A Computational Workbench Environment
for Virtual Power Plant Simulation

Quarterly Progress Report

Reporting Period Start Date: April 1, 2001
Reporting Period End Date: June 30, 2001

Mike Bockelie, REI
Dave Swensen, REI
Martin Denison, REI

July 30, 2001

DOE Cooperative Agreement No: DE-FC26-00NT41047

Reaction Engineering International
77 West 200 South, Suite 210
Salt Lake City, UT 84101

Disclaimer

Abstract

This is the third Quarterly Technical Report for DOE Cooperative Agreement No: DE-FC26-00NT41047. The goal of the project is to develop and demonstrate a computational workbench for simulating the performance of Vision 21 Power Plant Systems. To demonstrate the capabilities of the workbench and identify software design improvements, the Year One effort is focused on developing a prototype workbench for the DOE Low Emission Boiler System (LEBS) Proof of Concept (POC) design. During the last quarter good progress has been made. An "alpha" version of the prototype workbench for the LEBS POC is available for use. A project meeting was held with DOE personnel involved with Vision 21 to present an overview of current project status and to outline future work.

Table of Contents

1

Executive Summary

The work to be conducted in this project received funding from the Department of Energy under Cooperative Agreement No: DE-FC26-00NT41047. This project has a period of performance that started October 1, 2000 and continues through September 30, 2003.

The goal of the project is to develop and demonstrate a computational workbench for simulating the performance of Vision 21 Power Plant Systems. The Year One effort is focusing on developing a *prototype workbench* for the DOE Low Emission Boiler System (LEBS) Proof of Concept (POC) design. The LEBS prototype workbench will include the boiler (furnace and steam-side), particulate collection and Selective Catalytic Reduction (SCR) systems. LEBS is a system with which we are familiar and thus provides the opportunity to demonstrate the capabilities of the workbench and identify software design improvements before starting work on the Vision 21 workbench.

The main accomplishments during the last three months include:

- An "alpha" version of the *prototype workbench* has been assembled and is being tested;
- Completed integration into the workbench of the GLACIER CFD furnace model and reactor models for the SCR and baghouse.;
- Acquisition of the source code for an ESP model;
- Continued enhancement of the infrastructure within the **SCIRun** software system that is being used as the platform to create our computational workbench;
- Meeting with DOE to discuss project status and REI plans for developing component models to be used to simulate a Vision 21 energyplex.

Each of these topics is discussed in the following sections.

Experimental Methods

Within this section we present brief discussions on the many sub-tasks that must be addressed in developing the workbench. For simplicity, the discussion items are presented in the order of the Tasks as outlined in our detailed Work Plan.

Task 1 – Program Management

On May 14-16, 2001 members of the project team attended the 16th International Conference on Fluidized Bed Combustion held in Reno, Nevada. Attending this bi-annual meeting provided the opportunity to review many "applied research" projects and determine the state-of-the practice for modeling fluidized bed systems for power generation applications.

On June 4-7, 2001 members of the project team attended the ASME International Joint Power Generation Conference 2001 held in New Orleans, Louisiana. The purpose in attending the conference was to participate in a Panel Session for the DOE Vision 21 program. The session was organized by Dr. Larry Ruth, the DOE Vision 21 Program Manager. REI made a short presentation that provided meeting attendees an overview of our Vision 21 project.

On June 26, 2001 members of the project team attended a project meeting at DOE-NETL (Pittsburgh). Meeting attendees included the DOE Project Manager, the DOE Vision 21 Program Manager and several other DOE personnel involved with the DOE Vision 21 Program. Presentations by REI personnel included overviews of: current project status; software design issues being addressed in the project; models that have been developed for the LEBS workbench and plans for developing the models required for simulating a gasifier based Vision 21 plant; issues related to working with collaborators (foreign and domestic) and working with commercial organizations that have proprietary data or models that could be of use to this project. In addition, a short "movie" that showed the operation of the LEBS workbench was presented.

Informal discussions have been held with organizations that are interested in potential collaboration. The Black Coal Combustion Research Center in Newcastle, Australia has significant knowledge, experience and data for pilot and laboratory scale coal gasification systems. Several of their recent PhD projects have focused on developing physical sub-models that could be of use in our gasifier CFD model. The National Fuel Cell Research Center at the University of California – Irvine has a Vision 21 project investigating hybrid fuel cell systems. Models developed at the NFCRC could be of use to this project.

Task 2 – Virtual Plant Workbench I

The objective of this task is to demonstrate the capabilities of the computational workbench environment by evaluating the performance of a virtual LEBS power plant. For the many sub-tasks contained under Task 2, the work effort is being performed by software engineers from Reaction Engineering International (REI) and Visual Influence (VI).

Task 2.1 Software Design

The main focus of this sub-task has been to create an initial software design, which allows testing of basic workbench capabilities and provides a path to transition to more sophisticated designs as we finalize Workbench I.

