# CCSI

Carbon Capture Simulation Initiative

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U.S. Department of Energy
National Energy Technology Laboratory

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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**

**National Labs**

Pacific Northwest National Laboratory · NETL · Los Alamos National Laboratory · Lawrence Livermore National Laboratory

**Academia**

Carnegie Mellon · Princeton University · West Virginia University · Boston University · The University of Texas at Austin

**Industry**

ADA · Alstom · B&W · GE · EPRI Electric Power Research Institute · Fluor · Southern Company · Phillips 66 · American Electric Power · Southern California Edison · Chevron · ExxonMobil · Air Products · URS · Eastman · ANSYS · aspentech · invensys · PSE

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## Goals & Objectives

- **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 32D
  - Solvent system
- **Deploy** the CCSI Toolset to industry
  - Support initial industry users
  - Obtain feedback on features and capabilities
  - Arrange for long term commercial licensing



## CCSI Timeline

- Organizational Meetings: March 2010 - October 2010
- **Technical work initiated: Feb. 1, 2011**
- **Preliminary Release of CCSI Toolset: September 2012**
  - Initial licenses signed
- CCSI Year 3 starts Feb. 1, 2013
  - Began solvent modeling/demonstration component
- **2013 Toolset Release: October 31, 2013**
  - **Multiple tools and models released and being used by industry**
- **Future**
  - **2014 Toolset Release: October 31, 2014 – planned**
  - **Final release and workshop late 2015**
  - **Commercial licensing late 2015 or early 2016**

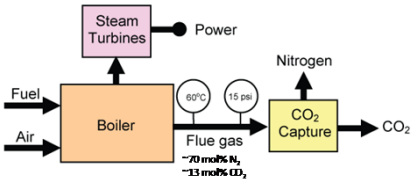
## Challenges associated with carbon capture

- Fossil energy systems currently generate
  - 67% of the US electricity
    - 42% coal, 25% natural gas
  - 65% worldwide electricity
- Large-scale problem
  - 2 billion tons/year $CO_2$ emitted from coal by 2020 in US
  - Flue gas: 5 million lb/hr for 550MW PC plant (630 kg/s)
- No existing economical solution
- Need for process optimization to fully evaluate technology options

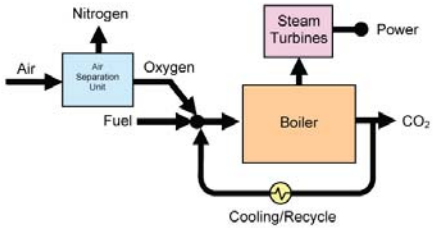
U.S. Energy Information Administration, Annual Energy Outlook 2013 Early Release Overview. Report Number: DOE/EIA-0383ER(2013), http://www.eia.gov/forecasts/aeo/er/pdf/0383er%282013%29.pdf (2013).
U.S. Energy Information Administration, International Energy Outlook 2011. Report Number: DOE/EIA-0484(2011), http://www.eia.gov/forecasts/ieo/pdf/0484%282011%29.pdf (2011).



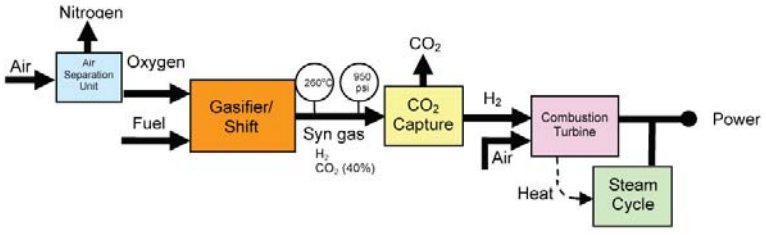
## Post-combustion capture (PC)



