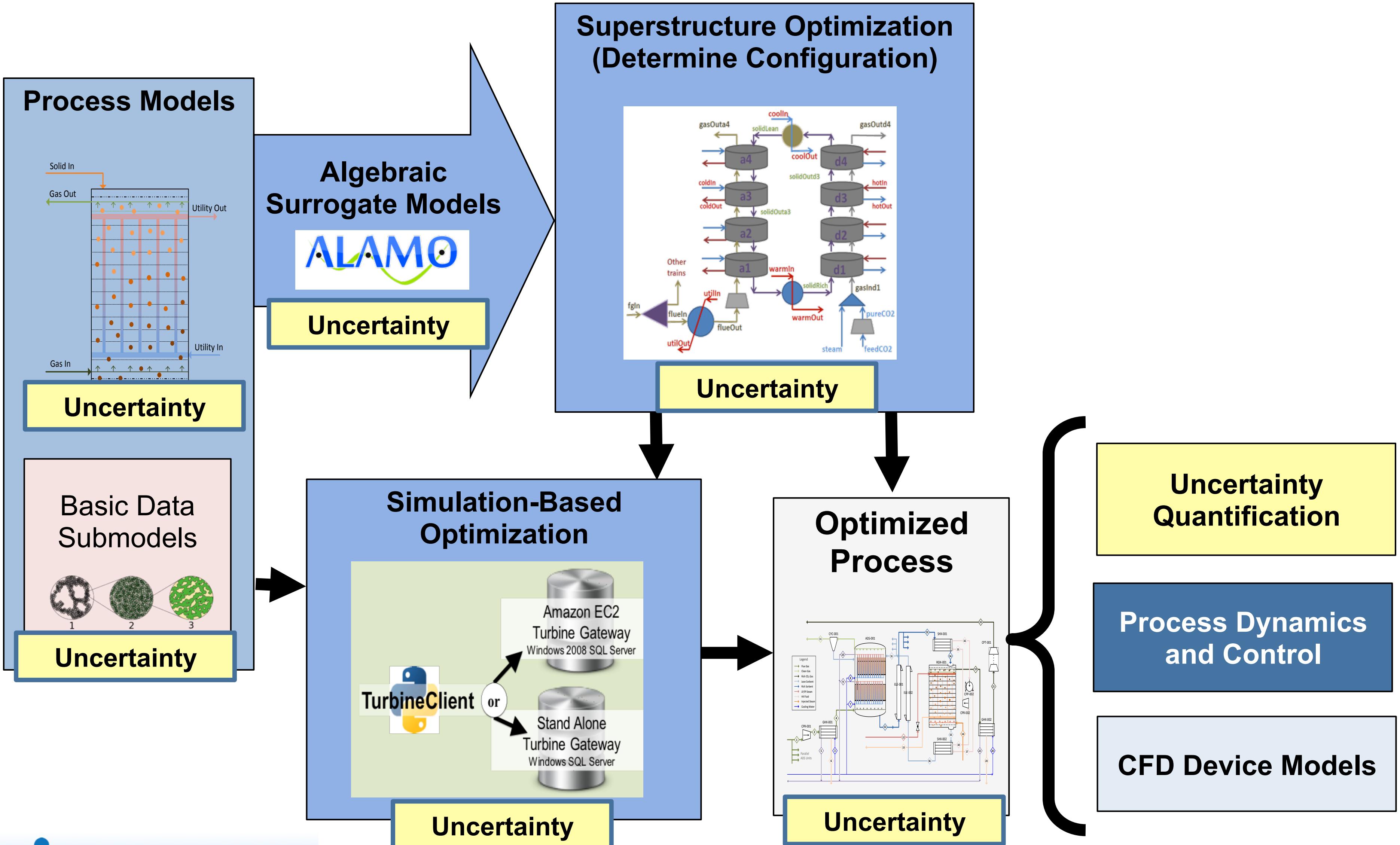
Tools to develop an optimized process using rigorous models



