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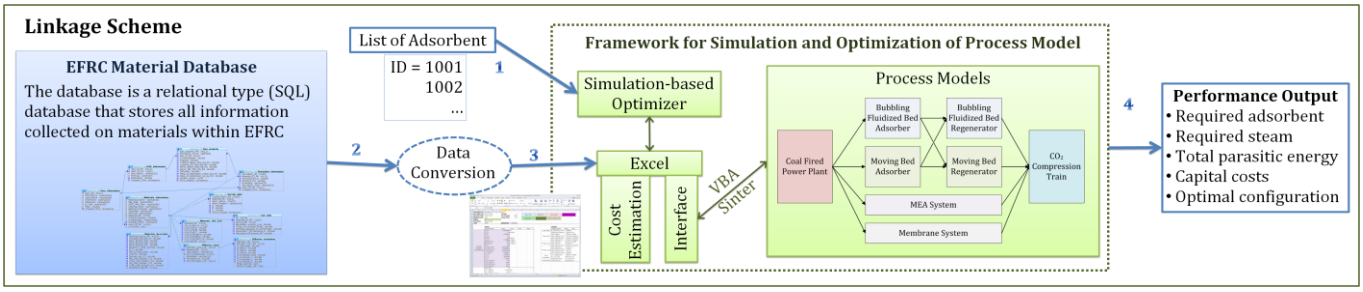

Annual Report: Carbon Capture Simulation Initiative (CCSI)

30 September 2012

NETL Technical Report Series

Office of Fossil Energy

NETL-TRS-CCSI-2012

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Cover Illustration: Schematic of the link among EFRC database, optimization framework and process models.

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Annual Report: Carbon Capture Simulation Initiative (CCSI)

Office of Research and Development, National Energy Technology Laboratory

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Acronyms, Abbreviations, and Symbols

Acronym	Descriptive Name
ACM	Aspen Custom Model/Modeler
ALAMO	Automated Learning of Algebraic Models for Optimization
AM	Activity Manager
AOD	Additive Output Disturbance
ARRA	American Recovery and Reinvestment Act of 2009
API	Application Programming Interface
BFB	Bubbling Fluidized Bed
BOD	Board of Directors
CCS	Carbon Capture and Storage
CCSI	Carbon Capture Simulation Initiative
CFD	Computational Fluid Dynamics
CMU	Carnegie Mellon University
CO_2	Carbon Dioxide
DOE	Department of Energy
EFRC	University of California at Berkeley Energy Frontier Research Center
FAL	Focus Area Lead
FWP	Field Work Proposal
FY	Fiscal Year
IAB	Industry Advisory Board
ICP	Industrially-Relevant Challenge Problem
IEA	International Energy Agency
IPT	Integrated Project Team
LANL	Los Alamos National Laboratory
LBNL	Lawrence Berkeley National Laboratory
LLNL	Lawrence Livermore National Laboratory
MFIX	Multiphase Flow with Interphase eXchanges
MMPC	Multiple Model Predictive Control
MOF	Metal-Organic Framework
MPC	Model Predictive Control
MW	Megawatt Thermal
MWe	Megawatt Electric

Acronym	Descriptive Name
MWh	Megawatt Hours
NETL	National Energy Technology Laboratory
ORD	Office of Research and Development
PC	Pulverized Coal
PDE	Partial Differential Equation
Penn State or PSU	The Pennsylvania State University
PID	Proportional-Integral-Derivative
Pitt	University of Pittsburgh
PMP	Project Management Plan
PNNL	Pacific Northwest National Laboratory
RC	Release Candidate
R&D	Research and Development
ROM	Reduced Order Model
RSI	Random Step-Input
RUA	Regional University Alliance
SARS	Safety Analysis and Review System
SCC	Strategic Center for Coal
SOPO	Statement of Project Objectives
TC	Technical Coordinator
TLT	Technical Leadership Team
TM	Technology Manager
TMo	Technical Monitor
UQ	Uncertainty Quantification
URS	URS Corporation
VUQ	Validation and Uncertainty Quantification
WBS	Work Breakdown Structure
WVU	West Virginia University

1.0 EXECUTIVE SUMMARY

The Carbon Capture Simulation Initiative (CCSI) is a partnership among national laboratories, industry and academic institutions that is developing and deploying state-of-the-art computational modeling and simulation tools to accelerate the commercialization of carbon capture technologies from discovery to development, demonstration, and ultimately the widespread deployment to hundreds of power plants. The CCSI Toolset will provide end users in industry with a comprehensive, integrated suite of scientifically validated models, with uncertainty quantification (UQ), optimization, risk analysis and decision making capabilities. The CCSI Toolset incorporates commercial and open-source software currently in use by industry and is also developing new software tools as necessary to fill technology gaps identified during execution of the project. Ultimately, the CCSI Toolset will (1) enable promising concepts to be more quickly identified through rapid computational screening of devices and processes; (2) reduce the time to design and troubleshoot new devices and processes; (3) quantify the technical risk in taking technology from laboratory-scale to commercial-scale; and (4) stabilize deployment costs more quickly by replacing some of the physical operational tests with virtual power plant simulations.

CCSI is organized into 8 technical elements that fall under two focus areas. The first focus area (Physicochemical Models and Data) addresses the steps necessary to model and simulate the various technologies and processes needed to bring a new Carbon Capture and Storage (CCS) technology into production. The second focus area (Analysis & Software) is developing the software infrastructure to integrate the various components and implement the tools that are needed to make quantifiable decisions regarding the viability of new CCS technologies. CCSI also has an Industry Advisory Board (IAB). By working closely with industry from the inception of the project to identify industrial challenge problems, CCSI ensures that the simulation tools are developed for the carbon capture technologies of most relevance to industry.

CCSI is led by the National Energy Technology Laboratory (NETL) and leverages the Department of Energy (DOE) national laboratories' core strengths in modeling and simulation, bringing together the best capabilities at NETL, Los Alamos National Laboratory (LANL), Lawrence Berkeley National Laboratory (LBNL), Lawrence Livermore National Laboratory (LLNL), and Pacific Northwest National Laboratory (PNNL). The CCSI's industrial partners provide representation from the power generation industry, equipment manufacturers, technology providers and engineering and construction firms. The CCSI's academic participants (Carnegie Mellon University, Princeton University, West Virginia University, and Boston University) bring unparalleled expertise in multiphase flow reactors, combustion, process synthesis and optimization, planning and scheduling, and process control techniques for energy processes.

During Fiscal Year (FY) 12, CCSI released its first set of computational tools and models. This pre-release, a year ahead of the originally planned first release, is the result of intense industry interest in getting early access to the tools and the phenomenal progress of the CCSI technical team. These initial components of the CCSI Toolset provide new models and computational capabilities that will accelerate the commercial development of carbon capture technologies as well as related technologies, such as those found in the power, refining, chemicals, and gas production industries. The release consists of new tools for process synthesis and optimization to help identify promising concepts more quickly, new physics-based models of potential capture equipment and processes that will reduce the time to design and troubleshoot new systems, a framework to quantify the uncertainty of model predictions, and various enabling tools that provide new capabilities such as creating reduced order models (ROMs) from reacting multiphase flow simulations and running thousands of process simulations concurrently for optimization and UQ. The components of the CCSI Toolset in this initial release include:

- SORBENFIT: Sorbent kinetic/equilibrium model fitting code for the 1st-generation sorbent model.

- 1 Megawatt Thermal (MW) adsorber and regenerator computational fluid dynamics (CFD) models for a solid sorbent carbon capture system.
- 1-D steady state Bubbling Fluidized Bed Reactor Model: a solid sorbent based moving bed reactor model implemented in Aspen Custom Modeler (ACM) that can be used to simulate an adsorber or a regenerator for carbon capture process.
- 1-D Steady State Moving Bed Reactor Model: a solid sorbent based moving bed reactor model implemented in ACM that can be used to simulate an adsorber or a regenerator for carbon capture process.
- 1-D Steady State Multi-stage Centrifugal Compressor Design Point Simulation for inline and integral gear multistage centrifugal compressors.
- 1-D Steady State Hollow Fiber Gas Permeation (HFGP) Membrane Model.
- 650 MW Supercritical Pulverized Coal (PC) Power Plant model (reference case).
- Complete process simulation examples for solid sorbent, membrane and solvent systems.
- ALAMO – Algebraic Surrogate Model Generator to enable detailed models to be used for large scale optimization.
- Superstructure Formulation for determining the optimal configuration of carbon capture processes utilizing algebraic surrogate models.
- Simulation Based Optimization Framework to rapidly determine the best design and operating conditions for a given process configuration.
- Dynamic Process and Control Models for Solid-Sorbent Bubbling Fluidized Bed Carbon Dioxide (CO_2) Capture Adsorber and CO_2 Compression.
- REVEAL: Reduced Order Modeling Tool for CFD simulations.
- AspenSinter library to assist running process simulations on Windows.
- Turbine Science Gateway environment for running and managing scientific applications and storing and archiving results.
- EFRC (sorbent database) Connector.
- UQ Framework GUI to evaluate and propagate uncertainty in both model parameters and model form.
- Financial Risk Model.

