A Computational Workbench Environment for Virtual Power Plant Simulation

Quarterly Progress Report

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Abstract

This is the fifth 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. Within the last quarter, our efforts have become focused on developing an improved workbench for simulating a gasifier based Vision 21 energyplex. To provide for interoperability of models developed under Vision 21 and other DOE programs, discussions have been held with DOE and other organizations developing plant simulator tools to review the possibility of establishing a common software interface or protocol to use when developing component models. A component model that employs the CCA protocol has successfully been interfaced to our CCA enabled workbench. To investigate the software protocol issue, DOE has selected a gasifier based Vision 21 energyplex configuration for use in testing and evaluating the impacts of different software interface methods. A Memo of Understanding with the Cooperative Research Centre for Coal in Sustainable Development (CCSD) in Australia has been completed that will enable collaborative research efforts on gasification issues. Preliminary results have been obtained for a CFD model of a pilot scale, entrained flow gasifier. A paper was presented at the Vision 21 Program Review Meeting at NETL (Morgantown) that summarized our accomplishments for Year One and plans for Year Two and Year Three.

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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 on 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 focused on developing a *prototype workbench* for the DOE Low Emission Boiler System (LEBS) Proof of Concept (POC) design. The Year Two effort is focused on developing a more advanced workbench environment for simulating a gasifier based Vision 21 energyplex.

The main accomplishments during the last three months include:

- Presentation of a paper at the Vision 21 Program Review Meeting that summarized our accomplishments for Year One and plans for Year Two and Year Three.
- Meeting with DOE and other DOE contractors developing plant simulation tools to discuss the issue of establishing a common software interface, or protocol, for model developers to use to ensure interoperability of the different tools being developed. From this meeting, a Vision 21 energyplex configuration was selected by DOE that can be used for testing and evaluating the impacts of different model interface methods. The case configuration consists of an entrained flow gasifier, gas clean up system, SOFC fuel cells, gas turbines, heat recovery steam generator and a steam generator.
- Completion of a Memo of Understanding with the Cooperative Research Centre for Coal in Sustainable Development (CCSD) in Australia. The MOU will facilitate collaborative efforts on developing sub-models, gasification kinetics and other research topics pertinent to modeling gasification systems.
- A component model has successfully been implemented using CCA protocols and has been interfaced to our now CCA enabled workbench.
- Preliminary results have been obtained for a CFD model of a pilot scale, entrained flow gasifier.

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 November 6-7, 2001 members of the project team attended the DOE Vision 21 Program Review held in Morgantown, WV. Meeting attendees included the DOE Vision 21 Program Manager, DOE personnel involved with the Vision 21 Program, project team members from Vision 21 contractors and researchers from universities and national laboratories. REI presented a paper [Bockelie et al, 2001] that described our accomplishments in Year One and outlined our plans for Year Two and Year Three. The paper included a thorough description of the models included in the workbench, the capabilities and functionality of the workbench and the software tools and techniques used to create the workbench. The proceedings of the Program Review meeting will be made available on the DOE Vision 21 Program web page (http://www.netl.doe.gov/coalpower/vision21/**).**

On November 5, 2001, prior to the Vision 21 Program Review meeting, an informal working meeting was held at NETL-Morgantown that included DOE Vision 21 personnel and non-DOE R&D groups that are developing “plant simulator” tools under DOE funding. The purpose of the meeting was to discuss the need to establish a common software “protocol” to be used by component model and simulator developers, to allow these tools to communicate in a seamless manner. REI project team members assisted DOE in organizing this meeting. Findings of the meeting have been documented and distributed by DOE to all meeting attendees. From this meeting, the DOE Vision 21 Program Manager has selected a Vision 21 energyplex configuration (see discussion for Task 3) that can be used by the two Vision 21 projects focused on developing plant simulator tools to evaluate the impact of employing different software “protocols”. The two protocols, or software interface standards, of main interest are CAPE_Open, which is being developed by the chemical process engineering community, and CCA, which is being advocated by researchers in the scientific computing community. A follow-up meeting is tentatively planned for late Spring, 2002 to discuss progress on the evaluation process.

On October 24, 2001, Prof. Mark Bryden of the Iowa State University Virtual Reality Applications Center (ISU-VRAC), and a consultant to this project, visited with REI. During his visit he provided an overview of the virtual reality work for the power generation industry being performed at ISU-VRAC. Discussions were held on how this project could potentially leverage some of the work being performed at ISU-VRAC. Last, Prof. Bryden conducted a review of the LEBS-POC workbench that was developed by REI during Year One of this program. His findings were documented in a report to REI and are be incorporated, to the extent possible, into our development plans for the workbench effort in Year Two.

