

CCSI and the role of advanced computing in accelerating the commercial deployment of carbon capture systems

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Abstract. The Carbon Capture Simulation Initiative (CCSI) is developing state-of-the-art computational modeling and simulation tools to accelerate the commercialization of carbon capture technology. The *CCSI Toolset* consists of an integrated multiscale modeling and simulation framework, which includes extensive use of reduced order models (ROMs) and a comprehensive uncertainty quantification (UQ) methodology. This paper focuses on the interrelation among high-performance computing, detailed device simulations, ROMs for scale-bridging, UQ and the integration framework.

1. Introduction

The *Carbon Capture Simulation Initiative* (CCSI) is a partnership among national laboratories, industry, and academic institutions that is developing 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 resulting *CCSI Toolset* will provide end users in industry with a comprehensive, integrated suite of scientifically validated models with uncertainty quantification, optimization, risk analysis, and decision-making capabilities. The CCSI Toolset will incorporate commercial and open-source software currently in use by industry and will develop new software tools as necessary to fill technology gaps identified during execution of the project. 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 a virtual power plant.

CCSI is part of DOE/NETL's comprehensive CCS RD&D program, part of the president's plan to overcome the barriers to the widespread, cost-effective deployment of CCS within 10 years [1]. It has been estimated that using today's commercially available CCS technologies will add approximately 80 percent to the cost of electricity for a new pulverized coal (PC) plant and approximately 35 percent to the cost of electricity for a new advanced gasification-based plant. Thus, an important part of the CCS RD&D effort is the development of the next generation of technologies for carbon capture that have the potential to reduce these costs to less than a 30 percent increase in the cost of electricity for PC power plants and less than a 10 percent increase in the cost of electricity for new gasification-based power plants [2]. For PC plants, the majority of the increased costs result from the parasitic loads (steam and power) required for the CO₂ capture and compression processes, which decrease the power generating efficiency (and the net output) by approximately one third.

Taking promising new power plant technologies from concept to commercial scale could take 20–30 years because of the need to manage the overall risk of the scale-up process. Typically, several incremental steps are taken during scale-up, ensuring that the risk in each step is as small as possible. CCSI will provide validated simulation tools that will accelerate the commercial deployment technologies developed under the CCS RD&D program. Science-based models will be used in conjunction with pilot-scale data to allow larger steps to be taken earlier with greater confidence, thereby reducing the time and expense required for achieving commercial deployment of carbon capture technology.

Recent experience in other industries such as aerospace and the automotive industry has demonstrated that simulations can be used to accelerate the development of technology [3–5]. The challenge addressed by CCSI is to use the recent advances in simulation technology and to develop a science-based capability to assess and mitigate the risk of scaling up carbon capture technologies.

The CCSI Toolset will incorporate high performance computation capabilities, high-resolution device-scale simulations and uncertainty quantification. The device-scale simulations will allow study of fine-scale and complex characteristics. Reduced-order models (ROMs) will be developed from the high-resolution simulations to enable scale-bridging and to develop detailed, computationally efficient models that will ultimately run on end-user computers. Uncertainty quantification, reduced-order model development, and validation of reduced order models will require high-performance computing resources. This paper describes the overall goals and approach of CCSI. It then provides a detailed discussion of the computational approach for high-resolution device-scale simulations and uncertainty quantification. The final section describes our approach for developing the integration framework that ties together the multiple simulation packages, uncertainty quantification tools, reduced-order model development tools, and the supporting computational architecture we are building to support these activities.

2. Overview of CCSI

The CCSI Toolset is being developed around three industrial challenge problems (ICPs) applicable to existing PC power plants, which generate nearly half the electricity in

the United States and emit about a third of all CO₂ from U.S. sources. Ninety-five percent of the coal-based CO₂ emissions projected to be released from 2010 through 2030 will originate from existing PC power plants, and a recent analysis suggests that roughly 325 coal-fired generating units accounting for roughly two-thirds (200 GW) of current U.S. coal-based generating capacity are suitable for carbon capture.