CCSI held one meeting with its IAB (April 2012) at which it reported progress on the development of the CCSI Toolset. CCSI completed planning for the fall meeting in October 2012 at which the initial tools were released.

CCSI also completed its transition from American Recovery and Reinvestment Act of 2009 (ARRA)-funded activities to Advanced/Crosscutting Research (AR)-funded activities during this reporting period. This report describes only the AR portion of this initiative.

2.0 TECHNICAL HIGHLIGHTS AND KEY RESULTS

CCSI is organized around Technical Elements that consist of integrated development teams with personnel from the five national labs and universities. Table 11: shows the national labs contributing to each Technical Element as well as their roles.

Table 11: Summary of CCSI Elements

Element	NETL	LANL	LBNL	LLNL	PNNL
1: Basic Data	Contributing	Lead	Contributing		
2: Particle & Device Scale Models	Co-Lead	Contributing			Lead
3: Process Synthesis & Design	Lead				
4: Plant Operations & Control	Lead				
5: Integration Framework	Contributing		Lead	Contributing	Contributing
6: Uncertainty Quantification		Contributing		Lead	Contributing
7: Risk Analysis		Lead		Contributing	Co-Lead
8: Software Development Support			Lead	Contributing	Contributing
9: Industry Advisory Board			Lead		

Element 1: Basic Data and Models

Element 1 provides physicochemical data and models as needed for Particle and Device Scale Models (Element 2), the Process Synthesis and Design (Element 3), and Plant Operations and Control (Element 4).

Solid Sorbent Models. Element 1 is developing a hierarchy of solid sorbent (PEI/silica) models (PEI is poly[ethyleneimine]), with each generation adding more detail to the previous generation. The 0th gen model was an ideal equilibrium model with no chemical kinetics. The 1st gen is a lumped kinetic model with ideal, 1st-order kinetics:

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

A tool, called *sorbentfit*, was recently added to the CCSI Toolset. It contains a fitting routine and parametric study for the 1st-gen model. The 2nd-gen model will include transport (diffusion) effects and site-competitive adsorption of water. Finally, the 3rd gen model will consider non-ideal thermodynamics effects. The fitting routine in the *sorbentfit* tool utilizes a particle swarm optimizer (PSO) to fit the model to thermogravimetric analysis (TGA) data. The output of the routine is a set of model parameters corresponding to the CCSI 1st-generation sorbent model, which represents a best fit (in a least-squares sense) of the model to the data provided. The routine should be appropriate for any amine-based solid sorbent. Additionally, the package provides the capability of evaluating the 1st generation model for arbitrary sets of parameters and an arbitrary profile of temperatures and gas compositions. The model considers the chemisorption of CO_2 to form carbamate, the physisorption of water, and the formation of

bicarbonate from a gaseous CO_2 molecule and an adsorbed water molecule, assuming that the kinetics of each are dominated by a single, ideally-behaved chemical reaction.

Prior Information and Model Discrepancy. A statistical methodology for UQ in amine-based solid sorbent models has been developed and demonstrated on the 0^{th}- and 1^{st}-gen models. Prior information on values for model parameters derived from quantum chemical calculations was combined with model form discrepancy functions based on Gaussian processes in a Bayesian analytical framework. Markov chain Monte Carlo routines for generating posterior distributions for model parameters in dry conditions were implemented in R and C++. It was found that the prior information reduced the parameter uncertainty evident in the posterior distributions for both 0^{th}-and 1^{st}-generation models. Preliminary results suggest that parameter uncertainty in the kinetic parameters of the 1^{st}-generation model is very high (no reliable prior information on those parameters is available due to their empirical nature), motivating the effort to include more accurate models for sorbent kinetics embodied in the 2^{nd}- and 3^{rd}-generation models. Model form discrepancies are proposed as a potential solution to the problem of uncertainty propagation in extrapolation. We can greatly improve the accuracy and utility of our sorbent models by incorporating independent information about model parameters, and by considering existing data when we make model predictions. The former is accomplished using quantum chemical (QC) calculations of model parameters, such as adsorption enthalpies and entropies.

In conjunction with Elements 3 and 6, the results of the 0th- and 1st-generation sorbent particle model were used to develop a method for propagation of uncertainty, including model-form uncertainty, up to the process scale. The process used for this demonstration was a simple moving bed adsorber. For a given process set point, probability distributions for the capture rate were obtained. A new, iterative methodology for producing these distributions in the context of model-form uncertainty was implemented, and the benefits of including model-form error in uncertainty propagation were demonstrated. The analysis will help to reduce uncertainty by aiding in the design of new TGA experiments for the chemical characterization of solid sorbents.

Berkeley EFRC. The Berkeley team has continued to work on the development of the Hierarchical Materials Design capability and extending the EFRC Database to include more CCSI-relevant data, particularly diffusion of CO_2 and water. A diffusion model for gases adsorbed in micro-porous materials (zeolites and metal-organic frameworks (MOFs)) has been created at the Berkeley EFRC, predicting with reasonable accuracy the diffusion properties of methane but requiring less time than existing analysis methods. Initial comparison between the self-diffusion coefficient values obtained from our model and the MD simulations of systems for 80 IZA zeolite structures indicates very good agreement especially in slowly diffusing materials (i.e. relatively small diffusion coefficient values) where TST is applicable. The use of graphics processing units (GPUs) allows a single self-diffusion coefficient value to be obtained in just a few seconds, making it possible to characterize the diffusive behaviors of a very large database of porous materials within a reasonable amount of time. During FY12, we extended the models to other molecules like CO_2 and N_2. In parallel, a process model was developed at NETL to investigate carbon capture behavior in a more realistic system with site-limited diffusion behavior, finite adsorbent particle size, and transient dynamics. This process model uses material properties to predict the efficiency of a carbon capture process that uses that material to selectively adsorb CO_2 from a mixture, and release it later sequestration.

With respect to water in solid sorbents, we have worked on preparing and validating a force-field to predict water adsorption isotherms with molecular simulations. The force-field provides good match with experiment and can be now used in high-throughput characterization of zeolite-based sorbents. Water exhibits a highly nonideal adsorption isotherm with a convex isotherm at low temperatures showing a discontinuity with an infinite slope. This behavior is part of what makes water difficult to model accurately. Water molecules attract each other, meaning that once a few water molecules are present, additional water molecules can enter the system more easily. This system is predicted to exhibit

hysteresis. Once the water model is validated, it can be applied to various materials to predict adsorption selectivity for CO_2 over water. For example, the Henry coefficients of water and CO_2 have been considered Zeolitic Imidizolite Frameworks (ZIFs) with various different molecular linkers.

We completed a prototype Application Programming Interface (API), which now allows the CCSI community to use the Berkeley EFRC Materials database (e.g., search and retrieve materials and basic data via the Materials JSON object). We extended the Materials JSON format to include both equilibrium and transport-related parametric data obtained by atomistic simulations. The Material JSON can be obtained from the database with a set of http queries, which are controlled by Excel, and can automatically populate the data in a spreadsheet. Then, a site-limited continuum model implemented in ACM can be executed to perform material performance analyses. Figure 11 presents the dataflow through our setup.

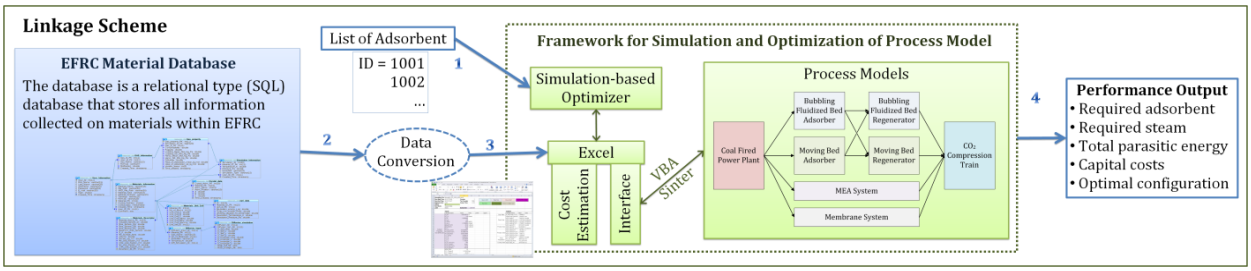


Figure 11: Schematic of the link among EFRC database, optimization framework and process models.

