Development of Technologies And Analytical Capabilities For Vision 21 Energy Plants

QUARTERLY PROGRESS REPORT

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DISCLAIMER

ABSTRACT

This is the eleventh Quarterly Technical Report for DOE Cooperative Agreement No: DE-FC26-00NT40954. The goal of the project is to develop and demonstrate a software framework to enable virtual simulation of Vision 21 plants.

During the last quarter much progress was made in software development. The CO wrapper for the integration of Alstom Power proprietary code INDVU was upgraded to CO V1.0.0 and was successfully integrated with an Aspen Plus flowsheet. The V21-Controller and the Fluent CO wrapper were upgraded to CO V.1.0.0, and the testing and debugging of the upgraded V21-Controller was completed. Two Aspen Plus analysis tools (sensitivity analysis and optimization) were successfully tested in an integrated simulation. Extensive testing of the integrated software was continued. A list of suggested enhancements was given to the software development team. Work on software documentation was started. Work on preparing the release version progressed: Several enhancements were made in the V21-Controller and the Fluent Configuration Wizard GUIs. Work to add persistence functionality to the V21-Controller was started.

During the last quarter good progress was made in software demonstration. Demo Case 1 simulations were completed. This case, a conventional steam cycle with a CFD model representing the boiler module, was successfully demonstrated at 9 distinct load points from 33 MW to 19 MW. Much progress was made with Demo Case 2. Work on adding a CO wrapper to the HRSGSIM code was completed, and integrated simulations with the HRSGSIM code were conducted. The CFD heat exchanger model for Demo Case 2 was calibrated with HRSGSIM results.

An Advisory Board meeting was held in Manchester, NH on May 6 during the Fluent Users Group Meeting. The preparation of the project final report was started.

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EXECUTIVE SUMMARY

The CO wrapper for the integration of Alstom Power proprietary code INDVU was upgraded to CO V1.0.0 and was successfully integrated with an Aspen Plus flowsheet (Task 2.15). The V21-Controller and the Fluent CO wrapper were upgraded to CO V.1.0.0, and the testing and debugging of the upgraded V21-Controller was completed (Task 2.17). Two Aspen Plus analysis tools (sensitivity analysis and optimization) were successfully tested in an integrated simulation (Task 2.20). Extensive testing of the integrated software was continued. A list of suggested enhancements was given to the software development team (Task 2.21). Work on software documentation was started (Task 2.22). Work on preparing the release version progressed: Several enhancements were made in the V21-Controller and the Fluent Configuration Wizard GUIs. Work to add persistence functionality to the V21-Controller was started (Task 2.24). Demo Case 1 simulations were completed. This case, a conventional steam cycle with a CFD model representing the boiler module, was successfully demonstrated at 9 distinct load points from 33 MW to 19 MW (Task 4.1). Work on adding a CO wrapper to the HRSGSIM code was completed, and integrated simulations with the HRSGSIM code were conducted. The CFD heat exchanger model was calibrated with HRSGSIM results (Task 4.2). An Advisory Board meeting was held in Manchester, NH on May 6 during the Fluent Users Group Meeting (Task 5.0). The preparation of the project final report was started (Task 7.0).

EXPERIMENTAL

Task 2.0 Software Integration

Task 2.15 Proprietary Model

The CO Wrapper for the INDVU code was upgraded to CO V1.0.0. The Aspen Plus flowsheet, with the INDVU code instantiated as a CO block, is now functioning and is providing the same answers as it did when the INDVU code was integrated as a user subroutine. This task has been completed.

Task 2.17 – COM-CORBA Bridge 2

The FLUENT CO wrapper has been successfully upgraded to support the new CORBA IDL specification – CO V1.0.0. The V21-Controller has been demonstrated to be working correctly in transferring reaction kinetics data from Aspen Plus to FLUENT.

A new Aspen Plus kit (115), which incorporates a couple of bug fixes in connection with the CalcProp and CalcEquilibrium methods of the COM ICapeThermoMaterialObject interface, was received. A critical time-out bug emerged during regression testing of the upgraded COM-CORBA Bridge with Aspen Plus kit 115. The defect is that the Vision 21 Controller CO block becomes invalid in about 270 seconds after connecting the streams to the block. This phenomenon happens before or during an integrated simulation provided the streams have been left connected for about the specified time-out period. This problem could not be replicated with kit 111, which is also based on CO V1.0.0.