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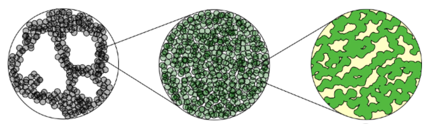
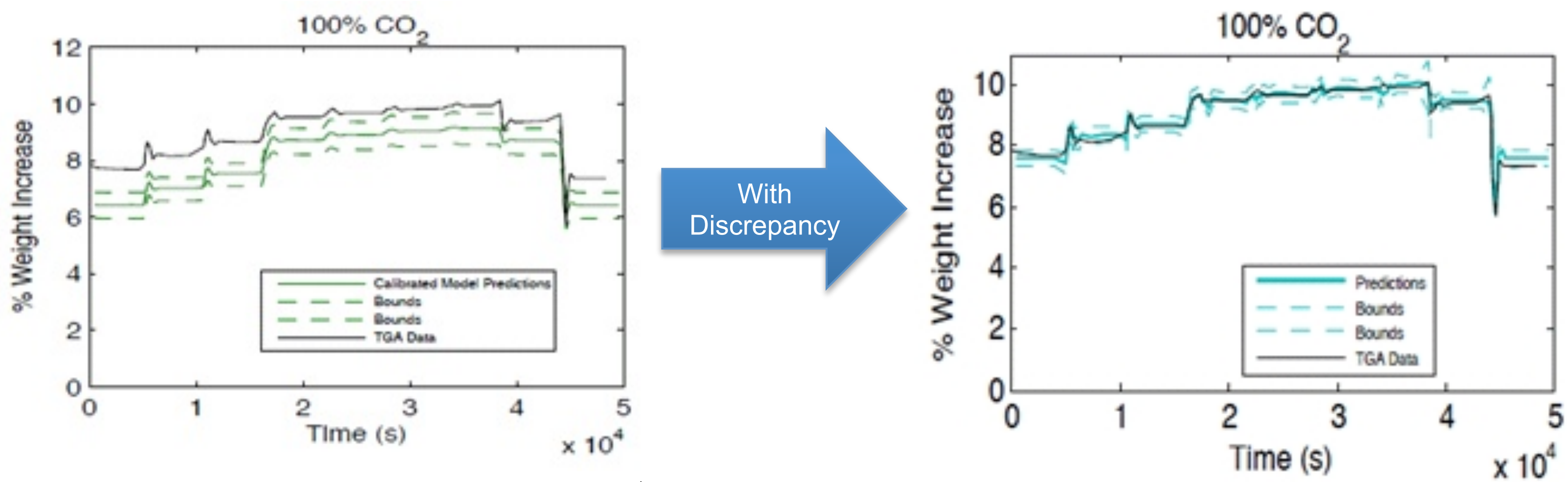
PEI-Impregnated Silica Sorbent Reaction Models

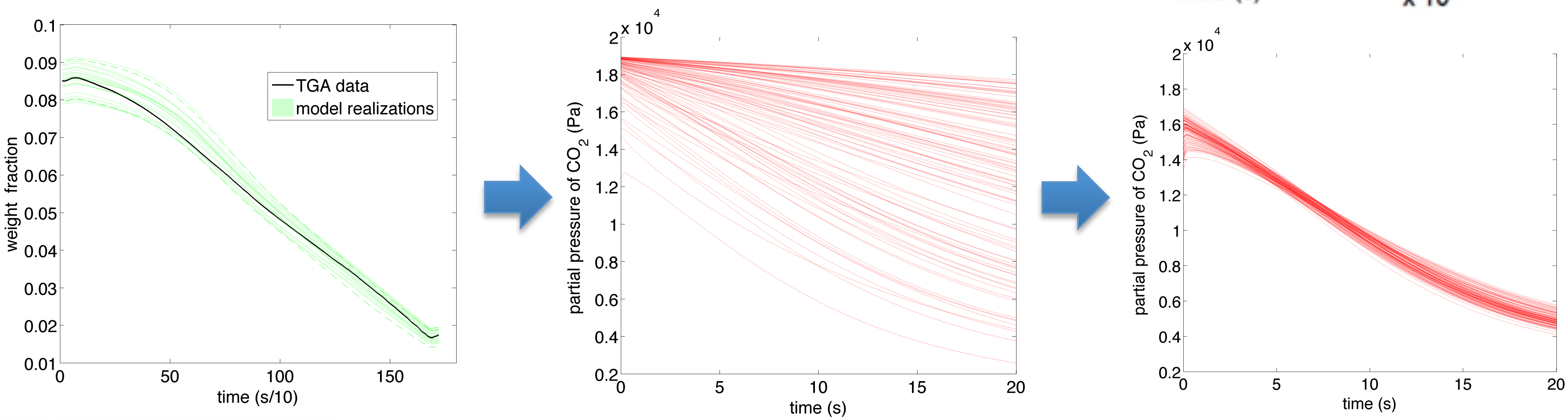


$$2R_2NH + CO_2(gas) \rightleftharpoons R_2NCO_2^- + R_2NH_2^+$$

$$R_2NH + H_2O(phys) + CO_2(gas) \rightleftharpoons HCO_3^- + R_2NH_2^+$$

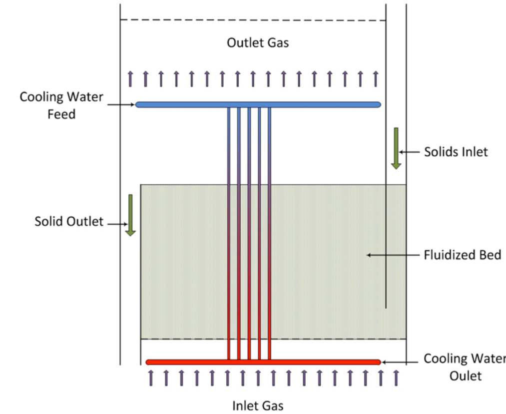
$$H_2O(gas) \rightleftharpoons H_2O(phys)$$