Attrition Models. To support the development of a model for the attrition of amine-impregnated mesoporous sorbents (see Element 2) we have focused on techniques to estimate the mechanical properties of the materials. In the sorbent material, individual grains of the sorbent consist of a silica aerogel, the structure of which is somewhat dependent on the method of synthesis. However, the aerogel can be viewed as spherical agglomerates (50 nm-2μ m) of smaller silica nanoparticles (2-50 nm) linked by thin silica strands. This creates a structure that is highly porous with the pores being almost entirely filled with PEI. The polymer is thought to interact with the external surfaces of the silica agglomerates through proton transfer from the silanol groups and the amines on the polymer chain. We expect two possible sources of attrition: (1) attrition arising from impacts of the particles in the entry jet, and (2) attrition arising from wear abrasion in the bed. During FY12, we concentrated on the latter, although Boerefijn and co-workers suggest that this is only a minor contribution to particle breakdown. According to literature related to pharmaceutical compacts, the porosity of the materials causes the rate of wear to increase. It provides several relations to quantify the wear process, including abrasion and impact. The final equation relating the rate of mass loss to mechanical properties is $dm/dt \sim H/E\ \rho\ m/K_c^{3/2}$, where H is the hardness, E is the elastic modulus of the crystal, ρ is the density and K_c is the fracture toughness. Using these formulae, an extension to the current simulation protocol could be made if appropriate values of the hardness and fracture toughness could be obtained for the sorbents.

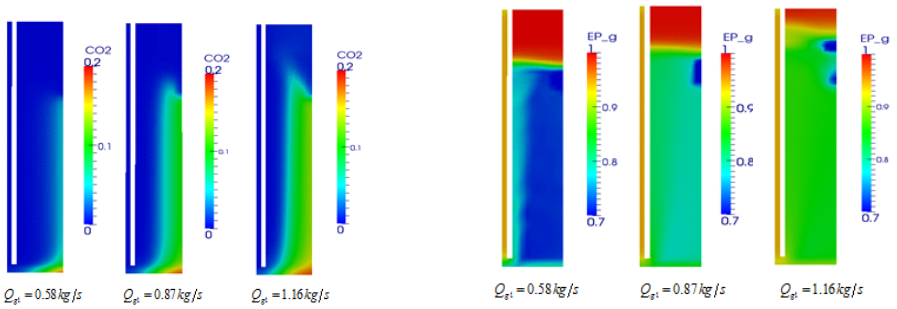
Flue gas contains significant moisture that strongly influences the performance of a carbon capture system both beneficially and adversely. A kinetic model was developed to provide process developers with a more complete understanding of the behavior of sorbent particles to enable better designs. This capability supports the Fossil Energy Clean Coal Technology Program's mission by enabling a more complete understanding of potential capture technologies, particularly how the a sorbent material behaves as a process is scaled up. The CCSI Technical Team is currently reviewing recommendations from the October 2012 IAB meeting and developing detailed plans and priorities for the next project year (Feb 2013 – Jan 2014).

Element 2: Particle and Device Scale Models

The development and validation of a device-scale modeling capability are critical in reducing the time and cost of scale up and optimization of any novel carbon capture technology. Major accomplishments in FY12 include:

Developed and delivered CFD models of multiphase reactive flow simulations for the adsorber and regenerator of a 1MW pilot scale solid sorbent system. We have developed MFIX multiphase flow simulation models of the 1MW adsorber and regenerator based on the initial design provided by Element 3. The initial and boundary conditions of sorbent composition, as well as the initial and boundary conditions of temperature, are set up according to the conceptual design of 1MW solid sorbent system. The multiphase flow model is formulated based on conservation of mass, momentum, and energy for each individual phase in the flow. Particle-level reaction kinetics developed by Element 1 have been implemented in the MFIX simulations to predict the CO_2 adsorption and desorption efficiency of the adsorber and the regenerator, respectively. These models (with theory and user manuals) have been included in the September 2012 CCSI product release, and the results have been presented and discussed at the IAB meetings in poster format.

For example, Figure 22(a) shows the predicted gas voidage distribution for various gas flow rates, and Figure 22(b) shows the predicted CO_2 mass fraction distribution for the 1MW adsorber. The CO_2 capture percentages for different gas flow rates have also be studied for the adsorber for different cooling tube efficiencies, see Figure 33. Consistent trends have been obtained between the CFD models and the process models for different gas flow rates. The results also indicate that the process model predictions (Element 3) are closer to the detailed CFD predictions with no cooling; therefore, they may underestimate the overall capture efficiency of the actual adsorber with cooling tubes.



(a) (b)

Figure 22: Predicted distributions of gas voidage (a) and CO_2 mass fraction (b) for the 1MW adsorber for different gas flow rate.

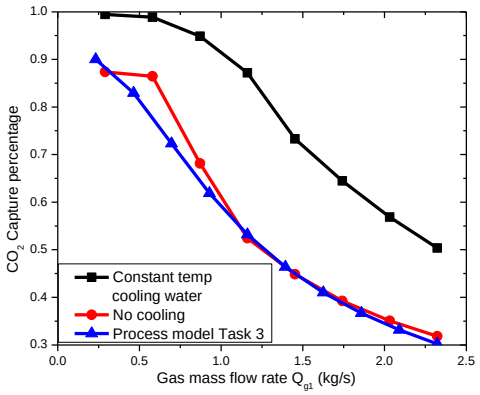


Figure 33: CFD and process model predicted CO_2 capture percentage for different gas flow rates.

Developed and began implementation of a hierarchical validation plan for multiphase reactive flow simulations in CCSI. In FY12, incorporating the recommendations from the IAB, Element 2 developed a CCSI validation plan by working with Element 6, Boston University, Princeton University, University of Utah, and industry (Babcock & Wilcox). The hierarchical validation plan with UQ was delivered to the IAB in September 30, 2012, and the approach was also presented in poster format in the April and October IAB meetings, see Figure 44.

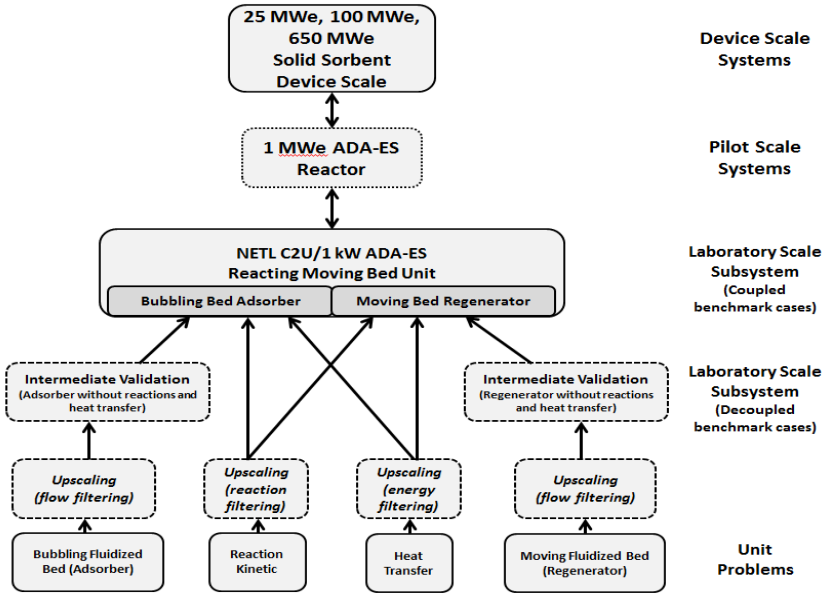


Figure 44: CCSI Validation Hierarchy

Developed a sub-grid 'filtered' model for cooling rods in the adsorber. In FY12, we developed the model for the sub-grid drag by performing highly resolved 2D simulations of the flow around a few tubes in a periodic domain. Results from a large number of finely resolved CFD simulations have been analyzed to determine the drag model and estimate the parameters in model. Based on recent results, a cylinder-

suspension drag of the form, $f_{\text{drag}} = \beta\left(-v_s|v_s|\right)+\gamma$ is proposed, where v_s is the average sorbent velocity, and β and γ are fitting parameters which depend on the solid fraction ϕ_s (Figure 55) and cylinder geometry. Additional simulations are currently being performed to verify the proposed drag relationship.

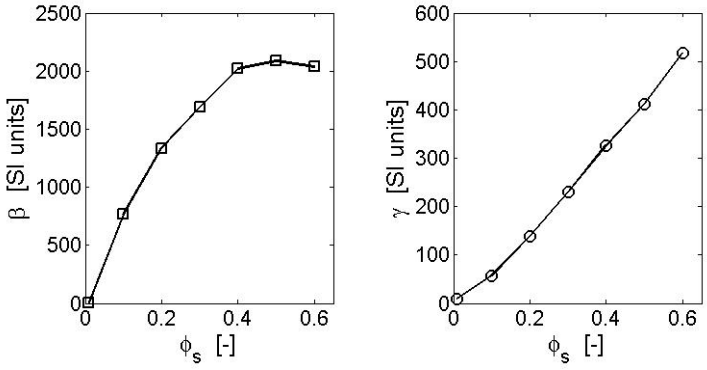


Figure 55: Dependence of the model parameters β and γ on the domain averaged solid fraction ϕ_s.