A Memo of Understanding (MOU) has been completed between REI and the Cooperative Research Centre for Coal in Sustainable Development (CCSD) located at Newcastle University in Australia (formerly the Black Coal Research Centre). The CCSD is one of the premier academic groups performing research on coal gasification. They have substantial experience and data on gasifier operation, fuel conversion and ash/slag issues. The CCSD researchers have used this data to develop sub-models for items such as high pressure reaction kinetics and slagging that would be of use to our V21 project. This collaborative effort will provide our project with early access to research and reports from CCSD. Note that both organizations will cover their own costs associated with this collaborative effort.

Task 2 – Virtual Plant Workbench II

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 commence work on Workbench II.

Component Interfaces

During the last performance period, Visual Influence (VI) delivered to REI a locally implemented version of a CCA framework and an accompanying component module based on the SCR model developed in Year One. The delivered CCA framework existed only as a standalone and thus modifications to SCIRun were performed by REI to make CCA components an integral part of the workbench. What was required was the creation of a SCIRun module able to take advantage of the provided CCA framework, and thus, any existing CCA components. The resulting module connects to the CCA SCR component (which can be on the local machine, a machine across a network or one accessed from the web) via CCA data "ports". Through these ports, the CCA component is able to take data from the workbench, run the simulation, and return the data to SCIRun where it is then reintroduced to the workbench's dataflow network. The power of CCA integrated into the workbench is easily seen, even at this early stage, in that CCA compliant models residing on geographically distributed computers can incorporated into the workbench with little regard to the complexity of the data structures being shared or to any computational resource that the model may require.

At present, a significant amount of user interaction is required to allow a workbench module to access a CCA component. In the future, we will hide these details from the workbench user by implementing a graphical based tool for connecting CCA components to the workbench.

Task 2.2 Visualization

The main focus of this task has been to implement the enhanced visualization capabilities of OpenDX within SCIRun and complete development of advanced visualization techniques.

SCIRun and OpenDX Coupling:

To access OpenDX within the workbench, the user selects the button labeled "3D" located on the module icon, this creates the connection between the SCIRun module and OpenDX via the DXLink library. Once the connection is made, the user is given access to a GUI to create and control various visualization techniques. The graphical user interface seen by the engineer is written with TCL/TK and belongs to the workbench itself – this separation of the GUI and OpenDX provides the user with a seamless user interface. The sophistication of the visualization is limited only by the experience of the user, as the full power of OpenDX – beyond the provided GUI's – is accessible to any user that desires it.

OpenDX networks, graphical user interfaces and the coupling to SCIRun for the following types of scientific visualizations have been implemented:

- Data Slices (xyz, ijk): produces a plot of a slice through a data field.
- Iso-surface: displays level surface of a scalar value within the data field.
- Streamlines: the path of a particle through the vector field.
- Particle Tracking: displays particle data from CFD model.

The user interfaces for these plotting tools are illustrated in Figures 1-5. Examples of the types of plots that can be generated are illustrated in Figures 6-8.

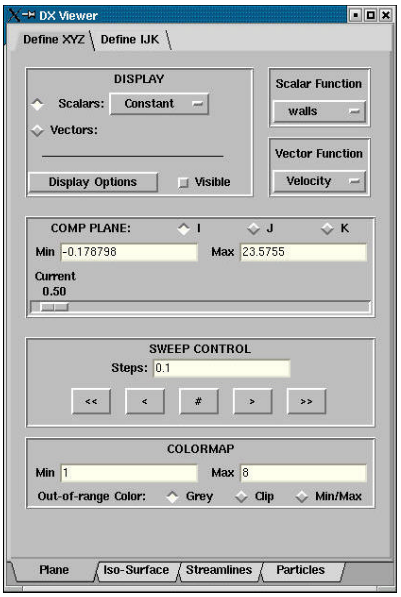


Figure 1. The xyz-slice GUI.

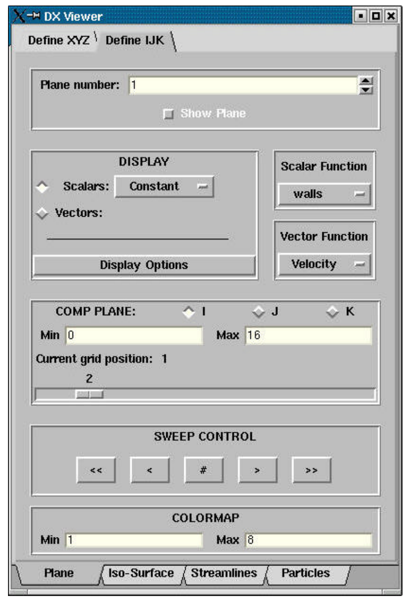


Figure 2. The ijk-slice GUI.

Figure 3. The iso-surface GUI.

