Computational Workbench Environment for Virtual Power Plant Simulation

Mike Bockelie, Dave Swensen, Martin Denison
Reaction Engineering International
77 West 200 South, Suite 210
Salt Lake City,UT 84101
bockelie@reaction-eng.com http://www.reaction-eng.com

ABSTRACT

In this paper we describe our plans for creating a computational workbench for performing virtual simulations of Vision 21 power plants. The workbench will provide a framework for incorporating a full complement of models, ranging from simple heat/mass balance reactor models that run in minutes to detailed models that can require several hours to execute. The workbench will be developed using the SCIRun software system.

INTRODUCTION

One of the goals in the DoE Vision 21 program is to significantly increase efficiency and reduce emissions from energyplex systems that will be developed in the 21st century [DOE,1999]. The Vision 21 roadmap places a strong emphasis on the use of computer based virtual demonstrations to reduce the time, cost and technical risk of developing these new energyplex systems. The virtual demonstration will require the integration of component models of various complexities in a way that allows cost effective computer simulations to be performed.

Currently available software systems do not contain models and functionality to meet the future demands that will be placed on plant simulations. For performing overall process simulation within a power plant, there are commercial software systems available (e.g., ASPEN, HYSYS, ACSL, MMS). These software packages typically have an intuitive graphical user interface that allows a non-specialist to lay out the major components in a plant. The included component models are usually limited to only heat, mass and energy balance reactor models. These models provide great insight into how energy plants will behave during normal operation. Likewise, software packages that allow for dynamic modeling can be invaluable for simulating unplanned upsets and devising control strategies [Ricketts et al, 1998]. Although the current state-of-the-practice software systems are very useful, they cannot predict many of the performance goals identified by DoE. Detailed models are required to predict pollutant emissions, spatial heat flux and three dimensional flow effects. The DoE Vision 21 Virtual Demonstration program that has been awarded to the FLUENT-ASPEN team will attempt to address this issue by allowing more detailed models to be interfaced to process engineering software systems. The computational workbench described in this paper addresses these needs by creating an environment with the power and flexibility required for next generation power plant simulations.

As part of a DoE Vision 21 project, Reaction Engineering International (REI) is developing a computational workbench that will provide a ***framework*** for integrating models of the many components that will be required to create a virtual power plant that can simulate the performance and emissions of energyplex systems. The workbench is being constructed as a tightly integrated problem solving environment, with plug and play functionality, that contains an array of tools and models that communicate in a seamless manner. The workbench will be designed for use by the non-specialist and will provide the capability to interrogate a virtual power plant simulation at multiple levels of detail. It will include models ranging in complexity from simple heat/mass balance models to sophisticated Computational Fluid Dynamics (CFD) based models. Models will be created (or obtained) for simulating key energy plant components, including boilers, fluidized beds, gasifiers, combustors, fuel cells and clean-up process components. Some of these models will tax the limits of the computer power readily available to most engineers.

We are using the SCIRun problem solving environment as the platform on which to build our workbench concept. SCIRun is an ideal development platform for this project. From inception it has been designed to support High Performance Computing (HPC) applications. It contains a wide range of state-of-the-art capabilities for running, analyzing and visualizing computationally intensive simulations.

Within our DOE project, two workbench systems will be developed. The first workbench will be based on the DOE Low Emission Boiler System (LEBS). This is a conventional power plant for which REI has modeling experience and thus will provide a good prototype workbench. Based on the findings from building and using the LEBS workbench, a workbench for a Vision 21 energyplex will be developed.

In the remainder of this paper we outline our plans for developing the workbench. We discuss, in order, the functionality of the workbench, software design issues and the component models to be included in the workbench.