Sorbent Particle Attrition Modeling. This is a new activity started in FY12. We made significant progress on the prediction of mechanism-based sorbent particle attrition. We have completed a literature survey on particle attrition and erosion and have identified methods that can be implemented in CFD models. We are considering two primary attrition mechanisms: impaction and abrasion. We selected an impaction method and have successfully implemented the method in the MFIX discrete element method (DEM). This model exploits the forces calculated in the DEM model and calculates the fracture volume due to particle-particle and particle-wall collisions. We have run simulations for a single particle in free-fall and the collision with a horizontal wall. The results are consistent with published data and models. We also simulated a 2D fluidized bed of mono-disperse particulates and calculated the resultant size distribution due to the attrition forces using the DEM model. Preliminary results for a 2D fluidized bed with 2400 particles are shown in Figure 66. We have also discussed with Element 1 how to define the mechanical properties of the NETL32D sorbent. In particular we have requested material properties for Young's modulus, shear modulus, toughness, hardness and density of the sorbent particles.

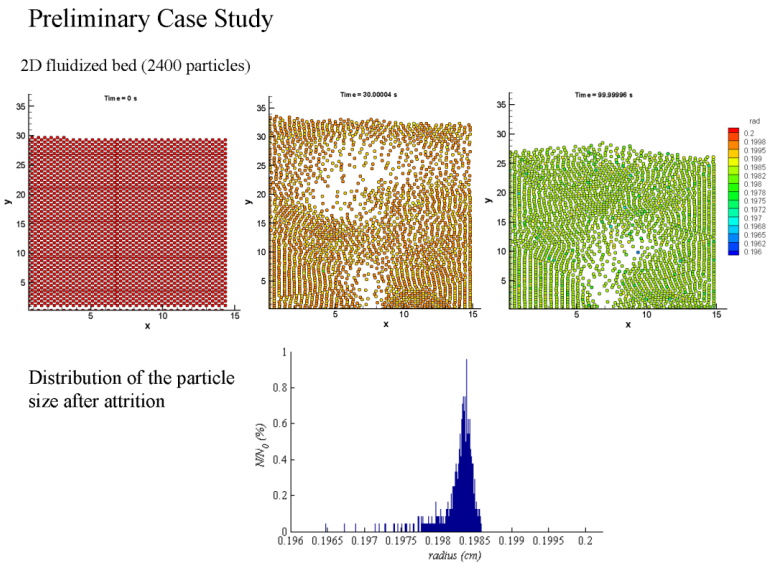


Figure 66: Initial results of attrition model for a 2D fluidized bed.

These computational tools and models will enable industry to more rapidly and effectively scale up and troubleshoot carbon capture technologies in support of the Fossil Energy Clean Coal Technology Program's mission.

In addition to the originally planned technical scopes, Element 2 has incorporated recommendations of the IAB while developing the CCSI CFD validation and UQ plan in collaboration with Element 6 and industry. We implemented the suggestions from the IAB and have begun development of a computational framework for particle attrition predictions for CCSI sorbents. These changes are necessary in order to keep stakeholders and industry engaged in the project in order to meet the Fossil Energy Clean Coal Technology Program's mission. We are currently in the process of refining and re-defining our research activities/deliverables for the next CCSI project year in order to keep the high level industrial engagement and relevance.

Element 3: Process Synthesis and Design

The major accomplishment this year involved preparing many of the Element 3 components of the CCSI Toolset for their initial release at the end of the September. Each tool includes detailed documentation, and tutorial. The tools released by Element 3 include the following:

- Process Models
  - 1-D Bubbling Bed Model (ACM)
  - 1-D Moving Bed Model (ACM)
  - 1-D Membrane Model (ACM)
  - 1-D Compressor Model (ACM)
  - Solvent System Model (Aspen Plus)
  - Reference Power Plant (Thermoflex)
- System Examples

  - Solid sorbent (hybrid, moving bed)
  - Membrane System
- Optimization Tools
  - ALAMO – Algebraic Model Development Tool
  - Superstructure to determine optimal configurations
  - Simulation-based optimization framework

Other significant accomplishments are described below.

We developed a 1 MW pilot scale design and simulation based on the 650 Megawatt Electric (MWe) design and simulation that was previously developed under the ARRA project. A brief report on this pilot scale design was prepared and transmitted to Element 2, which has used this as a basis for the development of detailed CFD simulations of the proposed adsorber and regenerator.

A multi-scale moving-bed reactor model which implemented a micro-scale dimension of an intra-particle phase was developed to explain a microscopic site-limited diffusion phenomenon for zeolite or MOF particle. The framework to link it with the University of California at Berkeley Energy Frontier Research Center (EFRC) material database was also developed. This framework can be used for screening candidate materials or investigating the correlation between the material properties and reactor performance.

The moving bed model now has two options for describing the reaction rate (Kinetic or Mass transfer limitation) and the flow directions for internal heat exchanger (upward for cooling water or downward for steam). A new initialization procedure now automatically changes to an initial model with no reaction, no heat transfer between gas and solid phase, and no heat transfer with tubes to a converged full-model by invoking a series of homotopy runs. The modeling environment, including pre-defined tables and figures for the important modeling variables, were embedded for the convenience of the end user.

Preliminary comparative studies have been completed with collaboration from Element 2 to validate the results of the process models with the 2D CFD models for the bubbling fluidized bed (BFB) adsorber and MB regenerator. Results are described in the accomplishments under Element 2.

A UQ analysis of the BFB absorber model, the MB regenerator model, and the complete hybrid capture system was completed in conjunction with Element 6. Results are described under Element 6's accomplishments.

The compressor model design constraints were updated. Minimum and maximum diameter, limits on impeller stress, and limits on impeller tip Mach number where added. The constraints should provide a good initial design with reasonable operating conditions and a good estimate of efficiency. A user manual was written and two multistage ACM models where created for an integral gear and inline compressor with TEG drier. Multistage gPROMS compressor models were also made, but they do not yet include drying. The design point compressor model should be nearly final.

We updated the benchmark MEA system model and re-optimized the system. The most important changes were the addition an inter-heater to the stripper and the ability to generate some of the stripping steam by flashing the lean solvent stream leaving the stripper at a lower pressure and recompressing it. The best cost of electricity was found to be $114./MWh, given the process variables that were optimized.

Two versions of ALAMO (Automated Learning of Algebraic Models for Optimization) were prepared for release: one to be run inside the Matlab environment and a standalone compiled Windows version. Packaged with the ALAMO suite are several modeling methods: the standard ALAMO model builder mixed integer problem best-subset method, the lasso regularization, and ordinary least squares regression.

The adaptive sampling routines available include the standard ALAMO error maximization sampling method as well as Latin hypercube sampling. ALAMO allows for diversified simulation inputs: fixed data set, pre run initial sampling set, ALAMO guided initial design of experiments, Matlab script simulation wrapper, and executable simulation wrapper. Along with complete documentation, the ALAMO release includes several example cases to help users run ALAMO in a variety of settings.

As part of development of the simultaneous synthesis method, improvements were made in comparison with the typical water networks considered in literature. The selection of a single wastewater treatment unit among multiple options is allowed for the removal of each type of contaminant. Also, uncertainties involved in the quantity of contaminant released in the water-using process units were modeled using a multi-scenario scheme. Finally, short-cut models were developed to replace simplified models to describe wastewater treatment units. These modifications increase the problem size and complexity quite significantly; as a result, there arises the need for more efficient algorithm to solve the formulation. To this end, a Lagrangean relaxation-based algorithm has been developed to solve the new formulation and we can show that the new algorithm indeed improves the solution time. We have implemented this model in a refinery example. Results show that reasonable saving can be achieved in freshwater consumption and wastewater discharge using this method.

Several publications and presentations were made, including:

- Yang, L., and Grossmann, I.E., "Water Targeting Models for Simultaneous Flowsheet Optimization," *Industrial & Engineering Chemistry Research*. Article ASAP. Publication Date (Web): July 19, 2012

- Eslick, J. C. and Miller, D.C., "Optimization of Water Use and Cost of Electricity for an MEA Carbon Capture Process," University of Texas Carbon Capture and Storage Conference, Austin, Texas, January 25-27, 2012.

- Sahinidis, N.V., Cozad, A., and Miller, D.C., "Derivative-Free Optimization Enhanced-Surrogate Models for Energy Systems Optimization," *9th International Conference on Computational Management Science (CMS 2012)*, Imperial College, London, U.K., April 19-20, 2012.

- Yang, L., and Grossmann, I.E., "Mathematical Optimization of Water Integration for Subcritical Pulverized Coal Plant with CO_2 Capture," presented at the *11th Annual Conference on Carbon Capture & Sequestration*, Pittsburgh, PA, April 30-May 3, 2012.