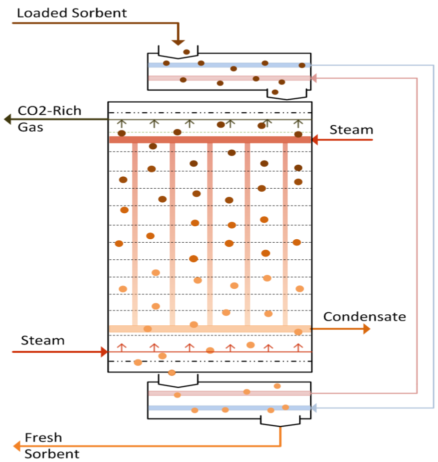


Process Models

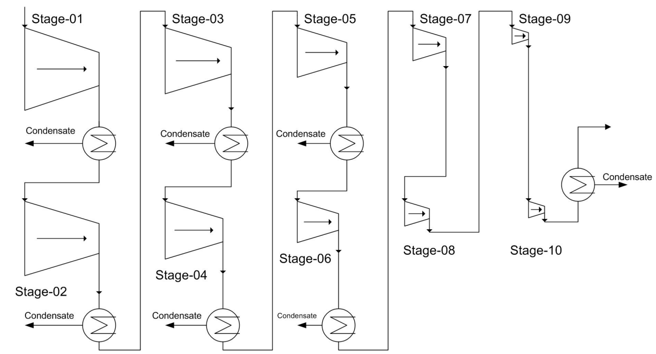
Bubbling Fluidized Bed (BFB) Model
- 1-D, nonisothermal with heat exchange
- Unified steady-state and dynamic
- Adsorber and Regenerator
- Variable solids inlet and outlet location
- Modular for multiple bed configurations



Moving Bed (MB) Model
- 1-D, nonisothermal with heat exchange
- Unified steady-state and dynamic
- Adsorber and Regenerator
- Heat recovery system



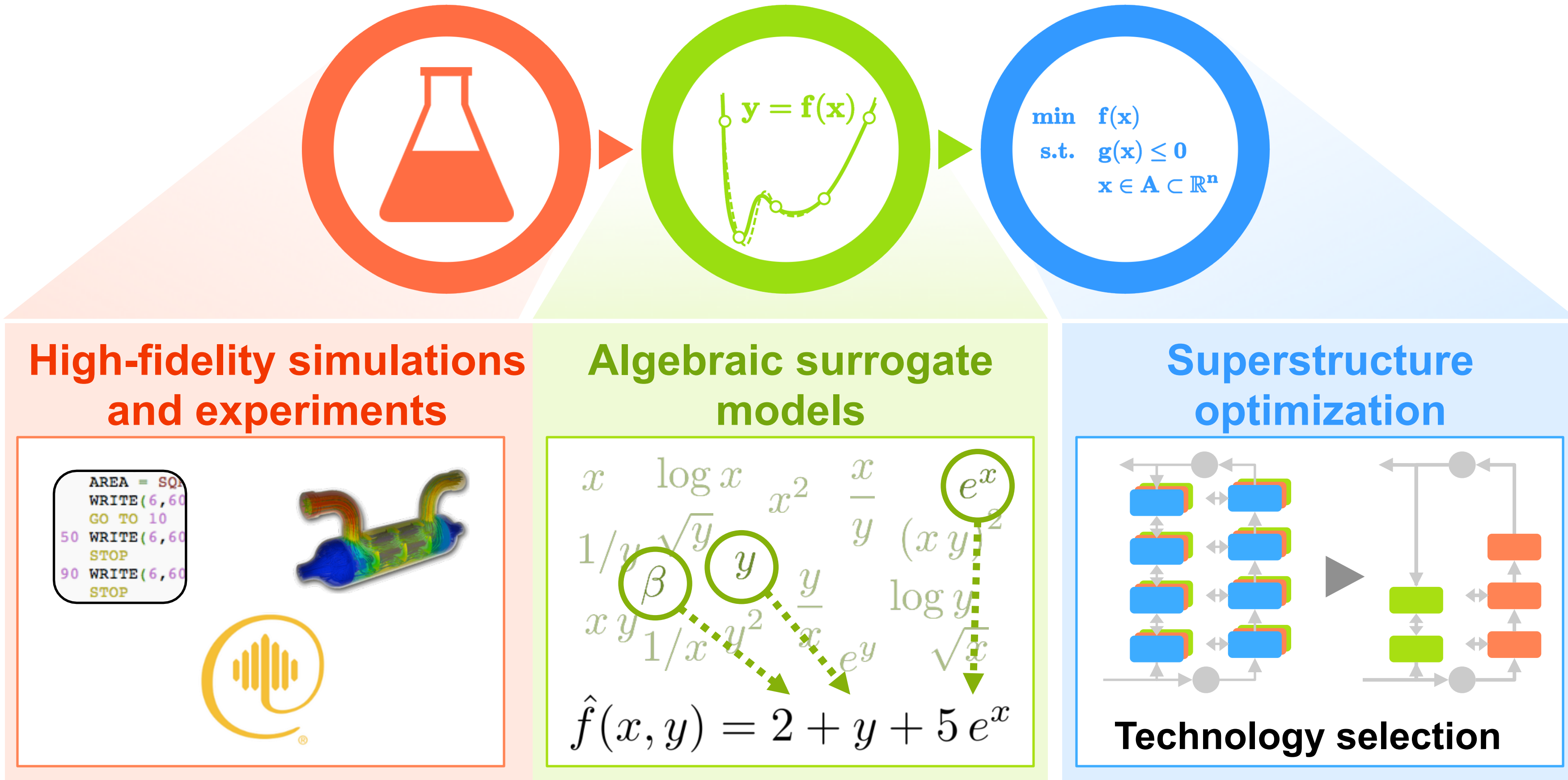
Compression System Model
- Integral-gear and inline compressors
- Determines stage required stages, intercoolers
- Based on impeller speed limitations
- Estimates stage efficiency
- CO_2 drying (TEG absorption system)
- Off-design performance.
- Includes surge control algorithm