Solid-sorbent-based post-combustion capture technology was chosen as the first ICP for CCSI because significant work remains to define and optimize the reactors and processes needed for successful sorbent capture systems. Sorbents offer an advantage because they can reduce the regeneration energy associated with CO₂ capture, thus reducing the parasitic load. Most of the work on sorbents has been restricted to developing the sorbent itself [6], with only recent studies considering the design of the reactor system and integration with the power plant [7]. Since *solid-sorbent systems are at the start of the traditional process development cycle*, this initial ICP will accelerate the analysis of options for this emerging technology. The CCSI Toolset will help identify promising solid-sorbent processes and accelerate the scale-up from 25 MWe to commercial demonstration scales.

Solvent-based postcombustion capture will serve as the second ICP. Commercial solvent developers have already completed process design and analysis for first-generation solvents, and these are being tested in various pilots; however, *advanced solvents are currently in the middle of the traditional process development cycle*, moving from pilot scale to commercial demonstration, so CCSI development can build logically on the prior developments for solid sorbents, chronologically matching current industrial development of advanced solvents. Oxy-combustion is the third ICP because of the expected timelines for oxy-combustion pilot and demonstration projects.

As shown in Table 1, the CCSI team is organized into three focus areas and ten Task Sets (TSs) to address the challenges in multiscale and multiphysics modeling and analysis, software implementation, and industrial applications.

Table 1 CCSI Task Sets by Focus Area

Physicochemical Models and Data	Analysis & Software	Industrial Applications
1. Basic Data and Models	5. Integration Framework	9. Industrial Challenge Problems
2. Particle and Device Scale Models	6. Uncertainty Quantification	10. Industrial Collaboration
3. Process Synthesis and Design	7. Risk Analysis and Decision Making	
4. Plant Operations and Control	8. Software Development Support	

The *Physicochemical Models and Data* focus area consists of four TSs that address the challenge of developing science-based modeling tools for various CCS processes considered in the ICPs. The models range from particle-scale reaction kinetics models, to device-scale CFD models, to steady-state process synthesis and design models, to dynamic plant operations and control models. Several commonly used commercial and open-source software such as FLUENT[®], Aspen Plus[®], DYNsIM[®], and MFIX will be used to build the models. Unlike other modeling efforts, the simulation and design activities at the different length scales (e.g., CFD and process system) will be integrated so that information and insight will continually flow between scales in order that each scale can benefit from insights

at the other scales. Much of this information flow will result from an integration framework being built by the second focus area.

The *Analysis & Software* focus area includes four TSs that will develop the capability to integrate different models and software packages, to quantify uncertainties in model predictions, to develop optimal designs based on integrated models, and to conduct risk analysis. An additional TS will support software development across all the TSs. Realizing the vision of an integrated and coherent multiscale software environment for the design, analysis, and optimization of carbon capture systems requires an approach that effectively enables the flow of information between the scales of interest.

In addition to technical risks, the development and deployment of new technology pose various economic and legal risks. Modeling and simulation can address some of the technical and economic risks through the use of predictive computer models, if the uncertainties inherent in the modeling process can be determined. Uncertainties that need to be addressed are related to the data used to describe the physicochemical models, coupling the results of one simulator to another, and in the extrapolation into poorly known regions of parameter space needed to explore new design scenarios. The assessment of economic and legal risks is possible only if a well-defined process is in place for assessing the propagation of uncertainties, sensitivity analysis, model reduction, model validation and calibration, and risk analysis of large-scale multi-physics technical models.

The *Industrial Applications* focus area consists of two TSs: Industrial Challenge Problems and Industrial Collaboration. The Industrial Collaboration TS is responsible for developing a strong collaboration between the industry partners and other CCSI partners and for ensuring that CCSI models are applied to support commercial decisions that will accelerate capture deployment. The Industrial Challenge Problems TS is responsible for working with industry partners to develop and refine the three ICPs. The ultimate objective of accelerating the deployment of capture technology requires that the tools and methodologies developed provide information necessary to support investment decisions by equipment suppliers and utility companies. Our industry partners will help ensure that CCSI understands these information requirements and can communicate simulation results in a manner appropriate to aid decision makers.