COMPUTATIONAL WORKBENCH - OVERVIEW

A *workbench environment* is more than just a set of software tools with a graphical user interface (GUI). The workbench contains all of the tools required for problem setup, running the models (steady or transient) and analyzing the simulation results. The computational models included in the workbench can be of arbitrary complexity and can be implemented in a wide variety of programming languages. The workbench provides all of the functionality required to pass data from one component to the next within the desired configuration. The computational workbench provides the engineer with the ability to visualize and interrogate the solution as it evolves, immediately make modifications to the computer model, and then intelligently restart the solution on the new configuration. In addition, the workbench provides the engineer the ability to interrogate the evolving solution within any component of the virtual plant to any desired level of detail at any time within the solution process. To make the workbench accessible to a large number of users it is being designed for use by the non-specialist. To ensure extensibility, enhanced functionality and functionality, the workbench is being designed and built using modern software design practices and object oriented software platforms.

Developing this new tool as a *workbench environment* will allow us to leverage other work being performed within the High Performance Computing (HPC) community. The requirements for coupling together a wide range of engineering models into a single system is not unique to analyzing power plants. There are several multi-disciplinary projects being funded in the HPC community where the focus is to conduct comprehensive simulations of complex systems or processes that employ many diverse engineering models. Here, the common thread is the need to have a powerful, easy to use simulation software system that will allow for a range of computational models to co-exist and interact. Not all of the models use the same numerical methods, provide the same level of detail, represent the physics in the same manner or use the same degree of computational resources. In the HPC community, the approach to creating a virtual simulation tool to meet these requirements is to develop a *computational workbench,* or *problem solving environment (PSE)* which provides a framework for coupling numerous, disparate computational components. These components exist as independent software entities, which can originate from any developer conforming to the component-architecture standards. The framework provides tremendous flexibility for instantiating the various components, dynamically coupling them to one another and for targeting their execution to specific, distributed computational resources

As stated previously, our workbench will include component models ranging from simple reactor models to detailed, CFD based models. Reactor models are limited in the physics considered, but run quickly. CFD based models provide much more detailed information about the component because they include the impact of localized mixing and heat transfer within the reactor. By necessity, the CFD models will be limited to the key components that will benefit with this type of detailed analysis. Flexibility will be provided for the engineer to choose whether to utilize a reactor or CFD model for any particular component. Using a combination of different model types will result in a cost effective analysis of a plant configuration.

By design, the workbench framework will be robust, flexible and extensible. It will be able to accommodate improvements in component models, computational methods and computer hardware that might become available after the completion of this project. For some components required to model an IGCC plant, the chemistry, physics and/or hydrodynamics of the system are poorly understood. As more experiments and improved computational models become available, they can be incorporated into the workbench.

SCIRun OVERVIEW

We are using the SCIRun software system to create our workbench. SCIRun is a continuously evolving product of the Scientific and Computational Imaging group, headed by Prof. Chris Johnson, in the Department of Computer Science at the University of Utah (UU/SCI). The latest SCIRun software represents the state-of-the-art in computational problem solving environments and is particularly well suited for cutting-edge, interdisciplinary computational projects [http://www.sci.utah.edu] [http://www.sci.utah.edu/pse/pse.html].

SCIRun offers several capabilities that make it attractive as the platform to support virtual simulations of energy plants. These are described below:

SCIRun Summary: SCIRun is a scientific programming environment that allows the interactive construction, debugging and steering of large-scale 3D scientific computations [Johnson, 1999], [Parker, 1998]. It contains a wide range of state-of-the-art capabilities for running, analyzing and visualizing computationally intensive simulations. By design, SCIRun provides a high level control over parameters in an efficient and intuitive way, through graphical user interfaces and scientific visualization. SCIRun can be thought of as a *computational workbench* in which an engineer can design and modify simulations interactively via a dataflow programming model. It enables engineers to interactively modify geometric models, boundary conditions, and physical and numerical model parameters. It provides the means for fully interactive control of the design, computation and visualization phases of a simulation. *Furthermore, SCIRun does not impose any inherent limitations on the type of computational model that can be used.*

Visual Dataflow Programming Model**:** SCIRun makes use of a visual dataflow programming model to connect various computational models and to route data to auxiliary modules for visualization and interrogation of results. The user of the workbench creates these connections in a plug and play manner by simply dragging the mouse between the outputs of one component to the input or inputs of other components. The dataflow paradigm naturally matches a physical process flow diagram.