- Miller, D.C., Sahinidis, N.V., Kim, H., Lee, A., Cozad, A., Yuan, Z.H., Konda, M., Eslick, J.C., and Morinelly, J.E., "Synthesis of Optimal Capture Processes using Advanced Optimization," presented at the *11th Annual Conference on Carbon Capture & Sequestration*, Pittsburgh, PA, April 30-May 3, 2012.

- Cozad, A. "Simulation Optimization: Why it's tough and how to deal with it," presented at *The 34th Annual Chemical Engineering Graduate Student Association Symposium*, Pittsburgh, PA., September 20-21, Winner of the 2012 Symposium Speaker Award.

- Presentations at the AIChE 2012 Annual Meeting, Pittsburgh, PA, October 28-November 2, 2012.
  - Alison Cozad, Nick Sahinidis and David C. Miller, Alamo: Automatic Learning of Algebraic Models for Optimization.
  - Alexander W. Dowling, Lorenz T. Biegler and David C. Miller, Coal Oxycombustion Flowsheet Optimization.
  - Hosoo Kim, Maciej Haranczyk, Tom Epperly, Mahmoud Abouelnasr, Joseph A. Swisher, Kuldeep Jariwala, David Mebane, Berend Smit, Joel Kress and David C. Miller. Integrating the Carbon Capture Materials Database with the Process Simulation Tools of the Carbon Capture Simulation Initiative.
  - Alison Cozad, Nick Sahinidis and David C. Miller, Surrogate-Based Optimization of Simulated Energy Systems.
  - Z.H. Yuan, A.L. Cozad, N.V. Sahinidis and D. C. Miller, Surrogate model based optimal synthesis of solid sorbent carbon capture process.
  - J. Morinelly and D.C. Miller, Post-Combustion Gas Permeation Carbon Capture System Models.

These process optimization and integration tools, coupled with the sophisticated process models, will enable potential concepts to be screened more rapidly and more optimal designs developed in support of the Fossil Energy Clean Coal Technology Program's mission.

The CCSI Technical Team is currently reviewing recommendations from the October 2012 IAB meeting and developing detailed plans and priorities for the next project year (February 2013 - January 2014).

Element 4: Plant Operations and Control

Element 4 released a one-dimensional (1D), partial differential equation (PDE), pressure-driven dynamic model (implemented in ACM) of a two-stage BFB reactor that is used to simulate an adsorber with overflow-type configuration for carbon capture using a solid sorbent. The model includes controls for regulating the sorbent and flue gas flowrates and a level controller for maintaining the level of the solids in the hopper. A schematic of the two-stage adsorber with control loops is shown in Figure 77. Control system models include traditional proportional-integral-derivative (PID), feedforward-augmented-feedback control and model predictive control (MPC) with two strategies for off-set free tracking. The software also contains a pressure-driven dynamic process model (implemented in Aspen Plus Dynamics) and controls for a CO_2 compression process consisting of a 10-stage inline centrifugal compressor with interstage coolers and a glycol tower for dehydration. A closed-loop control strategy was also developed for regulation of CO_2 capture by manipulating the sorbent inlet flowrate.

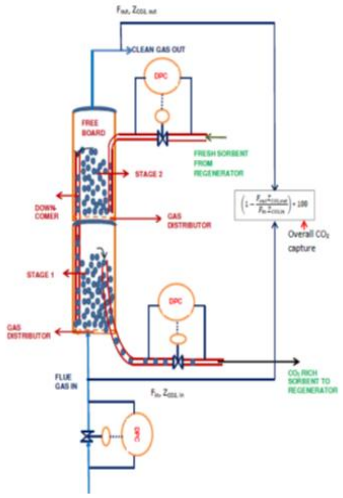


Figure 77: Schematic of 2-stage adsorber with controllers (open-loop CO_2 capture).

A coupled model of the adsorber-regenerator system (Figure 88) was also developed neglecting the dynamics of the solid-sorbent transport between the adsorber and regenerator. Simplified models of the feed and exit hoppers were developed neglecting vapor disengagement. Pre- and post- heat exchangers were added along with a valid pressure-flow network. In addition, a flow-driven model was developed for the solid sorbent preheating and heat recovery system. The transient response of the coupled system was studied by using a conventional PID controller for maintaining the CO_2 capture rate.

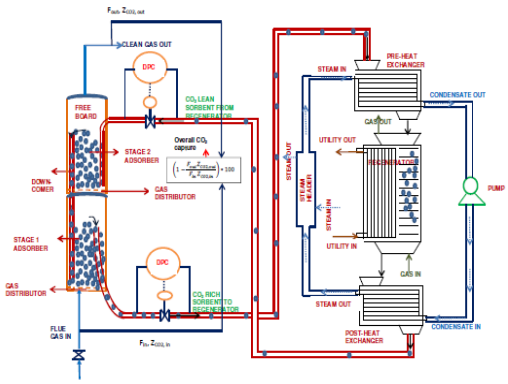


Figure 88: Schematic of coupled 2-stage BFB adsorber-reactor and moving-bed regenerator-reactor systems.

A multiple model predictive control (MMPC) strategy was developed, implemented, and applied to the solid sorbent-based adsorber capture model in ACM. MMPC is required given that performance of MPC operating on a single disturbance model deteriorates when the form of disturbance (whether step or ramp etc.) is not known *a-priori*. In such cases, a trial-and-error method has to be adapted to achieve good control performance by testing different disturbance models (output disturbance, random step input, random ramp input and even periodic ones). The MMPC algorithm uses a model-bank with different built-in disturbance model(s) so that it can continuously adapt. In Figure 99 the advantages of using MMPC strategy is highlighted, where a 20% step-input is provided to the disturbance (flue-gas flowrate). When a step increase in disturbance is provided, the algorithm automatically prioritizes the random step-input (RSI) disturbance over the additive output disturbance (AOD) initially to reduce the overshoot time but switches to AOD for smooth elimination of overall CO_2 capture offset. A clear advantage is seen during a step decrease in flue-gas flowrate, where RSI is automatically preferred all the way since offset is nullified very early during transients (compared to AOD).

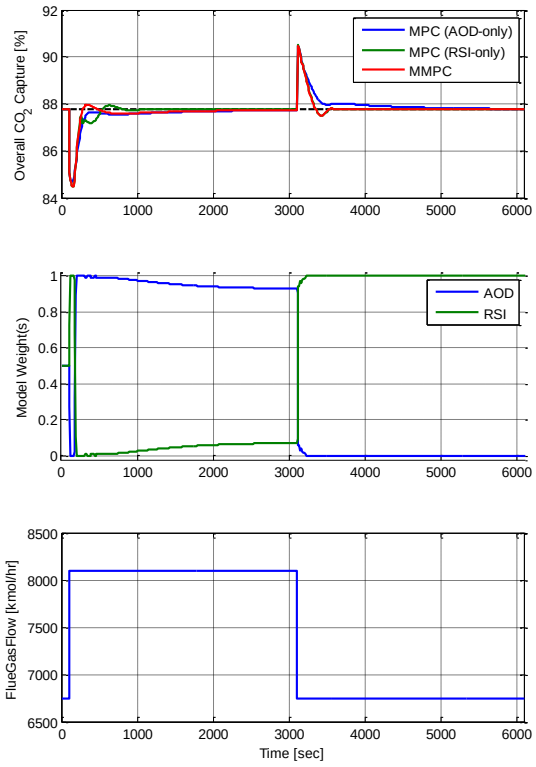


Figure 99: Comparison of different control algorithm responses for 20% step changes in flue-gas flowrate. MPC/MMPC parameters: P = 50, M = 10, Wy/Wu = 4.67e9, Q/R (RSI) = 0.01.

Several publications and presentations were made, including:

- Modekurti, S., Bhattacharyya, D., and Zitney, S.E., "Dynamic Modeling and Transient Analysis of a Solid-Sorbent Adsorber for CO_2 Capture," *Proceedings of the 29th Annual International Pittsburgh Coal Conference*, Pittsburgh, PA, October 15-18, 2012.

- Modekurti, S., Bhattacharyya, D., and Zitney, S.E., "Dynamic Modeling and Control of a Solid-Sorbent CO_2 Capture Process with Two-Stage Bubbling Fluidized Bed Adsorber-Reactor," Presented at the *AIChE 2012 Annual Meeting*, Pittsburgh, PA, October 28 – November 2 (2012).

These computational tools and models will enable industry to more rapidly evaluate potential operational aspects of integrating a carbon capture system with a power plant. The ability to understand the dynamic system response and evaluate potential control strategies is essential for accelerating the commercial development of carbon capture technology, a key component of the Fossil Energy Clean Coal Technology Program's mission.

The CCSI Technical Team is currently reviewing recommendations from the October 2012 IAB meeting and developing detailed plans and priorities for the next project year (Feb 2013 – Jan 2014).

