A Computational Workbench Environment For Virtual Power Plant Simulation

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ABSTRACT

In this paper we describe our progress toward creating a computational workbench for performing virtual simulations of Vision 21 power plants. The workbench provides 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 is being developed using the SCIRun software system. To leverage a broad range of visualization tools the OpenDX visualization package has been interfaced to the workbench. In Year One our efforts have focused on developing a prototype workbench for a conventional pulverized coal fired power plant. The prototype workbench uses a CFD model for the radiant furnace box and reactor models for downstream equipment. In Year Two and Year Three, the focus of the project will be on creating models for gasifier based systems and implementing these models into an improved workbench. In this paper we describe our work effort for Year One and outline our plans for future work. We discuss the models included in the prototype workbench and the software design issues that have been addressed to incorporate such a diverse range of models into a single software environment. In addition, we highlight our plans for developing the energyplex based workbench that will be developed in Year Two and Year Three.

INTRODUCTION

Virtual simulation of advanced systems will play an important role in reducing the time, cost and technical risk of developing a DOE Vision 21 energyplex [DOE,1999]. It is our belief that virtual simulations of these systems will require the use of a broad range of component models that will require new ways of conducting these simulations to perform them in a cost effective manner.

In our DOE Vision 21 project, Reaction Engineering International (REI) is developing a computational workbench that will provide a ***framework*** for integrating the range of models and visualization methods that will be required to perform simulations to predict energyplex performance and emissions. The workbench is being developed 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 is designed for use by the non-specialist and provides the capability to interrogate a simulation at multiple levels of detail. The models contained in the workbench can range in complexity from simple heat/mass balance models to sophisticated CFD based models. Through the course of this program, models will be created for simulating key energy plant components, including boilers, gasifiers, fluidized beds, 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.

The workbench is being constructed using the SCIRun software system. SCIRun was developed by the Scientific and Computational Imaging group at the University of Utah. From inception, SCIRun has been designed in an object oriented manner with the intent of supporting interdisciplinary projects in which High Performance Computing (HPC) models are needed. SCIRun places no inherent limitations on the physics, numerical technique or programming language used within a model. SCIRun supports component-based software techniques and allows for distributed computing. In addition, it is possible to interface additional software packages to SCIRun. To enhance the inherent visualization capabilities of SCIRun, REI has incorporated the OpenDX data visualization software package into the workbench. OpenDX is a popular package being used by researchers in a variety of disciplines that must visualize, analyze and explore large data sets.

For Year One, the focus of our project has been to develop a prototype workbench based on a conventional pulverized coal combustion plant, the DOE Low Emissions Boiler System Proof of Concept (LEBS-POC) facility. LEBS-POC is a system with which we are familiar and thus provides an opportunity to quickly evaluate many software design issues for the workbench. The prototype workbench uses a CFD model for the radiant furnace box. Reactor models have been implemented to simulate steam generation, the air pre-heater, NOx reduction with a Selective Catalytic Reduction (SCR) unit and particulate removal using a baghouse or an Electric Static Precipitator (ESP). In Year Two and Year Three, the focus of the project will be on creating models for gasifier based systems and implementing these models into an improved workbench.

In this paper we describe our work effort for Year One and outline our plans for future work. Discussed, in order, are: our workbench concept; the software systems and software design used within the workbench; the functionality of the workbench; the models contained within the Year One prototype workbench; a demonstration of using the workbench to evaluate the impact on downstream operations of changes in the boiler firing conditions; and last, the planned model development to occur in Year Two and Year Three that will lead to simulating a Vision 21 energyplex system.

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 non-specialists. To ensure extensibility 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 the integration of a wide range of coupled 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.

Traditionally, power plant simulation has been performed using either spreadsheet, flowsheet or CFD models. Spreadsheet models typically utilize algebraic models, or correlations, based on historical data (or multiple runs of more detailed models) to create a simple representation of the plant components. Spreadsheet based models are easy to use, run quickly but contain only limited accuracy with respect to predicted performance. The IECM tool [http://www.IECM-online.com] would be an example of a spreadsheet model. A flowsheet is a second approach commonly used to simulate a plant. A flowsheet typically contains mass and energy balance models, also called process or reactor models, for the equipment components within the plant. Although reactor models are limited in the physics that are considered, they are more accurate than correlations and run quickly. Flowsheets are good tools for analyzing the impact of equipment or process changes, evaluating control strategies and studying the dynamic response of the plant to upset conditions. Example commercial packages for flowsheet systems are Aspen, Hysys and GTPro. All of the commercial packages have simple interfaces and extensive user support. Computational Fluid Dynamic (CFD) models are a third type of model. 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. However, at present CFD models are typically used only for key plant components due to the computational expense and difficulty in using these more sophisticated models. In addition, the CFD models are typically run in a "stand-alone" mode and the impact of upstream or downstream equipment must be accounted with additional computations performed by the user, off-line from the CFD simulation.

The computational workbench being developed in our Vision 21 project will provide a significant improvement over analysis, or plant simulation, tools currently available. As stated previously, our workbench will include component models ranging from simple reactor models to detailed, CFD based models. Where feasible, multiple choices for model types will be provided. The reactor models will include simple algebraic models as well as mass/energy balance models. Where appropriate, reaction kinetics will also be included. The use of reactor models created as look-up tables from CFD modeling results will also be investigated. For key components in the plant, CFD models will be included. For all of the models, simple User Input panels will be provided that contain appropriate default values. The workbench will contain the flexibility for the engineer to choose whether to utilize a reactor or CFD model for any particular component. The CFD models will be implemented in such a manner to make these models to be easy to use. 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.

WORKBENCH – SOFTWARE

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]. A key aspect of SCIRun is the ability it provides to “bridge” the SCIRun system to other software packages to provide enhanced capability.

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]. 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. SCIRun does not impose any inherent limitations on the type of computational model that can be used or the programming language used to create the model. In addition, SCIRun contains the flexibility to “bridge” the SCIRun system to other software packages to provide enhanced functionality or capability.

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.

Computer Platform Flexibilty: During the design of SCIRun, careful consideration was given to computer platform flexiblity. In particular, notoriously platform dependent elements such as threading and GUI were either abstracted or implemented using platform-flexible packages. As a result of this effort, SCIRun, and modules developed for it, can easily be used on a large number of Unix and Linux-based computer platforms.

Extensibility**:** SCIRun was designed to be highly extensible. This capability exists 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, and SCIRun itself can be modified to provide additional capabilities. In addition, a SCIRun developer can leverage the large number of existing modules and dataflow types, which have already been created. This results in significant code reuse and a corresponding reduction in development effort.

Bridging Capabilities**:** As a result of SCIRun's extensibility features, it is possible to create software bridges to nearly any external software package. Currently, we use a software bridge to couple the OpenDX visualization software with SCIRun. Future bridges may include a link to 3DStudioMax, which would allow the comprehensive workbench models to share a common database of geometric information of plant components.

High Performance Computing Emphasis**:** From inception, SCIRun has targeted high performance computing applications. This emphasis is reflected in its heavily multithreaded architecture and attention to performance details such as efficient dataflow handling mechanisms and state-of-the-art algorithms.

Model Integration

The issue of model integration is of up most importance to the Vision 21 program. Proper model integration techniques can provide significant advantages, most notably model interoperability among the various Vision 21 teams and third-party developers.

The following sections detail the techniques used for model integration for the prototype workbench (Workbench I), along with plans for a more sophisticated approach for the Vision 21 Energyplex workbench (Workbench II). A robust and functional model integration paradigm is a key element of Workbench II being developed during Year Two and Year Three of this program.

Workbench I Model Integration Paradigm: During the development of the LEBS Workbench I, we have focused on a proven, traditional method of integrating the models into the SCIRun environment. This has involved the creation of C++ wrapper classes, which encapsulate the model of interest. This wrapper performs several functions, including abstracting model inputs and outputs, providing execution controls and providing SCIRun-to-model communication mechanisms. The instantiation of the resulting wrapper class yields a SCIRun compliant module, which is capable of being composed as part of a dataflow network program.

While using the aforementioned mechanism of model integration was the natural choice for the LEBS Workbench I, it does have shortcomings as a final solution. The most significant issue is that of interoperability of the wrapped models. This method generates modules which will only function within the SCIRun system. It is not possible to move these modules to other frameworks or to use modules developed for other frameworks inside SCIRun. In addition, the method places limits on model programming languages and provides no inherent parallelism.

Workbench II Model Integration Paradigm: To address the functional requirements of Workbench II, model integration will need to be performed using the methods of component architectures with standardized interfaces. Component architectures alone offer numerous advantages when compared with conventional programming techniques. These advantages include programming language and platform independence, location transparency (and hence parallelism) and reuse. When these core advantages of component architectures are coupled with standardized interfaces, reuse becomes interoperability.

For Workbench II, our intention is to allow interoperability of models through two emerging component architecture-based standards: CAPE-OPEN and CCA. These standards are discussed in the following sections:

CAPE-OPEN [http://www.colan.org] is a set of standards created 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. This standard has been well received by the process engineering community. Numerous simulation environments have already been modified for CAPE compliance (Aspen Plus, HYSYS). Although CAPE provides much functionality and interoperability, it alone does not fully address the needs of Workbench II model integration. CAPE has limitations due to its narrow targeting of process engineering problems, and its reliance on COM and CORBA which are currently not acceptable for high performance computing applications.

Common Component Architecture (CCA): 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 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.

By supporting both the CAPE-OPEN and CCA standards, Workbench II would benefit from the development of models in both the HPC and process engineering arenas. Plans to make SCIRun CCA 0.5 compliant and to implement CAPE functionality are being formulated.

As a first step to embracing component architectures in the workbench, REI software engineers have created a prototype SCR wrapper module which makes use of CORBA to provide platform and language independence and location transparency. This module has been demonstrated both on REI's LAN of Linux machines and across the internet on a geographically remote computer running a different operating system. Although the component-based test module was implemented using raw CORBA, the fundamental issues involved in developing the module will be directly applicable to the proposed hybrid CAPE-OPEN/CCA paradigm for Workbench II.

OpenDX for Visualization

Workbench Visualization Engine: During development of Workbench I, it was recognized that creating a link between SCIRun and OpenDX would give the workbench user access to the large range of visualization and data analysis capabilities possible with OpenDX. Since the creation of a link between SCIRun and OpenDX could be accomplished in a clean, robust manner, and could be done within the scope of our workbench visualization tasks, it was decided to develop this link. It should be emphasized that access to OpenDX functionality from within the workbench is not intended to be a replacement for the SCIRun visualization engine, but rather as an alternative. Such a paradigm provides the workbench user the "best of both worlds".

What is OpenDX? DX was originally developed by IBM. Its long history as a commercial software package shows in its polished core visualization capabilities and extensive documentation. Since being released to open source, DX has been widely accepted as the visualization package of choice for research groups in national laboratories, universities and large industrial research laboratories. The large user base for DX ensures that modules exist to manipulate, transform, process, realize, render and animate data based on points, lines, areas, volumes, images or geometric primitives. These modules can be quickly arranged to provide popular data analysis tools, such as: display point values (point probe); one (XY), two (carpet/surface plots) and three dimensional plots; line and solid shaded contours, iso-surface extraction, data and vector value slices, solid particle trajectories through flow fields. More complicated networks can be built for nearly every conceivable visualization task. Thus, OpenDX provides all of the capabilities of commercially available data visualization packages, plus additional state-of-the-art capabilities to visualize, interrogate, explore and analyze data sets. Further information about OpenDX is available on the web at: http://www.opendx.org.

SCIRun and OpenDX Coupling: The coupling between the workbench and OpenDX is accomplished using a library called DXLink. This package is distributed with the OpenDX software suite. DXLink allows a remote application to maintain fine-grained control of all aspects of OpenDX. Anything that can be accomplished using the dedicated DX user-interface can also be accomplished remotely with DXLink.