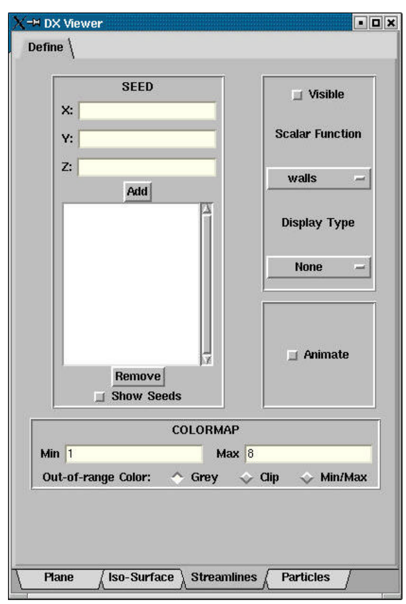


Figure 4. The streamlines GUI.

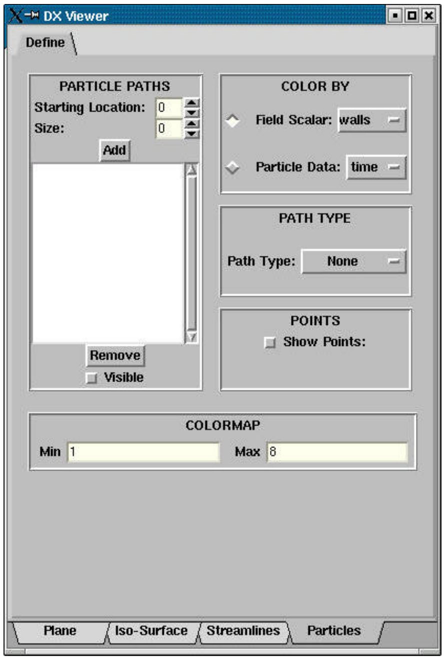


Figure 5. The particles GUI.