3. Device-Scale Simulation and ROMs

Since most of the proposed concepts for carbon capture [11] have multiphase reactive flow at the core of the system, we will use multiphase computational fluid dynamics (CFD) to simulate the device-scale performance in terms of flow properties, outlet composition, temperature, and pressures. The CFD predicted device-scale performance under different operating conditions will be used in creating device-scale ROMs for the subsequent tasks in process synthesis, control, and uncertainty quantification. We focus our discussions in this paper on our first industrial challenge problem (ICP-A), namely, carbon capture with solid sorbent. For ICP-A, the gas-particle device under investigation may be a fluidized bed [12], packed bed, or moving bed; and the simulation tool developed should permit analysis of all these different options. In general, CFD approaches for modeling multiphase reactors can be categorized into two types [13]:

1. An implicit multifluid Eulerian-Eulerian (EE) formulation in which both the fluid (carrier) phase and the particulate (dispersed) phase are treated as interpenetrating continua. This “multifluid” approach treats each phase as a fluid field fully coupled (i.e., interpenetrating).

2. An Eulerian-Lagrangian (EL) formulation in which the particle phase is discretely tracked and the each particle follows Newton's laws.

The EL formulation can be further classified into a resolved discrete particle model (RDPM) and an unresolved discrete particle model (UDPM). In RDPM the near-particle gas flow (e.g. particle boundary layer) is resolved. This would imply a simulation technique in which the resolution of the gas phase conservation equations is smaller than the particle size. UDPM is reliant on sub-models (e.g., drag, heat, and mass transfer correlation) to account for interactions between the particle phase and the gas phase. In most cases the discrete element method (DEM) [14] would be classified under UDPM. These classifications are depicted in Figure 1.

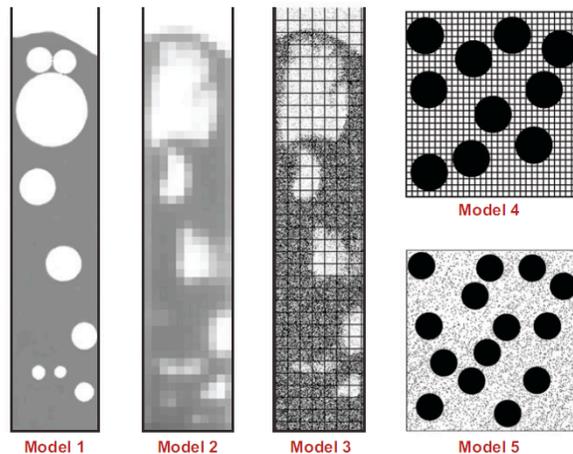


Figure 1. CFD model classification: (1) discrete bubble, (2) Eulerian-Eulerian, (3) UDPM, (4) RDPM, and (5) Lagrangian-Lagrangian (from van der Hoef et al. 2008).

Clearly, the scientific challenge in accurately modeling a full-scale reactor is the large disparity of physical scales in the reactor. The overall flow structure can be characterized in the order of meters, yet these overall flows are influenced by the particle-level properties such as particle size, particle-particle collision, and particle-gas reaction rate. Since the reactor may contain hundreds of millions of physical particles, it is neither computationally feasible nor physically necessary to have one single simulation to cover the entire reactor and represent all the time and length scales. Hence, the computational challenge is to develop a coarse-graining strategy that can accurately and efficiently pass the particle-scale reactions and interactions to the overall device scale flow simulations.