An important design consideration of the SCIRun-to-DX link is the visualization user interface. Forcing the user to move between the SCIRun user interface panels and those of DX would be cumbersome and confusing. To eliminate this difficulty, the user interface for the OpenDX visualization engine is being written using TCL/TK and integrated with the SCIRun workbench. This will provide the user a seamless user interface experience, while DXLink is being used to transparently move information and commands to and from DX. The visualization module is accessed by selecting a button labeled "3D" located on a module icon. The visualization user interface has a "look and feel" comparable to that employed in commercial CFD visualization tools. Non-specialist users will not be aware that OpenDX is being used. However, sophisticated workbench users will have access to powerful data visualization and analysis tools.

WORKBENCH - USER INTERFACE AND FUNCTIONALITY

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 using 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.

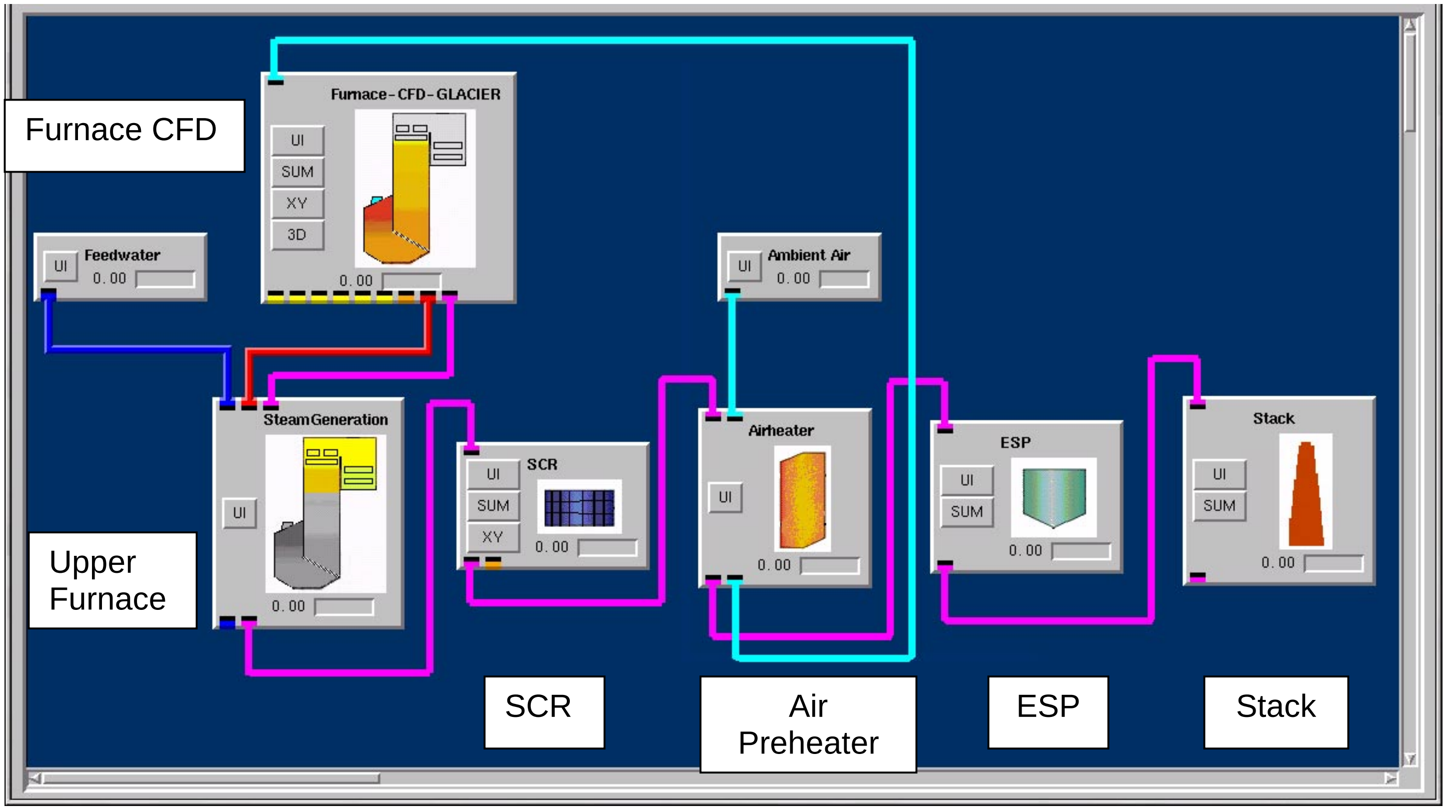
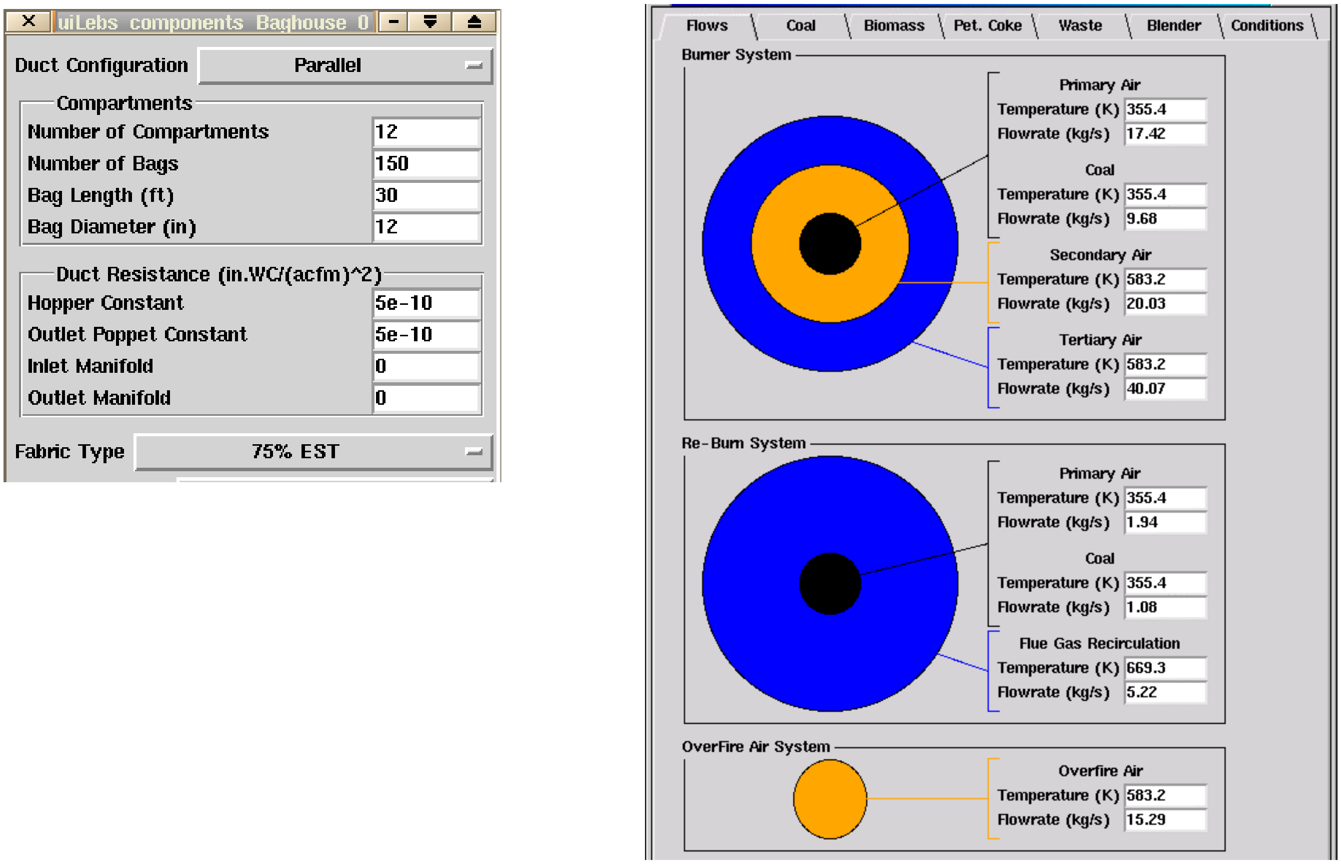


Figure 1. User Interface for prototype workbench (Workbench I).

Model Inputs: Located on each SCIRun module is a button labeled “UI”. Selecting the UI button will cause a TK-based user input dialog box, such as illustrated in Figure 2a, to appear on the screen. Using this dialog, the engineer can alter the model parameters that would impact module performance. The input dialog uses a combination of simple type-in boxes and other standard user-interface elements that request information in terms (and units) typically used in the combustion community.

To make operation of the workbench as robust and user-friendly as possible, default values are provided for all model inputs, and all inputs are checked for errors prior to allowing the user to close the dialog. Note that, at present, the defaults provided for the user in the model dialog boxes are configured specifically for the LEBS POC. However, the software design of the user-interface allows these defaults to be easily changed to match alternative facilities.



Duct Configuration: Parallel

Compartments
Number of Compartments: 12
Number of Bags: 150
Bag Length (ft): 30
Bag Diameter (in): 12

Duct Resistance (in.WC/(acfm)^2)
Hopper Constant: 5e-10
Outlet Poppet Constant: 5e-10
Inlet Manifold: 0
Outlet Manifold: 0

Fabric Type: 75% EST

Burner System
Primary Air
Temperature (K): 355.4
Flowrate (kg/s): 17.42
Coal
Temperature (K): 355.4
Flowrate (kg/s): 9.68
Secondary Air
Temperature (K): 583.2
Flowrate (kg/s): 20.03
Tertiary Air
Temperature (K): 583.2
Flowrate (kg/s): 40.07

Re-Burn System
Primary Air
Temperature (K): 355.4
Flowrate (kg/s): 1.94
Coal
Temperature (K): 355.4
Flowrate (kg/s): 1.08
Flue Gas Recirculation
Temperature (K): 669.3
Flowrate (kg/s): 5.22

OverFire Air System
Overfire Air
Temperature (K): 583.2
Flowrate (kg/s): 15.29

Figure 2a. Example dialog boxes for inputting model data.

Model Outputs: A full range of techniques are available for displaying model results. The most basic form of output is a simple summary table of values. Typically the summary data consists of the 5-10 key items for that model. The tabular output, or summary data, is accessed by clicking on the SUM button on the module icon and is displayed in a window. For a CFD furnace model, typical items displayed in the summary data window would be average values at the furnace exit for the gas temperature, gas composition (O_2, CO, NO), fuel conversion (%), etc (See Figures 5b, 7, 9, 10). Model output information can also be displayed as XY, or 1D, plots. This information is accessed by selecting the XY button on the module icon. The plotted values are model dependent (see Figures 5b, 7). For the CFD furnace, the average gas temperature along the furnace axis in the upflow section is displayed. For the baghouse model, the predicted pressure drop as a function of time is displayed. Model output information can also be displayed using 3D visualization methods. As discussed above, the OpenDX package has been implemented into the workbench. This provides the user the ability to perform all of the standard CFD visualization methods (see Figure 2b). It is accessed by selecting the "3D" button on the module icon. The combination of OpenDX and SCIRun also provides the ability to perform some low cost virtual reality methods, such as stereoscopic visualization using "stereo glasses", volume rendering and "fly-through" scenarios. The ability of SCIRun to "bridge" to other software packages also opens the possibility of interfacing the workbench to other virtual reality tools. Some possible linkages are: 3DstudioMax, a professional 3D modeling package that can be used to create plant walk-through scenarios; and VR-Juggler, a software package used to drive large scale immersive environments such as the C-2, C-4 and C-6 at the Iowa State University Virtual Reality Applications Center.