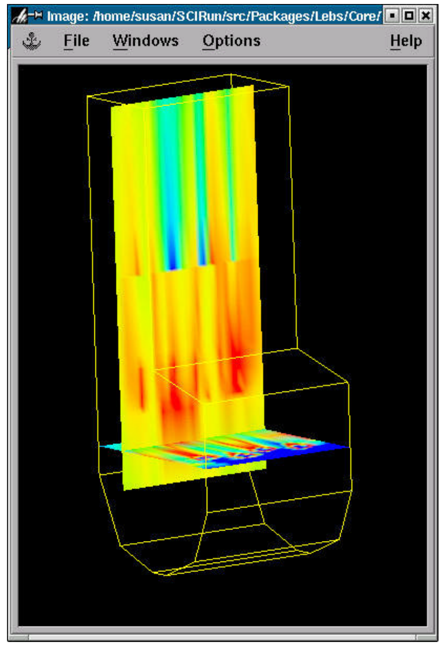


Figure 6. Example of viewing two data slices

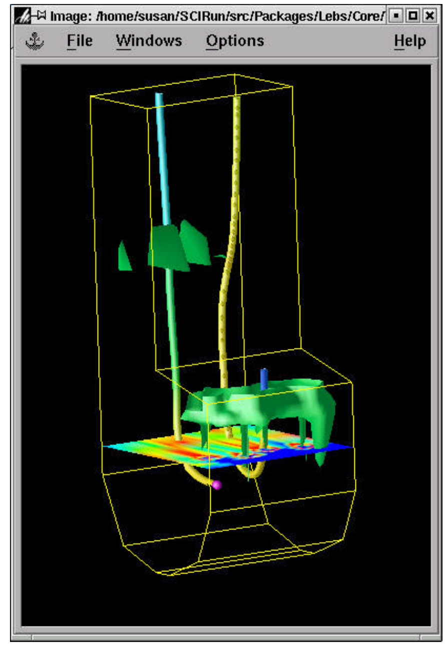


Figure 7. Data slices, Iso-surfaces and particles

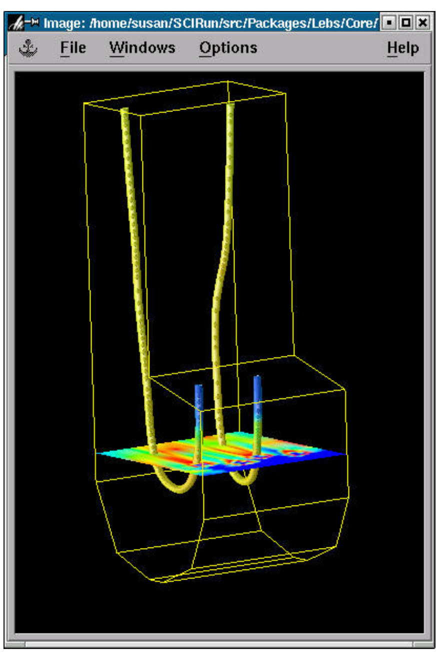


Figure 8. Example of viewing a data slice and particles

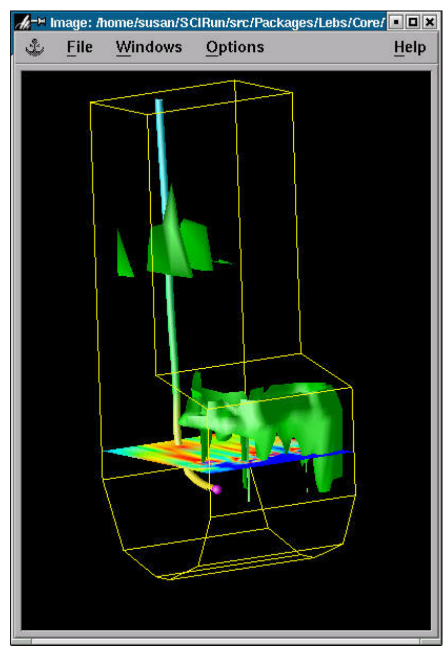
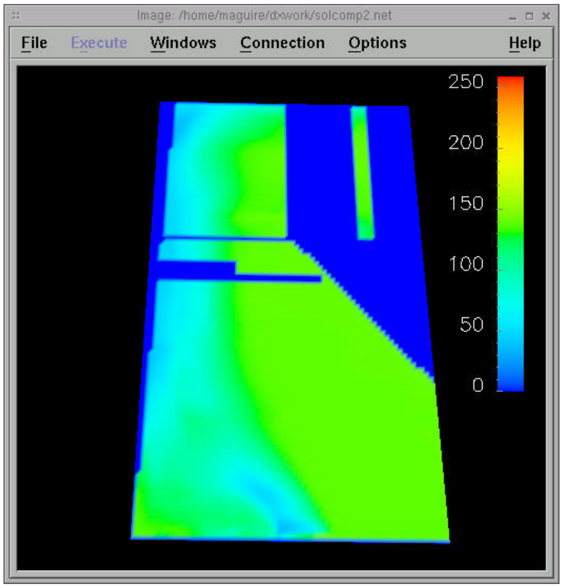


Figure 9. Example of viewing an iso-surface, data slice and streamline

Solution Comparison

Comparing two data sets using standard visualization techniques often involves generating two separate views, placing them next to each other, and using the researcher's eye to identify any differences and similarities, such as in Figure 10. While laborious, this works well for many data sets, especially ones that have clear regions of difference.



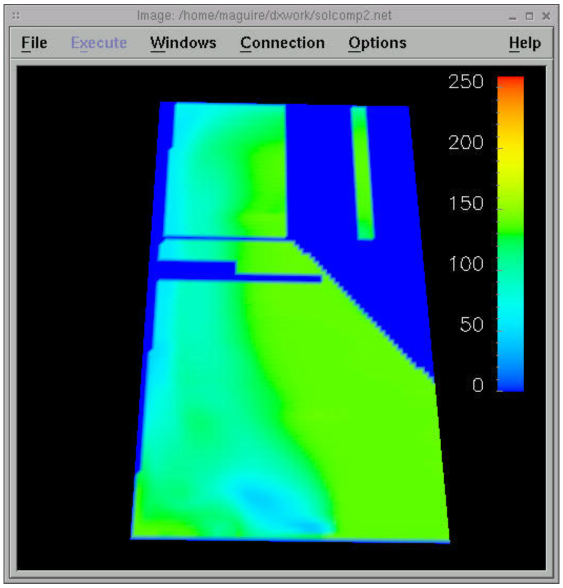


Figure 10a, b. Side by side comparison of two CFD solutions for predicted NOx due to two slightly different SNCR injector strategies.

For data that does not exhibit this behavior or that has small relative differences, this method often is impractical and important differences may escape the notice of the engineer. Alternate methods of viewing data that highlight (isolate) differences are required. Because there are so many different data sets that could be analyzed, a single tool (method), which would generate a visualization that aids the researcher in one case, may be useless in another. What is required is a set of techniques which that the researcher can combine as needed, guided by the data and their own knowledge, to produce a visualization that better illustrates the similarities and differences of the two solutions. Several such techniques have been implemented and are described below. However, it should be noted that many of these techniques require a "live" demonstration to fully appreciate the functionality:

> Difference: Subtracts one data set from another (see Figure 11). This gives immediate and concrete feedback on regions that vary, but doesn't work well for data with small relative differences, or for data that doesn't vary in clearly defined regions.

> Interpolation: The data set viewed is an interpolation from data sets A to B. A slider bar is used to "morph" between the data sets. This method has the same advantages and disadvantages as Difference, but the animation provided as the data varies across the screen greatly simplifies identifying subtle differences between the solutions.

Split Slab: A slice of both data sets, with solution A on one side of a dividing line and solution B on the other. A slider bar is used to move the dividing line through the domain. This is an excellent method for viewing before/after type situations when performing parametric CFD studies.

Multiple Techniques Concurrently: Viewing combinations of data sets and techniques (scalar, contour, etc.) can produce valuable insight. For example, in Figure 12 solution A is viewed as a scalar data field, overlaid with a contour map of the difference between solution A and solution B.

Deformed Slice (Rubbersheet): Deforming the slice with the difference between two solutions provides a striking visualization where even regions that have small relative changes fail to escape the attention of the user (see Figure 13).