Scale bridging

We are developing predictive capabilities at three distinctive scales with ROMs as the scale-bridging methodology (Figure 2). First, we are developing a detailed single-particle model in which the inhomogeneity within the particle is explicitly resolved; the pore structure and composition changes resulting from the interaction with the external environment will be modeled, including the possibility that such changes at the interior of the particle are nonuniform. These morphological changes affect the accessibility of the reaction sites and hence the overall reaction rate. The particle properties to be considered include

diameter, pore morphology, bulk density, specific area, composition, heat conductivity, and heat capacity, as well as its diffusion properties and reaction kinetics with CO₂ as obtained from ab initio calculations provided and possibly lattice Boltzmann simulations of nanopores.

Next, we will develop effective lumped models with a *cloud* of particles that incorporate the parametric results obtained from the detailed single particle model. The size of the simulation domain (cloud size) is comparable to the grid size in typical coarse grid reactor CFD simulations with the particles fully resolved. The periodic gas-particle flow domain will be subjected to various thermal hydrodynamic conditions, and the outcome of this task will be a law, that is, a reduced order model, relating the effective reaction kinetics of a cloud of particles to the average particle phase volume fraction and the prevailing local hydrodynamic conditions. Results on various cloud size will also elucidate the required computational resolution needed in the device scale CFD simulations for various types of solid sorbents and under different hydrodynamic conditions. A similar subgrid strategy was demonstrated by [15] for a coarse-grid simulation of gas-particle flow using MFI_X to account for the effects of the unresolved mesoscale instability structures.

The ROM will be validated against experimental data. The approach is to propose a candidate lumped kinetic model based on the results in this task and validate it with some controlled experiments. Any directly measured model parameters will be input into the model. The other parameters will be calculated to minimize the error between the model behavior and experimental measurements. For a particular solid sorbent with specific properties, reaction parameters from experiments include system pressure, CO₂ and H₂O partial pressure, flow rates, and temperature or heat input. These require temporally resolved measurements of exit gas temperature, exit gas composition, particle mass, and particle temperature.

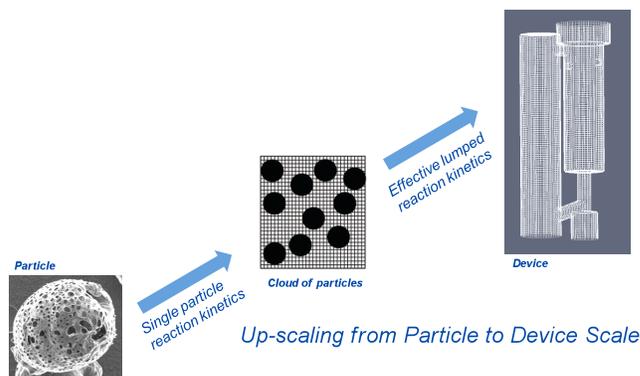


Figure 2. Approach for up-scaling from particle scale to device-scale CFD models.

On the reactor scale, coarse-grid CFD simulations will be performed. At this scale, each simulation cell is assumed to have uniform thermal hydrodynamic and reaction properties, and the particles within each cell are assumed to evolve identically with the lumped reaction kinetics laws obtained from the cloud model. Similarly subgrid or (subfilter) closures for the Eulerian fields are necessary for tractable simulations of these larger systems. These subgrid models would include phenomena such as turbulence and gas-solid drag. Models such as MPIC [16] or Dense DPM [17] represent a hybrid model in which the motion

of the particles are treated in a Lagrangian sense but some of the interactions and particle-collisions, in the case of MPIC, are treated in an Eulerian sense.

From the device-scale CFD results, ROMs will be generated to relate the device scale performance measures to the design parameters such as reactor geometry and sorbent properties and the operational parameters such as temperature, flow rates, and chemical and physical compositions of the feed streams. The complexity of the ROM to capture the performance at the device scale will have to be determined on a case-by-case basis depending on the features of a given device scale design and on the specific needs of the process scale.