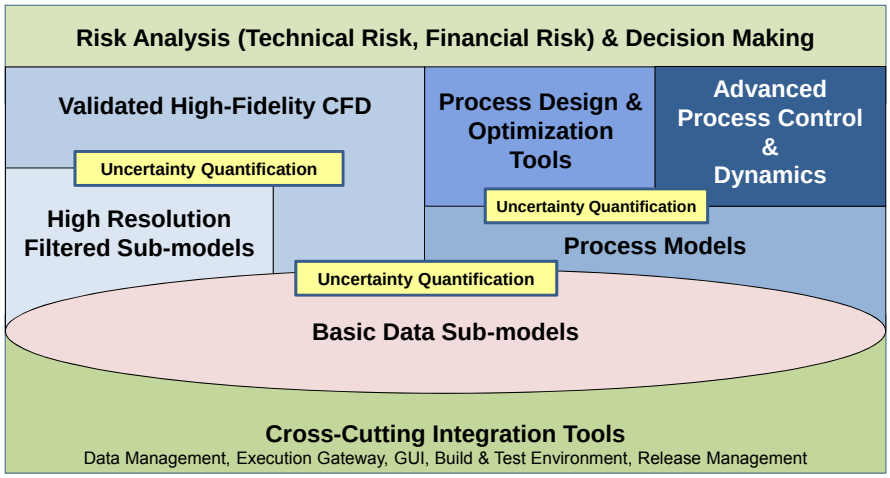

## Oxycombustion (PC)




## Pre-combustion capture (IGCC)



## Advanced Computational Tools to Accelerate Carbon Capture Technology Development

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## Carbon Capture (and other process) Simulation Grand Challenges

- **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 tools 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

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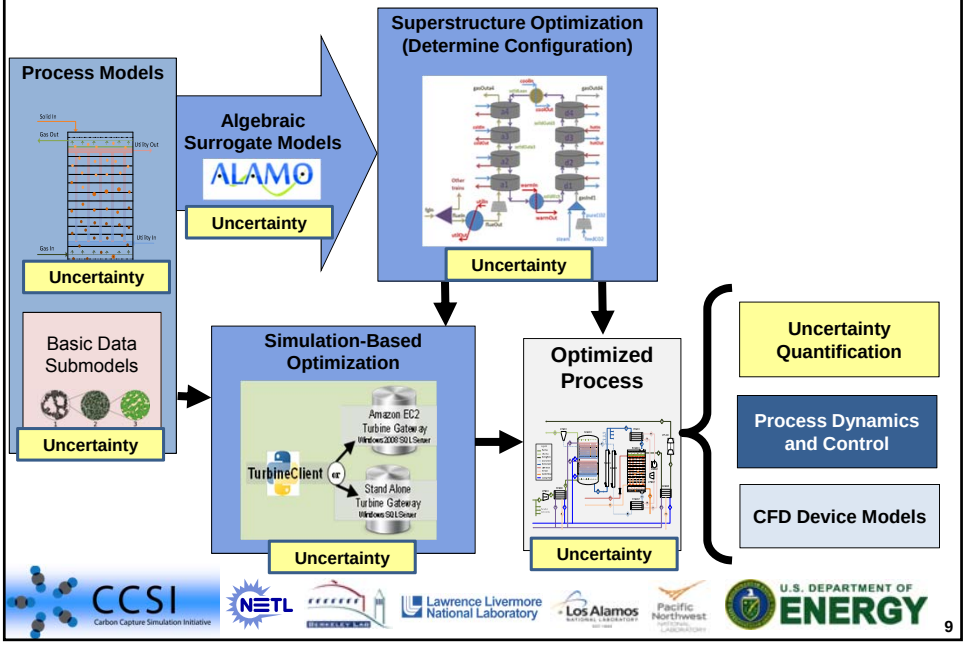
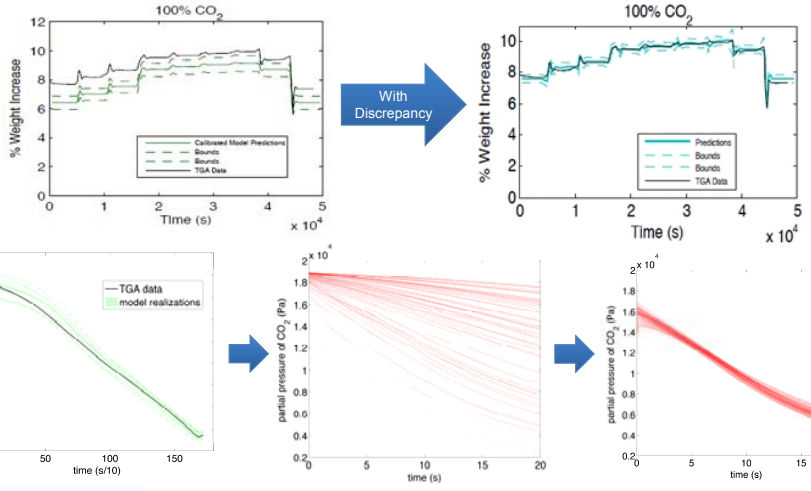
## Tools to develop an optimized process using rigorous models