<u>Update on Component Interfaces</u>: As stated previously, component interfaces define how the individual **SCIRun** modules communicate with their underlying computational modules. At present, all of the function-based component interfaces for Workbench I have been identified and designed and used in Task 2.3 Module Implementation/Integration. Note that work will continue in this area as we begin transitioning modules to component architectures for Workbench II.

<u>Abstract Datatypes:</u> The identification and design of abstract datatypes is an ongoing task, which defines the data structures which are used throughout the workbench modules and supporting software infrastructure. These types provide abstractions for numerous concepts including threads, process control, file I/O, database and data conversion. While this sub-task is nearly complete for Workbench I, the design of abstract types will continue as we proceed with Workbench II and manage its increased complexity.

<u>Port Interrogation Capabilities</u>: In a dataflow environment such as SCIRun, it is important for the user to be able to interrogate the dataflow network at any point to determine what information is being passed. In the past, this need has been addressed by creating special modules, which allowed a user to display the network information graphically or in a table. While this method was functional, it required the user to connect a separate module whose sole purpose was display the properties of the network stream in question. Now, a TCL display class can be defined for a given network stream data type, and network execution populates this display with data from the module. All of this is done internal to the module, omitting the necessity of a separate display module. Work is currently being performed to generalize this functionality for all modules and all data types.

<u>Online Help System:</u> 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.

Task 2.2 Visualization

The main focus of this task has been to identify and begin implementation of enhanced visualization capabilities for **SCIRun**. Many of these visualization capabilities are based on emerging technologies and will provide leading edge visualization capabilities, some of which provide a modest degree of Virtual Reality functionality. Our current focus is on: enhanced transient visualization, enhanced volume rendering, and solution comparison capabilities.

Update on Enhanced Transient Visualization: Software engineers at Visual Influence are continuing development of enhanced transient visualization capabilities in SCIRun. As discussed in the last quarterly report, the design currently being implemented involves creation of a collector module, which manages the transient data sets and feeds downstream visualization modules.

Update on Enhanced Volume Rendering: Software engineers from Visual Influence have completed an initial implementation of an enhanced volume-rendering module. This module makes use of the latest advances in computer graphics hardware and should provide a tool for performing cutting-edge visualization. We are currently in the process of acquiring the hardware necessary to run this module on a Linux machine. This hardware includes the just-released nVidia Gforce3 graphics card and also a stereoscopic system from StereoGraphics Corporation.

Update on Solution Comparison: Visual Influence is continuing development of solution comparison capabilities for SCIRun. These new capabilities will allow us to perform highly visual comparisons of complicated data sets using user controlled rapid graphics switching techniques. This will allow the user increased insight into differences in the field data.

During the last performance period, we have also developed capabilities to create a "video" of the workbench operation and to simplify the user interface to the inherent visualization tools within SCIRun:

Ability to Capture Computer Screen in to a Movie File:
A need that has frequently arisen during this project is the ability to generate a highly portable demonstration of the workbench. Because of the hardware and software requirements of the workbench, it is difficult to show during presentations at remote sites, and difficult to send a demonstration of the workbench to remote parties. The movies are created using publically available (i.e., no cost) software tools for high-speed frame capture (xvidcap) and video encoding (RAD video tools). The movies generated using these tools are easy to view on multiple operating systems, laptops and can easily be sent electronically to remote sites. This method was used to provide a demonstration of the workbench capabilities for the NETL Vision 21 project meeting in June 2001.

Enhanced Visualization Module Usability: While basic SCIRun scalar and vector field visualization capabilities are more than adequate, the user interface and control elements tend to favor more sophisticated users. To help make the capabilities of these visualization modules more accessible to general users, software engineers from REI have made modifications to these visualization modules. These changes include the addition of user-interface elements that provide a convenient and intuitive means of controlling visualization parameters.

Task 2.3 Module Implementation/Integration

The focus of this sub-task has been to continue the development of component wrappers needed for the Year One workbench computational components and to integrate the LEBS component models into **SCIRun**.

Update on Component Wrappers: Development of the component wrappers for the LEBS Workbench I is now complete. Wrappers exist for the lower furnace, steam-side model, air preheater, baghouse, SCR and ESP. Wrapper development will continue as we begin implementing standard and component-based modules for Workbench II.

Update on Component Model Integration: Component models have been integrated into the workbench for the lower furnace (GLACIER steady-state CFD model), steam-side model, air preheater, baghouse and SCR. Integration efforts are now focused on an additional model for the LEBS furnace (AIOLOS transient CFD model) and an Electrostatic Precipitator (ESP) Model. AIOLOS is parallel-capable on both SMP and distributed architectures and is therefore challenging to integrate with the SCIRun LEBS Workbench. The ESP model, which was obtained as hard copy printouts, is currently being debugged.

Task 3 – Model Vision 21 Components

The purpose of this task is to develop the reactor and CFD models for the components that will be included in the workbench. Oftentimes, these models are developed in a "stand-alone" form and then subsequently integrated into the **SCIRun** environment.