4. Uncertainty Quantification

Uncertainty quantification (UQ) is now recognized as an essential component of the computational investigation of complex, multiphysics, multiscale system behavior. UQ is the study of the accuracy and reliability of scientific inferences and provides quantified confidence measures that can be used to inform decision making involving simulations such as those that will be produced by the CCSI. CCSI is leveraging the significant advances and expertise from the DOE National Nuclear Security Administration Advanced Simulation and Computing Program and the Office of Science Advanced Scientific Computing Research programs. The main objective of these efforts will be to develop a set of computational tools for UQ to be integrated into current simulators.

Uncertainties can arise in many different forms. First, there are uncertainties associated with the set of governing equations to describe the physical or chemical processes. Then, there are uncertainties in how one subsystem should be coupled to the rest of the system. Moreover, many parameters to describe material properties are computed from data generated from independent experiments, and uncertainties abound in these data sets. In addition, some physical processes may not be adequately accounted for in the simulation model, giving rise to the “missing physics” uncertainties. Furthermore, uncertainties arise when one uses simulators to extrapolate from well-known regions of parameter space to other regions of interest as for example when one is exploring new design scenarios. Quantifying uncertainties can be a monumental task that requires major advances in high-performance hardware and software technologies.

The first step in a UQ study is to identify all possible sources of uncertainties in the system to be modeled. This is followed by the characterization of these uncertainties as model or parameter forms. Parametric uncertainties can further be classified as aleatoric (associated with some probability distribution) or epistemic (the probability distributions are not known). Subsequently, different methods are used to propagate these uncertainties through the model. The uncertain model outputs of interest then are analyzed and the effects of uncertainties assessed. In performing these steps are needed, many numerical and statistical techniques such as those for forward uncertainty propagation, sensitivity analysis, dimension reduction, response surface analysis, and model calibration.

UQ approaches are often categorized as nonintrusive and intrusive. For a generic multiphysics application characterized by both linear and nonlinear components, nonintrusive methods use sampling or collocation procedures, which typically employ a (large) number of deterministic simulations to generate output statistics. On the other hand, intrusive methods, such as generalized polynomial chaos, typically require a reformulation of the mathematical models and thus may require substantial code modification. Since the CCSI simulator will heavily leverage existing modeling codes, most of which do not contain embedded UQ capabilities, the program must initially focus on nonintrusive UQ methods to understand

sensitivities of each simulator component to its input parameters and data, as well as the uncertainties associated with other causes.

In order to facilitate a UQ study, three components are essential: a well-defined UQ strategy, a relevant UQ toolkit, and an adequate hardware/software infrastructure to handle the logistics of large ensemble calculations and analyses. In the following subsections, we illustrate each of these three components in more details.

4.1. UQ Strategy

Having a UQ strategy at the beginning phase of the project is critical to the success of a UQ study. Conclusions that can be made about the model are valid only with respect to the assumptions made in the beginning. Without a well-thought-out plan, much manpower and computer cycles can be wasted. For example, a UQ study performed on CCSI models can be formalized into the following phases:

1. Define the objectives of a UQ study, and identify the model to be studied.
2. Identify the sources of uncertainty to be propagated, and characterize them (this includes the available experimental data and their uncertainties).
3. Design computer experiments to propagate uncertainties.
 - If the model has many uncertain parameters, dimension reduction may be needed.
 - If the model is expensive to evaluate, response surfaces/surrogates are needed.
 - Accurate and efficient designs are always needed to propagate uncertainties.
 - “Importance” sampling for calibration with experimental data may be needed.
 - Specialized designs for sensitivity analysis may be needed.
4. Analyze the impact of uncertainties on model prediction.
 - Probability of system failure or non-compliance with regulations.
 - The ability to predict a “hold-out” (from calibration) system accurately.
5. Conduct expert review and publish findings.

We will tailor this general methodology for three ICPs, each modeling a different physical process: solid solvent, liquid solvent and oxy-combustion. In each case we follow a gradual approach for the development of the full-scale model, at each step introducing complexities such as number of devices in the design, the complexity of each device, and a dynamic (instead of static) process. The development of the UQ capabilities follows a similar path: we will first demonstrate the applicability of UQ tools to individual components or devices of a given model, followed by an extension to components of higher internal complexity and to process designs consisting of multiple devices. This workflow will be applied to each of the case studies, hardening the UQ tools and ensuring the general applicability of the developed capabilities.