## PEI-Impregnated Silica Sorbent Reaction Models

$$2R_2NH + CO_2(gas) \rightleftharpoons R_2NCO_2^- + R_2NH_2^+$$
$$R_2NH + H_2O(phys) + CO_2(gas) \rightleftharpoons HCO_3^- + R_2NH_2^+$$
$$H_2O(gas) \rightleftharpoons H_2O(phys)$$

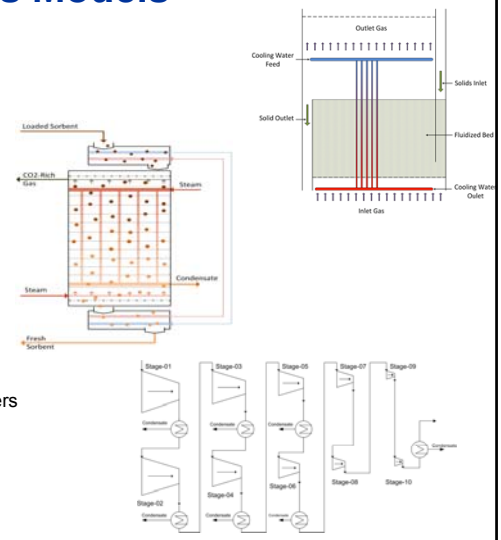


# Process Models

**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

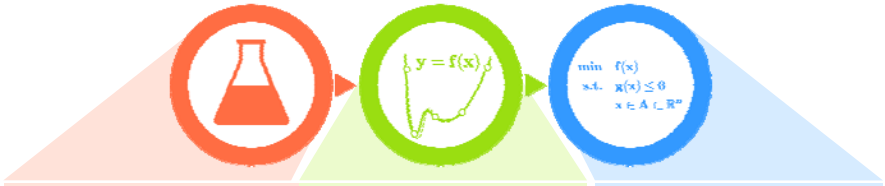
**Compression System Model**
- Integral-gear and inline compressors
- Determines stage required stages, intercoolers
- Based on impeller speed limitations
- Estimates stage efficiency
- $CO_2$ drying (TEG absorption system)
- Off-design performance.
- Includes surge control algorithm





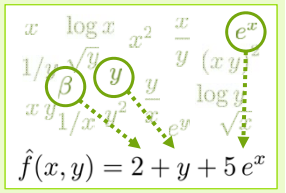

ALAMO
Automated Learning of Algebraic Models for Optimization

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

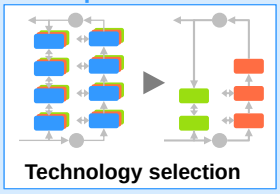



**High-fidelity simulations and experiments**

**Algebraic surrogate models**

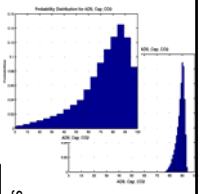



**Superstructure optimization**



**Technology selection**

# FOQUS/Turbine/SimSinter



***Output*** *— Best variable and objective values*

***Input*** *— Initial guess, problem definition*

***FOQUS Engine: DFO and/or UQ***

*Samples*

*Results*

***Meta-flowsheet*** *Evaluation — executed in parallel, may include rigorous heat integration*

***Heat Integration Tool****: Solves LP transshipment model in GAMS, takes stream and equipment information from flowsheet, and returns heat integration results*