Task 3.1 LEBS Components

Progress has been made on the following LEBS component models:

***GLACIER* POC Furnace Module (Steady State) :** During this performance period, *GLACIER* has been integrated into the LEBS Workbench. The User Interface (UI) for this model 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.

***AIOLOS* POC Furnace Module (Transient/Steady State):** The integration of *AIOLOS* with the workbench is nearly completed. The UI is identical to that used for the *GLACIER* module. *AIOLOS* is a CFD tool that is parallel-capable on both SMP and distributed architectures, can employ multi-domain grids and perform time dependent coal combustion simulations and thus provides some capabilities not available in *GLACIER*.

Steam Side Module: Integration of the steam side module into the LEBS workbench has been completed. 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. The outputs contained in the UI include a Summary Data panel for the steam properties (e.g., flow rate, temperature, pressure). The UI also includes an on-line Help panel that contains a short description of the model and basic instructions for running the module.

Air Heater: The integration of this module into the LEBS Workbench has been completed. 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. At present, the UI does not contain a summary data panel for this model because the output can be viewed with the gas-data-stream viewer module. The UI does contain a simple on-line Help panel.

SCR Module: The integration of this model into the LEBS Workbench is complete. The UI for the SCR model includes the following inputs: NH3/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. A simple on-line Help panel has been implemented that includes a short description of the model and basic instructions for running the module.

Baghouse Module: The integration of the baghouse module into the LEBS Workbench has been completed. 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 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 the time-averaged pressure drop across the baghouse. A simple on-line Help panel has been implemented.

ESP Model A listing of the source code for an Electro-Static Precipitator (ESP) model developed at the Southern Research Institute and subsequently enhanced at Clean Air Engineering (CAE) has been provided 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. CAE no longer has an electronic copy of the source code for this model. Hence, REI has manually reentered the program from a company report provided by CAE. The initial entry has been completed. However, at this point in time, the resulting executable program does not reproduce the predictions in the CAE report. Work is continuing to remove code entry errors.

Task 3.2 Fluidized Bed Models

We intend to incorporate both simple reactor models and a CFD based model into the workbench. This will allow users of the workbench to choose the model that they feel best represents the system they are analyzing.

At present we are reviewing three CFB reactor models. Based on our review, we will implement one of more of these models.

- A CFB model available from the International Energy Agency (IEA) [Hannes,1993], [Hannes,1995] has been obtained. At present our efforts are focused on understanding the physical sub-models contained within the IEA code and how to run the code. This is a 1.5-dimensional steady-state model (annulus-core model) for coal combustion in an atmospheric circulating fluidized bed. The model describes gas and solid flows, development of coal/char particle size distribution, coal conversion, homogeneous and catalytic gas reactions and heat transfer to the furnace wall. Reduction of sulfur dioxide using limestone/dolomite was also taken into account. The model predicts coal conversion, cyclone efficiency, temperature profile in the furnace and emissions of CO, CO_2, NO, N_2O and SO_2 from the furnace.

- A second reactor model being reviewed is a model developed at DOE NETL (Morgrantown) [Shadle, 2001]. This model has two versions: one is a steady-state model and the other a dynamic model. The steady-state model was based on mass and energy balances, assuming instantaneous devolatilization and combustion, and kinetically limited gasification reactions in a continuously stirred tank reactor. A one-dimensional lumped parameter model was used for the riser and standpipe (return leg) in the dynamic version of the model. The model predicts the solids distribution and operating regimes from operating conditions, including particle properties and gas flow rates. The model has been validated against available data in the literature. Both versions of this model are limited to cold flow simulations, and thus may not be applicable to this project.

- The third reactor CFB model is based on work previously done by REI project team members. This is a 1.5-dimensional dynamic model (annulus-core model), based on energy balance and species mass balance equations. The model simulates coal combustion in an atmospheric or elevated-pressure circulating fluidized bed combustor. The circulating fluidized bed model is based on the model developed by Yang (1988), which describes the characteristics of the riser, cyclone, return leg and the solids flow control valve. The hydrodynamics associated with the bubbling zone in the CFB is taken from the results reported by Glicksman *et al*. (1991). Char combustion chemistry and a single particle model are adopted from Shakti *et al*. (1995) and Goel *et al*. (1996). It is assumed that volatiles and moisture in the feed coal release instantaneously once coal particles enter the CFB; the combustion of the volatiles and char then takes place simultaneously in the riser only. It is also assumed that temperature in the gas and solid phases is the same; it is uniform in the radial direction, but may vary along the axial direction. The temperature of particles from the solids flow control valve is specified. Addition of dolomite/limestone to the CFB for reduction of sulfur dioxide will also be taken into consideration. The model can thus predict flow dynamics, temperature profile, coal burnout and emissions of different gas species, including green house gases, nitrogen oxide and sulfur dioxide. We have written a white paper that outlines the proposed model and it is currently being reviewed by Prof. Glicksman (MIT) who is a consultant to this project.

