Development of Technologies And Analytical Capabilities For Vision 21 Energy Plants

QUARTERLY PROGRESS REPORT

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DISCLAIMER

ABSTRACT

This is the tenth 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 template was developed for the integration of Alstom Power proprietary code INDVU. The session management tasks were completed. The multithreading capability was made functional so that user of the integrated simulation may directly interact with the CFD software. The V21-Controller and the Fluent CO wrapper were upgraded to CO v.1.0. The testing and debugging of the upgraded software is ongoing. Testing of the integrated software was continued. A list of suggested GUI enhancements was made. Remote simulation capability was successfully tested using two networked Windows machines. Work on preparing the release version progressed: CFD database was enhanced, a convergence detection capability was implemented, a Configuration Wizard for low-order models was developed, and the Configuration Wizard for Fluent was enhanced.

During the last quarter good progress was made in software demonstration. Various simplified versions of Demo Case 1 were used to debug Configuration Wizard and V21-Controller. The heat exchanger model in FLUENT was calibrated and the energy balance was verified. The INDVU code was integrated into the V21-Controller, and the integrated model is being debugged. A sensitivity loop was inserted into Demo Case 2 to check whether the simulation converges over the desired load range. Work on converting HRSGSIM code to run in batch mode was started. Work on calibrating Demo Case 2 was started.

Project personnel attended and gave presentations at The 29th International Technical Conference on Coal Utilization & Fuel Systems, Clearwater, Florida, March 10-14, 2003 and the AIChE Spring National Meeting, March 30 - April 3, 2003, New Orleans, LA.

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EXECUTIVE SUMMARY

The CO wrapper template was developed for the integration of Alstom Power proprietary code INDVU (Task 2.15). The session management tasks were completed. The multithreading capability was made functional so that user of the integrated simulation may directly interact with the CFD software (Task 2.16). The V21-Controller and the Fluent CO wrapper were upgraded to CO v.1.0. The testing and debugging of the upgraded software is ongoing (Task 2.17). Testing of the integrated software was continued. A list of suggested GUI enhancements was made. Remote simulation capability was successfully tested using two networked Windows machines (Task 2.21). Work on preparing the release version progressed: CFD database was enhanced, a convergence detection capability was implemented, a Configuration Wizard for low-order models was developed, and the Configuration Wizard for Fluent was enhanced (Task 2.24). Various simplified versions of Demo Case 1 were used to debug Configuration Wizard and V21-Controller. The heat exchanger model in FLUENT was calibrated and the energy balance was verified. The INDVU code was integrated into the V21-Controller, and the integrated model is being debugged (Task 4.1). A sensitivity loop was inserted into Demo Case 2 to check whether the simulation converges over the desired load range. Work on converting HRSGSIM code to run in batch mode was started. Work on calibrating Demo Case 2 was started (Task 4.2). Project personnel attended and gave presentations at The 29th International Technical Conference on Coal Utilization & Fuel Systems, Clearwater, Florida, March 10-14, 2003 and the AIChE Spring National Meeting, March 30 - April 3, 2003, New Orleans, LA (Task 7.0).

EXPERIMENTAL

Task 2.0 Software Integration

Task 2.15 Proprietary Model

A CO CORBA wrapper template for proprietary codes has been developed and was made available to Alstom Power for wrapping up the INDVU code so that the code can be integrated with the V21-Controller. (The wrapper needs to be upgraded as the V21-Controller is upgraded to CO version 1.0 in Task 2.17). The development has been completed, but the testing and debugging cannot be completed until Task 2.17 is completed.

Task 2.16 Session Management

The development of SolutionStrategy classes was finished. All required classes were debugged, integrated into V21Controller, and tested. Two modifications of SolutionStrategy classes were introduced: (a) Check simulation conditions before executing a solver (b) Allow a choice of multiple solvers. A new method skipStep() was added to the SolutionStrategy class to support switching to the next solver when the low-order solver cannot provide a solution. Modified the Calculate() method to switch to the next solver if low-order solver returns an exception because of insufficient data for interpolation.