Net efficiency:
33.8% → 36.4%

***Turbine****: Simulation queuing/execution, error and result management*

***SimSinter****: standard .NET interface for simulation software, graphical tool*

***Simulation****: Aspen Plus, Aspen Custom Modeler, gPROMS, Microsoft Excel*

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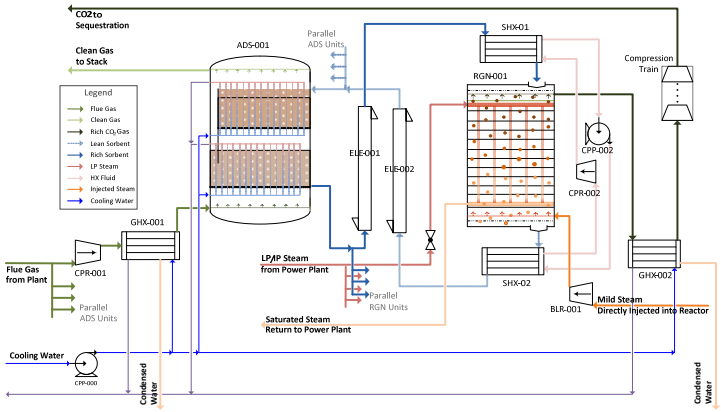
# Optimized Process Developed using CCSI Toolset




***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 $CO_2$) | 1.82 | 1.48 | 1.48 |
| Q_Vap (GJ/tonne $CO_2$) | 0 | 0.61 | 0.74 |
| Q_Sen (GJ/tonne $CO_2$) | 0.97 | 1.35 | 0.68 |
| Total Q | 2.79 | 3.44 | 2.90 |

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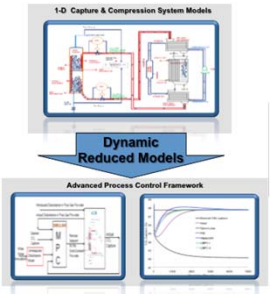
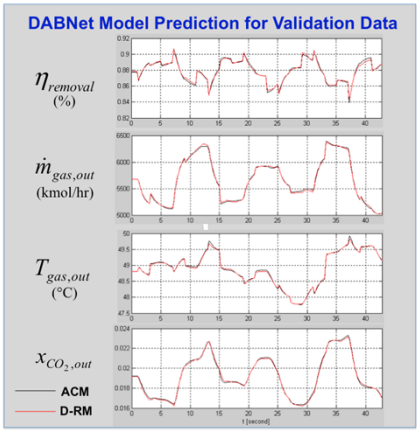
# Dynamic Reduced Model Builder




## Example (BFB Reactor/Adsorber)


## DABNet Model Prediction for Validation Data




- **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)

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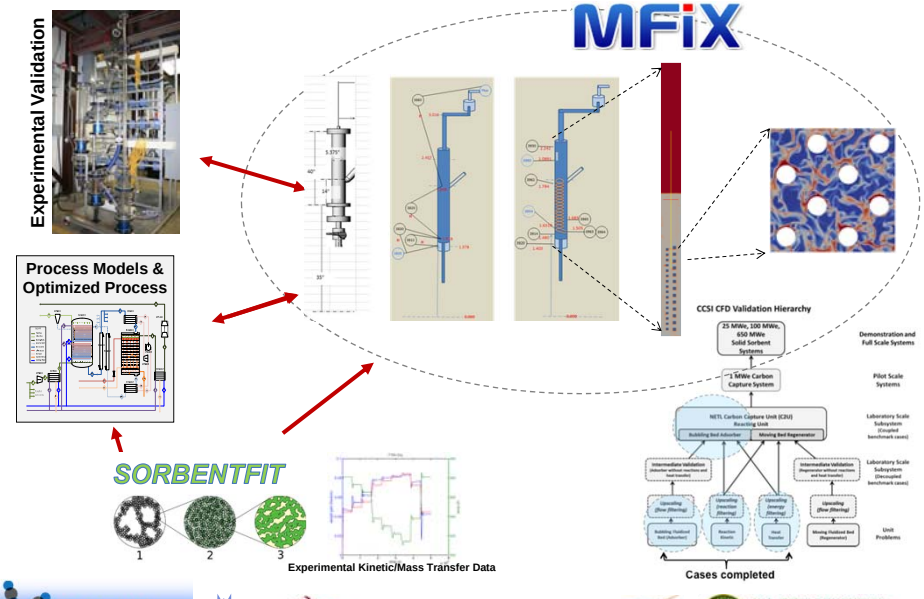
# Simulation & Experiments to reduce time for design/troubleshooting