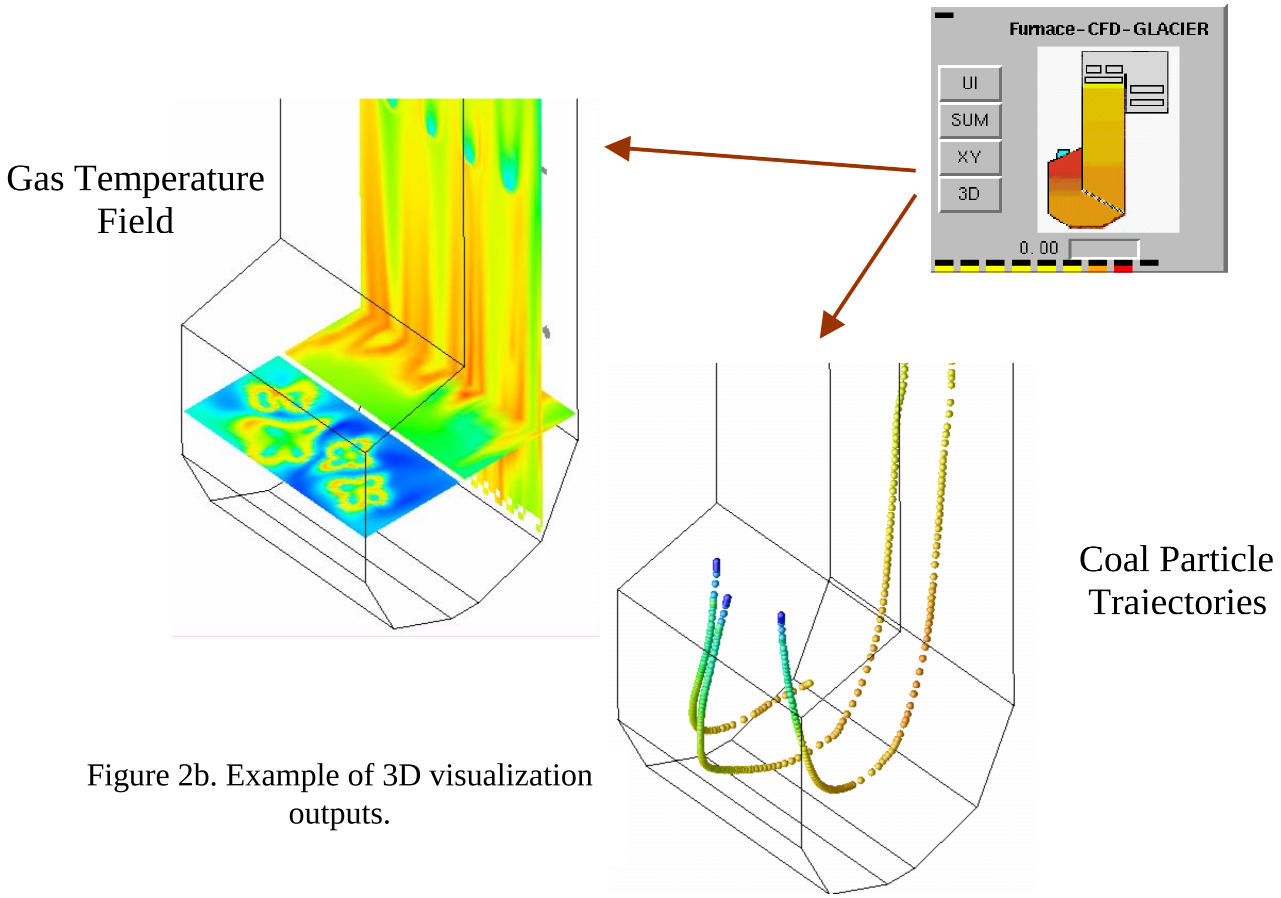
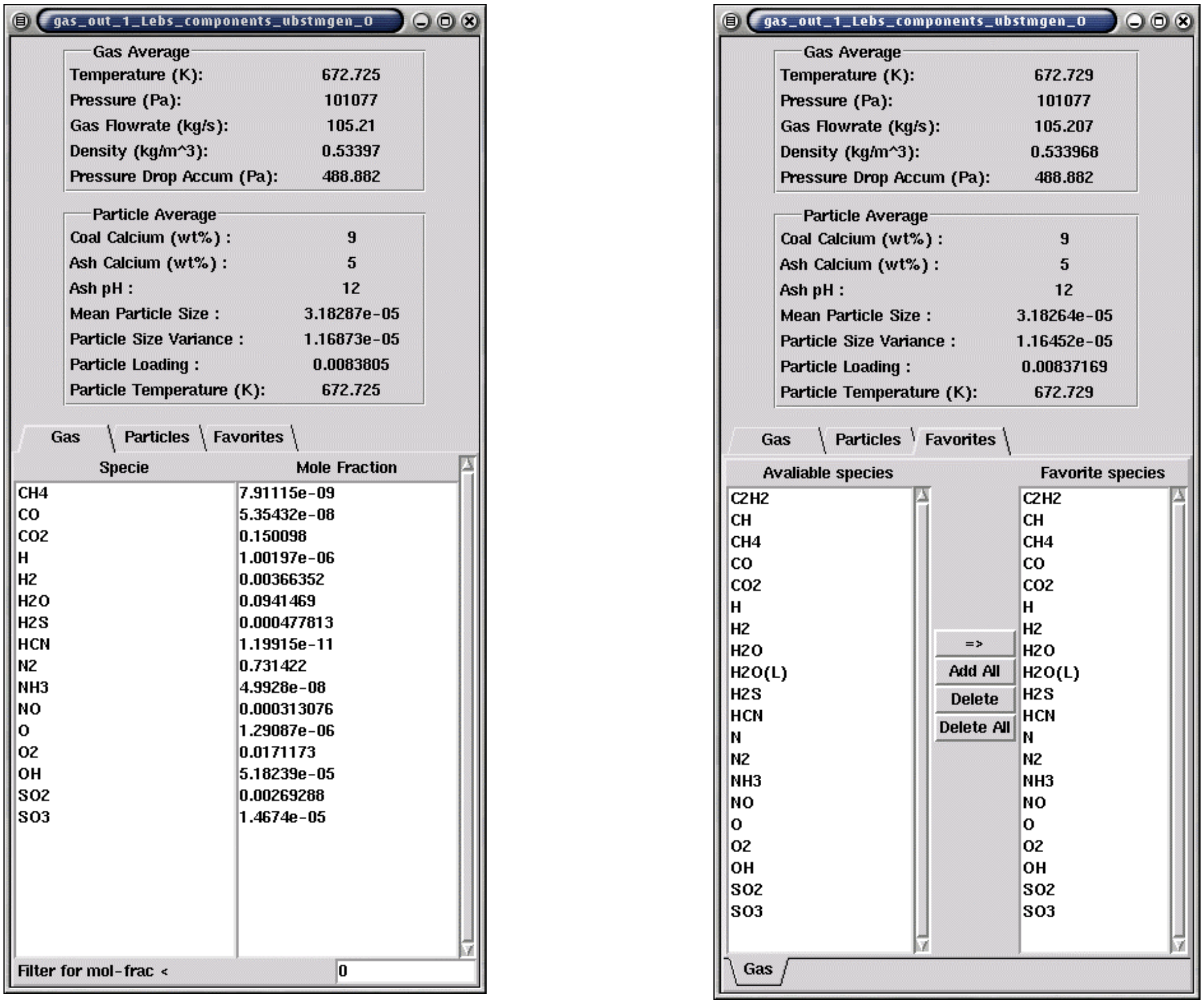


Figure 2b. Example of 3D visualization outputs.

Port Interrogation: Port Interrogation provides the user with a mechanism, or tool, to display all of the data contained within the gas and solids stream data structure that is passed between different workbench modules. With this tool, the user can view detailed information about the composition, temperature, etc. for the gas and solids at any point within the module network. The Port Interrogation tool provides the ability to list only "favorite" gas species and has a data threshold capability to limit the displayed species to major species. The Port Interrogation can be performed for any module by placing the cursor over the desired data port and performing a right mouse click. The Port Interrogation tool has been implemented by defining a TCL display class for a datatype, such as gas or solids. When a module executes, the display is populated with data from the module. All of the code required for this functionality exists within the module, omitting the necessity of having a separate, dedicated display module. Illustrated in Figure 3 is an example of the data displayed by the Port Interrogation tool.



Gas Average

Temperature (K):	672.725
Pressure (Pa):	101077
Gas Flowrate (kg/s):	105.21
Density (kg/m^3):	0.53397
Pressure Drop Accum (Pa):	488.882

Particle Average

Coal Calcium (wt%) :	9
Ash Calcium (wt%) :	5
Ash pH :	12
Mean Particle Size :	3.18287e-05
Particle Size Variance :	1.16873e-05
Particle Loading :	0.0083805
Particle Temperature (K):	672.725

Specie	Mole Fraction
CH4	7.91115e-09
CO	5.35432e-08
CO2	0.150098
H	1.00197e-06
H2	0.00366352
H2O	0.0941469
H2S	0.000477813
HCN	1.19915e-11
N2	0.731422
NH3	4.9928e-08
NO	0.000313076
O	1.29087e-06
O2	0.0171173
OH	5.18239e-05
SO2	0.00269288
SO3	1.4674e-05

Gas Average

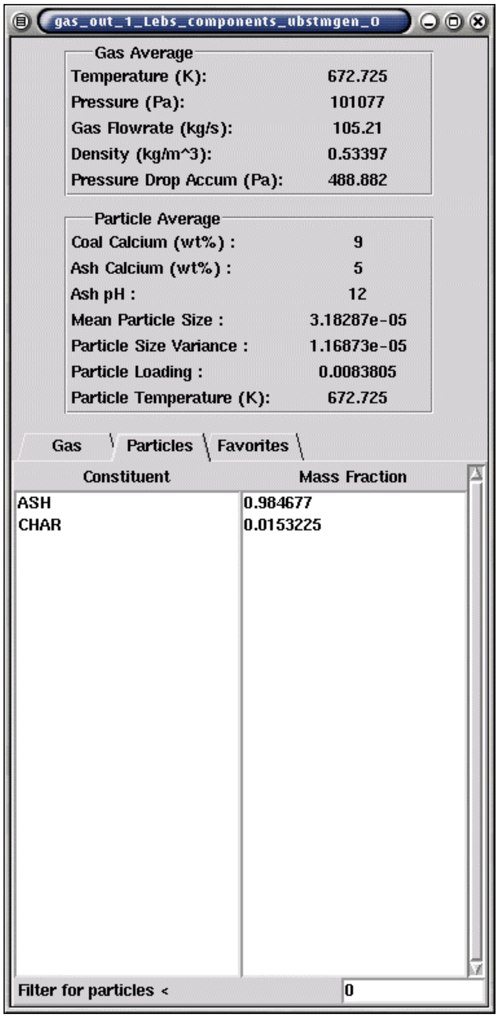
Temperature (K):	672.729
Pressure (Pa):	101077
Gas Flowrate (kg/s):	105.207
Density (kg/m^3):	0.533968
Pressure Drop Accum (Pa):	488.882

Particle Average

Coal Calcium (wt%) :	9
Ash Calcium (wt%) :	5
Ash pH :	12
Mean Particle Size :	3.18264e-05
Particle Size Variance :	1.16452e-05
Particle Loading :	0.00837169
Particle Temperature (K):	672.729

Avaliable species	Favorite species
C2H2	C2H2
CH	CH
CH4	CH4
CO	CO
CO2	CO2
H	H
H2	H2
H2O	H2O
H2O(L)	H2O(L)
H2S	H2S
HCN	HCN
N	N
N2	N2
NH3	NH3
NO	NO
O	O
O2	O2
OH	OH
SO2	SO2
SO3	SO3

Figure 3a. Port Interrogation windows showing detailed information about the flue gas stream (left) and "favorite" species for the flue gas stream (right).