For a CFD based model we are currently evaluating the MFIX code developed at the NETL-Morgantown facility [Symalal,1993]. MFIX is a comprehensive CFD research code that solves for mass, momentum, energy and species for interacting granular and fluid phases. MFIX has been used to model a wide range of fluidized bed systems. The MFIX code has been obtained. At present our efforts are focused on repeating the DOE provided tests cases to learn more about the capabilities and limitations of MFIX.

Task 3.3 Gasifier Models

A literature review is being conducted to identify potentially useful sub-models and possibly available data. A report available from the IEA that reviews recently published gasification models has proved quite useful [IEA, 2000]. Discussions are on-going with organizations on the possibility of collaborating on developing the gasifier model.

Our plan is to develop a CFD based model for an entrained flow, oxygen blown gasifier. We intend to develop the model using REI's combustion CFD codes with appropriate modifications as needed. 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 and slagging. The planned gasifier model will have the flexibility to simulate a wide range of conditions and options. The engineer will have the ability to easily change process conditions (e.g., fuel properties, slurry composition), gross burner characteristics and overall column geometry.

Results and Discussion

During the last quarter, an "alpha" version of the prototype workbench for the LEBS POC has been assembled. The prototype workbench can be used for performing steady state simulations of the LEBS facility, using a CFD model for the furnace and reactor models for the steamside, SCR, air heater and baghouse. Using the workbench makes it possible to do a more extensive analysis than could be done previously. In particular, it simplifies studying the impact of changes to the boiler firing conditions on the performance of other equipment located upstream and downstream of the boiler. In the following we highlight some of the capabilities that are currently available in the workbench.

Illustrated in Figure 1 is the User Interface (UI) that an engineer using the LEBS Workbench would see on the computer screen. Note the presence of a series of "boxes" and "pipes". The "boxes" with an icon represent the different modules that contain engineering models of different equipment or processes at the LEBS POC (e.g., the Furnace CFD model). The "boxes" that do not have an icon are general purpose modules for performing functions such as specifying additional air streams to equipment or interrogating simulation results. The "pipes" provide a mechanism for the flow of data in-to and out-of the different modules, much like material flows between equipment at a power plant.

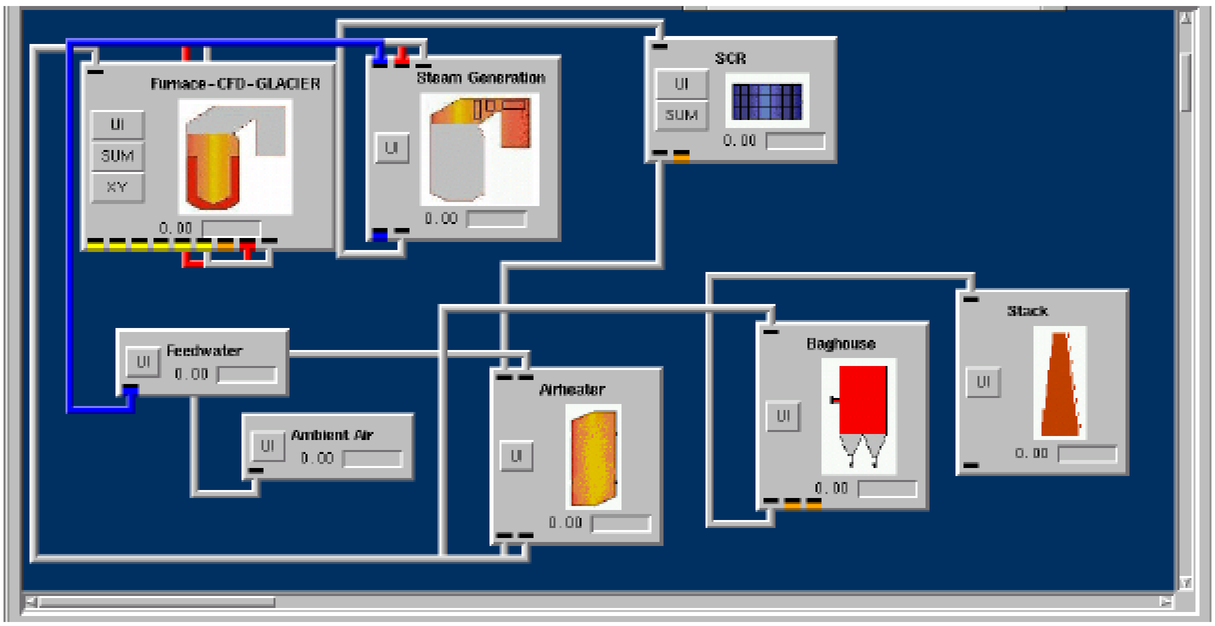


Figure 1. LEBS Workbench User Interface

The UI for the LEBS workbench provides a large degree of flexibility. The LEBS layout can be easily modified: modules can be deleted (e.g., delete the SCR unit to analyze a plant that does not have a SCR) or re-ordered within the data network. However, the workbench does not check for erroneous configurations, such as placing the baghouse unit ahead of the air heater (the flue gas entering the baghouse would be too hot in such a configuration).