Some of the UQ objectives are to identify the most important sources of uncertainties, to study the effect of uncertainties on the effectiveness of CO₂ capture, to inform our risk assessment team of potential vulnerability, and to guide subsequent uncertainty reduction efforts.

4.2. UQ Toolkit

The selection of methods and tools is an important part of our UQ effort. Inappropriate choices of methods will result in wrong conclusions. For example, many classical sensitivity methods such as standardized regression coefficients (SRCs) are based on the assumption that the model input-output relationships are linear, and violation of this assumption may result in faulty conclusions. For our carbon capture process and device models, we anticipate

nonlinear input-output relationships with unknown functional form. Thus, our selected UQ methods will largely be nonparametric. However, we do expect the function to be somewhat smooth.

We anticipate that our more sophisticated simulations will have a large number of uncertain parameters. Thus, we will need screening methods to down-select the parameters to a manageable number (say, ~ 10). Again, classical methods such as SRC and perturbation methods are largely inadequate. We will use nonparametric screening methods such as the Morris design and other stratified designs for this purpose.

To construct response surfaces or surrogates (these are sometimes also called reduced order models), we need space-filling designs together with effective and efficient interpolation schemes. Many space-filling designs exist, such as quasi-Monte Carlo, Latin hypercube, orthogonal arrays, and spectral collocations. For interpolation schemes, we will investigate Gaussian process and cubic splines (we may use polynomial regression if appropriate). We will adaptively increase the sample size and use rigorous validation techniques to ensure the accuracy of the response surfaces.

The choice of model output uncertainty representation depends on the nature of the uncertainties. For aleatoric uncertainties, the proper choice is the posterior probability distributions. For epistemic uncertainties, the upper and lower bounds for the model outputs may be more informative, even though the distributions may still enable insights. Propagation of uncertainties will be through the cheap surrogates, and thus the sample size is usually not a major concern.

Bayesian inferences are popular for model calibration. The idea is to first prescribe initial distributions for the uncertain parameters (called priors). Then a likelihood function is developed relating model prediction and data. These are then combined in the Bayes formula to compute the posterior distributions. Again, for epistemic uncertainties, the posterior bounds may be more relevant.

Global sensitivity analysis methods based on variance decomposition are more suitable for nonlinear models since they are nonparametric methods. Since these methods require large sample sizes for accuracy reasons, they are generally analyzed on the cheap surrogates. The major sensitivity indicators from these methods are first-order, second-order, and total-order sensitivity indices, which express numerically the percentage of the model output variance attributed to each uncertain parameter.

Another form of uncertainty has not been addressed above, namely, model form uncertainties. For expensive models that rely on response surfaces, this type of uncertainty may introduce added complexity. One research task is to investigate how to efficiently propagate this type of uncertainty.

To employ the methods described above, we need an enriched set of statistical tools. Instead of developing our UQ toolkit, our approach will be to leverage, as much as possible, existing state-of-the-art UQ tools. Some of these tools are available at the DOE national laboratories and they include, for example, the DAKOTA framework from Sandia National Laboratories and the PSUADE toolset from Lawrence Livermore National Laboratory, as well as other efforts in development. If existing tools do not provide appropriate capabilities, it will be important to understand those limitations and to develop new approaches for characterizing uncertainty.

4.3. UQ Hardware/Software

The need to run large ensemble of simulations implies the great extent to which high-performance computers will be needed for UQ studies. In addition to computer cycles, a great deal of logistics is involved in managing large numbers of runs ranging from job scheduling and monitoring to I/O and storage, fault tolerance, and user interfaces. Thus, in order to facilitate easy access to the UQ tools and to manage a large number of simulation runs, a framework for workflow management is needed. Advanced scientific computing techniques will be valuable in the development of such an end-to-end UQ engine for CCSI.