Element 5: Integration Framework

Realizing the potential of CCSI depends on having an integrated carbon capture simulation environment that enables multi-scale simulations, UQ, decision support, and optimization. Element 5 is developing the software framework needed to enable interoperability of the underlying simulation tools.

ROM development was a major focus of our work this year. Element 5 in coordination with Element 2 designed and implemented a reduced-order modeling tool. The tool enables the creation of a simplified model of CFD simulations suitable for integration into process models. During development of the ROM, a user specifies input ranges where the ROM needs to be valid. The CFD is run on a sample of the input range and the extracted results are used to build response surfaces using various regression methods that represent the ROM for the simulation. The resulting ROM can be easily integrated into ACM and AspenPlus (Figure 1010).

Java classes for ROM generation were developed, which can be used to extract the boundary conditions and model parameters from an MFIX data file or an ANSYS Fluent case file and generate the data for CAPE-OPEN COM and ACM code for the unit operation model. The main revision included the data related to the chemical species involved and the solid phase data in a multiphase flow CFD. The Java class contains a method to convert and export the data in the format that the CAPE-OPEN COM library can read when the ROM model is added to an Aspen Plus flowsheet. It also contains a method to export the data and the algorithms for enforcing the mass and energy balances in forms of variables and equations in ACM script language, which can be imported in by ACM as a unit operation module.

A paper describing the ROM Builder, the underlying approach and technologies used for designing the Reveal ROM Builder tool was published. The Reveal ROM Builder tool was demonstrated at the October 2012 IAB meeting. In addition, an installer that integrates all of the packages associated with the Reveal ROM Builder into a single install was developed.

Figure 1010: Dataflow for ROM builder.

We also completed and released the Optimization software in coordination with Element 3. This optimization package enables the optimal configuration of a process simulation flow sheet to be determined using a wide variety of tools including SciLab, ModeFrontier, and other tools.

In support of the process simulation optimization and UQ work in CCSI, the Element 5 team continued to improve their Turbine Gateway and AspenSinter tools. These tools connect the optimization and UQ tools with cluster or cloud resources to enable the large numbers of parallel process simulations needed by both tools. The Turbine Gateway and AspenSinter capabilities have been deployed and have been used by the CCSI team during the course of the development and have now enabled 500,000 CCSI process simulations to be run.

We continued to develop AspenSinter, which integrates the AspenTech process simulators into the CCSI framework and enables interaction with the gateway. It was refactored to support the JSON configuration

files and to make vectors work properly. We also designed and wrote schemas for the JSON-based sinter configuration files and added support for JSON sinter configuration files to AspenSinter. We created tools to go with it, such as a converter from the old format to the new format. ExcelSinter, which allows sinter to run Excel files (including macros) was created. This is useful for running some simulators, such as Thermoflow, but it is also useful for testing and post processing.

We completed the EFRCConnector to collect sorbent information from the EFRC database and input them to ACM simulations. In particular, the EFRCConnector enables communication between an Excel spreadsheet and the web interface to the EFRC database. This technology was demonstrated at the IAB meeting.

One of the roles of the integration framework is to provide the ability to convert values between differing units of measurement. For example, it should be able to convert an energy value in BTUs (British Thermal Units) to a value in Joules. Element 5 personnel developed a Microsoft COM interface to the open source UDUnits2 package. This COM interface makes UDUnits2 available to Excel and other integration framework software in a variety of languages.

Improvements to the versatility of the Turbine execution gateway have broadened the set of databases that the gateway works with and allow the gateway to be run locally on a desktop machine. This allows the same simulation execution commands to be used regardless of whether the user is running a single simulation or a large number of simulations. An MSI installer was created along with user manuals and installation manuals. Automated testing of the gateway was also implemented. A test environment that can serve as a simple continuous integration testing tool using AWS S3 and EC2 was developed. The gateway architecture is shown in Figure 1111. The Turbine gateway and AspenSinter capabilities were released in September 2012.

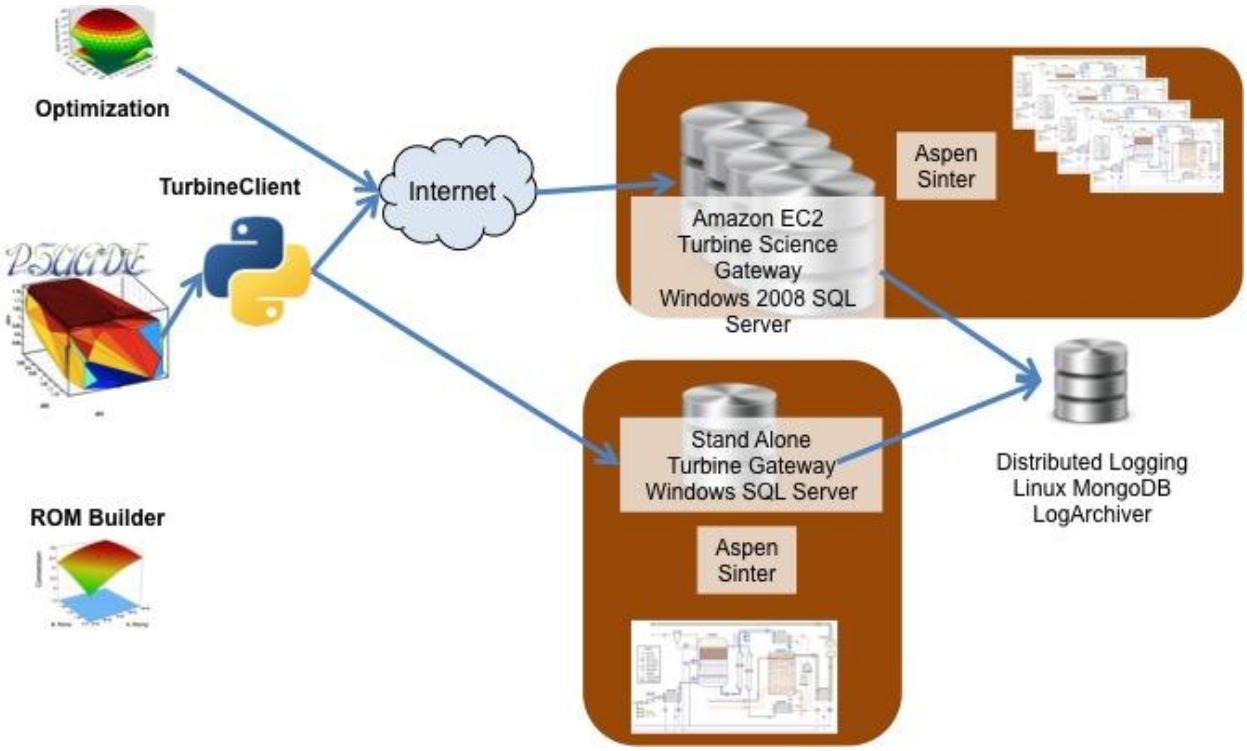


Figure 1111: Process Optimization, Turbine Gateway and AspenSinter in operation.

An important challenge will be enabling effective generation of ROMs for long-running CFD simulations. The current ROM technology requires a large number of simulations to build the ROM. We are investigating adaptive techniques and other options for efficient building of ROMs. In addition, the Turbine Gateway enables large numbers of simultaneous simulations; however, the current licensing model of the simulation software does not typically allow this type of use. We are working with vendors to address this issue but it has been a slow process.

The key Element 5 Research and Development (R&D) accomplishments Turbine, Reveal, Sinter, EFRCConnector, and Optimization directly relate to developing a suite of technologies critical to meeting the Fossil Energy Clean Coal Technology Program's mission.

The CCSI Technical Team is currently reviewing recommendations from the October 2012 IAB meeting and developing detailed plans and priorities for the next project year (Feb 2013 – Jan 2014).

Element 6: Uncertainty Quantification

The role of UQ is to provide a rigorous methodology and computational capabilities for assessing the prediction confidence of computer models simulating different carbon capture technologies in view of the many uncertainties in the models and in the experimental data. During FY12, the major milestones for Element 6 were the development of the V2 UQ framework for applying UQ to solid sorbent carbon capture process simulations connected with basic physicochemical properties and the documentation of the application of UQ methodology for process simulations using the baseline solid sorbent capture simulation (A650.1). In accomplishing these milestones, the CCSI UQ team collaborated with: (1) Element 3 and 5 to perform UQ analysis of the full-scale design A650.1 solid sorbent process model; (2) with Element 1 to quantify uncertainties (including model form) for several chemical kinetics models; and (3) with Element 5 in developing a graphical user interface to facilitate uniform access to a wide variety of UQ tools. In addition, the UQ team also collaborated with Element 2 to develop a process for hierarchical Validation and Uncertainty Quantification (VUQ) methods to study uncertainties in the CFD models and to demonstrate this approach in the context of a specific unit problem.