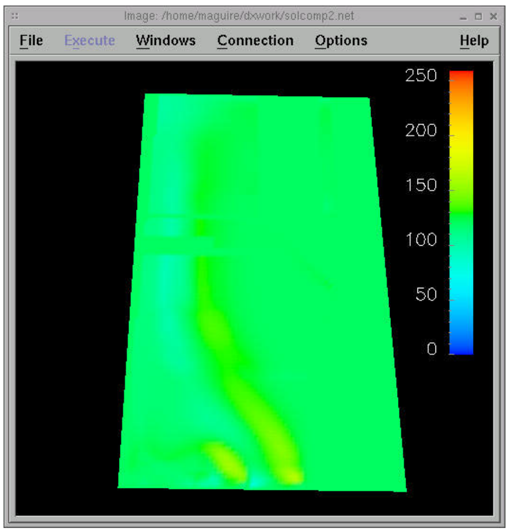


Figure 11. Example of using the solution difference capability for the two solutions shown in Figure 10.

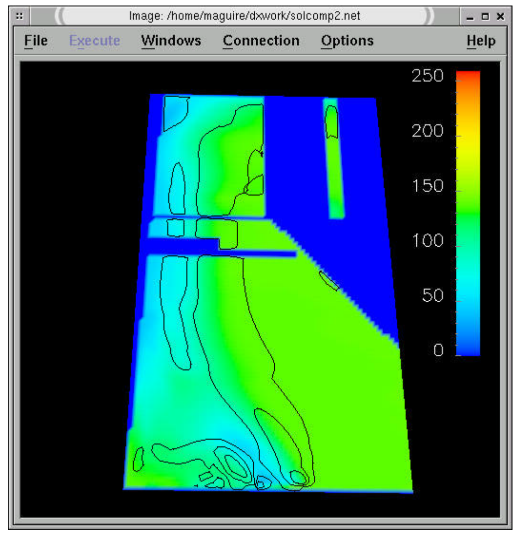


Figure 12. Example of using the contour overlay capability for the two solutions shown in Figure 10.

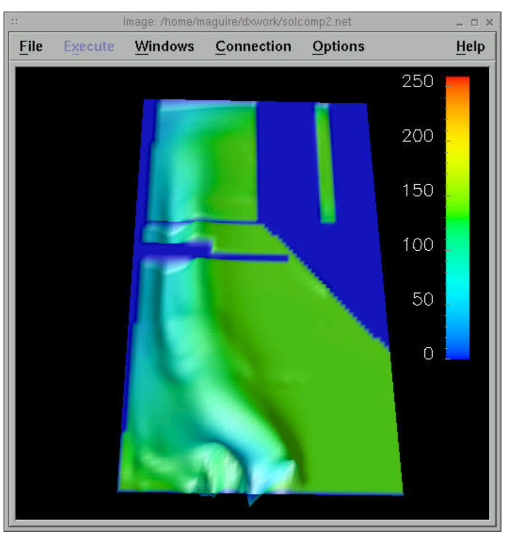


Figure 13. Example of using the rubbersheet deformation capability for the two solutions shown in Figure 10. Note that the deformation is performed using the difference between the two solutions.

Stereovision

Using stereovision on the target development platform, Linux/XFree86, is tricky at best, and nearly impossible with the new breed of cheap, ultra fast consumer video hardware such as the ATI Radeon and Nvidia GeForce chipsets. Often, support for stereovision from the manufacturers is limited to Windows 98 only, excluding even Windows NT/2000.

For this project, we have developed a simple and inexpensive "workaround" to this difficulty by using a new OpenDX Stereo module. This module seamlessly duplexes a left and right field of vision of a single view onto the top and bottom halves of a CRT monitor (or alternatively the left and right sides of the CRT), halving the aspect ratio in the affected direction, and independent of any stereo GL capability (or lack thereof) in software video drivers. At this point, solutions from a number of hardware vendors serve to convert the output into a stereo view. A simple setup involves the use of Stereographics' StereoEyes eyewear in conjunction with that company's EPC-2 sync-doubling emitter module, which watches the vertical sync signal from the video card, exactly doubles the frequency of the signal, then outputs the new sync signal back out the VGA cable to the CRT monitor as well as to the StereoEyes glasses in the form of an IR (infrared) pulse. When activated, the CRT monitor then displays the (former) top half of the screen containing the left-eye image onto the full screen, syncs back to the top of the field, and draws the (former) bottom half of the screen containing the right-eye image onto the full screen. The StereoEyes glasses then use the sync-doubled frequency to alternately shutter the left or right eye using simple LCDs, creating the stereo effect. Owing to the independence of this technique from the video card, operating system, and video drivers, this solution is therefore easily implemented across a broad range of computing platforms and takes advantage of further developments in inexpensive video hardware without further development, while still allowing the use of large, dedicated 3D stereo environments. With our approach, the cost for a workbench user to obtain the required hardware and software to perform stereovision is about $1K.