The time-out problem was fixed. The problem was traced to an inadvertent call from the ACE CORBA library to the Controller DLL to request a pre-mature unloading of the Controller DLL. As a result, the code to unload the ACE CORBA library has been migrated to a safer location: destruct function in the ICapeUnit class implementation. (It is still, however, unclear as to why this problem does not occur whilst running on a Windows NT operating system, and why this call was being made prematurely when a request to shut down the application has not been made by the user.)

A number of other bugs reported in Controller v0.9.5 were fixed:

- The crash that occurs when placing two CO blocks on the flow sheet and trying to activate the second block has been fixed.
- Additional iterations can now be requested after convergence of a flow sheet, with the CFD solver responding in an expected manner.
- A new CO block can now also be placed on the flow sheet after convergence of an initial CO block without the occurrence of any crashes or error messages.

With these fixes, the work required to upgrade the Controller to CO V1.0.0 is now complete.

<u>Task 2.20 Aspen Plus analysis tools</u>

A sensitivity analysis was run for the CSTR example over FLUENT shaft speeds ranging from 85 to 400 rpm and the results were plotted directly in Aspen Plus.

An Aspen Plus optimization was run for the CSTR example. The objective was to determine the optimum shaft speed for maximizing the product yield. Aspen Plus found the optimal yield of 19567.487 lb/hr at 189.804 rpm, which is consistent with the results of the sensitivity analysis. This completes Task 2.20.

<u>Task 2.21 Test Integrated Software</u>

The software is undergoing extensive testing. Five new V21 Controller kits, as they became available from the Vision 21 development team, have been tested. Feedback on the testing results was provided to the software development team.

<u>Task 2.22 – Documentation</u>

A demonstration of the software was given to Kelly Griggs, Fluent documentation team manger. A preliminary draft of the user manual was also given to Kelly. Thus the documentation effort has been kicked off.

<u>Task 2.23 – Software Support</u>

Software support is being provided to ALSTOM Power. MOO collaborated with DGS to ensure that the CORBA wrapper template for the demo cases is being correctly implemented, and that the simulations are running smoothly.

<u>Task 2.24 Prepare release version</u>

Several enhancements were made in the V21-Controller and the Fluent Configuration Wizard GUIs:

- Select the solvers to be launched for a given block in the Edit Model GUI rather than in the Model Selection GUI.
- Bug fixes and enhancements in the Domains and Parameters Pages of the Configuration Wizard GUI.
- In the Edit Model GUI re-implemented the Solution Strategy and fixed some bugs in the Advanced Parameters page.

- Support for the persistence of Solution Strategy, Basic Parameters and Advanced Parameters data in the Controller GUI.

Work to add persistence functionality to the V21-Controller was started. This will allow the user to restore a simulation session without having to reconnect streams anew or reconstruct a Solution Strategy from scratch. This functionality will also include the option to update the Fluent case and data with the current run data.

When only non-CFD models (e.g., INDVU) are available to represent a particular block in the flowsheet, a tool for generating XML files is needed. (When CFD models are available, the FLUENT Configuration Wizard generates the necessary master and solver XML files.) Work on developing a XML File Generator was started.

Fixed a minor bug in PreComputedResults class and changed get methods in PreComputedReader class to const. The PreComputedReader class was modified to support results generated from runs of a Vision 21 CAPE-OPEN block in different flowsheets with different number and type of species.

Task 4.0 Run Integrated Simulations

<u>Task 4.1 Simulations of Demo Case 1</u>

Jeff Ma at Fluent has completed the rp-var/tui/scheme files required to get the CFD case to work in tandem with Aspen Plus for Demo Case 1, and has provided a report. Prepared the CO parameters and manipulated variables (as a function of load) to be used in solving the INDVU and CFD versions of Demo Case 1. Outlined and planned all of the flowsheet modifications required for accommodating the new parameters.

Ideally, the boiler module for Demo Case 1, instantiated as a CFD block, should be coupled to the Aspen Plus flowsheet with both an inner and outer loop. In the inner loop, for a given and appropriate fuel feed rate, the bypass and excess air controls are adjusted until the superheat outlet temperature reaches the desired value. In the outer loop, the fuel feed rate is modified until the desired overall or total absorption is attained. It is anticipated that the inclusion of both loops would substantially increase the number of FLUENT executions required to complete the cycle simulation. Since the simulations of Demonstration Case 1 are being performed on a modest 500 MHz PC, it was decided to reduce the CPU time requirements of the run by eliminating the outer loop. This was done by decoupling the air preheater and hard-wiring the fuel flow rate and inlet air temperatures to the boiler as a function of the load. With only the inner loop in operation, Demo Case 1 was successfully demonstrated at 9 distinct load points from 33 MW to 19 MW.

