Development of Technologies And Analytical Capabilities For Vision 21 Energy Plants

QUARTERLY PROGRESS REPORT

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ABSTRACT

This is the twelfth 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 the software development was completed and the testing of the integrated software was completed. A user manual was written to complete software documentation. An installation CD-ROM including the following items was written: software installer, controller source code, proprietary CORBA wrapper templates for building local and remote servers, publicly available source code of the ACE/TAO CORBA library that needs to be built before compiling the controller source code, pre-built binaries of the publicly available XERCES XML library, and a PDF version of the software user's manual. The software was delivered to DOE.

During the last quarter software demonstration tasks were completed. A few additional load points of Demo Case 1 were solved. Integrated simulations of Demo Case 2 with the proprietary HRSGSIM code and FLUENT CFD model were completed. The final task report describing Demo Case1 and Demo Case 2 simulation results was written and delivered to DOE.

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EXECUTIVE SUMMARY

Testing of the integrated software was completed (Task 2.21). A user manual was written to complete software documentation (Task 2.22). An installation CD-ROM including the following items was written: software installer, controller source code, proprietary CORBA wrapper templates for building local and remote servers, publicly available source code of the ACE/TAO CORBA library that needs to be built before compiling the controller source code, pre-built binaries of the publicly available XERCES XML library, and a PDF version of the software user's manual. The software was delivered to DOE (Task 2.24). A few additional load points of Demo Case 1 were solved (Task 4.1). Integrated simulations of Demo Case 2 with the proprietary HRSGSIM code and FLUENT CFD model were completed (Task 4.2). The final task report describing Demo Case1 and Demo Case 2 simulation results was written and delivered to DOE (Task 4.3). The work on writing the project final report was continued (Task 7.0).

EXPERIMENTAL

Task 2.0 Software Integration

Task 2.21 Test Integrated Software

- Tested Controller v0.9.6 (based on CAPE-OPEN v1.0) with Aspen Plus 12.1 kit 115 and FLUENT 6.1.18 and provided feedback to the software development team.
- Tested the use of CAPE-OPEN CFD parameters in Aspen Plus analysis tools (i.e., optimization, case studies, sensitivity analysis). Used Aspen Plus to optimize overall process yield by manipulating impeller speed of FLUENT CSTR.
- Tested procedure for using the FLUENT Configuration Wizard (parameter rpvar option) to make FLUENT calculated variables (e.g., fuel cell voltage) available as parameters for use in Aspen Plus analysis tools.
- Carried out extensive integration testing using selected problems to assess the performance, reliability and robustness of the Controller.
- Tested several new versions of the Controller (v0.9.6b, v0.9.6c, and v0.9.7) with Aspen Plus 12.1 Release Candidate 8 and FLUENT 6.1.18.
- Tested the general Configuration Wizard and provided feedback to the software development team.

Task 2.22 – Documentation

A user manual was written. A PDF version of the manual is included in the installation CD-ROM.

Task 2.23 – Software Support

MOO collaborated with DGS to track down a perennial Aspen Plus CO error message that get thrown at some random load points during integrated simulations. MOO recommended an OS upgrade from Window NT to Windows 2000. The latter is the officially supported Windows platform and the recommendation appears to have cured the reported problems.

Task 2.24 Prepare release version

Implemented the functionality to update parameter values in the Edit Model GUI at run-time so that the user can be sure of what parameters were actually employed by the process simulator in the most recent COSE iteration. This feature is particularly useful in checking the value of

parameter(s) in the Edit Model GUI during coupled sensitivity analysis with an external unit operation model such as Fluent.

Completed the development of the Controller XML writer, which provides a parallel functionality to the Fluent configuration wizard for writing out both the Master and Solver XML files required by the Controller Edit Model GUI. This functionality would be particularly useful for presenting proprietary model parameters and other pertinent model information to the Controller subsystem.