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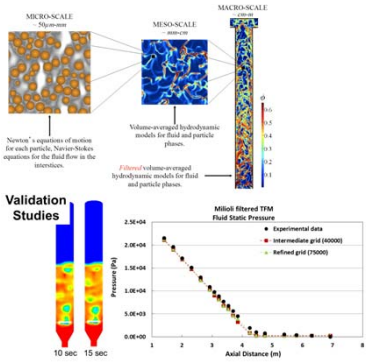
# High Resolution Filtered Models

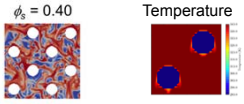
**Filtered Models for Gas-Particle Flows**



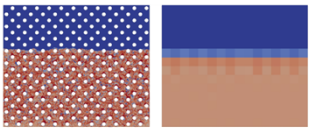

**Validation Studies**




**Flows and Heat Transfer with Cooling Tubes**

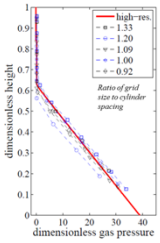



Bubbling Bed



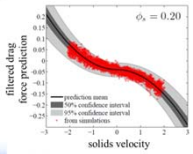
Highly-resolved "Exact solution" ~O($10^6$) cells

Coarse grid + Filtered models ~O($10^2$-$10^3$) cells

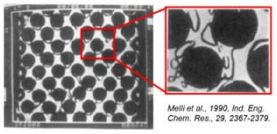



**Model-on-model verification**

**Validation and UQ of Filtered Models**



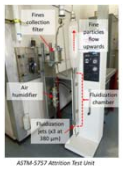

**Filtered Models for Solvent Systems**



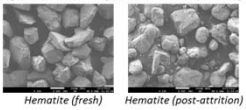



# CFD Modeling of Carbon Capture Sorbent Particle Attrition

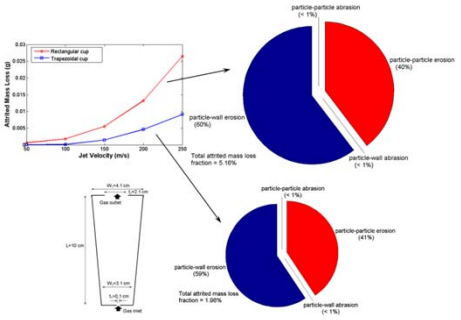
**Experimental Attrition Observation**




*SEM images show evidence of particle abrasion (rounding and fines)*

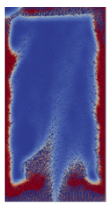


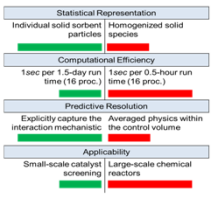

**Jet Cup Modeling: Understanding the Mechanisms of Attrition**




**Attrition Models**

CFD Discrete Element Model



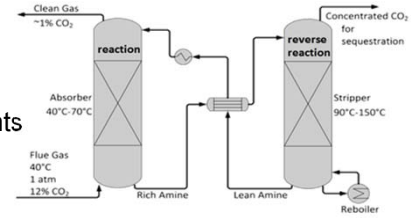


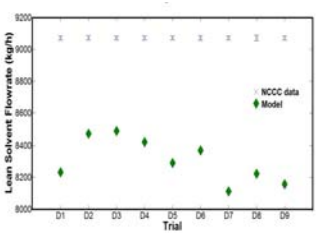

Population Balance Model

- Dominant attrition mechanism: erosive chipping
- Major attrition source: particle-wall interaction
- Critical operating factors: jet velocity and sorbent density