Advanced Scientific Visualization**:** SCIRun, having been designed for high performance computing applications, provides significant scientific visualization capabilities. These capabilities rival, if not exceed, available commercial visualization packages. SCIRun supports numerous mesh types, mesh visualization, vector field visualization, iso-surfaces, contour plots, cutting planes, volume rendering and other capabilities. SCIRun also supports less sophisticated data analysis tools such as tabular output of summary information and XY chart plots.

Computer Platform Independence**:** During the design of SCIRun, careful consideration was given to computer platform independence. As a result of this effort, SCIRun**,** and modules developed for it, can easily be used on a large number of computer platforms. These range from Windows NT/2K machines to virtually any flavor of Unix or Linux running on cutting-edge workstations.

Extensibility**:** SCIRun was designed to be highly extensible. This capability exists as a result of its support for a component-based architecture, and as a result of its wide-spread use of object-oriented programming concepts and methods. As a result, additional computational components can easily be added (dynamically), and SCIRun itself can be modified to provide additional capabilities. In addition, a SCIRun developer can leverage the large number of existing components, modules and dataflow types, which have already been created. This results in significant code reuse and a corresponding reduction in development effort.

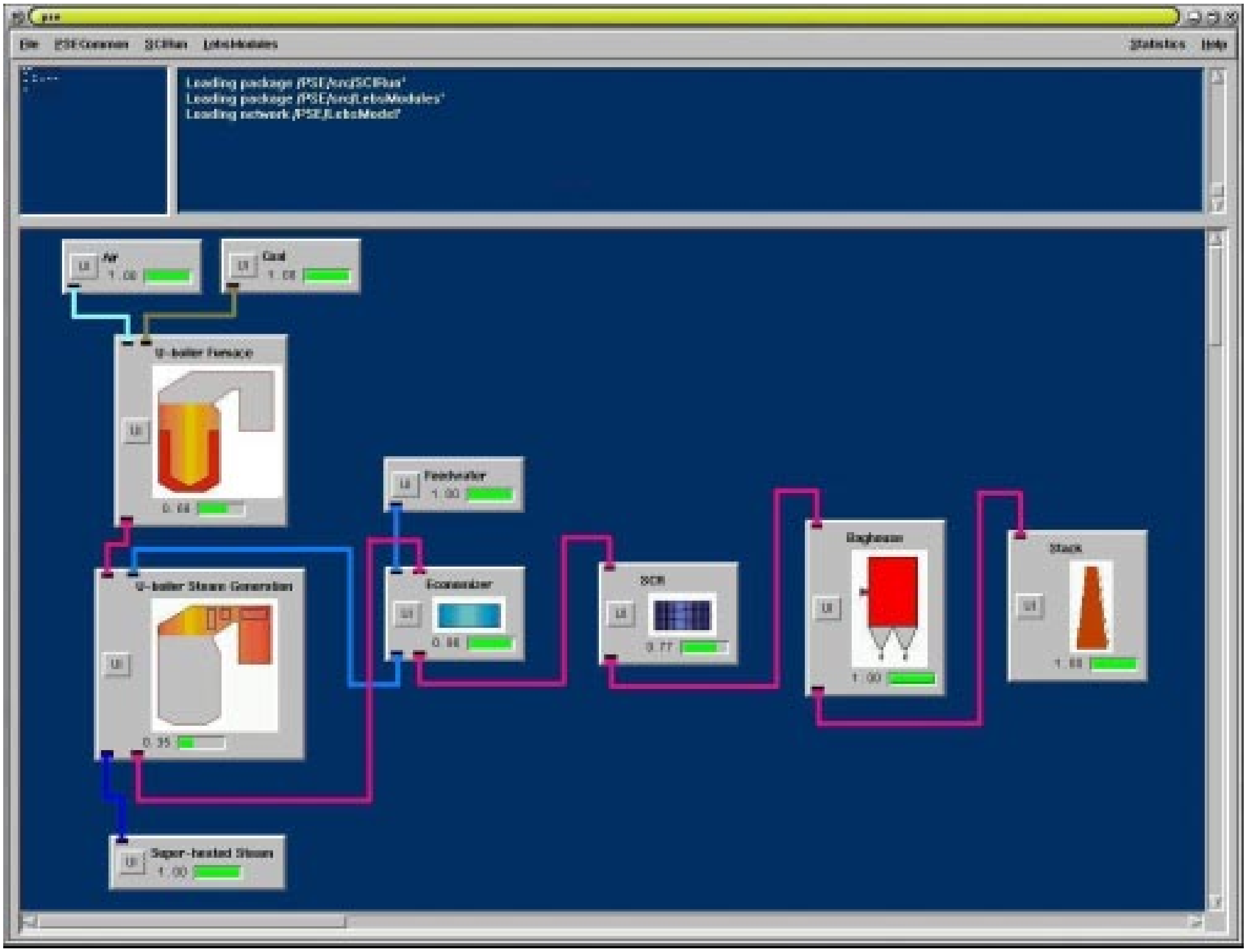
Component Architecture***:*** The complexity of the software required for a Vision 21 computational workbench creates the need for more flexible solutions than those offered by conventional programming techniques. The solution to this problem is component programming, which is based on encapsulating units of functionality as well as software and programming standards for specification of module interfaces. Component-based software development is an evolutionary step beyond object-oriented design [Armstrong et al., 1999] [Cleary et al., 1998]. Currently, various component architectures (COM/DCOM, CORBA) are successfully being used for business oriented