The UI for the models in the workbench make it very easy to alter process conditions and view model results. The functionality of the UI is accessed by using the screen cursor and mouse to select the desired module. As an example, shown in Figures 2-7 are a series of input, output and help windows from the UI for the SCR model. Comparable capabilities are provided for all of the models included in the workbench. The conditions used are the "baseline" firing conditions.

Illustrated in Figure 2 is the module for the SCR model. Located on the SCR module is a button labeled UI and some exit data ports along the bottom of the module. Selecting the UI button on the module will cause the user input dialog box illustrated in Figure 3 to appear on the screen. Using this panel the engineer can alter the model parameters that would impact the SCR performance, such as allowable NH3 slip, as well as parameters that control the accuracy and computational effort to execute the SCR model, such as the number of cells used to define the length of the catalyst. The input panel uses a combination of simple type-in boxes that request information in terms (and units) typically used in the combustion community. Default values are provided for all model inputs. At present, the defaults are configured for the LEBS POC. For the input panels for all the models, extensive data and error checking is performed.

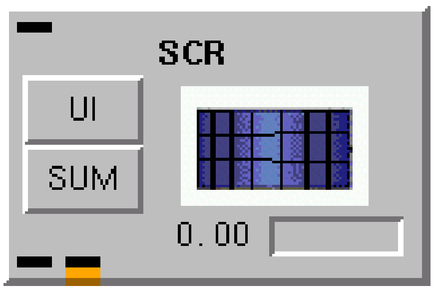


Figure 2. SCR module icon

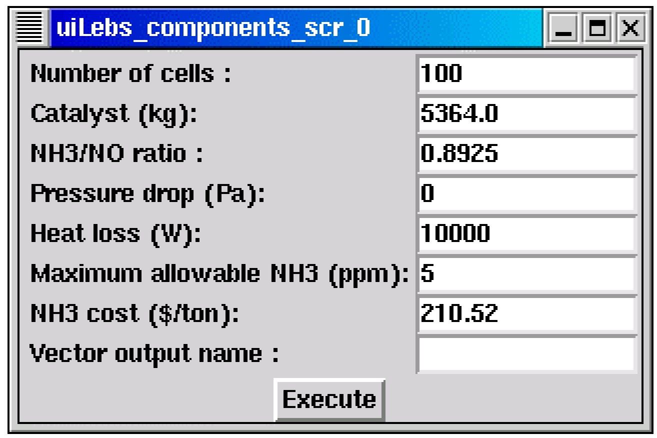


Figure 3. SCR module input dialog box.

To make the workbench more "user-friendly", each module contains an easily accessible on-line help system. Illustrated in Figure 4 is the "on-line" help panel for the SCR model. The Help content includes documentation on model input, model outputs usage and capabilities. The Help page is accessed by placing the cursor over the module, performing a right-click of the mouse, and then selecting the "help" item from the popup menu. Selecting the Help menu item activates a HTML viewer (much like a web browser window) which then displays the documentation for the module in question .