Gas Average

Temperature (K):	672.725
Pressure (Pa):	101077
Gas Flowrate (kg/s):	105.21
Density (kg/m^3):	0.53397
Pressure Drop Accum (Pa):	488.882

Particle Average

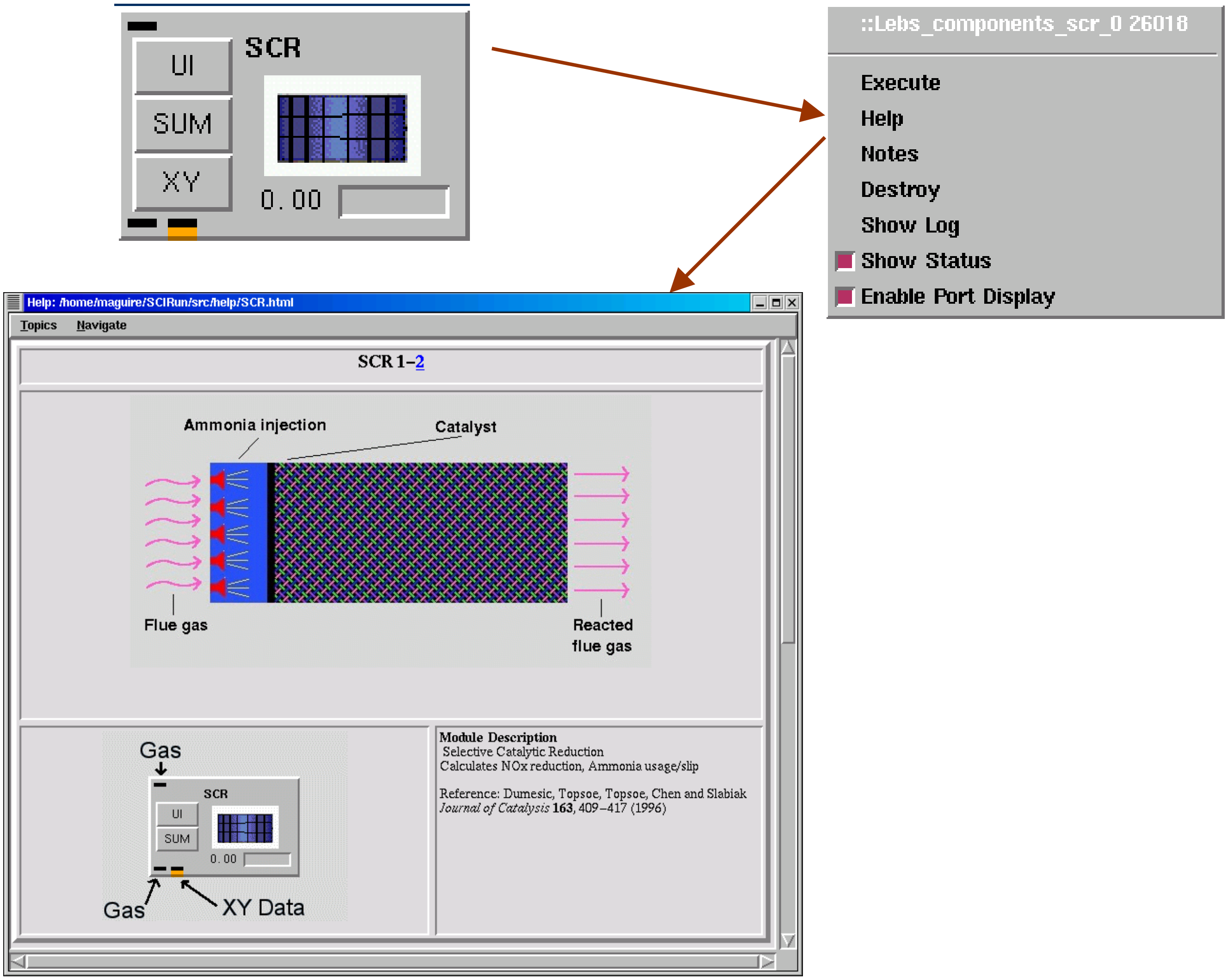
Coal Calcium (wt%) :	9
Ash Calcium (wt%) :	5
Ash pH :	12
Mean Particle Size :	3.18287e-05
Particle Size Variance :	1.16873e-05
Particle Loading :	0.0083805
Particle Temperature (K):	672.725

Constituent	Mass Fraction
ASH	0.984677
CHAR	0.0153225

Filter for particles < 0

Figure 3b. Port Interrogation window showing particle stream information.

Online Help System: A key element of a successful workbench is an easily accessible online help system. Such a system allows a user to quickly answer questions regarding model inputs, outputs, usage and capabilities. To address this need, software engineers from REI have implemented a help system within the SCIRun environment. The SCIRun help system uses HyperHelp, the internal iTCL html viewer, to display hypertext help files for each module. Help content includes instructions on usage of the module and a description of the module's ports. Help also contains a picture of the module's user interface, as well as a description of fields in the UI. To access help for a given module, the user simply uses the mouse to right-click on the module, and choose the "Help" item from the popup menu. Selecting this help menu item activates a TCL HTML viewer (much like a web browser window) which then displays the documentation for the module in question. Since the module documentation is created using HTML, the online help system is easy to create and maintain using the plethora of tools available for web development. An example Help panel is shown in Figure 4.



Module Description
Selective Catalytic Reduction
Calculates NOx reduction, Ammonia usage/slip

Reference: Dumesic, Topsoe, Topsoe, Chen and Slabiak
Journal of Catalysis **163**, 409–417 (1996)

Figure 4. Example of Online Help. Shown are windows for SCR module.

PLANNED WORKBENCH ENVIRONMENTS

Two workbenches will be developed. The first workbench is intended to be a prototype and includes component models required for simulating a current energy plant. The selected plant configuration is based on the DOE Low Emissions Boiler System Proof of Concept (LEBS-POC) facility. The second workbench will focus on a Vision 21 energyplex system.

Prototype Workbench

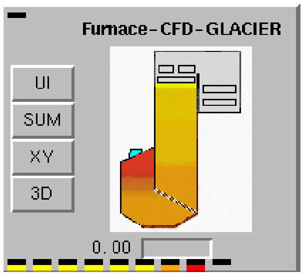
The LEBS-POC is a nominally 90 MW, down-fired unit. It contains four low NOx burners in a staggered arrangement in a U-shaped, wet bottom boiler and has provisions for OFA and reburning. The LEBS-POC plant configuration, as represented in the workbench, is shown in Figure 1. The prototype workbench uses a CFD model for the radiant furnace box. Reactor models have been implemented to simulate steam generation, the air pre-heater, NOx reduction with a Selective Catalytic Reduction (SCR) unit and particulate removal. Modules for a baghouse and an Electro-Static Precipitator (ESP) have been provided for modeling particulate removal.

For the firebox, two CFD modules have been implemented. One module is based on *GLACIER*, a comprehensive two phase CFD based combustion code. *GLACIER* has been used by REI to model a variety of utility boiler configurations [http://www.reaction-eng.com]. At present, *GLACIER* is limited to performing steady-state simulations. A module has also been implemented for *AIOLOS*, a comprehensive CFD combustion code developed at the University of Stuttgart that can be used for performing steady or unsteady simulations of coal fired utility boilers.

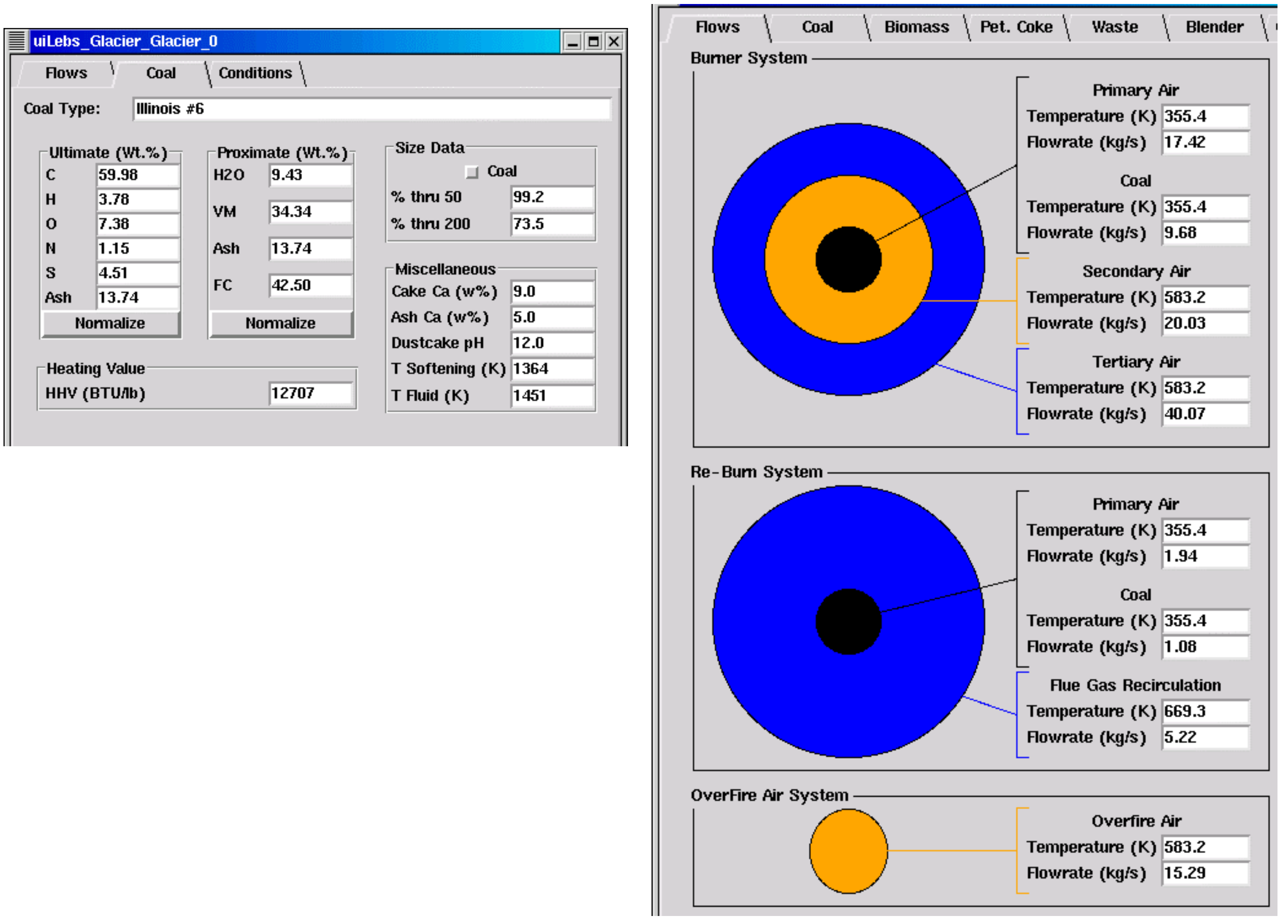
Below we briefly describe the modules that have been implemented. For each module, the functionality, model inputs and model outputs are described. It should be noted that for each module included in the workbench there is an on-line Help panel that contains a short description of the model and basic instructions for running the module (see Figure 4 in the Workbench-Interface section).

GLACIER POC Furnace Module (Steady State): The *GLACIER* CFD code is a comprehensive CFD modeling code that can be used to model a broad range of turbulent reacting flows. It is capable of modeling two-phase fuels for either gas-particle or gas-liquid applications. For establishing the basic combustion flow field, full equilibrium chemistry is employed. To compute NOx and other trace species, finite rate chemistry effects can be included in a post-processor mode. Turbulence chemistry coupling is accomplished using PDF methods. An important aspect of GLACIER is the tight coupling used between the dominant physics for utility boiler applications: turbulent fluid mechanics, radiation heat transfer, chemical reactions and particle/droplet dynamics. Further information on GLACIER is available at

http://www.reaction-eng.com/combustion.htm.



The User Interface (UI) for this module is illustrated in Figure 5a. It includes the inputs that control fuel, air, and re-circulating flue gas flows, temperatures, and coal properties. Outputs are available in: tabular format for summary data for predicted performance; XY plots to show axial variations of averaged values; and 3D field data formats for use with CFD visualization techniques. Linkages to Virtual Reality visualization techniques are being explored.