computing. In addition, the CAPE-OPEN project [http://www.global-cape-open.org] has established a set of standards to facilitate the use of COM and CORBA component software for process engineering problems. The CAPE-OPEN standard is specifically designed for process engineering problems and provides numerous capabilities. However, it is designed for and is limited to relatively simply computational models. It is based upon the COM/CORBA component architectures and thus suffers from their limitations. These architectures were not designed to handle the rigors imposed by the high-performance computing community which uses comprehensive three-dimensional models with extremely large datasets.

To address the need for component architecture for HPC, the Common Component Architecture (CCA) Forum was created [http://www.acl.lanl.gov/cca-forum/]. The creation of this forum was inspired by the DOE2000 initiative. The specification created by this group provides all of the benefits of the standard business oriented component architectures (interoperability, language independence, parallel capabilities), while addressing the issues of high-performance computing such as parallel communication channels between components and other elements required for dealing with extremely large data sets. Prof. Johnson and Prof. Parker are members of our project team and are members of the CCA Forum. SCIRun is currently in transition to become CCA 0.5 compliant. Support for this task was provided (in part) through the University of Utah's DoE ASCI program, CSAFE, and the University of Utah's NIH Center for Bioelectric Field Modeling, Simulation, and Visualization. The use of CCA allows widely disparate computational models written in a plethora of programming languages (including C/C++, FORTRAN, JAVA) to interact and communicate seamlessly as part of a larger simulation within SCIRun. Utilizing a CCA capable SCIRun provides the means to create a workbench where computational models describing various components can truly be used in a *plug-and-pl*ay manner. In addition to these capabilities, the component architecture sets the stage for large-scale, distributed computing where simulations may be monitored and controlled from anywhere on the internet using a web browser.