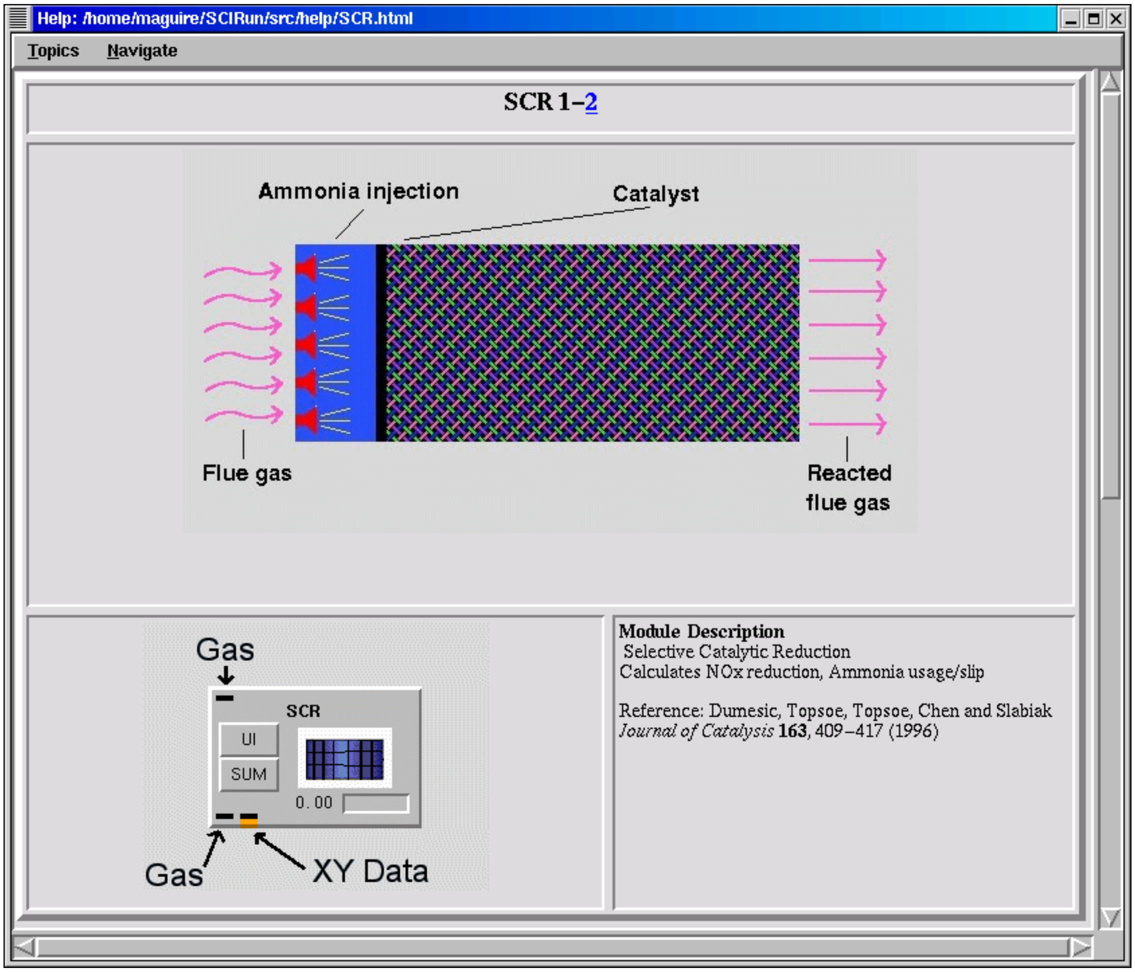


Figure 4a. SCR module on-line Help page – model description

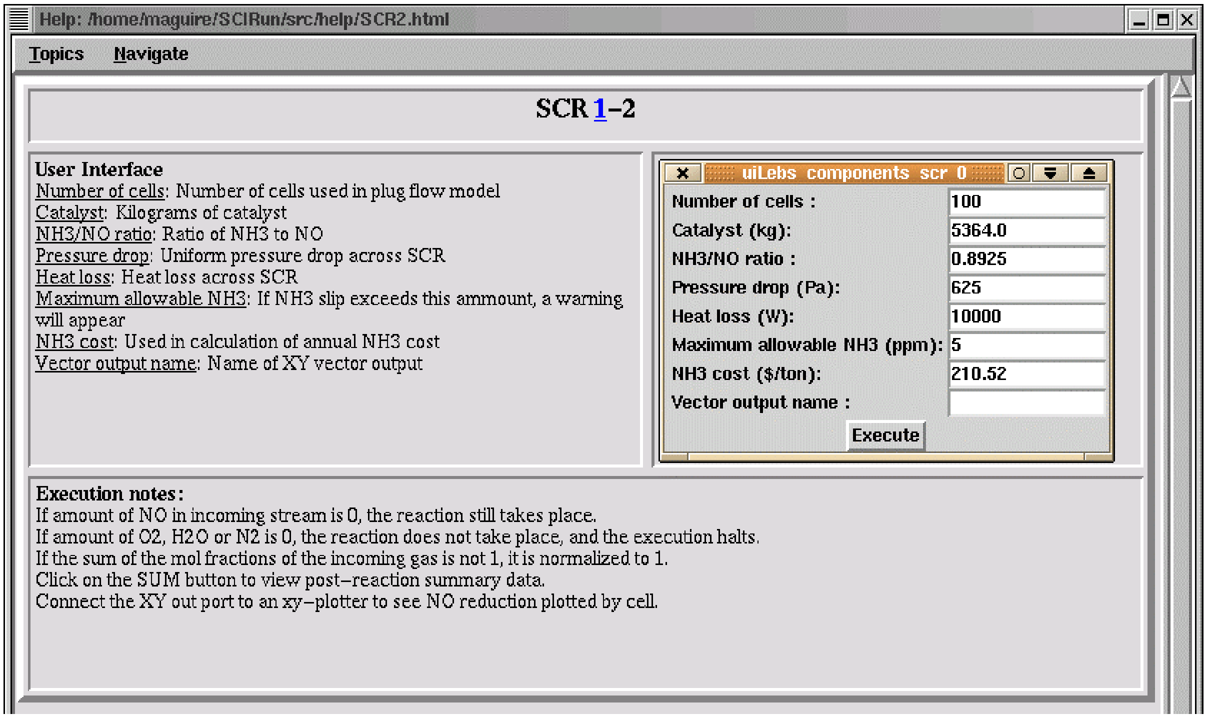
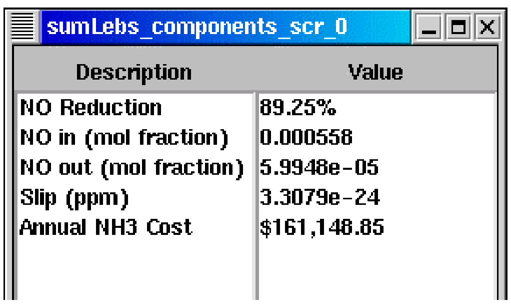