ALAMO

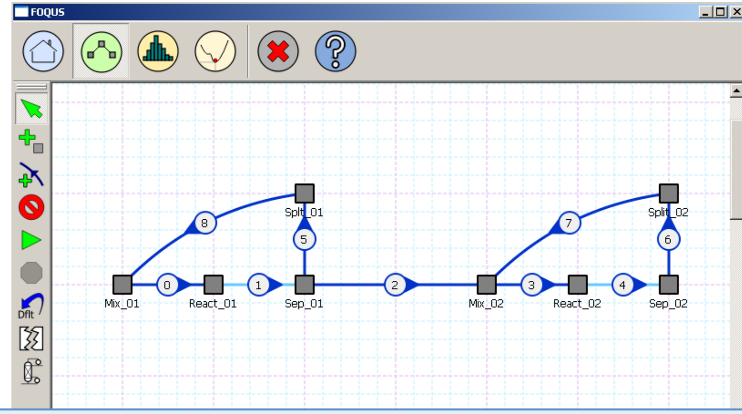
Automated Learning of Algebraic Models for Optimization

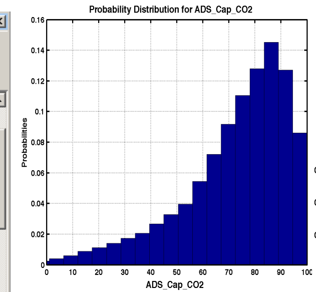
Simplifying the balance between optimal decision-making and model fidelity through tailored simple surrogate models

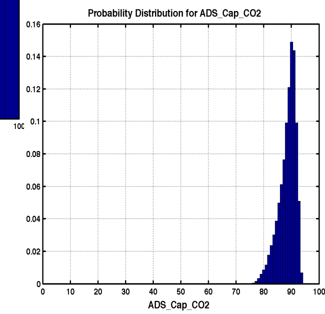


Framework for Optimization and Quantification of Uncertainty and Sensitivity

FOQUS







Derivative Free Optimization or Uncertainty Quantification Sample Generation

Sample Set

Result Set

Parallel Flowsheet Execution

Meta-Flowsheet

Meta-Flowsheet

Meta-Flowsheet

- Connects to Turbine/SimSinter to run simulations.