MODEL INTEGRATION

The workbench will use numerous computational models to represent the targeted plant components. Component models will be interfaced to the workbench using a SCIRun module and an associated software component where the model will actually reside. The process of creating a SCIRun module involves writing a new C++ class. The newly created class/module will then be able to communicate with the software component encapsulating the model. It is important to note that the software component represented by a module in SCIRun exists as a completely separate software entity. It could exist as a separate process on the same computer, or it could exist on a remote computer with a different hardware architecture and running a different operating system with access to the internet. Existing model code, proprietary libraries and binaries may be integrated into SCIRun by implementing a new module and an associated component which wraps the existing code/library/binary. While SCIRun handles passing data into and out of the modules and translating the data structures accordingly, at a lower level, the component architecture software provides automatic conversions of datatypes based on: 1) the type of computer platform SCIRun is operating on versus the platform that the software component is running on and 2) the programming language used to implement the software component. Each model component can be provided with custom visualization, data input and data output elements within SCIRun. After these necessary model components have been created, they are integrated within a SCIRun dataflow network. This network describes the overall interactions between the various software components.

USER INTERFACE



```
Loading package /PSE/src/SCIRun'
Loading package /PSE/src/LebsModules'
Loading network /PSE/LebsModel'
```

Figure 1. User Interface for LEBS POC Workbench.

Illustrated in Figure 1 is a SCIRun interface for the LEBS Proof of Concept (POC) unit (described below). Each rectangle in this figure denotes a module (or plant component) with encapsulated functionality. The pipes that connect the modules (or boxes) denote the transfer of model data between modules. Data flows from one component to the next, much in same way that “material” flows through an engineering process flow diagram Conversion modules will be used to allow “data massaging” as the data flows from one component to the next. These are needed because not all models require the same level of detail for their input data (i.e., a module using a detailed CFD simulation is connected to a module doing a simple heat/mass balance model). SCIRun provides the flexibility to perform all of the required functions. The inputs for any component model can be inherited from an upstream device or entered directly via input dialog boxes that can contain pull down menus, type-in boxes, radio buttons and menu selections as per standard GUI operation.

The visual programming capability within SCIRun allows an engineer to modify the *dataflow network* of the virtual power plant in a user-friendly manner. Additional modules can be instantiated at any time during a computational analysis, as can the connections between modules. The interface to SCIRun can best be described as a graphical programming environment with true plug-and-play functionality.

PLANNED WORKBENCH ENVIRONMENTS

Two workbenches will be developed. The first workbench is intended to be a prototype and will include component models required for simulating a current energy plant involving the LEBS firing system. The second workbench will focus on Vision 21 energyplex systems.

LEBS Workbench: The LEBS workbench will focus on a baseline firing conditions for the LEBS Proof of Concept (POC) design. The POC furnace is a nominally 86 MW, down-fired unit. It contains four low NOx burners in a staggered arrangement in a U-shaped, wet bottom boiler and has provisions for OFA and reburning. The LEBS plant configuration, as represented in the workbench, is shown in Figure 1. Below we briefly describe our planned modules:

<u>LEBS Proof of Concept (POC) Boiler:</u> This module will involve full reacting CFD simulations of the boiler fireside for the LEBS POC unit. Both steady state and time dependent simulations will be performed. REI is currently involved in modeling this boiler for the LEBS program so little development will be required for the steady state module other than interfacing with the workbench. Our fireside module can include models for NOx controls, such as SNCR, OFA and reburning. Illustrated in Figure 2 are representative results for the CFD model of the LEBS POC.

<u>Steam-Side model</u>**:** A simple steam-side model is being developed for which the steam flow rate and exit steam conditions will be calculated from thermodynamic steam calculations coupled with an integrated heat transfer rate to the steam from the CFD model for the POC boiler.

<u>Selective Catalytic Reduction (SCR) System:</u> A reactor model for a SCR system is being developed that will predict the catalyst temperature as well as poisoning and deactivation. We plan to use microkinetic models, rather than global rate models, because the range of applicability is greatly extended and is more readily adapted to different geometric configurations of the catalyst (Dumesic, et al., 1993; Komatsu et al., 1994).