In summary, a major UQ goal is to predict the performance within an operating envelope and quantify the uncertainty in the prediction in order to reduce the technical risk associated with the project. In order to accomplish this, it will be necessary to identify the critical performance parameters and develop a method for translating system simulation results into performance predictions with uncertainty. In addition, we will determine the sensitivity of performance predictions to the uncertainty in the component models and integration methods that constitute the system simulation in order to assess current state of uncertainty in the component models or integration methods that cause the most sensitivity. Case studies of failures in large-scale demonstrations will be used to identify gaps in component models and integration methods. We will then develop new or reduce uncertainty in existing component models and integration methods identified in the above steps.

5. Integration Framework

The integration framework in CCSI integrates the software tools implementing the simulation capabilities into a seamless, multiscale simulation environment. The services provided by the integration framework include data management, user interfaces, analysis capabilities, ROMs, and interaction among the CCSI software tools. The resulting CCSI software will enable the incorporation of a large number of pre-existing commercial and open-source software packages. The conceptual view of the resulting CCSI framework is shown in Figure 3.

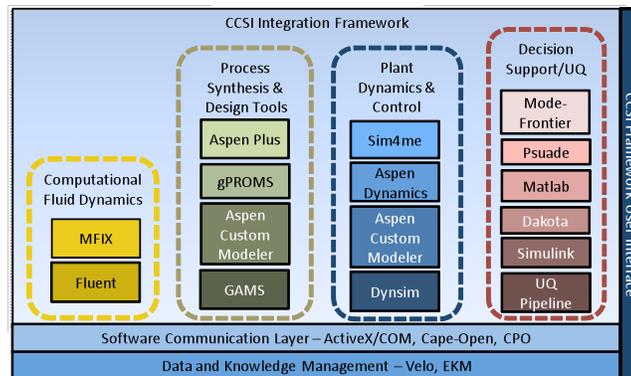


Figure 3. Conceptual CCSI Integration Framework showing examples of the software tools that will be integrated into the CCSI environment.

In this paper, we focus on the framework components to enable execution of CFD and process simulations in support of UQ and to enable ROM development. Our initial ROM development focus is on implementing and automating the PCA-based ROM development techniques laid out in [8] and the ROM development processes developed in the Advanced

Process Engineering Co-Simulator project [9–10]. The ROM techniques discussed in the device scale and UQ sections will also be implemented.

To understand the industry practice, we conducted a survey of the major industrial carbon capture participants to identify the set of software in normal use for simulation. The initial CFD tool identified as most broadly in use is Fluent, with AspenPlus and Aspen Custom Modeler being identified for process simulation. These commercial software tools along with MFIX (an open source CFD simulation capability) are the initial target for CCSI integration. Integration of these tools will enable users to quickly adopt the new CCSI software since they will be able to leverage their trained core of workers and long experience in using these tools as well as their libraries of simulations developed in the software. The CCSI Toolset will bring to their simulation environment new, higher-level capabilities such as optimization, uncertainty quantification, and reduced-order model development.

Dealing with existing commercial software technologies is a significant integration challenge because of hardware platforms, operating systems, and licensing diversity. For example, the AspenPlus software runs on Microsoft Windows and the uncertainty quantification software runs on Linux platforms, and some CCSI modeling and simulation capabilities can be run on a laptop while others will require larger-scale computing. UQ and ROM development both need the ability to run a large number of simulations in order to develop a mapping of the input space to the output space.

We are developing a web services-based, client-server framework to provide the infrastructure for the cross-tool simulation execution capability. The web-services framework will enable and manage both local and remote execution of simulations as well as data passing between components. Workflow software will provide the coordination and tracking of the executions. This design will allow the UQ and ROM development software to run a large number of simulations in order to test the design space using different input combinations and gather the resulting outputs without requiring the software packages to run on the same machine. It will also provide web-based interfaces for monitoring executions and results. CCSI is leveraging existing component interchange standards and formats such as CAPE-OPEN, ActiveX/COM, and SOAP to interconnect the framework and software tools.