Coal Type: Illinois #6

Ultimate (Wt.%)	
C	59.98
H	3.78
O	7.38
N	1.15
S	4.51
Ash	13.74

Proximate (Wt.%)	
H2O	9.43
VM	34.34
Ash	13.74
FC	42.50

Size Data
☐ Coal
% thru 50: 99.2
% thru 200: 73.5

Miscellaneous
Cake Ca (w%): 9.0
Ash Ca (w%): 5.0
Dustcake pH: 12.0
T Softening (K): 1364
T Fluid (K): 1451

Heating Value
HHV (BTU/lb): 12707

Burner System

	Temperature (K)	Flowrate (kg/s)
Primary Air	355.4	17.42
Coal	355.4	9.68
Secondary Air	583.2	20.03
Tertiary Air	583.2	40.07

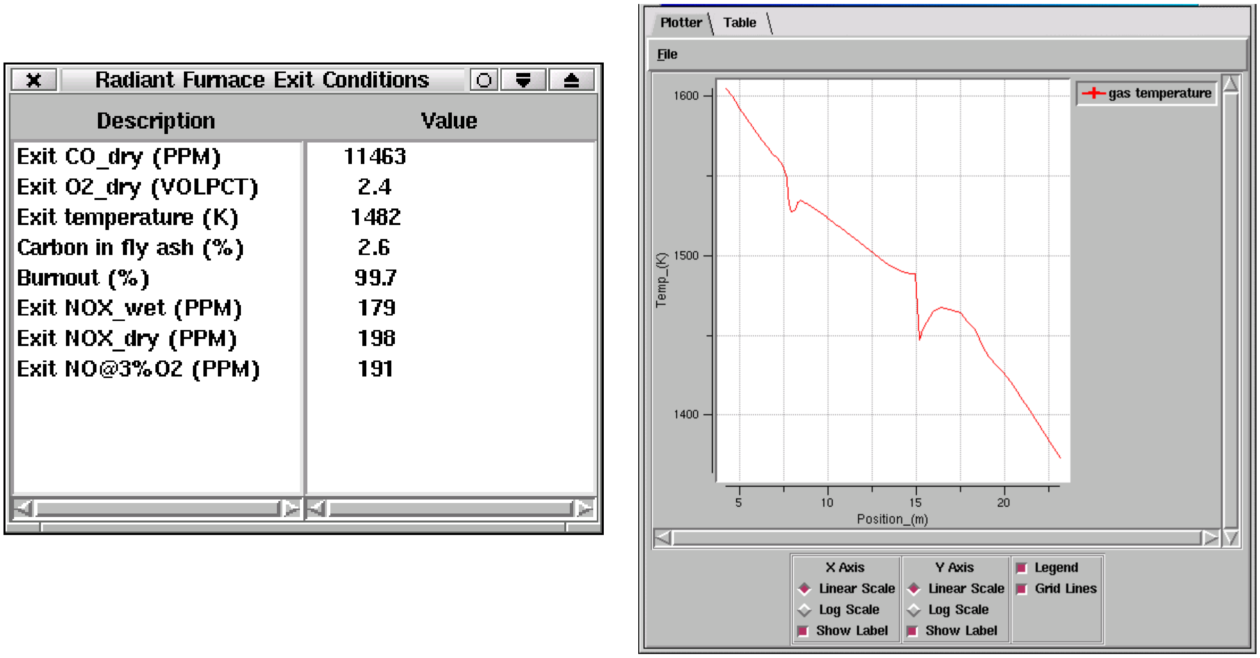
Re-Burn System

	Temperature (K)	Flowrate (kg/s)
Primary Air	355.4	1.94
Coal	355.4	1.08
Flue Gas Recirculation	669.3	5.22

OverFire Air System

	Temperature (K)	Flowrate (kg/s)
Overfire Air	583.2	15.29

Figure 5a. Windows showing example input dialog boxes for specifying coal composition (left) and air-fuel distribution (right).

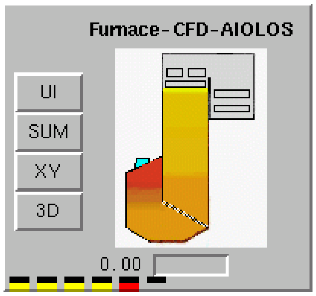


Radiant Furnace Exit Conditions

Description	Value
Exit CO_dry (PPM)	11463
Exit O2_dry (VOLPCT)	2.4
Exit temperature (K)	1482
Carbon in fly ash (%)	2.6
Burnout (%)	99.7
Exit NOX_wet (PPM)	179
Exit NOX_dry (PPM)	198
Exit NO@3%O2 (PPM)	191

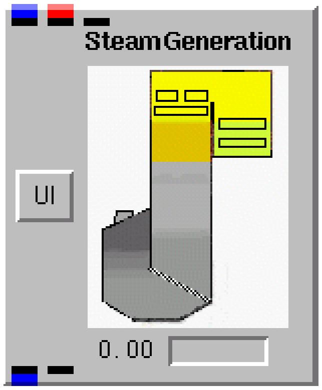
Figure 5b. Windows showing examples of the Summary Data output (left) and XY Plots of the mean Gas Temperature in the upflow section of the furnace (right).

<u>*AIOLOS* POC Furnace Module (Transient/Steady State)</u>: The *AIOLOS* CFD code is a comprehensive CFD modeling code that can be used to model a broad range of turbulent reacting flows. It can be used to model two-phase fuel applications, using either Eulerian-Eulerian or Eulerian-Lagrangian methods. *AIOLOS* employs an EDC technique for turbulence chemistry coupling. It can employ multi-domain grids and perform time dependent coal combustion simulations using either implicit or explicit time stepping. It can be used on virtually any level of hardware or operating system. *AIOLOS* is parallel-capable on both SMP and distributed architectures. It can be executed on single or dual cpu PCs/workstations, PC clusters and has been tuned for use on supercomputers. Further information on AIOLOS can be found on the web at: http://www.ivd.uni-stuttgart.de/english/aiolos_e_fh.html.

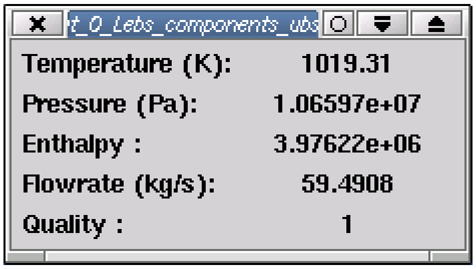


The User Interface (UI) for this module is identical to that used for the *GLACIER* module.

Upper Furnace Module**:** A simple model has been implemented to compute the steamside and CO burnout in the upper, or convective pass, of the furnace. For the steamside model, the steam flow rate and exit steam conditions are computed from thermodynamic steam calculations coupled with an integrated heat transfer rate to the steam from the CFD model for the POC boiler. The model is based on a tube bank heat exchanger model, with correlations taken from [B&W, 1992]. Included in the model is a stream property code. The module was tested by comparing predicted values versus design data for the LEBS-POC.



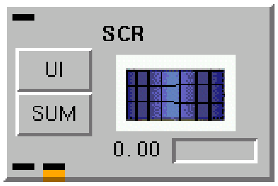
The module can be configured to model a variety of systems. Components available within the UI for building a heat transfer network include: Cavity, Steam Drum, Water Walls, Tube Banks, Atemperator and Superheater. This module could be used to model other plant heat transfer devices, such as a heat recovery steam generator (HRSG). The default values provided with the module in the prototype workbench are for the LEBS-POC facility. All of the remaining input items for this module (e.g., furnace flue gas flow properties) are obtained directly from the output of the CFD model of the furnace. Note that this module has two “exit ports”. One port is for the flue gas leaving the furnace convective pass. Applying a Port Interrogation tool to this port allows the user to view detailed information about the predicted composition of the flue gas at the exit of the economizer. A second port is used for the steam exiting the boiler – this is the steam that would be sent to the steam turbine. By clicking on the steam port, the steam properties (e.g., flow rate, temperature, pressure) can be viewed.



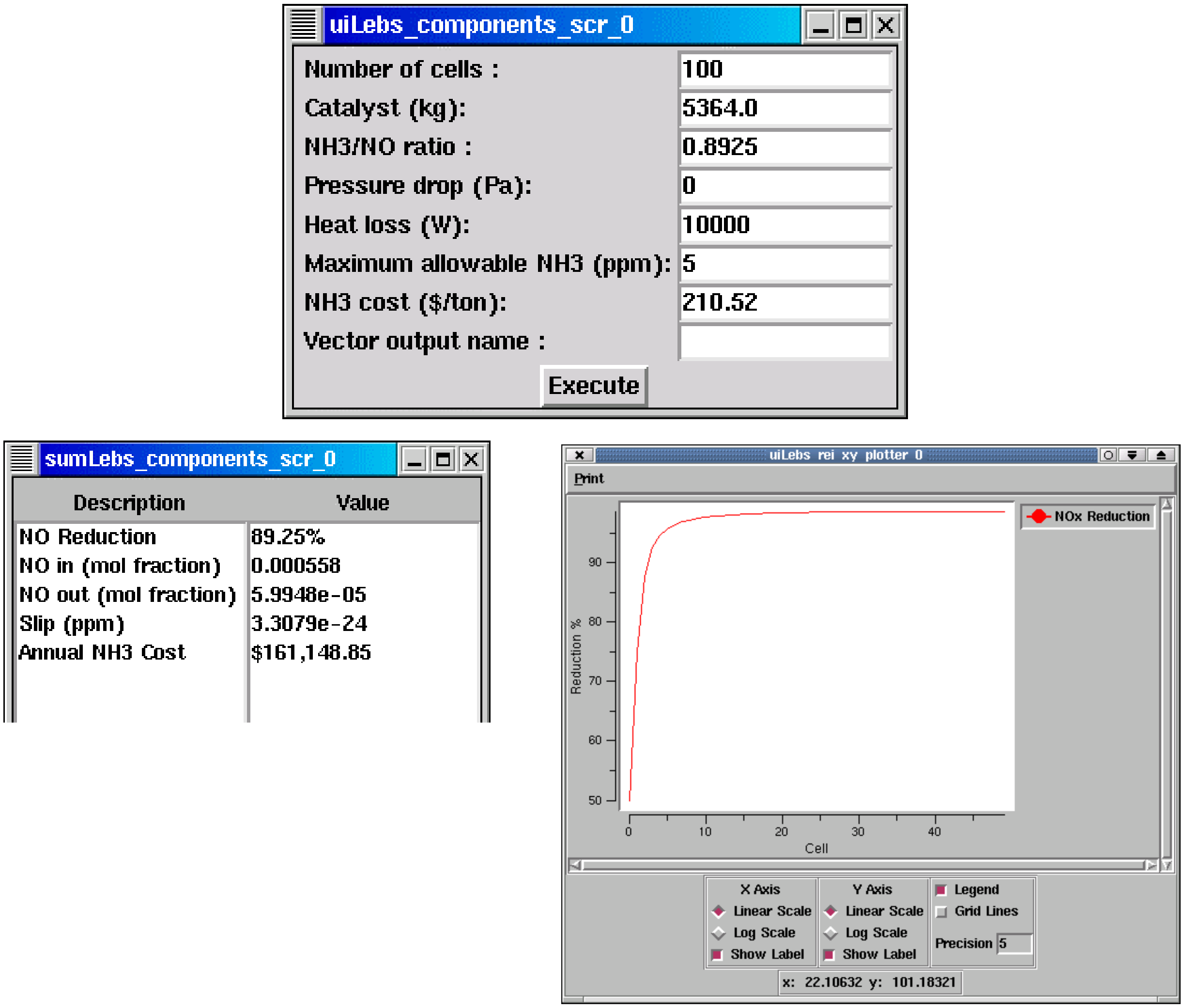
Temperature (K):	1019.31
Pressure (Pa):	1.06597e+07
Enthalpy :	3.97622e+06
Flowrate (kg/s):	59.4908
Quality :	1

Figure 6. Window showing the steam properties output from steamside model. Note that quality = 1 implies that pure steam is being sent to the turbine.