<u>Baghouse:</u> A simple zero dimensional (reactor) model for the baghouse is being created that will predict pressure drop, based on the amount of trapped solids.

<u>Demonstration:</u> The workbench will be demonstrated by predicting system performance with the coupled modules. Key points to the tests are to (1) exercise the user interface to determine the

degree of ease-of-use, and (2) determine the impact of coupling the additional equipment into the simulation. Performance will be measured on the integrated system - not only on what exits the boiler as with most current boiler modeling efforts.

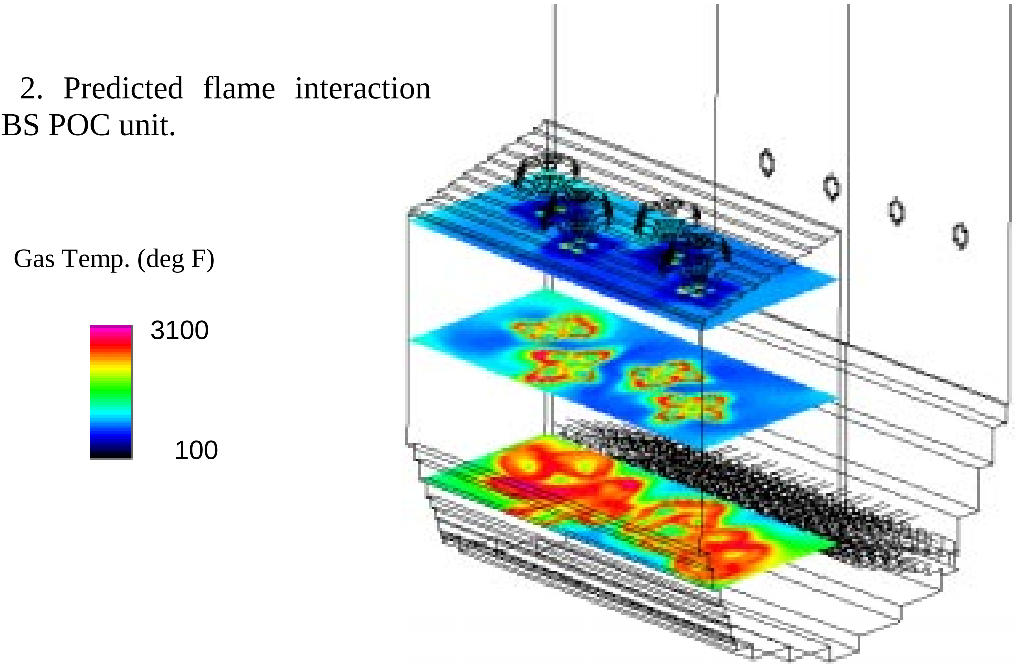


Figure 2. Predicted flame interaction for LEBS POC unit.

Vision 21 EnergyPlex Workbench: The second workbench will contain models for simulating a Vision 21 energyplex system. As noted in the Vision 21 Roadmap, at present there is not a preferred configuration. Thus, we intend to develop models for key components that will be common to different configurations. Where possible, we will try to acquire models being developed by other Vision 21 programs. The models we intend to include in the workbench are highlighted below:

Fluidized Bed: Models to simulate a Pressurized Fluidized Bed Combustor (PFBC) will be developed and incorporated into the workbench. Both a reactor model and a CFD based model will be included. Implementing two models will (1) provide users the option to use the model that best represents their system and (2) demonstrates the ability to interface models with different levels of complexity and detail into our workbench framework. The Reactor model has the advantage of being physically realistic and runs fast enough to be used for dynamic model response. Our reactor model will be based on previous work by [Glicksman et al, 1991] and [Goel, Sarofim et al, 1996]. For the CFD model we intend to use MFIX, a publicly available code developed at DoE FETC [MFIX], [Boyle, 1998], [O'Brien,1997]. MFIX is a comprehensive, unsteady CFD research code designed for modeling reacting flows in fluidized bed systems.