Further refining of the results of the simulation may be pursued if time and resources permit. Full running of more rigorous, CPU-intensive runs (e.g., with realistically sized meshes and the inclusion of nested loops around the CFD block) should await development of the remote running capability, so that the CFD executions can be performed on platforms (e.g., clusters) that better match the CPU requirements of the CFD cases.

<u>Task 4.2 Simulations of Demo Case 2</u>

Oleg Kukar has completed the CO wrapper for the HRSGSIM code. Simulations with the HRSGSIM code included as a CO block were conducted.

The gridding of the HRSG for Case 2 was completed, and a CFD case was developed. The HX model in the stand-alone FLUENT CFD case of the HRSG unit was calibrated to the HRSGSIM results. Temperature-dependent properties were turned off in the CFD run because the Aspen Plus properties transferred to FLUENT invalidated the HX calibration, which appears to be due to an error in Aspen Plus's C_p for O_2. The absorptions from the HX scheme file are still incorrect; the CFD block can be fully coupled to the Aspen cycle only after correcting this error.

Task 5.0 Advisory Board Activities

Prepared a demonstration of an Aspen Plus fuel cell system flowsheet integrated with two FLUENT 3D CFD models—solid-oxide fuel cell (SOFC) and a steam reformer. Reduced-order models (ROMs) based on a linear regression of pre-computed FLUENT CFD results were generated for both the SOFC and reformer.

Prepared a demonstration of an integrated simulation with two interconnected laptops, with the FLUENT CSTR model running on one laptop and the Aspen Plus simulation running on another laptop.

An Advisory Board meeting was held in Manchester, NH on May 6 during the Fluent Users Group Meeting. The above-mentioned integrated Aspen Plus-FLUENT simulations were demonstarted at the meting. A report containing meeting minutes was sent to the advisory board members and posted on the project website.

Task 7.0 Project Management

A software development wrap-up meeting was held on May 7 in Lebanon, NH, and was attended by MOO, MXS, KKT, and SEZ.

<u>Final report:</u> KJC, MXS and SEZ discussed and developed an outline of the final report. The outline was sent out to the team members and the DOE project manager for review.

For the Vision 21 final report, SEZ wrote an initial draft of a major section on Integrated Model Development and Use, along with a smaller sub-section on the use of the CAPE-OPEN Standard. SEZ provided these write-ups to the Fluent documentation group for use in preparation of V21-Controller documentation.

Created an updated version of the document on a design of the Vision 21 database (CFD database) and its current implementation. Generated Doxygen-style Reference Guide for all Vision 21 database classes. Wrote first draft of a section of the Final report for DOE on the CFD Database. Solution Strategy (Doxygen style) documentation finished. Reference with detailed overall description and examples was created.

Issues and Resolution:
Because of the delay in completing Task 2.17, as explained in the last quarterly report, the completion of tasks 2.21, 2.22, 2.24, 4.2, and 4.3 has been delayed until 8-30-03.

Progress forecast for the next quarter:

- Task 2.21 Test Integrated software
  - Conduct simulations with the integrated software as needed

- Task 2.22 Documentation

- Complete the work on documentation

- Task 2.24 Prepare release version
  - Complete the implementation of the persistence functionality that is being added to the new COM-CORBA bridge
  - Test the implementation of the Fluent CO wrapper for Linux OS, using the new CAPE-OPENv1-0-0 CORBA IDL specifications
  - Complete the XML File Generator
  - Design a new installation kit and test the new software functionality for remote deployment and execution on both Linux and Windows operating systems
  - Send the software and documentation to DOE

- Task 4.2 Demonstration Case 2 simulation
  - Integrate the FLUENT CFD case of the HRSG into the Aspen Plus flowsheet and solve over a range of loads

- Task 4.3 Report on Demonstration Case simulations
  - Complete the demonstration case report

- Task 5.0 Advisory Board Activities
  - Plan and conduct the final Advisory Board meeting

- Task 7.0 Project management
  - Complete the final report

Project Milestones:

Task	**Milestone/Deliverables**	**Completion Date**		
		Original	**Revised**	**Actual**
1.0	Project Management Plan	1-30-01		1-23-01
2.2	User Requirements Document (URD)	3-15-01		3-28-01
2.3	Software Requirements Specifications (SRS)	4-15-01		5-13-01
2.6	Software Design Documentation	5-15-01	7-15-01	8-10-01
2.7	Software Development Plan	6-30-01	1-21-02	1-21-02
2.7	Working Test Case 1	6-30-01	10-30-01	10-30-01
2.8	Demonstrate CFD database	9-30-02		9-30-02
2.10	Prototype with reaction kinetics data transfer	12-31-01		12-31-01
2.11	COM-CORBA bridge - 1	6-30-02		6-30-02
2.12	Transfer physical properties	12-30-02		9-30-02
2.13	GUI	6-30-02	7-31-02	8-31-02
2.14	CFD Viewer	9-30-02	12-30-02	12-30-02
2.15	Proprietary model template	12-30-02	5-15-03	6-15-03
2.16	Session Management	12-30-02	3-30-03	3-30-03
2.17	COM-CORBA bridge - 2	9-30-02	5-15-03	6-15-03
2.18	Configuration Wizard	6-30-02	9-15-02	9-15-02
2.19	Low Order model	9-30-02		9-30-02
2.20	Aspen Plus analysis tools	12-30-02	5-30-03	6-30-03
2.21	Test integrated software	12-30-02	8-30-03	

		Completion Date		
2.22	Documentation	3-30-03	8-30-03	
2.24	Prepare release version	6-30-03	8-30-03	
3.1	Demonstration Case 1 selection	1-31-01	5-15-01	4-30-01
3.2	Demonstration Case 2 selection	9-30-01	7-15-02	8-31-02
4.1	Demonstration Case 1 simulation completed	6-30-02	5-30-03	6-30-03
4.2	Demonstration Case 2 simulation completed	5-30-03	8-30-03	
4.3	Report on Demonstration Case simulations	7-30-03	8-30-03	
5.1	Advisory Board Meeting	3-31-01		6-6-01
5.2	Advisory Board Meeting	9-30-01	11-7-01	11-7-01
5.3	Advisory Board Meeting	3-31-02	6-12-02	6-10-02
5.4	Advisory Board Meeting	9-30-02	12-30-02	12-18-02
5.5	Advisory Board Meeting	3-31-03	5-6-03	5-6-03
5.6	Advisory Board Meeting	7-30-03		
7.0	Quarterly reports to DOE	Every quarter		1/30/01, 4/20/01, 7/20/01, 10/20/01, 1/29/02, 4/30/02, 7/30/02, 11/01/02, 1/30/03, 4/30/03, 7/30/03
7.0	Draft Final Technical Report	10-30-03		
7.0	Final Technical Report	12-30-03		

RESULTS AND DISCUSSION

During the last quarter we have continued development of the framework for integrating equipment (CFD and proprietary) and plant models. This being a software development and demonstration project there are no experimental or simulation results to report and discuss.

CONCLUSION

Much progress was made during the last quarter to develop a framework for integrating equipment and plant models. We expect to deliver the software to DOE in the upcoming quarter.

REFERENCES

1. Syamlal, M. and W.A. Fiveland, “Roadmap for the Development of a Vision 21 Simulator,” presented at The 29th International Technical Conference on Coal Utilization & Fuel Systems, Clearwater, Florida, March 10-14, 2003.

2. Syamlal, M. J.I. Madsen, W.A. Rogers, and S.E. Zitney, “Application of an Integrated Process Simulation and CFD Environment to Model Fuel Cell Systems,” Presented at the AIChE Spring National Meeting, March 30 - April 3, New Orleans, LA (2003).

LIST OF ACRONYMS AND ABBREVIATIONS

Personnel Name	Affiliation	Initials
Woodrow Fiveland	ALSTOM Power	WAF
John L. Marion	ALSTOM Power	JLM
David G. Sloan	ALSTOM Power	DGS
Herb Britt	AspenTech	HB
Randy Field	AspenTech	RF
Steve Zitney	AspenTech	SEZ
Joe Cleetus	CERC	KJC
Igor Lapshin	CERC	IBL
Lewis Collins	Fluent	RLC
Paul Felix	Fluent	PEF
Ahmad Haidari	Fluent	AH
Barb Hutchings	Fluent	BJH
Maxwell Osawe	Fluent	MOO
Krishna Thotapalli	Fluent	KKT
Madhava Syamlal	Fluent	MXS
Frank Joop	Intergraph	FJ
Philip Simon	Intergraph	PPS