Volume Rendering

OpenDX uses the "dense emitter" model to provide volume-rendering capabilities. A density emitter value (used to simulate light coming from translucent objects) is assigned to each point in the grid. Color and opacity at each data point is interpreted as the instantaneous rates of light emission and absorption per the volume per unit thickness respectively. Several OpenDX modules receive these emission and absorption values and use them to compute, and attach "color multiplier" and "opacity multiplier" attributes to the data field. Using the simple heuristics that OpenDX provides produces volume rendered data appropriate to the volume, but not necessarily helpful to a researcher. We are currently in the process of developing tools whereby the user is intuitively able to modify the color and opacity modifiers throughout the range of the data to produce more helpful visualizations.

Transient Data Sets

OpenDX's data model contains a series member. When a series is used to represent a single field sampled across some parameter. Exploiting this feature with time as the parameter allows us to visualize transient data. OpenDX provides many modules to manipulate and visualize series data. For example, there is a streakline module that calculates the movement of particles through vector fields as they change with time.

Video Movies

As the prototype workbench began to take shape and be used, it became quite apparent that in order to share information with other partners and to instruct others on the use of the workbench, a more dynamic form of demonstration would be necessary. Our solution was to develop a procedure to produce small movie “features”, each one demonstrating a specific workbench feature or capability, that can be difficult or confusing to explain with words. With this approach, a “library” of video clips can be developed which, with little effort, can then be spliced together to create a video to demonstrate the functionality of the workbench.

We use several programs and libraries to produce a movie: Xvidcap is used to capture continuous area at regular intervals; ImageMagick is a C++ library used for file conversion; Bink and Smacker further converts files to a video clip; Cinepak Codec by Radius for compression; and finally Adobe Premier is used for editing and splicing. All of this software is available at no-charge on the internet, except for Adobe Premier which sells for about $500. Open-DX provides it’s own modules for automatic movie production.

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. In general, these models are first developed in a "stand-alone" form and then subsequently integrated into the workbench environment.

At a meeting held at NETL-Morgantown on November 5, 2001 with DOE Vision 21 personnel, it was suggested that DOE select an energyplex configuration that could be used by the different DOE funded R&D teams that are working on developing energyplex simulator tools. The DOE Vision 21 Program Manager has suggested using the energyplex configuration illustrated in Figure 14 below. This configuration consists of an entrained flow gasifier, gas clean up system, gas turbines, heat recovery steam generator, steam turbine and SOFC fuel cells. The layout shown below, taken from a DOE contractor report, contains a hot gas clean up. DOE has suggested that this be replaced with a warm gas clean up system. Work is in progress to evaluate the impact this change would have on the mass and energy balances. At present we are formulating plans to develop the models and software infrastructure within the workbench environment to create a workbench for this configuration.