Entrained Flow Gasifier: This is one of the most important systems in an IGCC cycle because the gasifier converts a solid fossil fuel into more environmentally attractive hydrocarbon fuel or feed stock. Many different types of systems (e.g., Lurgi, Fluidized Bed, Entrained Flow) have been used in pilot scale plant demonstrations. At present, it is not clear which unit will be used in the 21st Century Power Plant. However, if one considers the commercial units that are operational or in development, there appears to be a trend toward entrained flow processes [NRC, 1995]. Hence, for demonstration purposes, in this project we will focus on entrained flow gasifiers. With some extensions and modifications, we feel that our existing (dilute phase) CFD combustion tools can be used to model entrained flow gasifiers. Our models have been proven highly useful for evaluating large-scale industrial furnaces operating over a wide range of temperatures, stoichiometries, fuel types, and particle loadings. Many of our simulations have successfully described sub-stoichiometric environments of relevance to gasification. However, modeling the controlling phenomena in a system designed for entrained flow gasification will require the development of additional information and extensions to existing physical sub-models. Most of the validation of coal conversion phenomena depends upon experience gained at atmospheric pressure. To develop an effective gasifier model will require establishing appropriate parameters for the chemistry and physics of coal conversion phenomena at pressure and under gasification conditions. Planned model improvements include: pyrolysis kinetics/yields; kinetic rates for gasification conditions; soot formation/destruction; particle fluid dynamics for high particle loadings; NOx model for gasification conditions; and radiation for high optical thickness. Included in this effort is locating data for reaction processes under pressure.

Turbine Combustor **:** A combustion CFD model for a turbine combustor will be included in the workbench. Models will be included to allow studying the impact of clean, lean burn conditions (i.e., natural gas) and dirty, syngas conditions such as would be generated in a gasification/PFBC system. To improve the predictive capability of the CFD model for the syngas simulations, reduced kinetic mechanisms specifically designed for the syngas fuel will be created for use in the combustion and NOx simulations. It is anticipated that using reduced mechanisms will provide significant improvement over more standard methods such as using global mechanisms [Chen, 1997][Montgomery et al., 1999] [Cremer & Montgomery et al, 2000].

Fuel Cell **:** Fuel Cells could potentially play an important role in Vision 21 energy plants. Hence, we will include within our workbench a heat/mass balance reactor model for a Solid Oxide Fuel Cells (SOFC) for simple geometric configurations that exhibit the important fluid dynamics, heat transfer, chemical and electrochemical reactions, species transport, etc. This model will provide a simple test platform to understand the gross effects for SOFC cells. More accurate models could be developed, but would require resources beyond that available in this project.

Additional Clean Up Components: Zero dimensional reactor models will be included for an assortment of clean-up equipment, such as: candle filters, H_2S removal, particulate removal. In addition models for a SCR and a Heat Recovery Steam Generator will be included. The models will be based on information and correlations available in the open literature.

Demonstration: We will work with DOE to identify energyplex configurations that are of greatest interest. At this stage of the project, the workbench will have significantly more functionality and capability than was available in the prototype system. As with the LEBS workbench, the demonstration will be to predict system performance with the coupled modules. Key points to the tests will be to (1) exercise the user interface to determine the degree of ease-of-use, (2) exercise the improved analysis capabilities and (3) determine the impact of coupling the additional equipment into the simulation.

CONCLUSIONS

In this paper we have outlined our approach for developing a computational workbench for performing virtual simulations of power plant systems. Descriptions have been provided on the functionality of the workbench and the software platform, tools and models that will constitute the workbench. An important element in our design is the combined use of fast running reactor (process) models for some components and detailed CFD models for key components that require a detailed model. A prototype workbench will first be created capable of simulating a conventional power plant containing a LEBS firing system, after which a second workbench will be created for simulating Vision 21 energyplex systems.

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