Figure 4b. SCR module on-line Help page – UI and execution notes

The tools in the workbench provide the capability to observe the performance of each piece of equipment, or process, modeled and to view results at different levels of detail. For the SCR model, both summary data (tabular) and plotted data can be viewed. Shown in Figure 5 is a dialog box containing gross performance data. This panel is accessed by selcting the SUM button located on the module icon. Listed are the predicted model results, which include the predicted NO reduction, ammonia slip and the annual cost for the ammonia consumption. More detailed information for this model can be obtained by connecting a XY-plotter module to one of the data ports along the bottom of the module (note that in the future this feature will be accessed through a XY button placed on the module icon as per the SUM button). The SCR model uses a plug flow approximation that accounts for axial variation in the gas composition along the SCR. Illustrated in Figure 6 is a plot of the predicted NO reduction along the axis of the SCR.



sumLebs_components_scr_0

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

Figure 5. SCR module – table of summary output data

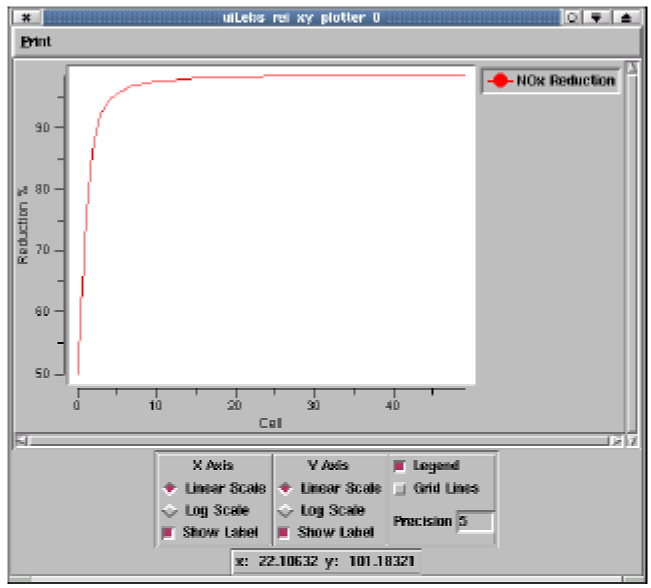


Figure 6. SCR module – plot of NO reduction as a function of axial position

The performance of the SCR unit can also be reviewed by comparing the composition and properties of the gas stream (flue gas) entering and exiting the SCR. A special module has been developed that can be applied to any location along a data "pipe" to obtain a table listing of the flue gas stream properties at that location. Illustrated in Figure 7 is an example of such an analysis.