Each pre-existing software tool is integrated into the web-services framework using its available interface capabilities. In the case of Aspen Plus, we are using the ActiveX interfaces to set inputs, monitor the simulation process, and gather outputs. A typical Aspen Plus process simulation has thousands of parameters, inputs, and outputs. However, only a small number of these variables can actually be varied and need to be monitored. The Aspen Plus graphical interface makes it relatively easy to find the parameters, inputs, and outputs that can be varied; however, programmatically they are difficult to separate from the rest of the variables, and the allowed operating range of these variables is even harder to find. The framework will provide a user interface to allow the designer of the simulation to specify the parameters, inputs, and outputs of the simulation as well as the operating range for each variable. The results of this specification process get stored in a configuration file with the simulation. When the simulation is run within the CCSI framework, this configuration file guides the programmatic interface to the correct variables and parameters within Aspen Plus. The configuration file also enables automation of the interfaces to the higher-level tools such as UQ by defining the interesting variables and parameters along with their operating ranges. The UQ and ROM software use that information to design and execute their simulations.

The remaining unresolved issue in this architecture is the ability to run a large number of simultaneous simulations. Many of the commercial simulation vendors assume that simulations are run sequentially on a small number of resources, and their per seat licensing restricts the number of simultaneous simulations that can be executed. We are working with vendors to identify appropriate licensing models and ease these restrictions, which are otherwise limiting the ability for high-resolution simulations to be run in large numbers simultaneously. The alternative and parallel solution we are pursuing is ROM development. Although a large number of high-resolution simulations are required to develop the ROM, once the ROM is available, it can significantly reduce the number of additional high-resolution simulations needed to support UQ, optimization, and decision support.

The initial, smaller-scale demonstration problems, as well as initial uncertainty quantification, optimization, and risk management computations will be run primarily using institutional computational resources at PNNL's NW-ICE system (20 teraflops IBM system); LANL's 20, 100, and 200 teraflops systems accessed through the Institutional Computing Program, LLNL's 43.5 Teraflops Ansel Linux cluster; and NETL computer clusters. For the more computationally intensive, full-scale simulations, the CCSI team will use the resources at NETL's Simulation-Based Engineering User Center (SBEUC), which will provide over 200 teraflops of computing power starting in 2012. The primary purpose of SBEUC is to facilitate CCSI and a project in storage simulation. In addition, we are in the process of obtaining high performance computing resources through DOE's National Energy Research Scientific Computing program. We anticipate that peak computational resource requirements will be 100 million CPU-hours per year.

6. Summary

CCSI is using advanced computing to support its overall goals of accelerating the commercial development of carbon capture technologies. Advanced computing is supporting the development of detailed, multiscale device models through the development of detailed ROMs that enable computationally efficient scale-bridging from the particle scale to device scale. In addition, advanced computing is critically important for conducting the large numbers of simulations required for conducting comprehensive UQ of both device models as well as complicated systems. This comprehensive, end-to-end UQ methodology is essential for identifying, quantifying, and ultimately reducing technical risk, thus facilitating commercial decision-making. To enable these activities, we are building an integration framework to manage connectivity among various cross-platform software tools consisting of simulators and UQ tools.

Thus, over five years, CCSI will develop an integrated, validated suite of models and computational tools for accelerating the development and deployment of carbon capture technology. CCSI will address the key industrial challenge of quantifying and reducing the level of uncertainty in simulation results and will enable the prototyping of designs with greater confidence and provide a uniform platform for evaluating options. More important, the CCSI Toolset will support decision making to move to larger scales, more quickly and with better designs, thereby considerably reducing the cost and time required for the commercialization of carbon capture technology. Throughout the CCSI project, we are working closely with end-users in the carbon capture industry to obtain input to and regular feedback on products.

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