SCR Module**:** The purpose of the SCR is to reduce NOx emissions in the boiler flue gas. Ammonia is injected into the flue gas immediately upstream of the SCR. Within the SCR, the ammonia enriched flue gas then passes through an array of catalysts that induce catalytic reactions that in-turn reduce the NOx in the flue gas. A plug flow SCR model has been developed based on the microkinetic mechanism of Dumesic et al. (1996) (also known as the Topsoe mechanism) for NOx reduction with vanadia/titania catalysts. This is the most common SCR catalyst used by utilities and is the catalyst that will be used in the LEBS POC facility. The model was verified through comparisons of predicted values and values presented in Dumesic et al. (1993).



The UI for the SCR model includes the following inputs: NH_3/NO ratio of ammonia injection, ammonia cost, maximum allowable ammonia slip, number of computational cells, heat loss from the SCR, and pressure drop. Other inputs required by the model, such as gas flow rate and composition, are obtained from the gas data passed from upstream modules. For outputs, the UI contains a summary data dialog box that lists the predicted NOx reduction, ammonia slip and annual ammonia costs; and a XY plot that illustrates the predicted NOx destruction along the axis of the SCR unit. The module will flash a warning message if the predicted ammonia slip exceeds the prescribed maximum level.



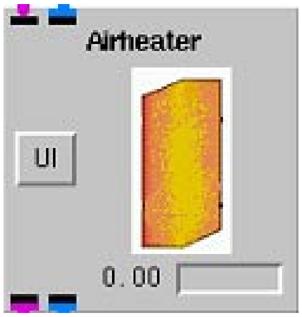
Number of cells :	100
Catalyst (kg):	5364.0
NH3/NO ratio :	0.8925
Pressure drop (Pa):	0
Heat loss (W):	10000
Maximum allowable NH3 (ppm):	5
NH3 cost ($/ton):	210.52
Vector output name :	

Description	Value
NO Reduction	89.25%
NO in (mol fraction)	0.000558
NO out (mol fraction)	5.9948e-05
Slip (ppm)	3.3079e-24
Annual NH3 Cost	$161,148.85

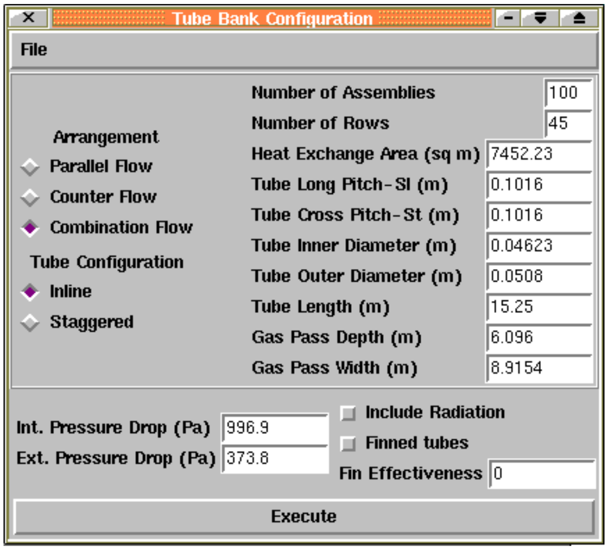
X Axis: ● Linear Scale ○ Log Scale ☑ Show Label
Y Axis: ● Linear Scale ○ Log Scale ☑ Show Label
☑ Legend ☐ Grid Lines
Precision 5
x: 22.10632 y: 101.18321

Figure 7. For SCR module, example input dialog box, output dialog box and 1D plot of predicted NOx reduction along axis of SCR unit.

Air Heater Module: The air preheater is a heat exchanger that uses hot effluent gas from the furnace to heat the secondary and tertiary combustion air and over fire air (OFA). The air heater module was created by re-using the tube bank heat transfer model developed for the steam side module.



The UI for this module includes a dialog box to prescribe the properties of the incoming external (cold) air. Note that the properties for the (hot) furnace flue gas are extracted from the flue gas properties in the workbench data flow network. This module has two “exit ports”. One port is for the flue gas leaving the air heater and the second port is for the pre-heated air that is sent to the boiler. Applying a Port Interrogation tool to the flue gas exit port allows the user to view detailed information about the predicted composition of the flue gas. Likewise, applying a Port Interrogation tool to the pre-heated air exit port allows the user to view detailed information about the pre-heated air exiting the air preheater device.

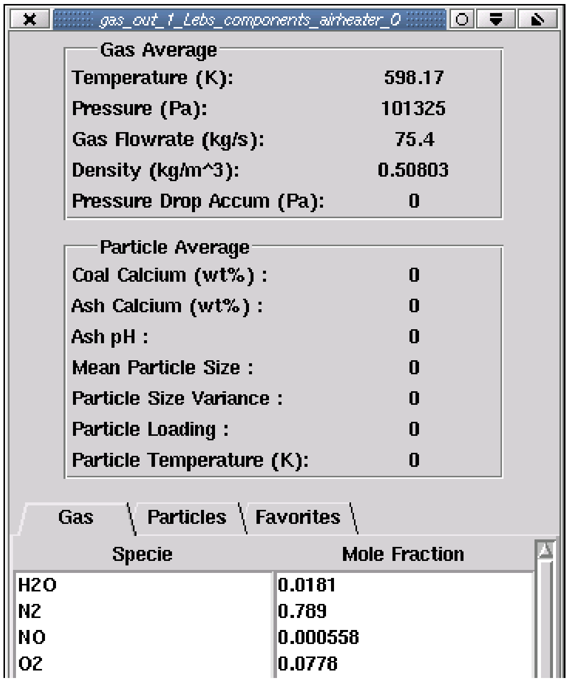


Arrangement
○ Parallel Flow
○ Counter Flow
● Combination Flow

Tube Configuration
● Inline
○ Staggered

Number of Assemblies	100
Number of Rows	45
Heat Exchange Area (sq m)	7452.23
Tube Long Pitch-SI (m)	0.1016
Tube Cross Pitch-St (m)	0.1016
Tube Inner Diameter (m)	0.04623
Tube Outer Diameter (m)	0.0508
Tube Length (m)	15.25
Gas Pass Depth (m)	6.096
Gas Pass Width (m)	8.9154
Int. Pressure Drop (Pa)	996.9
Ext. Pressure Drop (Pa)	373.8

☐ Include Radiation
☐ Finned tubes
Fin Effectiveness 0



Gas Average

Temperature (K):	598.17
Pressure (Pa):	101325
Gas Flowrate (kg/s):	75.4
Density (kg/m^3):	0.50803
Pressure Drop Accum (Pa):	0

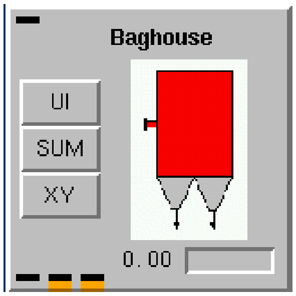
Particle Average

Coal Calcium (wt%) :	0
Ash Calcium (wt%) :	0
Ash pH :	0
Mean Particle Size :	0
Particle Size Variance :	0
Particle Loading :	0
Particle Temperature (K):	0

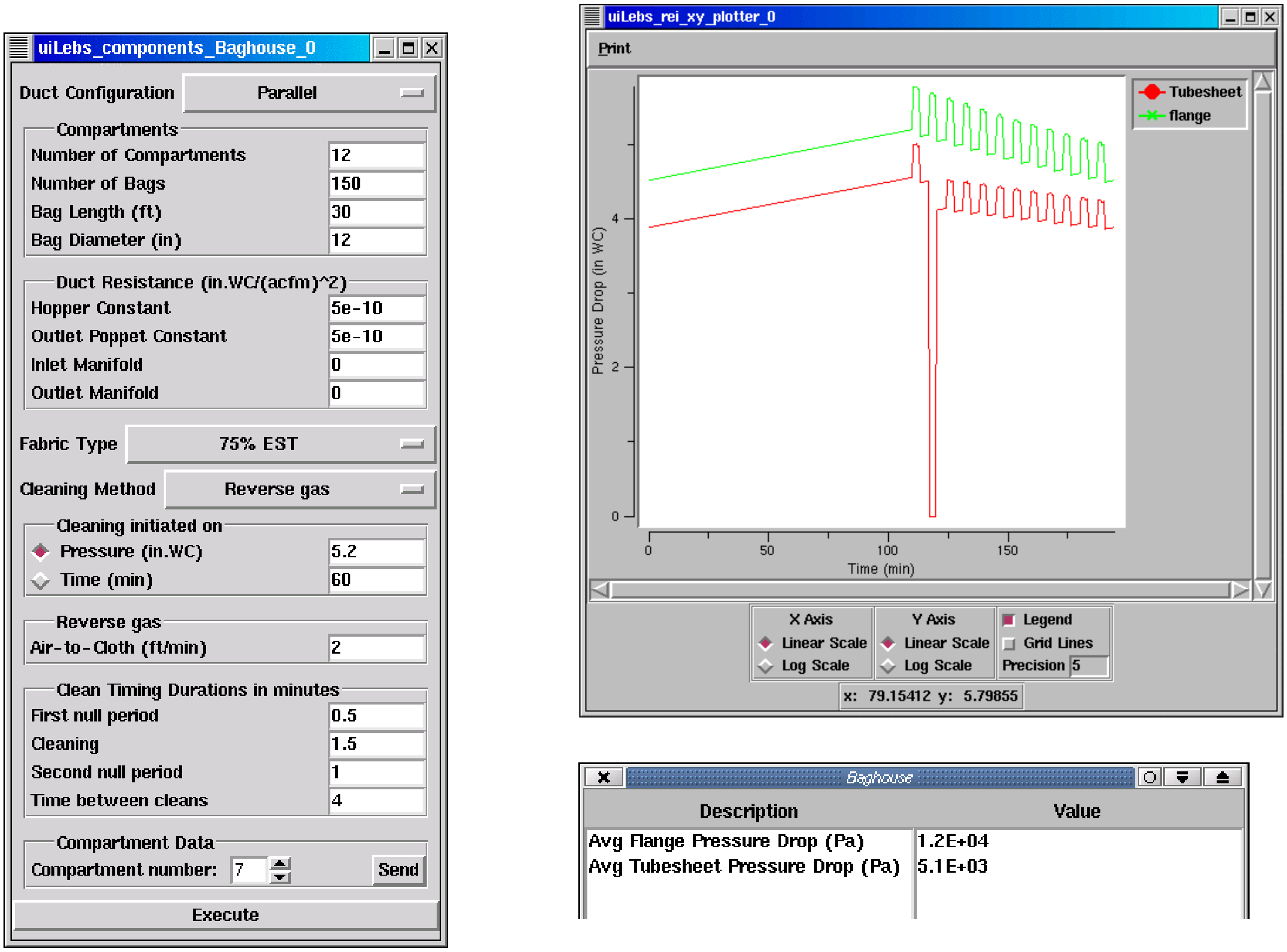
Specie	Mole Fraction
H2O	0.0181
N2	0.789
NO	0.000558
O2	0.0778

Figure 8. For Air Heater module, shown are the input dialog window (left) and Port Interrogation window (right) when applied to the exit port for the pre-heated air.

Baghouse Module: A baghouse is a device that uses fabric filters to remove particulates from effluent coal combustion gases. A simple zero dimensional (reactor) model has been implemented that computes capture efficiency and pressure drop, based on the amount of trapped solids. The pressure drop calculations are important to establish fan requirements. The baghouse model used here is based on a model provided to REI by the Southern Research Institute [Pontius, Robinson & Vann Bush, 1992].



The UI includes inputs for the number of filter compartments and their arrangements, and cleaning frequency and method. Ash properties pertinent to dust cake buildup in the baghouse are input with the coal properties in the furnace UI (i.e., the UI for *GLACIER* and *AIOLOS*). All other flue gas properties required by the model are obtained directly from the gas data output from the upstream module. The output for the model consists of the time-averaged pressure drop across the baghouse.