The multithreading capability was made functional. With this capability the user will be able to directly interact with a FLUENT process that is running within a process simulation.

Task 2.17 – COM-CORBA Bridge 2

The CAPE-OPEN v1.0 interface specifications were reviewed for upgrading the V21-Controller, the Fluent CO wrapper, the low-order model wrapper and the proprietary model wrapper template. The V21-Controller and the FLUENT CO wrapper were upgraded. The testing and debugging of the upgraded version is on going.

Task 2.21 Test Integrated Software

Using the reaction-separation-recycle and fuel cell system test cases, the integration tools are undergoing testing. To improve the usability of the GUIs, a list changes required in the Configuration Wizard, Model Selection and Model Edit GUIs has been developed.

Remote simulation has been successfully tested using two networked Windows machines using CORBA Implementation Repository Service, and will be replicated and tested for a Linux server as soon as the Linux shared library is fully implemented using the new CORBA interface specifications.

Task 2.24 Prepare release version

Some progress was made with the code reviews. The effort on this task was reduced because of other higher priority tasks.

Several enhancements were made in the CFD database. Support for separate databases for each CapeUnit was developed. Designed API for PreComputedRange class, which provides info on ranges of stored data in pre-computed database. The 'Server' class was updated with addServer() method.

A convergence detection capability, which can determine if a given FLUENT run converged or not, was added to V21-Controller subsystem. This new functionality ensures that only converged CFD results are written to the database for developing a low-order model.

A Configuration Wizard for low-order models was developed. This will allow users to configure low order models so that they may be linked V21-Controller. New database classes were developed to support a write-function in the low-order model Configuration Wizard.

The low-order model was converted into a lightweight DLL executable to improve performance and to preclude the need for an occasional manual deletion of a separate process.

A printing capability was added to the CFD viewer, to enable the printing of CFD graphics. The functionality to transfer CFD graphics over the LAN was developed. Thus the graphics from a CFD run executed on a remote server can be displayed in the integrated process simulation environment.

Several modifications were made in the Fluent Configuration Wizard: Segregated the generation of the Master and the Solver XML files as required in a modified database structure, added the functionality to specify the Service Information so as to facilitate remote execution of a solver.

Support for multiple solver XML files and for the selection of a remote server were added to Model Selection GUI.

Task 4.0 Run Integrated Simulations

Task 4.1 Simulations of Demo Case 1

Using various simplified constructions of Case 1, along with an Aspen Plus gas-only cycle, work continued to focus on assisting the debugging of the Configuration Wizard and V21-Controller in order to be able to instantiate and run the CFD block. The V21-Controller converts the mass flow rate from Aspen Plus into an axial velocity in FLUENT. A UDF was utilized to calculate a tangential velocity for each nozzle (based on a local cylindrical cross section). This allows Case 1, which has 24 inlet ports to be instantiated and connected to the flowsheet streams. One gas phase iteration must occur before the UDF sees the changes in mass flow rate from the CO stream.

Galen Richards tested the new version of the Heat Exchanger model in FLUENT, with heat balance information and a corrected DO radiation model source term. He recalibrated a few of the Case 1 load runs and found the energy balancing to be satisfactory.

Eric Johnson completed the work on the CO wrapper for the INDVU code and Maxwell Osawe integrated it into V21-Controller. However, during testing with Aspen Plus, it became apparent that the same input translation error that precludes the running of the CFD cases is also preventing the running of the legacy codes. Fluent is working to resolve this issue.

Fluent is working on the scheme files required to get the CFD case to work in tandem with Aspen Plus for Demo Case 1.

Task 4.2 Simulations of Demo Case 2

A sensitivity loop was inserted into the Case 2 cycle and work has ensued to ensure that the simulation converges over the desired load range (with Sequential Modular only), and that the results are reasonably similar to the HRSGSIM results.