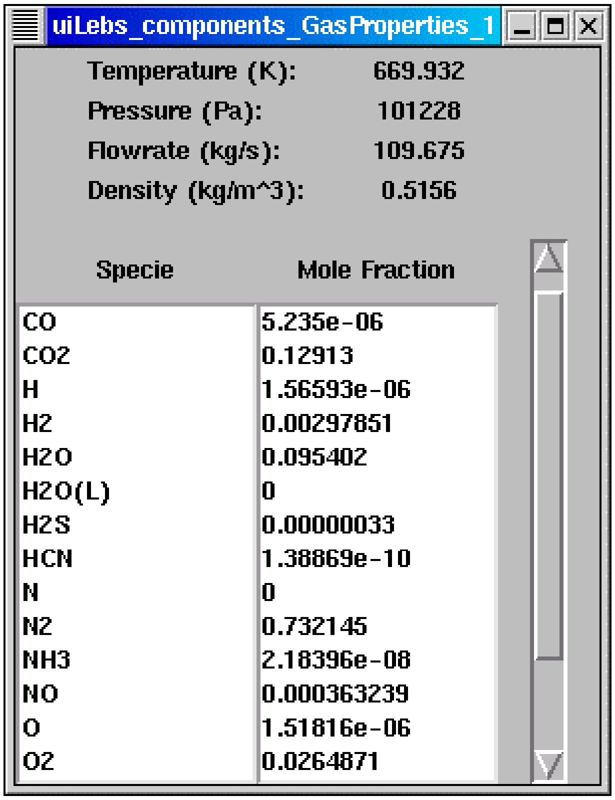


Figure 7a. Predicted gas stream properties upstream of SCR module

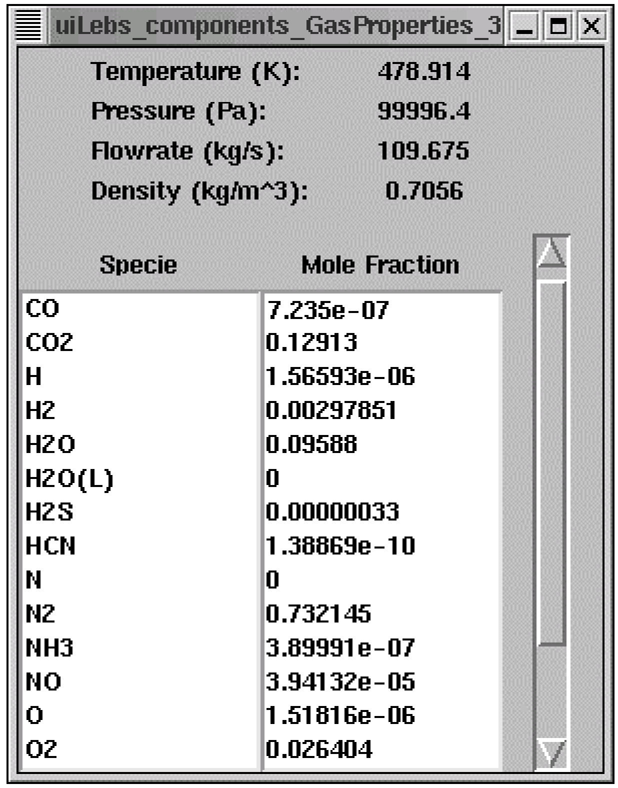


Figure 7b. Predicted gas stream properties downstream of SCR module

Using the SCR model, it would now be possible to alter the amount (weight) of catalyst in the SCR, allowable ammonia slip or ammonia cost to "optimize" the performance of the SCR for a given set of upstream conditions. Note that such a study would not require re-executing the upstream modules.

Conclusions

Good progress has been made in the last quarter. An "alpha" version of the prototype workbench has been completed and is being tested. Modules required to perform a steady state simulation are fully integrated into the workbench. However, additional modules and capabilities remain to be integrated into the workbench environment. Preliminary results from using the prototype workbench were presented to DOE in a project meeting held at NETL-Pittsburgh.

The rate of expenditures has approached the desired level. Software engineers recently hired by REI to be a part of the project team have helped accelerate the pace of development.

Plans for the next quarter will focus on two efforts. First, we will push forward to complete the development and integration of models required for the prototype workbench for the LEBS POC. Second, we will commence some of the preliminary work needed for developing a second version of the workbench that will be targeted for simulating Vision 21 energyplex systems.

References

Bockelie, M.J., Swensen, D.A., and Denison, M.K., and Sarofim, A.,"A Computational Workbench for Simulating Power Plant Systems", Presented at the ASME International Joint Power Generation Conference 2001, New Orleans, Louisiana, June 4-7, 2001.

Glicksman L.R., Yule T. and Dyrness A., 1991, *Chem. Eng. Sci.*, **46**, 1561-1571.

Goel S.K., Beer J.M. and Sarofim A.F., 1995, *Proc of 13th Intl Conf Fluidized Bed Comb.*, ASME, 887-898.

Goel S., Sarofim A., Kilpinen P. and Hupa M., 1996, *26th Symp (Int) on Combustion*, the Combustion Institute, 3317-3324.

Guenther C., T.J. O'Brien and M. Syamlal (2001), A numerical model of silane pyrolysis in a gas-solids fluidized bed", *proceedings of the International Conference on Multiphase Flow 2001*, New Orleans, Louisiana, May 27-June 1 2001.

Hannes J.P., K. Svoboda, van den Bleek and U. Renz (1993), Mathematical modeling of CFBC: An overall modular programming frame using a 1.5-dimensional riser model, *proceedings of the 12th International Conference on Fluidized Bed Combustion*, (L.N. Rubow ed.), San Diego, CA, 455-463.

Hannes J.P., C.M. van den Bleek and U. Renz (1995), The IEA-Model for circulating fluidized bed combustion, *proceedings of the 13th International Conference on Fluidized Bed Combustion*, (K.J. Heinschel ed.), Orlando, FL, 287-296.

IEA, *Modeling and simulation for coal gasification*, IEA Coal Research 2000, ISBN 92-9029-354-3, December, 2000.

Syamlal M., W. Rogers and T.J. O'Brien (1993), "MFIX documentation: Theory guide". Technical Note, DOE/METC-94/1004 (DE94000087), National Technical Information Service, Springfield, VA.

Shadle L., E.R. Monazam and M.L. Swanson (2001), Coal gasification in a transport reactor, to appear in *Industrial & Engineering Chemistry Research*.

Yang W.C., 1988, *Circulating Fluidized Bed Technology II*, Oxford, Pergamon Press, 181-191.