Duct Configuration: Parallel

Compartments
Number of Compartments: 12
Number of Bags: 150
Bag Length (ft): 30
Bag Diameter (in): 12

Duct Resistance (in.WC/(acfm)^2)
Hopper Constant: 5e-10
Outlet Poppet Constant: 5e-10
Inlet Manifold: 0
Outlet Manifold: 0

Fabric Type: 75% EST
Cleaning Method: Reverse gas

Cleaning initiated on
● Pressure (in.WC): 5.2
○ Time (min): 60

Reverse gas
Air-to-Cloth (ft/min): 2

Clean Timing Durations in minutes
First null period: 0.5
Cleaning: 1.5
Second null period: 1
Time between cleans: 4

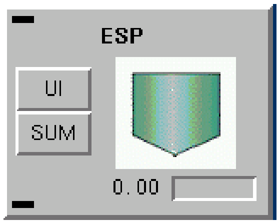
Compartment Data
Compartment number: 7

X Axis: ● Linear Scale ○ Log Scale
Y Axis: ● Linear Scale ○ Log Scale
☑ Legend ☐ Grid Lines
Precision 5
x: 79.15412 y: 5.79855

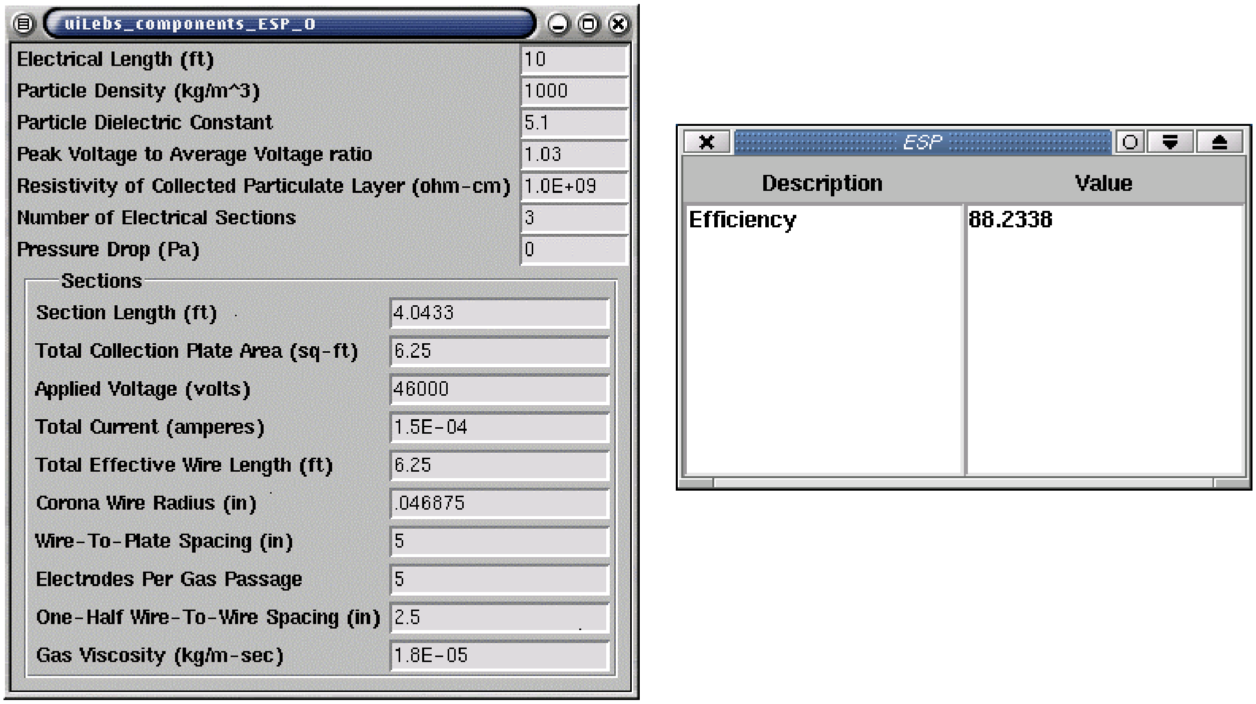
Description	Value
Avg Flange Pressure Drop (Pa)	1.2E+04
Avg Tubesheet Pressure Drop (Pa)	5.1E+03

Figure 9. For baghouse module, shown are windows for input dialog box (left), Summary output (lower right) and 1D plot of time dependent pressure drop (including cleaning event) (upper right).

ESP Module: An Electro-Static Precipitator (ESP) is a device for removing dust particles from a gas stream. Within the ESP, an electro-static charge is induced on the particles, causing the particles to be deposited onto a plate with an opposite charge. The model implemented into the workbench is based on a model provided by Clean Air Engineering (CAE). The model was originally developed at the Southern Research Institute and then subsequently enhanced by CAE. The model calculates the voltage-current characteristics and electric potential, electric field, and space charge density distributions on a two dimensional grid. These fields are in turn used to predict the particulate removal efficiency. The resistivity of the particulates is a key input in determining charge accumulation.



The UI includes inputs for the precipitator geometry, voltage-current relationships, ash dialectric constant and particle layer resistivity. Ash particle size distribution is input based on the coal size distribution in the furnace (note: coal size distribution is available from the inputs for the furnace CFD model) and a predetermined size reduction factor for the ash from an ash formation model developed under DOE funding [Bool et al., 1995]. All other properties of the flue gas that are required by the model are obtained directly from the gas data output from the upstream module. The output for the model consists of removal efficiency as a function of particle size and the ash particle concentration of the outlet stream.



Electrical Length (ft)	10
Particle Density (kg/m^3)	1000
Particle Dielectric Constant	5.1
Peak Voltage to Average Voltage ratio	1.03
Resistivity of Collected Particulate Layer (ohm-cm)	1.0E+09
Number of Electrical Sections	3
Pressure Drop (Pa)	0

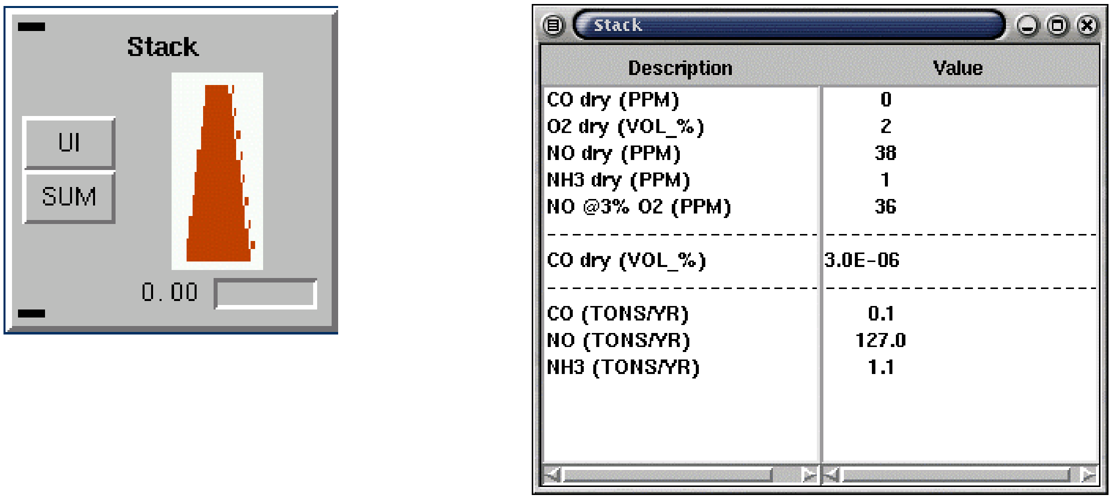
Sections

Section Length (ft)	4.0433
Total Collection Plate Area (sq-ft)	6.25
Applied Voltage (volts)	46000
Total Current (amperes)	1.5E-04
Total Effective Wire Length (ft)	6.25
Corona Wire Radius (in)	.046875
Wire-To-Plate Spacing (in)	5
Electrodes Per Gas Passage	5
One-Half Wire-To-Wire Spacing (in)	2.5
Gas Viscosity (kg/m-sec)	1.8E-05

Description	Value
Efficiency	88.2338

Figure 10. For ESP module, shown are windows for input dialog box, summary output and 1D plot of time dependent pressure drop (including cleaning event).

Stack Module. For completeness, the LEBS workbench includes a stack. At present, the stack module does not contain any models. However, models could be included to predict items such as aerosol formation, stack opacity or particulate dispersion in the local environment. In the current configuration, the stack module provides a simple summary output dialog (see Figure 11) that provides gross properties of the flue gas exiting the stack (e.g., CO_2, CO, NO, particulates). Alternatively, using the Port Interrogation data viewer, the user can obtain detailed information about the predicted conditions of the flue gas at the stack (see Figure 1 in Section 2.1 for example of data available with the Port Interrogation tool).



Description	Value
CO dry (PPM)	0
O2 dry (VOL_%)	2
NO dry (PPM)	38
NH3 dry (PPM)	1
NO @3% O2 (PPM)	36
CO dry (VOL_%)	3.0E-06
CO (TONS/YR)	0.1
NO (TONS/YR)	127.0
NH3 (TONS/YR)	1.1

Figure 11. Icon and Summary information for Stack.

Demonstration – Prototype Workbench

To demonstrate the functionality of the prototype workbench for the LEBS-POC facility, simulations have been performed to study the impact of changes to the boiler firing conditions on the performance of other equipment located downstream of the boiler.

LEBS-POC Steady State Demonstration: For the test, the Overfire air and Reburn ports in the up-flow portion of the furnace have been "turned off" and the impact on the downstream equipment studied. Note that the air and fuel flows through the burners were correspondingly increased to maintain the same overall firing rate and stoichiometry.

Table 1 illustrates the type of information that can be obtained. From the table it can be seen that the changed firing conditions result in reduced LOI, increased furnace exit gas temperature and a slight increase in the steam flow rate and steam temperature. For both firing conditions, the flue gas temperature at the economizer exit is about the same.

The simulations also predict that the modified firing conditions increase the NOx levels at the furnace exit. In both simulations, the SCR model was run in an "iterative" manner so that the ammonia flow rate was automatically adjusted to the desired NOx level at the SCR exit (it is assumed that the NOx and ammonia levels in the flue gas exiting the SCR do not change between the SCR and the stack). For these tests, the target NOx level at the stack is the anticipated NOx regulation limit of 0.15lb/mmBTU. From Table 1, it can be seen that the SCR operation can be modified to ensure that both firing configurations achieve the desired NOx level at the stack. However, the modified firing condition requires more ammonia to be used in the SCR. Assuming an ammonia cost of $200/ton, the increased ammonia usage results in ammonia costs increasing from $30,000/year to $54,000/year.

Table 1. Comparison of Predicted Values for Baseline Firing Conditions and Turning Off the OFA and Coal Reburn

	Baseline	**OFA & Reburn OFF**
Furnace Exit NOx, ppm dry (lb/mmBTU)	200 (0.25)	257 (0.33)
Stack NOx, ppm dry (lb/mmBTU)	119 (0.15)	119 (0.15)
Ammonia Slip, ppm dry	< 1	< 1
Ammonia Cost, $/yr	$30,000	$54,000
Steam Flow Rate, kg/s	60	66
Steam Temperature, K	1019	1025
Heat Transfer to Water Walls, MW	68	76
LOI, %	2.6	1.6
Furnace Exit CO, ppm dry	11460	7492
Furnace Exit Temperature, K	1482	1572
Economizer Gas Outlet Temperature, K	674	679
Air Heater Outlet Air Temperature, K	598	606

LEBS-POC Transient Demonstration: To demonstrate the transient capability of the *AIOLOS* reacting CFD model a simulation for a 50% load turndown of the POC furnace has been performed. For this simulation, it is assumed that the unit is operating at 100% load and then at time t = 0, the burner fuel and air flow rates are instantaneously turned down to 50% load. The integration of the solution through time was performed in a time accurate mode. This simulation was performed by project team members at RECOM Services.

Figure 12 shows the transient response of furnace exit gas temperature. Note that the load change is also shown in the figure. The simulation involved a real time integration of about 24 seconds. A unit of this size (90 MW) responds quickly to the load reduction. The predicted exit temperature is seen to be approaching steady state at 24 seconds.