Heat Integration

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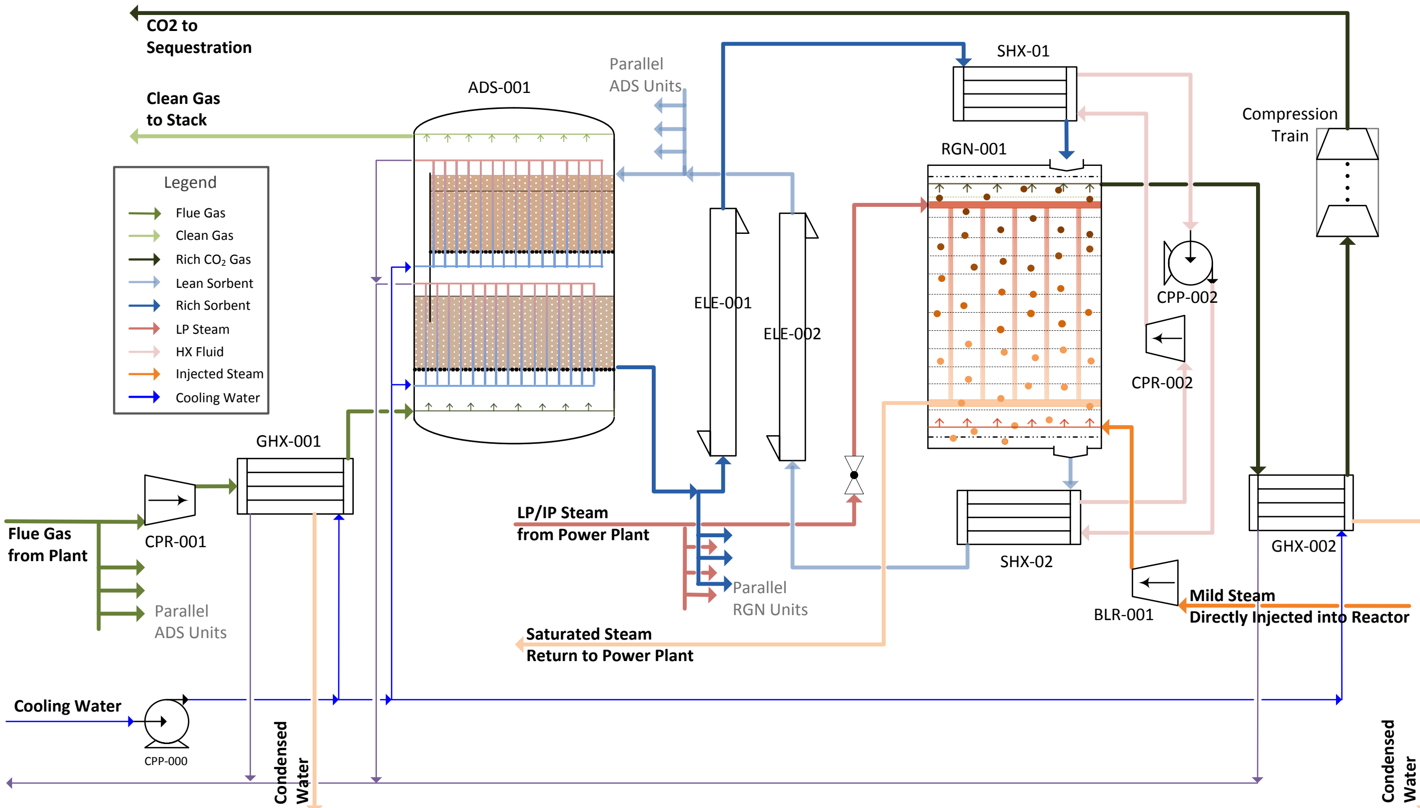
Optimized Process Developed using CCSI Toolset



ΔLoading
1.8 mol CO2/kg
0.66 mol H2O/kg

	Solid Sorbent	MEA (Δ10°C HX)	MEA (Δ5°C HX)
Q_Rxn (GJ/tonne CO2)	1.82	1.48	1.48
Q_Vap (GJ/tonne CO2)	0	0.61	0.74
Q_Sen (GJ/tonne CO2)	0.97	1.35	0.68
Total Q	2.79	3.44	2.90