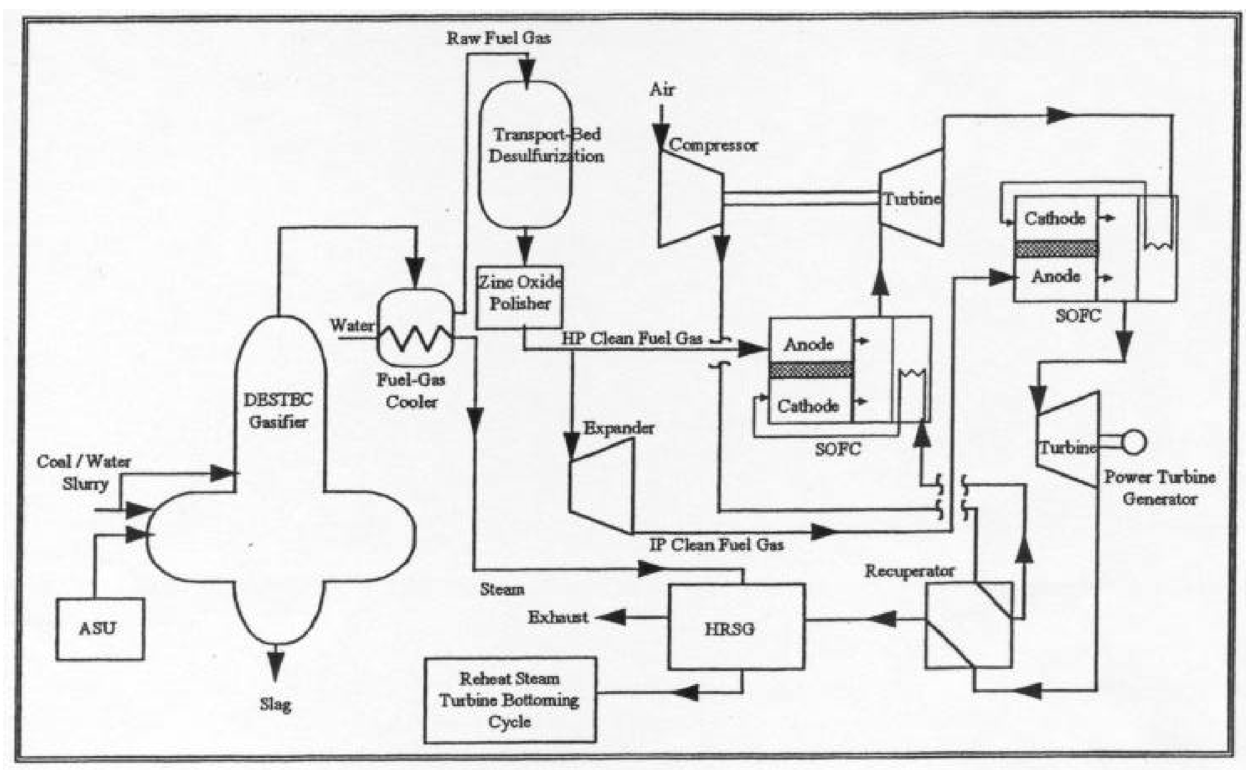


Figure 14. DOE selected Vision 21 test case configuration.

Task 3.3 Gasifier Models

We have continued development of a generic gasifier model. The effect of pressure on coal combustion and gasification is not well understood. Efforts have been made to compare available kinetic data on the pressure effect in the literature. Six sets of coal combustion kinetics have been compared under a broad range of conditions. It was found that gasification rate might change several orders of magnitude from one set of kinetics to another. In our test case presented below we use the kinetic parameters from Lupa and Kliesch (1979) since that work involved validation in a pilot scale gasifier similar to what we have modeled. We will continue to monitor advances in gasification kinetics, an effort that will be facilitated with our interactions with the Collaborative Research Centre on Sustainable Development in Australia.

We have selected a slagging model developed under the High Performance Power Generating System (HIPPS) program (United Technologies Research Center, 1995). The model predicts slag flow, slag thickness, and heat transfer through the walls of the gasifier. The thickness of the frozen ash is also predicted. The equations used to describe the ash layer are the conservation equations for momentum, energy, and mass. The model is two-dimensional. The slag thickness is calculated as a function of vertical distance down the walls. At each vertical location, the temperature profile is calculated through the layer thickness. The model is being integrated into our CFD coal combustion code being extended to gasification. The code predicts the gas side composition, temperature, heat transfer, and particle deposition rate, which will feed into the slagging model. The slagging model will be made three-dimensional by applying it for every vertical column of wall computational cells. We are planning to integrate the slagging model to be fully coupled with gasification code. The slagging model was originally developed for use in an air heater with the air-side temperature calculated from an energy balance. This boundary condition will be modified an external ambient temperature. As a first step we will integrate the model to operate as a post process. Ultimately the wall thermal resistance in the gasification model will be updated based on the calculated slag layer thickness and temperature.

Results and Discussion

We have commenced development of a generic down-fired, entrained flow gasifier. Described below are preliminary CFD model results.

Demonstration of the Gasifier Model

As a test case, CFD calculations using *GLACIER* have been performed to simulate the detailed gasification behavior in a down-fired single-staged, pressurized, entrained flow reactor into which oxygen and a slurry of coal in water are continually injected through a central nozzle located at the top of the gasifier. All the streams are heated as they travel down the reactor with coal undergoing devolatilization to form pyrolysis gases and char which then combusts and gasifies. A computational grid for a pilot-scale gasifier has been built based on the geometry given in Schneyer et al. (1982). Kinetic parameters for coal combustion and gasification have been taken from Lupa and Kliesch (1979). These coal reaction kinetics were obtained based on information in the literature for coal combustion and gasification at atmospheric pressure, and were verified through comparison with actual pilot plant data on four different coals.

Simulations have been performed for two disparate sets of operating conditions. Both tests were performed assuming the gasifier operates at 25 atm. In the first test, to obtain a particle residence time comparable to that of a full scale gasifier, we specified a relatively low gas and particle inlet velocity (i.e., 7.6 m/s). However, as noted in [Marion et al., 1972], in applications the inlet gas velocity is much higher (30 to 135 m/s was recommended for the down-fired gasifiers) and thus calculations have also been conducted using a gas velocity of 125 m/s. For the low and high inlet velocity cases the coal particle burnout and volatile yield are over 98% and 80%, respectively. Gas temperature is relatively uniform and oxygen is consumed completely in the gasifier. Figures 15, 16 and 17 show overall configuration and the distribution of CO and H_2 in the gasifier. From Figure 2 and 3 it can be seen that we predict very high and roughly uniform CO and H_2 concentrations.