## Solvent Systems: Validation & High Viscosity

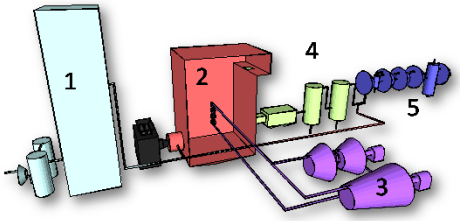
- **National Carbon Capture Center**
  - Pilot Scale Data
- **MEA System Model "Phoenix"**
  - UT Austin pilot plant & experiments
- **Utilize UQ Tools**
  - Physical property models
  - Reaction models
  - Process models
  - Model parameters
  - Experimental data
- **Effective prediction of high viscosity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





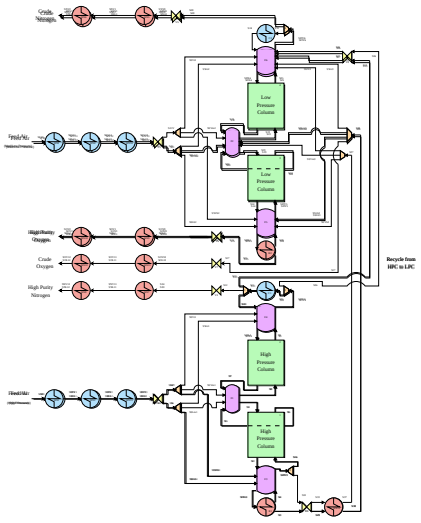

## Oxy-combustion Process Synthesis: Fully Equation-Based




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

- OxyBoiler Model
- CO2 processing unit (CPU)
- Steam turbine model
- Oxycombustion flowsheet optimization framework by optimizing the entire power plant

### Air Separation Unit



| CCSI Release 2013.10.2 | |
|---|---|
| ***Basic Data Submodels*** | High viscosity solvent model |
| | SorbentFit – Kinetic/diffusion basic data fitting tool with UQ |
| ***High Resolution Filtered Submodels*** | Attrition Model |
| | Cylinder Filtered Models with quantified uncertainty bounds |
| ***Validated high-fidelity CFD models & UQ tools*** | 1 MW Adsorber and Regenerator CFD Models (validated) |
| | Large scale adsorber and regenerator CFD Models |
| | Statistical Model Validation Tool for Quantifying Predictions |
| | REVEAL: Reduced Order Modeling Tools for CFD and ROM Integration Tools |
| ***Process Models*** | Bubbling Fluidized Bed Reactor Model |
| | Moving Bed Reactor Model |
| | Multi-stage Centrifugal Compressor Model |
| | Membrane $CO_2$ Separation Model |
| | Reference Power Plant Model |
| ***Optimization and UQ Tools*** | FOQUS – Optimization & Quantification of Uncertainty |
| | ALAMO – Surrogate models for optimization |
| | Process Synthesis Superstructure |
| | Oxy-Combustion Process Optimization Model |
| ***Dynamics & Control*** | D-RM Builder |
| ***Risk Analysis Tools*** | Technical Risk Model |
| | Financial Risk Model |
| ***Crosscutting Integration Tools*** | SimSinter – Links simulation files to FOQUS/Turbine |
| | Turbine Science Gateway – Runs hundreds of thousands of simulations |



## Toolset Deployment

- Initial licensees:
- Additional licensees:
- Others licenses in progress….
- CRADA: in development
- Support: Help available for installation and use issues

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