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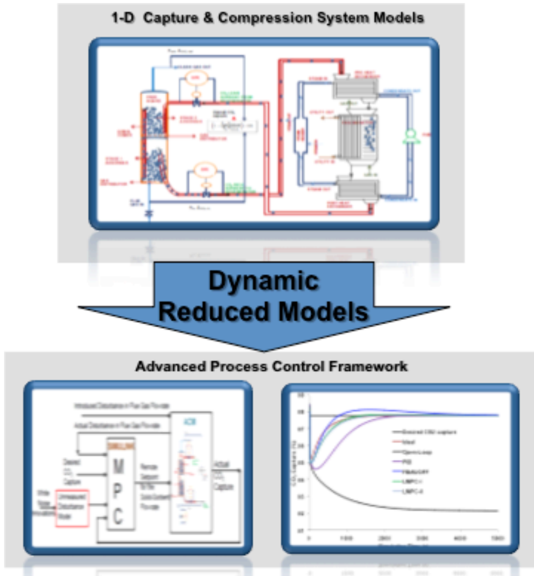
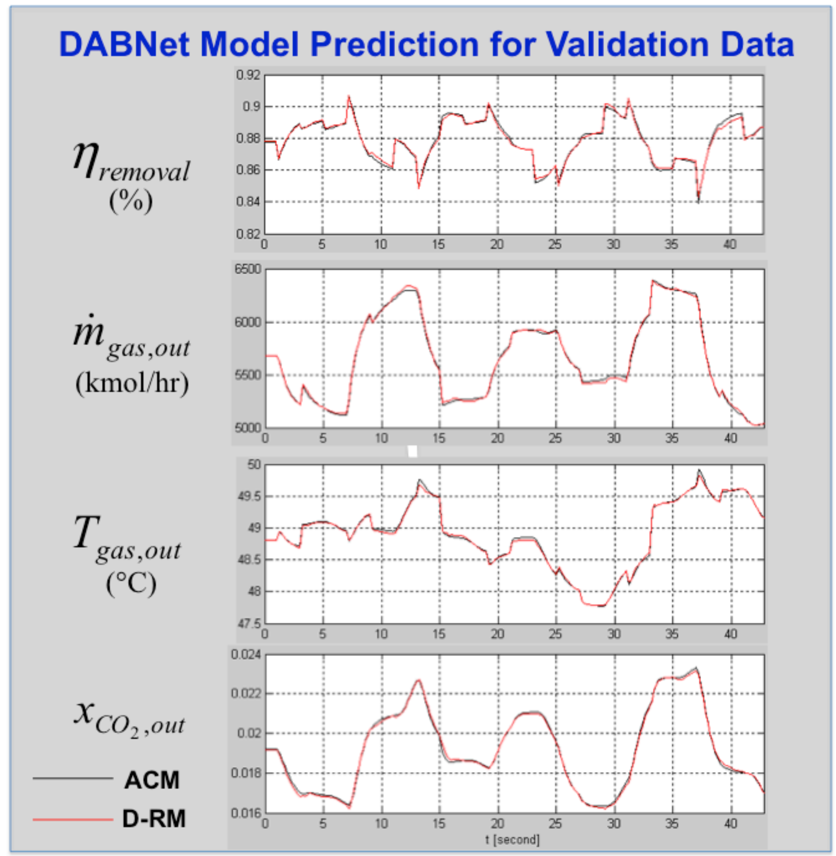
Dynamic Reduced Model Builder



- **Automatic D-RM Generation**
  - Use high-fidelity ACM/APD models embedded in Simulink to create data-driven black-box D-RMs as MATLAB script files (.m files)
- **GUI Driven Workflow**
- **Data-driven Black-Box Methods**
  - Nonlinear Autoregressive Moving Average (NARMA) based on Neural Networks
  - Decoupled A-B Net (DABNet)

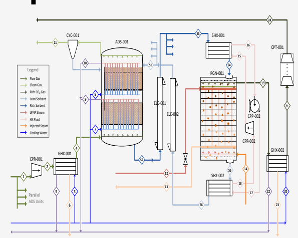
Example (BFB Reactor/Adsorber)