In our UQ analysis of the A650.1 process model, we followed a structured approach, beginning with interaction with subject matter experts in Element 3 to understand the physics and identify sources of uncertainties in the adsorber and regenerator models. The team identified about 40 uncertain parameters associated with chemical kinetics, heat transfer and mass transfer coefficients, and a few other quantities. Element 1 and 3 scientists also helped us to characterize the initial (prior) probability distributions of these identified parameters. Due to the complexity of the process model, it was decided that the UQ analysis should be divided into two phases: separate UQ studies for adsorber and regenerator, followed by UQ studies for the full system. The next step consisted of sampling the uncertain parameter distributions to compute uncertainties and sensitivities. Subsequently, thousands of ACM simulations were run with the help of Element 5 personnel using the Turbine Gateway for launching many simultaneous simulations. The simulation results were analyzed using various uncertainty and sensitivity analysis methods. It was found that the chemical kinetic parameters were the most sensitive in inducing model output uncertainties. In addition, significant correlations were detected for the chemical kinetic parameters. For example, the heat of reaction and entropy parameters in the formation of carbamic acid are highly correlated. Furthermore, the regenerator model was found to be much less tolerant to variations in chemistry parameters than initially anticipated. The results of sensitivity analysis indicated that we needed better characterization of uncertain parameters, especially the sorbent chemistry parameters. As such, more refined probability distributions from ongoing UQ analyses of the chemical kinetics models (more details about below) were employed in our final analysis, which yielded better uncertainty results (smaller prediction uncertainty). The overall UQ approach and results have been documented.

To better characterize the chemistry parameter uncertainties, some members of Element 6 have been working with NETL on a series of models that have been proposed for solid sorbents. A simplified Lumped Kinetic Model has been the primary focus of recent UQ investigation, building on previous collaborative work for both a dynamic model and an equilibrium model. A Bayesian calibration approach is being used to generate a joint distribution on the model parameters that is consistent with experimental data. This approach also provides predictions and associated uncertainties that can be compared to the actual data. In addition to the calibration work, sensitivity analysis techniques are being used to identify appropriate parameter regions and to explore which variables are important drivers in the uncertainty present in the model output. Posters were also prepared for the Conference on Data Analysis held in Santa Fe at the end of February and a DOE Industry-National Laboratory Workshop on Modeling and Simulation held in March. Our calibration approach and sensitivity analysis results were also presented at the Joint Statistical Meetings in August. In addition, to handle model deficiencies that may cause significant uncertainties in upscaling, efforts have been expended in incorporating model form uncertainties in the form of discrepancy models. However, model form uncertainty analysis was not incorporated into the results presented for the A650.1 study this year.

We also completed a new version of the UQ framework with user manual and installation guide. The graphical user interface of this framework was developed in the MATLAB environment. This framework connects the ACM simulation server, allowing running hundreds of simulations simultaneously, with the PSUADE UQ software for sampling and analysis. As such, this framework provides many UQ capabilities such as parameter screening, response surface analysis, basic uncertainty analysis, global sensitivity analysis, and Bayesian inference. This framework has been released as part of the CCSI product release in September, 2012.

Element 6 has also been investigating the use of UQ for CCSI CFD models with Element 2. As a part of this effort, some team members are participating in the CFD Validation/UQ Subteam which developed an integrated plan for carrying out VUQ Activities for CCSI CFD models. The UQ team has contributed to planning to use experimental data from NETL's C2U for validation. This includes development of statistical experimental designs for data collection to assess the impacts of different variables and to understand variability and uncertainties that are present.

Element 6 has also been investigating UQ in the modeling of multiphase flow in a full-scale regenerator. Due to the high computational cost, a Gaussian process-based response surface methodology was used to quantify the relationship between the uncertain variables (bottom inlet gas flow rate, particle size) and output quantities of interest such as pressure drop gradients and solid fraction. Parametric uncertainty studies show that 1) gas velocity and particle size are the two most significant parameters; 2) smaller particles will have uniform fluidization but allow small gas flow rates; 3) larger particles will allow larger gas flow rates but tend to form dense clusters. These results were presented at the 2012 ASME Meeting (Guang Lin, Alex Konomi, Avik Sarkar, Emily Ryan, Xin Sun, Uncertainty Analysis for the Full-scale Regenerator Model as a Post-combustion Carbon-Capture Unit, ASME 2012 Fluids Engineering Summer Meeting, July 11, 2012, Puerto Rico, USA.) Also: G. Lin, B. A. Konomi, A. Sarkar, X. Sun, J. Bao, C. Tong, J. Wendelberger, K. S. Bhat, L. Moore, B. Ng, D. Miller, and M. Khaleel, "Solid Sorbent Simulation: Early Development and UQ Evaluation Tools," was presented at the 11th Annual Conference on Carbon Capture and Sequestration, Pittsburgh, Pennsylvania, April 30-May 3, 2012.

One of the major hurdles in conducting our UQ studies has been the characterization of uncertainty in parameters because of the limited information available for developing defensible probability distributions (called priors) or ranges for the uncertain parameters. If the priors are too narrow, they may not reflect the true uncertainty of the parameters. If they are too large, they may inadvertently over-stress the simulation models, in the sense that some parameter combinations are not physically or numerically realizable even though they are in the feasible parameter space. This is further compounded by difficult-to-characterize parameter correlations and the presence of difficult-to-detect model form uncertainties.

Our experience with UQ analysis of the A650.1 model further demonstrated that UQ is valuable not just for quantifying our confidence in model predictions, but also for identifying potential model improvements.

The UQ methodology is essential for assessing uncertainty present in carbon capture models and establishing quantifiable confidence in parameter estimates and model predictions. This means prescribing error bars for model predictions to reflect our confidence in view of various sources of uncertainties. The key results have led to a better understanding of limitations in our current modeling process and helped to identify significant issues and drivers requiring additional information and model development. Progress this year has addressed technical challenges associated with several component models as well as the integration of some key coupling processes required for understanding overall system behavior. These results will inform further work in the CFD arena requiring ROMs for simulations with extended run times and scale-up to industrial process scale.

The CCSI Technical Team is currently reviewing recommendations from the October 2012 IAB meeting and developing detailed plans and priorities for the next project year (Feb 2013 – Jan 2014).

Element 7: Risk Analysis and Decision-Making

As part of the first software release for the CCSI project, the Element 7 team released the Financial Risk Model (FRM) spreadsheet. The FRM is an Excel Workbook that quantifies financial risk for a coal power plant retrofitted with a carbon capture system based on key technical and financial factors believed to be important determinants of the expected profitability of carbon capture, subject to uncertainty. The model calculates the expected profitability of investments in carbon capture and measures risk in terms of variability in expected net returns from these investments. The key features of the model are:

- An estimate of the Discounted Net Present Value (NPV) of receipts over the lifetime of the plant to assess the merits of the CCS retrofit.
- Incorporation of uncertainty for key CCS parameters to assess the risk associated with uncertainties in the technology.
- A regression analysis to assess the relative importance of the uncertain parameters.
- Model inputs and key outputs are assembled in a single worksheet. The NPV estimates are contained in additional worksheets for three separate cases – a coal plant without the retrofit and two cases with CCS retrofits using different approaches for incorporating uncertainty. The FRM takes two kinds of model inputs, user input (point estimates for retail and wholesale electricity prices, discount rate, as well as federal and state tax rates) and process parameter distributions (1: CCS parasitic power requirements; 2: drop in capacity factor due to CCS; 3: carbon capture percentage; 4: CCS construction costs; and 5: CCS fixed O&M costs). The initial point estimates of these values are taken from the Element 3 process design, but the actual distributions will be taken from the UQ and other CCSI Technical Elements.

A Wiki-based expert elicitation system has been developed to automate input and development for the Technical Readiness Level (TRL) model. A technology, such as carbon capture for a PC fired power plant, is made up of several processes (e.g., adsorber, regenerator, CO_2 compression train). Each process contains its own challenges in new technologies, scale, and overall maturity. The goal of a risk

assessment which includes technical maturity modeling should include an estimate of the maturity of each process and the combined system level maturity. To estimate the current maturity level, we utilize the technology readiness level (TRL). Our technical maturity model incorporates the process-level TRL into a system-level maturity model that feeds into the technical risk model. Combining results from different experts we estimate the likelihood of the technology being within each maturity level. For each maturity level (1-9), an uncertainty or confidence bound can be developed and used to simulate an uncertainty estimate (e.g., cost multiplier). The goal is to combine information from the TRL elicitation and likelihood model to obtain the most realistic estimate of uncertainty from lack of knowledge or maturity. Progress in the development of this tool was presented during FY12:

- Engel, D.W., Letellier, B.C., Edwards, B., LeClaire, R., and Jones, E., "New Technical Risk Management Development for Carbon Capture Process," presented at the *11th Annual Conference on Carbon Capture & Sequestration*, Pittsburgh, PA, April 30-May 3, 2012.