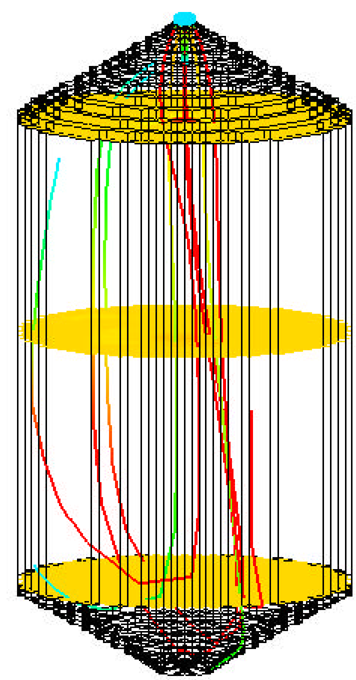


Figure 15. Pilot Scale Gasifier with coal

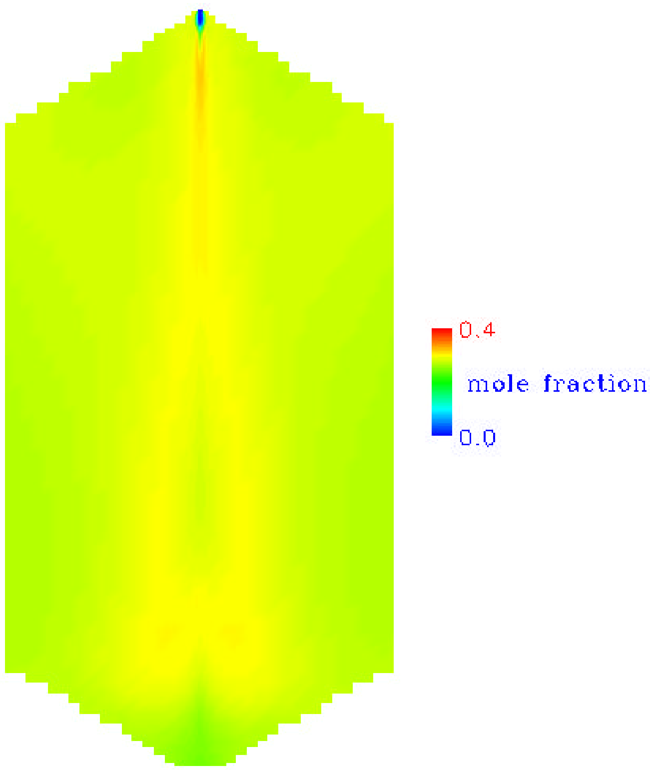


Figure 16. Hydrogen concentration in a plane across the centerline of the gasifier

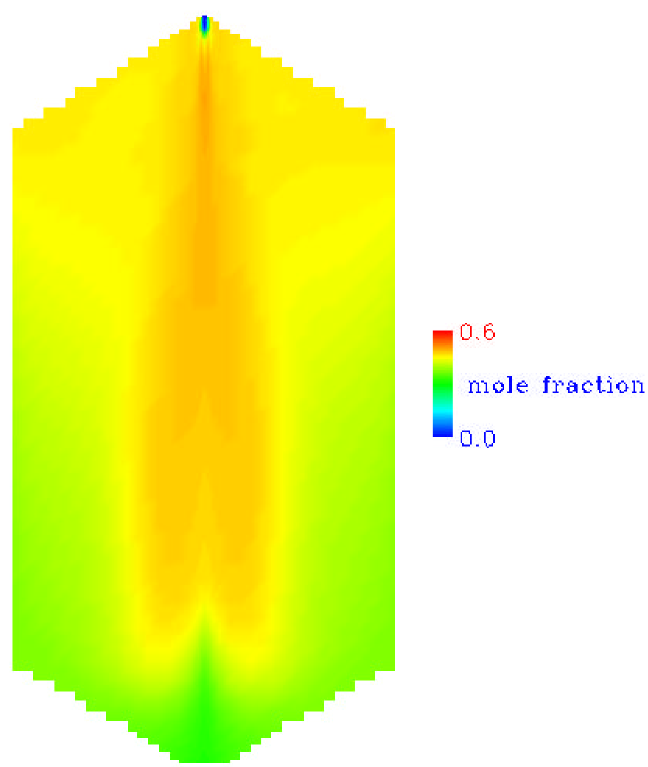


Figure 17. CO concentration in a plane across the centerline of the gasifier

Conclusions

All development efforts are being focused on creating an IGCC energyplex workbench. Preliminary results for a gasifier model have been presented. A first test of using CCA implementation for the workbench has been completed. Tests have successfully been performed using a CCA version of a SCR component module in which the CCA component was executed remotely and communicated with the workbench using a CCA protocol. An overview of the advanced visualization capabilities developed during Year One has been provided. Results from Year One of the project were presented at the DOE Vision 21 Program Review meeting held at DOE-NETL (Morgantown). An energyplex case configuration has been suggested by DOE that will be used to evaluate the IGCC workbench that will be developed in Year Two.

Plans for the next quarter will focus on: developing models required for the energyplex case configuration suggested by DOE, with continued focus on improving our gasifier model; 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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