Illustrated in Figure 13 are three snapshots in time of the gas temperature field, at t = 0, t = 6 sec, and t = 24 sec, respectively. The highest temperatures in the flame are seen to move closer to the burner plane as time progresses.

The computer run time required for this simulation was quite large - 76 real time hours on a single “8-processor node” of a Hitachi SR8000. The Hitachi is a hybrid supercomputer that distributes computations and memory across nodes. Within each node, the computations are performed in a SMP parallel mode across eight processors. Another high performance computer is available for these computations - the NEC SX-5 vector machine. The single node of a Hitachi is comparable to a single processor of a NEC SX-5. Using 4 NEC SX-5 processors in parallel would reduce the real time to perform this simulation by a factor of 4.

It would not be practical to perform this type of simulation on a standard desktop workstation due to the long run-time required. Although *AIOLOS* is fully integrated into the workbench, to perform this simulation AIOLOS was run in “standalone” mode on the supercomputer. One of the goals of this project is to implement into the workbench environment the ability to perform cpu intensive computations on remote computers connected via a network. REI has demonstrated this capability for a relatively small model (i.e., the SCR model) using CORBA based components. In future work we will investigate enhancing this capability to allow running large, cpu intensive simulations on a remote supercomputer or PC cluster. Here, the issues are not so much technical, but rather deal with firewalls and other security measures used at supercomputer centers.

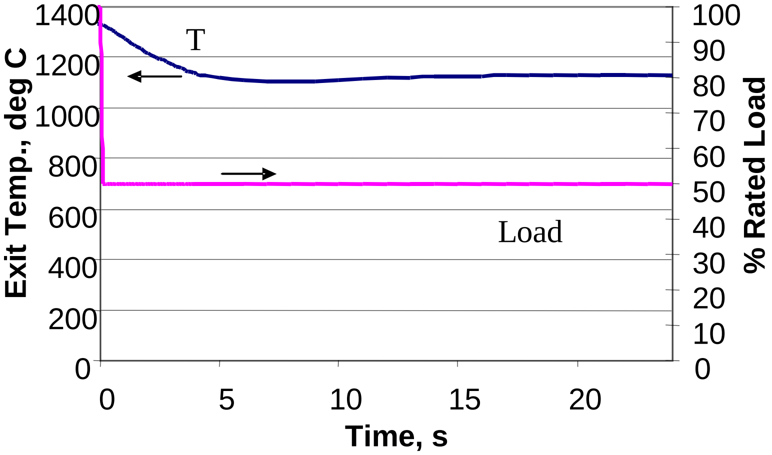
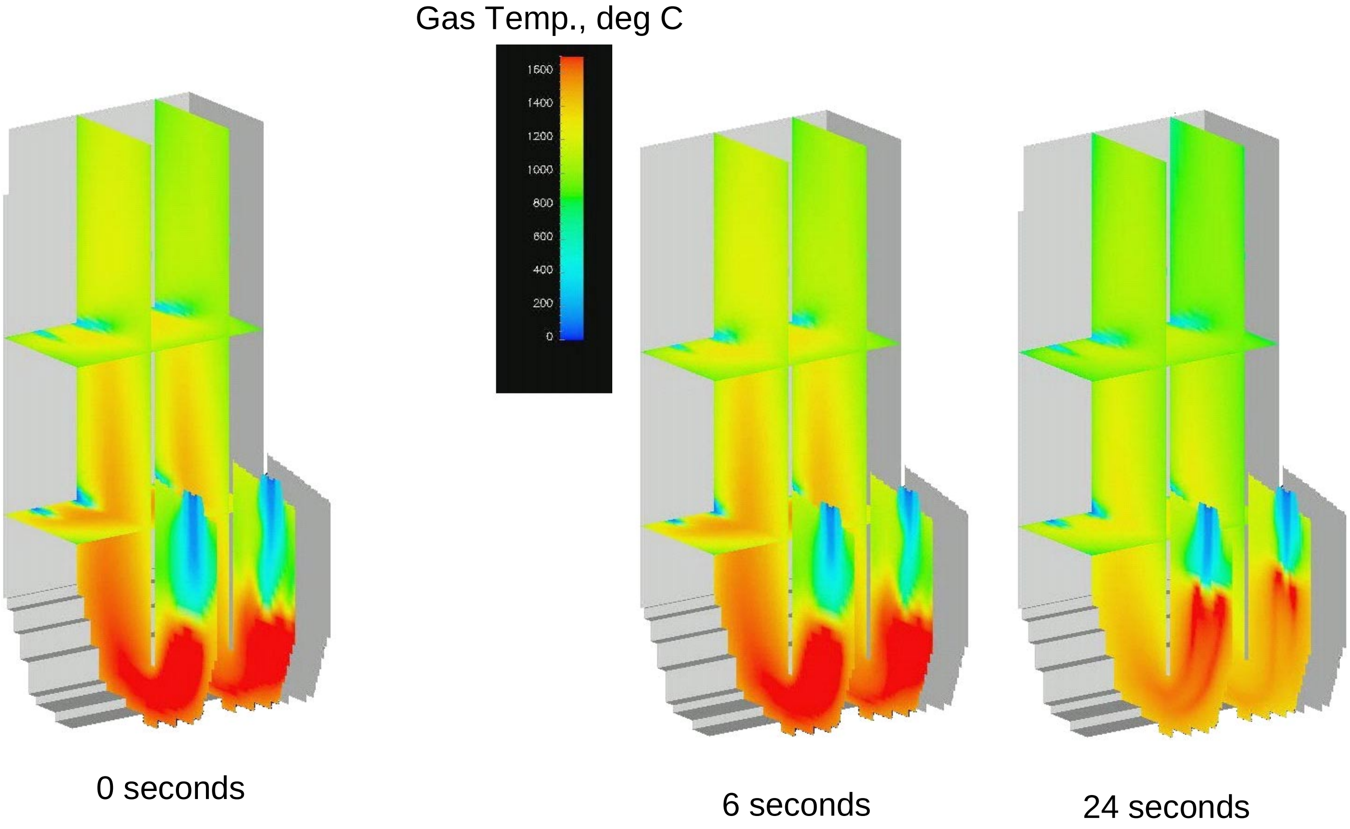


Figure 12. Furnace exit temperature as a function of time for transient turn-down to 50% load.



0 seconds

6 seconds

24 seconds

Figure 13. Gas temperature field at three instances of time for transient simulation.

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:

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 [Simbeck and Johnson, 2001], [Holt, 2001], [IEA, 2000]. Hence, in this project we will focus on oxygen blown, 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. We anticipate having to incorporate extensions to our models to account for high pressure effects on the reaction kinetics and possibly the impact of the heavier particle loading. Additional models might be required to also include predictions for ash, slagging and air toxics.

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. Here, we intend to collaborate with Prof. Terry Wall and other members of the Collaborative Research Center for Sustainable Development (CCSD) (formerly the Black Coal Co-operative Research Center) at the University of Newcastle, Australia. The CCSD group has extensive experience in gasification and has developed experimental data sets for pilot scale gasifier operation, reaction kinetics for high pressures and many sub-models to describe slag and ash behavior in a gasifier.

It is our intention to provide within the workbench the ability to model “generic”, cylindrical gasifier configurations (see Figure 14) for (1) single feed, down fired systems and (2) two stage systems with multiple feed inlets that could be opposed or tangentially fired. These systems are representative of the dominant, commercially available gasifier systems. The user will have the ability to: select different sub-models; perform limited modifications of the firing configuration, gross characteristics of the fuel injector and overall riser geometry; alter model inputs for feedstock (fuel), slurry composition and system pressure. Model outputs will include detailed information about the flowfield (e.g., gas and particle velocity, composition, temperature) and gross information about carbon conversion. The gasifier model to be developed here will allow workbench users to address many of the performance and operational problems currently hindering the operation of solid fuel gasifiers [Steigel et al, 2001], [Holt, 2001].

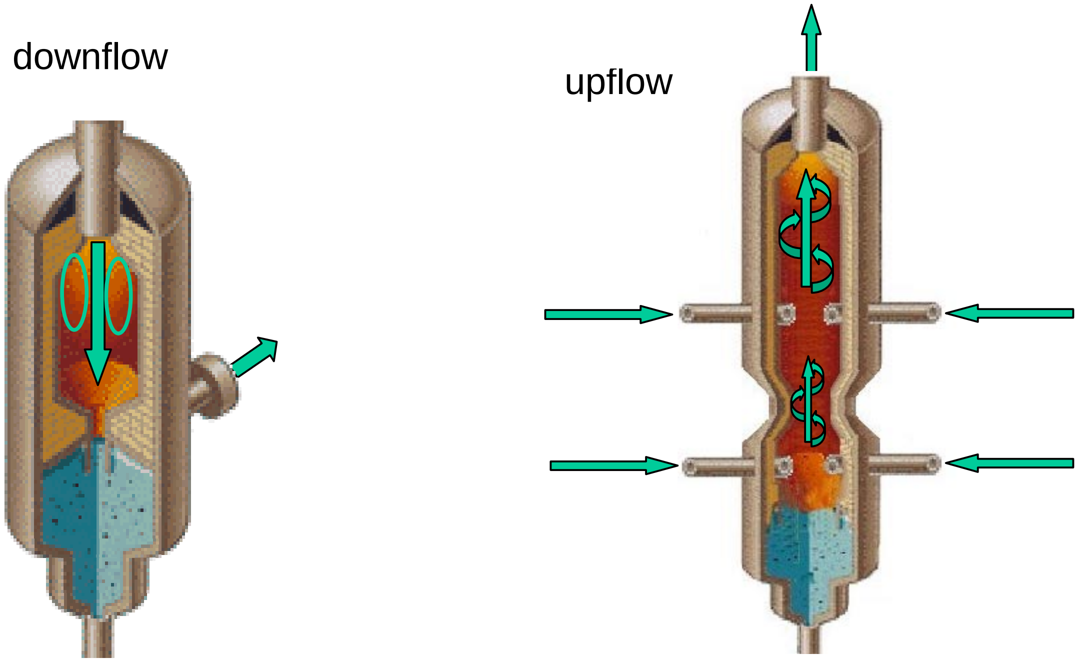


Figure 14. Generic gasifier configurations to be modeled.

Fluidized Bed: We intend to include in the workbench models to simulate circulating fluidized beds. Both a reactor model and a CFD based model will be included. Implementing two models will provide users the option to use the model that best represents their system. The reactor model has the advantage of being physically realistic and runs fast enough to be used for plant design studies and possibly dynamic model response. Our reactor model will be based on previous work by [Hannes, 1993], [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. The accuracy of the reactor and CFD based fluidized bed models will be tested on available data sets, such as [Monazam and Shadle, 2001], [Guenther et al, 2001].

Turbine Combustor**:** We plan to include a combustion CFD model and a reactor model for a turbine combustor 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 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 Cell (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, SCR and Heat Recovery Steam Generator. The list of models to be included will be dependent on the energyplex configuration of greatest interest to the DOE. The models will be based on information and correlations available in the open literature.

Demonstration – Vision 21 Energyplex Workbench

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 prototype 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 and progress 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 used in 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 based on the LEBS-POC facility has been developed and tested. All modules required to perform a simulation are fully integrated into the workbench. A set of steady-state simulations have been performed. A time accurate, transient simulation of the LEBS-POC furnace for dropping load has been performed. A remote computing capability has been demonstrated. In addition, two reviews of the workbench environment have been completed. An in-house review of the workbench software design and workbench functionality has been completed. A review of the software design and proposed plans for the next version of the workbench has been completed by the original developers of the SCIRun software system. The recommendations from these reviews have been prioritized and incorporated into the software development plan for the workbench.

With the development effort for the prototype workbench completed, efforts are now being focused on developing a workbench for IGCC based energyplex systems. Plans for the next year include a focused effort on the gasifier model and (to a lesser extent) evaluating fluidized bed models and implementing modifications to the workbench software infrastructure to support development of a second version of the workbench for simulating energyplex systems.

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