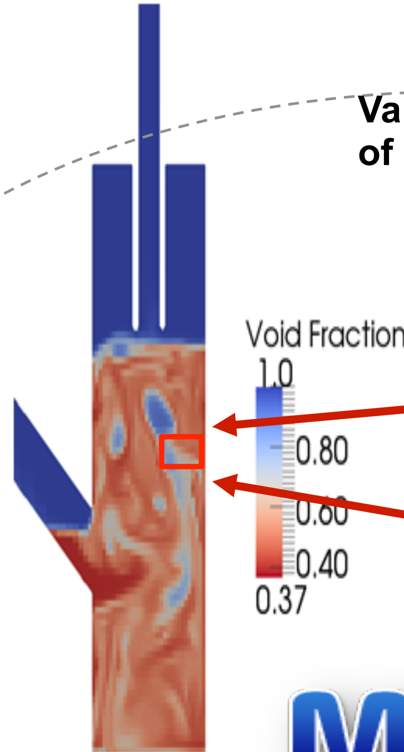


Simulation & Experiments to reduce time for design/troubleshooting

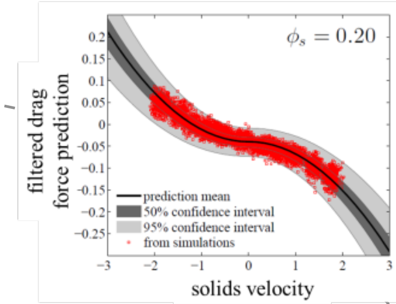
Experimental Validation

Process Models & Optimized Process

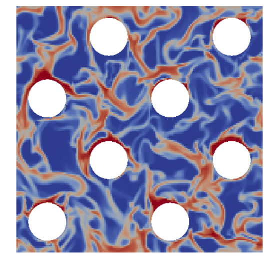




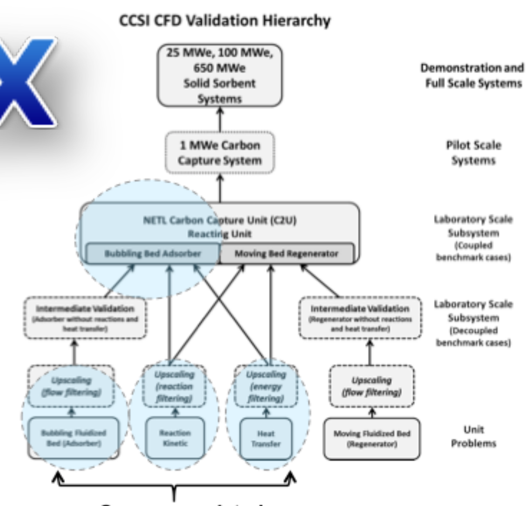
Validation and UQ of Filtered Models



$$f^*_{drag} = \beta^*\left(-v_s^*\left|v_s^*\right|\right) + \gamma^*$$

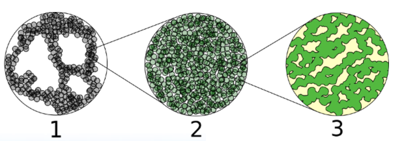


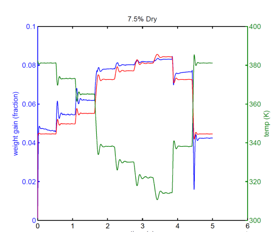
MFiX



Void Fraction along vertical center plane

SORBENTFIT

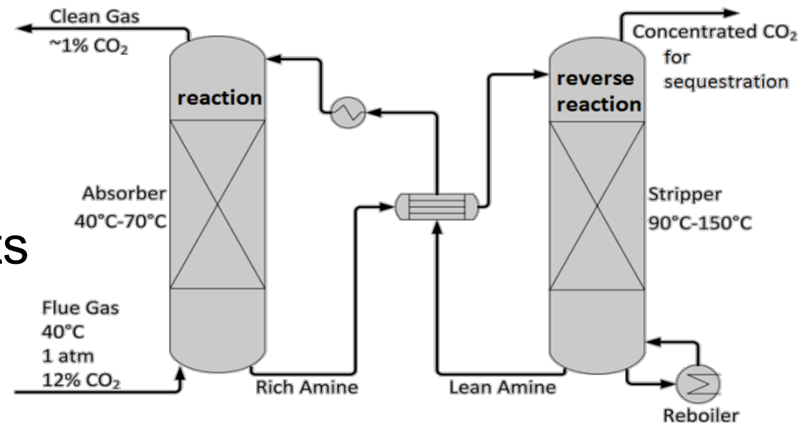


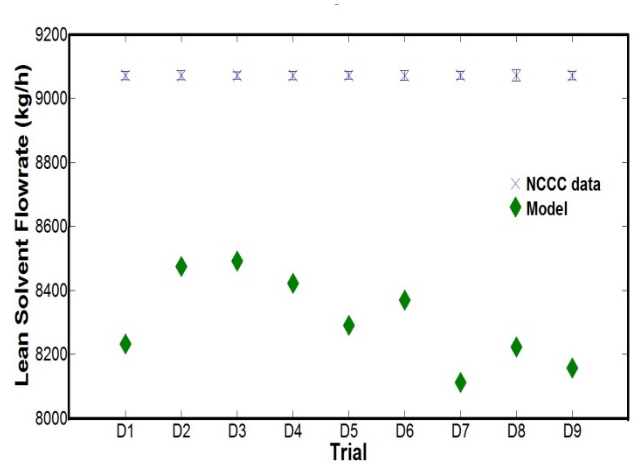


Experimental Kinetic/Mass Transfer Data

Solvent Systems: Validation & High Viscosity

- **National Carbon Capture Center**
  - Pilot Scale Data
- **MEA System Model "Phoenix"**
  - UT Austin pilot plant & experiments
- **Utilize UQ Tools**
  - Physical property models
  - Reaction models
  - Process models
  - Model parameters
  - Experimental data
- **Effective prediction of high viscosity systems**
  - 2-MPZ as a demonstration solvent