Name	Description
ActiveX	A Microsoft technology built on top of COM that extends the basic capabilities of OLE to allow components to be embedded in Web sites.
AHGO	Air Heater Gas Outlet (e.g., referring to the flue gas exit temperature from the air preheater)
AHAO	Air Heater Air Outlet (e.g., referring to the air gas exit temperature from the air preheater; after the air preheater, the heated air goes into the boiler)
API	Application Programming Interface.
C++	C++ programming language.
CERC	Concurrent Engineering Research Center, WVU.
CFD	Computational Fluid Dynamics.
CAPE-OPEN	Computer Aided Process Engineering – Open Simulation Environment Interface definitions for exchanging information with process simulation software (www.colan.org).
CASE	Computer Aided Software Engineering.
CO	CAPE-OPEN
CO wrapper	The code for implementing CO interfaces in a software.
COM	Component Object Model – Refers to both a specification and implementation developed by Microsoft Corporation that provides a framework for integrating software components.
CORBA	The Common Object Request Broker Architecture is a specification of a standard architecture for object request brokers (ORBs). A standard architecture allows vendors to develop ORB products that support application portability and interoperability across different programming languages, hardware platforms, operating systems, and ORB implementations (www.omg.org).

COM-CORBA Bridge	Software for translating COM objects to CORBA objects and vice versa. This component of the Vision 21 Controller will permit Aspen Plus running under Windows to exchange data with Fluent running under UNIX.
CORTEX	FLUENT's user interface engine.
COSE	CAPE-OPEN Simulation Executive (e.g., Aspen Plus).
CSTR	Continuous Stirred Tank Reactor.
DCOM	Distributed Component Object Model – An extension of COM that allows software components to be distributed over a network.
DLL	Dynamic link library. A collection of small programs, any of which can be called when needed by a larger program that is running in the computer.
DO	Discrete Ordinates (radiation model).
Doxygen	A documentation system for C++, Java, IDL (Corba/COM) and C.
DOE	U.S. Department of Energy.
EO	Equation oriented solution strategy for solving flowsheet models.
GCO	Global CAPE-OPEN, an extension of the CAPE-OPEN project. (www.global-cape-open.org)
GOF	Gang of Four – the four authors of a book, which originally categorized and described several software design patterns.
GUI	Graphical User Interface.
HEX	Fluent heat exchanger module.
HRSG	Heat recovery steam generator.
HRSGSYM	ALSTOM Power in-house code for simulating HRSG.
HX	Heat Exchanger
IDL	Interface definition language, which is used for defining the communications between software components linked through a middleware.
INDVU	ALSTOM Power in-house code for the analysis and design of the gas side of a powerplant.
Java	Java programming language.
LTSH	Low temperature super heater.
Middleware	Connectivity software that consists of a set of enabling services that allows multiple processes running on one or more machines to interact across a network.
NETL	National Energy Technology Laboratory.
OLE	Object Linking and Embedding. Builds on COM to provide services such as object "linking" and "embedding" that are used in the creation of compound documents (documents generated from multiple tool sources).
PFD	Process Flow Diagram.
Python	Python programming language.
QT	Software used for developing the *V21 Controller* GUI.
RP&L	Richmond Power and Light power plant.
RUP	The Rational Unified Process® – a web-enabled set of software engineering processes that provides guidance to streamline development activities.
Scheme	Programming language used in CORTEX (FLUENT)
SDD	Software Design Document.
SM	Sequential modular solution strategy for solving flowsheet models.
SRD	Software Requirements Document.
SDP	Software development plan
SGI	Silicon Graphics Inc.

Swing	A Java GUI tool kit.
UDF	User defined function. A program written in C for enhancing the functionality of FLUENT.
UGM	Users Group Meeting.
UML	Unified Modeling Language.
URD	User Requirements Document.
Use Case	The specification of a sequence of actions, including variants, that a system can perform, interacting with actors (users) of the system.
VB	Visual Basic programming language.
Visual Basic	Visual Basic programming language.
V21 Controller	The software being developed in this project for linking CFD and other proprietary equipment-level models with process simulation models.
WVU	West Virginia University.
XML	Extensible Markup Language: A metalanguage -- a language for describing other languages -- which lets one create their own markup language for exchanging information in their domain (music, chemistry, electronics, hill-walking, finance, surfing, CFD, process simulation).