In our initial design of our risk analysis and decision making framework, the major focus was on how the uncertainties and risks effected the overall financial risk model. The idea was that we pushed all of the risk and uncertainties up to the top level and focused the results mainly on financial issues as they affect the "Technology User." Since this initial design, we have worked with several collaborators and have identified two additional levels/scales for modeling risk. These two additional levels include the Technology Designers (optimization) and the Technology Creator (R&D). Collaboration with Eastman Chemicals and feedback from the IAB provided the impetus for this shift in direction.

On August 6-7, 2012, Element 7 team held a workshop at LANL, bringing together the team members from all of the participating labs for 1½ days of discussion with project leadership from NETL. The objectives of the workshop included identifying the uncertainty drivers behind the financial cost estimates, identifying key risk drivers for program performance, and laying out the framework for integrating the different types of program risk; technical, financial, and maturity. A key result coming from this workshop was the identification of a mechanism for introducing technical risk into the Element 3 process models. Simulation of process performance in off-nominal states can be used to generate a distribution of scenarios such that the high-risk scenarios can be identified and assessed for mitigation.

Following the April IAB meeting, the team began collaborating with Eastman Chemical Company, which is interested in contributing to the development of the risk analysis and decision support system. Following a visit to Eastman in Kingsport, TN August 28-29, we identified three unique stages or perspectives for technology development (maturation). Using consistent methodology, risk and uncertainty assessment techniques can be used to inform decision making at each stage of the design life cycle. These stages are Early R&D (Technology Creator), Design Refinement (Technology Designer), and Construction & Operation (Technology User).

Based on priorities to be established by the IAB and the CCSI leadership team, the following are development areas we could pursue:

- **Porting FRM to Matlab (or similar) -** Extending the FRM to a more flexible programming environment would allow for more readily performing parametric analyses. In addition to the parameters that are currently user input, liquid vs. solid sorbent could be considered, as well as alternative time horizons, types of plants being retrofit, etc.

- **Risk-based Optimization Modeling -** The team plans to couple technical component performance uncertainty into the Element 3 process models, to capture the system behavior under other than nominal conditions. This combination is anticipated to enable

a degree of risk identification that exceeds the speed and accuracy of a group of subject matter experts.

- **Risk-based R&D Integration -** The application of risk techniques to early R&D efforts has been identified as a need by IAB collaborators. A functional failure approach to risk analysis at the pre-component level of R&D is proposed. Combining a hazards analysis approach with a high-level functional description of a notional process, "anything that can go wrong" is identified as a risk. The consequences for each risk can be defined and evaluated for anticipated likelihood.

- **Technology Maturity Modeling -** Assigning risk to TRL transition questions as a means of prioritizing R&D. The proposed technique would need to be further adapted to capture the relative importance or consequence of each question. High risk, high importance items should have priority, but all medium and high risk items would need to be tracked under a risk mitigation plan.

- **TRL Uncertainty Model -** The goal of this model is to combine information from the TRL elicitation and likelihood model to estimate the most realistic estimate of uncertainty. To do this, we will incorporate the ability to model each process separately and then bring together for the final estimate.

- **Decision Making Framework** - A wiki based system would be developed to access all of our risk models within a single system (GUI). This system would be based on an existing architecture system to automatically pass information (results) between each model to analyze, report, and display key risk analysis results.

Element 8: Software Development Support

Element 8 provides comprehensive development support and incorporates comprehensive licensing, versioning, bug tracking, build, packaging, and test tools. Element 8 introduced JIRA (www.atlassian.com/software/jira) as the software project tracker for CCSI. JIRA provides bug and project tracking, and supports agile development methodologies, in particular scrum (www.scrum.org). Element 8 has adapted the scrum methodology to match CCSI geographic and personnel situation, and has used scrum to organize its internal work.

We continued updating and refining the CCSI Software Development Plan. The Software Development Plan describes how the CCSI software and modeling activities will meet or exceed future software quality assurance goals that inevitably will be established upon the successful completion of the initial phase modeling and simulation efforts. Specifically the document describes, the processes (consisting of activities, tools, work products and artifacts) that are implemented by CCSI to develop software and how they meet the required level of rigor based on risk level using a graded approach.

We started working toward our long-term objective to streamline, document, and, wherever practical, automate the build, test, and release procedures. We believe this is essential both for the CCSI agile development process, as automated build and testing will allow to integrate their work with others as

often as needed; and to achieve a reliable and reproducible release process. The potential challenge is that the requirements of automated building and testing may constrain the choices developers make when working with their codes, in particular when it comes to define their product dependencies on external software and the tools used to build their codes. We are in the process of defining a set of turn-key virtual machines which are ready to run build and test procedures for all CCSI software products on our target platforms.

The main accomplishment of Element 8 was our contribution to the September CCSI pre-release. We acted as integration testers for the 21 software products comprising the release. For each of the products, one or more members of Element 8 would follow, for each of the product supported platforms, the installation steps outlined in the product installation guide and run the examples and tutorials in the user guide. For each product we provided feedback on basic functionality, usability, and documentation, as well as making software engineering recommendations on coding and packaging where relevant. By taking the point of view of a user not familiar with the CCSI toolkit, and thanks to the fast response to our feedback from all product developers, we were able to identify over 50 issues (mostly minor) across all CCSI products. In addition to testing, our contribution to the release has been in defining release procedures and providing basic tools to support them:

1. We defined a common package structure and tagging scheme in CCSI SVN repository for the artifacts in a software product.
2. In collaboration with Element 5 we defined a product versioning scheme that encodes the status of the product from the testing and validation point of view. We defined what stages a product undergoes in the release integration stage (alpha, beta, release candidate) and gained experience in what kind of testing different CCSI products need during these stages.
3. In collaboration with the Tech Leads team we agreed on a simple procedure to report issues during the internal testing, and the future pre-release stages, by using the ccsi-support mailing list to encourage maximum feedback. For products which are being tracked on JIRA (the integration framework in particular) we have also used JIRA to formally track issue resolution
4. We added a Software Product database to the CCSI web site and implemented workflows to upload new products and new versions of existing products to it to make sure that all necessary information on a product was provided, and to notify testers about the uploads.
5. We defined access control groups on the CCSI web site for the initial alpha testing, and later on for the internal beta testing stage.

The scrum project management methodology has not yet been used outside Element 8. We believe this was due in part to the nature of the R&D work and of the deliverables of some CCSI Technical Elements, as well as the considerable time pressure under which most of CCSI developers have worked, which may have made them less willing to test a new development methodology. Over the course of next year we plan to reach out further to the other Technical Elements to promote the scrum methodology and to receive feedback on its suitability to CCSI work.

Another challenge is that the number of products we are testing, and the number of platforms we are potentially supporting them on can very quickly create a large test matrix (even when sparse). We have experienced this first hand during the September pre-release; hence, we will focus on streamlining and automating the testing procedures as much as possible. This problem should also be mitigated once, with the help of other Technical Elements, we will understand better how to package our software products and prioritize which platforms should be supported.

The CCSI Technical Team is currently reviewing recommendations from the October 2012 IAB meeting and developing detailed plans and priorities for the next project year (Feb 2013 – Jan 2014).

Element 9: Industry Advisory Board

This element transitioned from the ARRA-funded activities to Advanced/Crosscutting Research activities following the April meeting of the IAB. The major accomplishment was planning for the next meeting of the IAB in October 2012.

The bi-annual meetings of the IAB enable industry, the ultimate users of the CCSI Toolset, to have advance knowledge of new computational tools and capabilities, which they can employ to accelerate the development of carbon capture technologies. In addition, the meetings facilitate communication among industry and the technical team to ensure that the new computational capabilities are aligned with the most pressing and critical needs to meet the Fossil Energy Clean Coal Technology Program's mission.

3.0 TECHNOLOGY TRANSFER

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Bhat, K.S., Moore, L., Wendelberger, J., Kress, J., and Mebane, D., "Uncertainty Quantification in the Carbon Capture Simulation Initiative," presentations, Industry-National Laboratory Workshop on Modeling and Simulation, Austin, TX, March 7-8, 2012.

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Cozad, A., Sahinidis, N.V., and Miller, D.C., "Derivative-Free Optimization Enhanced-Surrogate Model Development for Optimization," presentation, RMS 2012, Phoenix, AZ, October 14-17, 2012.

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The National Energy Technology Laboratory (NETL) conducts cutting-edge energy research and technology development and analyzes energy systems and international energy issues for the U.S. Department of Energy. The NETL-Regional University Alliance (NETL-RUA) is an applied research collaboration that combines NETL's energy research expertise with the broad capabilities of five nationally recognized, regional universities: Carnegie Mellon University (CMU), The Pennsylvania State University (PSU), University of Pittsburgh (Pitt), Virginia Tech, and West Virginia University (WVU), and the engineering and construction expertise of an industry partner (URS). NETL-RUA leverages its expertise with current fossil energy sources to discover and develop sustainable energy systems of the future, introduce new technology, and boost economic development and national security.

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