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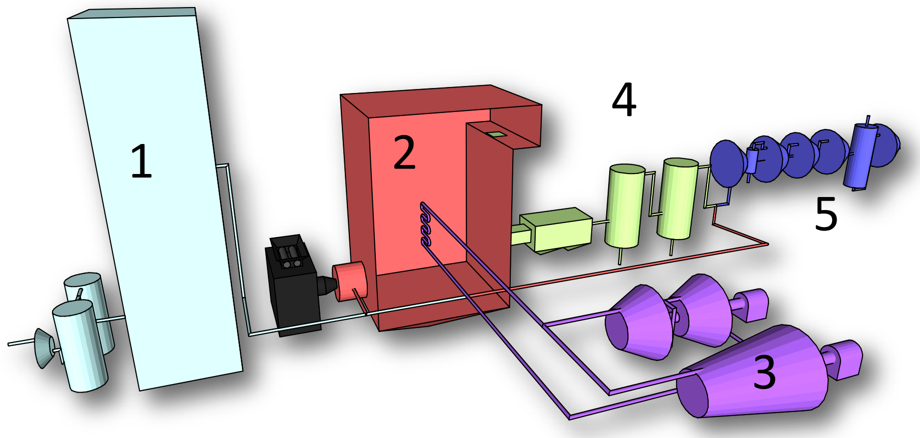
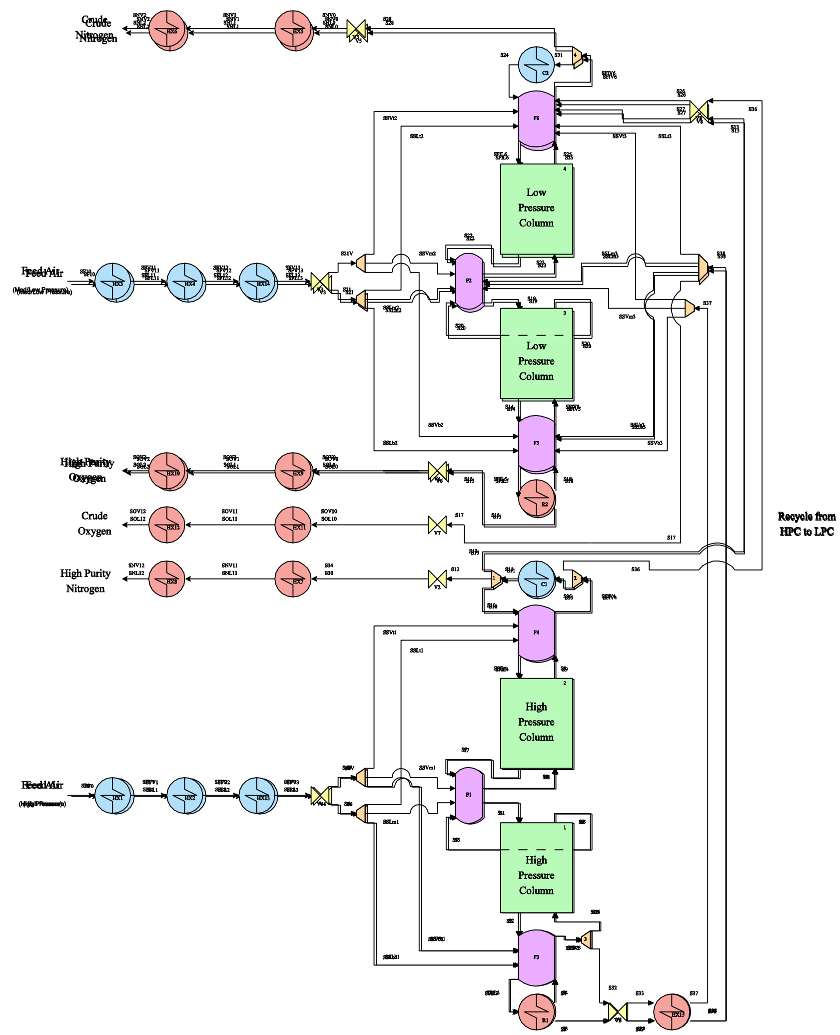
Oxy-combustion Process Synthesis: Fully Equation-Based



1. Air Separation Unit
2. Boiler
3. Steam Turbine
4. Pollution Controls
5. CO_2 Compression Train

- Rigorous models to capture trade-offs between subsystems
- Large scale optimization algorithms
- Energy consumption matches industry results
- Open models allow for integration with other systems

Air Separation Unit



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Status	Name	
NEW	High viscosity solvent model (2-MPZ)	***Basic Data Submodels***
UPDATED	SorbentFit	
NEW	Attrition Model	***High Resolution Filtered Submodels***
NEW	Cylinder Filtered Models	
	1 MW Adsorber and Regenerator CFD Models	***Validated high-fidelity CFD models & UQ tools***
NEW	AX Cold Flow MFIX CFD Models	
NEW	BSS-ANOVA-UQ Statistics Model Validation Tool	
UPDATED	Reduced Order Modeling Tools for CFD (REVEAL) and ROM Integration Tools	
UPDATED	Bubbling Fluidized Bed Reactor Model	***Process Models***
UPDATED	Moving Bed Reactor Model	
UPDATED	Multi-stage Centrifugal Compressor Model	
UPDATED	Membrane CO_2 Separation Model	
UPDATED	Reference Power Plant Model	
NEW	FOQUS (requires PSUADE for UQ)	***Optimization and UQ Tools***
UPDATED	ALAMO	
UPDATED	Process Synthesis Superstructure	
NEW	Oxy-Combustion Process Optimization Model	
NEW	D-RM Builder	***Dynamics & Control***
NEW	Technical Risk Model	***Risk Analysis Tools***
UPDATED	Financial Risk Model	
NEW	SimSinter (includes CCSIUnits)	***Crosscutting Integration Tools***
NEW	Turbine Science Gateway (Local)	
UPDATED	Turbine Client	

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