Completed the implementation of the Controller persistence functionality. The new feature would be tested with Aspen Plus 12.1 Release Candidate 7, which will hopefully contain bug fixes required for restoration of the persisted flow sheet file without crashes. With this new feature, a flow sheet file containing a CAPE-OPEN can now be saved and be fully restored in a new session, along with the automatic activation of the associated external solver process or processes without user intervention.

A few bugs that surfaced in the first release candidate build of the software were tracked down. One of the identified bugs, which has now been fixed, was such that a new page of the Edit Model tab dialog gets displayed on attempting to dismiss the GUI. As a result, the Controller is unable to activate the selected external unit operation process.

Prepared a release build of the proprietary Regression model.

Prepared the installation CD-ROM, which includes the following:

- Software installer
- Controller source code
- Proprietary CORBA wrapper templates for building local and remote servers
- Publicly available source code of the ACE/TAO CORBA library which needs to be built before compiling the Controller source code
- Pre-built binaries of the publicly available XERCES XML library
- A PDF version of the software user's manual.

Detailed instructions for using the supplied CORBA templates are contained in the user's manual. A copy of the Qt GUI library must be obtained from Trolltech (www.trolltech.com) to build the Controller source code.

The release version of the software was delivered to the DOE.

Task 4.0 Run Integrated Simulations

Task 4.1 Simulations of Case 1. After installing the new Windows 2000 operating system and the (almost complete) eradication of the ECape errors, it was possible solve Case 1 at the load points 19, 17, and 15 MW.

Task 4.2 Simulations of Case 2. (1) The proprietary HRSGSIM code was successfully run in conjunction with Aspen Plus. (2) The scheme file was set up to allow for transfer of information between Fluent and the steam cycle for Demo Case 2. The Fluent case was modified so that its species list corresponded to the species list in the Aspen Plus flow sheet. Attempts were made to run the case. (3) The presence of an unresolved error (ECapeError), which seriously interferes with the computations, is presumed to be due to the Windows NT operating system (OS) on the PC. The NT OS was replaced with Windows 2000, and all of the pertinent software was re-installed on the hard drive. The new OS permitted Case 2 to run without persistent ECape errors.

(4) A 3-minute time-out error was encountered, which precludes the reading in of larger steam tables. Only the 100x100 tables can be read in within the prescribed limit. (5) The CFD block has been manually sequenced (as many as 16 times in a series) in order to try to propagate the information throughout the cycle and get the superheat outlet temperature from the CFD case to stabilize. Ideally, more loops would be necessary in the sequence in order for the superheat outlet temperature to truly level out, but the 16 loops was sufficient for the code to successfully find a solution at the 6 discrete load points from 100% to 50% load. (Randy Field, Aspen Tech, proposed an alternate methodology that gives greater control to Aspen Plus.)

Task 4.3 Task Report of Case 1 and 2 Results. The final task report of the Case 1 and Case 2 simulation results has been completed. The report was delivered to DOE.

Task 5.0 Advisory Board Activities

No activity this quarter.

Task 7.0 Project Management

Final report:
Updated the section on Integrated Model Development and Use in the Vision 21 final report.

Issues and Resolution:

Task 5.0 Advisory Board: A final Advisory Board meeting is outstanding. In lieu of the regular advisory board meeting, the members of the board have been invited to attend a Web Seminar scheduled for October 30th, which will give the Advisory Board members a demonstration of the software. The Advisory Board members have been requested to e-mail their feedback to the project team. During the project extension period we may consider conducting another advisory board meeting.

Progress forecast for the next quarter:

- Task 7.0 Project management
  - Complete the final report
  - Plan the project extension

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

		Completion Date		
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	9-15-03
2.22	Documentation	3-30-03	8-30-03	9-25-03
2.24	Prepare release version	6-30-03	8-30-03	9-25-03
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	9-30-03
4.3	Report on Demonstration Case simulations	7-30-03	8-30-03	10-15-03
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		10-30-03
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 10/30/03
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 completed the 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

During the last quarter we completed the development of a framework for integrating equipment and plant models. The software and documentation were delivered to DOE.

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).