Oleg Kukar is converting the HRSGSIM code to work in batch I/O mode, so that it can be utilized in the same fashion as the INDVU code. Subsequently, he will work on the CO wrapper for the HRSGSIM code.

An effort was made to calibrate the Aspen Plus cycle for Demo Case 2 with the HRSGSIM results over the load range. The results match at max load, but they diverge from each other at lower loads, possibly indicating fundamental differences in the component models.

Task 5.0 Advisory Board Activities

There was no activity on this task during this reporting period.

Task 7.0 Project Management

Presentations

MXS and WAF coauthored the paper “Roadmap for the Development of a Vision 21 Simulator,” and presented it at the The 29th International Technical Conference on Coal Utilization & Fuel Systems, Clearwater, Florida, March 10-14, 2003.

WAF and SEZ attended The 29th International Technical Conference on Coal Utilization & Fuel Systems, Clearwater, Florida, March 10-14, 2003.

WAF and MXS gave a presentation to the DOE Morgantown/Pittsburgh on the Vision 21 (Phase I) and the benefits of continued work in this area.

MXS presented the following paper at the AIChE meeting: 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).

Issues and Resolution:

Task 2.17 COM-CORBA Bridge - 2
There has been much delay in making progress with this task because Aspen Plus 12.1 with CO v.1.0 (Beta3) kit was received only in the third week of March. So the full integration testing could not be carried out earlier. The testing has shown a DLL registration issue with the new Beta 3 kit. Fluent is consulting with Aspen Plus developers to resolve this issue.

The completion of Task 2.15 (Proprietary model), Task 2.20 (Aspen Plus analysis tools), Task 2.22 (Documentation), Task 2.21 (Test integrated software), and Task 4.1 (Simulations of Demonstration Case 1) has been delayed pending completion of Task 2.17.

Progress forecast for the next quarter:

- Task 2.15 Proprietary model
  - Test and debug the proprietary model hook up

- Task 2.17 COM-CORBA bridge 2
  - Upgrade the CORBA wrapper template to conform to CO v1.0 specifications
  - Test and debug the CO v1.0 implementation in V21-Controller

- Task 2.20 Aspen Plus Analysis tools
  - Demonstrate the use of Aspen Plus analysis tools in an integrated simulation.

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

- Task 2.22
  - Start work on documentation

- Task 2.24 Prepare release version
  - Complete the upgrade implementation of the low-order model (regression variant), using the new CO CORBA IDL specification –v1-0-0 (Task 2.19)
  - Complete the implementation of the Fluent CAPE-OPEN wrapper for Linux OS, using the new CAPE-OPENv1-0-0 CORBA IDL specifications
  - Continue to do code reviews and to make code enhancements

- Task 4.1 Demonstration Case 1 simulation
  - Conduct an integrated simulation for Demo Case 1 with the INDVU code hooked up
  - Conduct an integrated simulation for Demo Case 1 with CFD case hooked up

- Task 4.2 Demonstration Case 2 simulation

    - Include a CO wrapper in HRSGSIM code
    - Conduct an integrated simulation for Demo Case 2 with the HRSGSIM code hooked up
    - Conduct an integrated simulation for Demo Case 2 with CFD case hooked up

- Task 5.0 Advisory Board Activities
    - Plan and conduct an Advisory Board meeting in May

- Task 7.0 Project management
    - Start writing 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	
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	
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	
2.21	Test integrated software	12-30-02	5-30-03	
2.22	Documentation	3-30-03	6-30-03	
2.24	Prepare release version	6-30-03	7-30-03	
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	
4.2	Demonstration Case 2 simulation completed	5-30-03		
4.3	Report on Demonstration Case simulations	7-30-03		
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

		Completion Date		
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	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
7.0	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. There has been a delay in completing the task of upgrading the COM-CORBA Bridge to CO Version 1.0. This has caused delays in completing Demonstration Case 1. Fluent and AspenTech developers are working to resolve the issues in upgrading the software to CO Version 1.0. We expect to complete this task in the next 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
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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.
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).