DEVELOPMENT OF TECHNOLOGIES AND ANALYTICAL CAPABILITIES FOR VISION 21 ENERGY PLANTS

COOPERATIVE AGREEMENT NO DE-FC26-00NT40954

QUARTERLY REPORT FOR OCTOBER-DECEMBER 2002

FOR

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DISCLAIMER

1. Executive Summary

A software design review meeting was conducted (Task 2.0). A CFD Viewer was developed, to allow the process analyst to view CFD results from the process simulator (Task 2.14). Work on developing a CO wrapper for the INDVU code was continued (Task 2.15). The model-edit GUI was modified to allow the user to specify a *solution strategy*. Enhancements were made to the solution strategy implementation (Task 2.16). Testing of the integrated software was continued and several bug fixes and enhancements were made: ability to expose CFD parameters to the process analyst and support for velocity and pressure inlet boundary conditions (Task 2.21). Work on preparing the release version progressed: Version 0.3 of V21 Controller was released, a global configuration dialog was implemented, and a code review process was initiated (Task 2.24). The calibration of the tube bank CFD model for the RP&L case was completed. While integrating the tube bank CFD model into the flow sheet model, several development requirements were identified and communicated to the developers. The requirements of porting V21 Controller and Configuration Wizard to FLUENT 6.1, turning off the transfer of temperature dependent properties, exposing CFD parameters in Aspen Plus and supporting velocity boundary conditions have been implemented (Task 4.1). An initial grid for the HRSG component has been prepared (Task 4.2). A web-based advisory board meeting was conducted on December 18, 2003 (Task 5.0). Project personnel attended and gave presentations at the Aspen World Conference, October 28-30, 2002; AIChE Annual Meeting, November 8, 2002; and the Vision 21 Simulation meeting at Iowa State University, November 19-20, 2002 (Task 7.0).

2. Technical Accomplishments

Task 2.0 Software Integration

A software design review meeting was held Oct 9th and 10th in Lebanon, NH. The following topics were discussed at the meeting:

- Review current status of the development
- Finalize the demos for Aspen World (October 27, 2002) and the Advisory Board meeting
- Develop plans for code review
- Review the plans for completing software development

Task 2.14 CFD Viewer

The functionality for the automatic generation of graphic files depicting the distributions of computed velocity, temperature and species from a Fluent CFD model was implemented. The generated files can subsequently be viewed in the COSE environment using the CFD viewer.

An edit box “model view file” was added to the configuration wizard, which allows the CFD analyst to specify the file name that will persist a FLUENT model-view, which is a snapshot of the cross-section of the computational domain. The user-specified view is restored at run-time during an integrated simulation, and is employed by FLUENT for the generation of the required graphics files for subsequent display in the CFD Viewer. Graphics plots are only generated for user-specified views.

A selection dialog that allows the user to select a variable to be displayed by the CFD viewer was implemented. Event-handlers for displaying selected quantities in the CFD viewer were implemented.

Task 2.15 Proprietary Model

Eric Johnson (ALSTOM) met with Maxwell Osawe on Oct. 11th and received a tutorial on the CO wrapper (C++ template) for legacy codes. Eric Johnson has since been preparing the CO wrapper that will serve as the interface between Aspen Plus and the INDVU code.

Task 2.16 Session Management

The model-edit GUI was enhanced to include the Solution Strategy functionality. This GUI allows the process analyst to associate a combination of solvers to represent a CO block on a process flow sheet and have them activated in a specified sequence. The Session Management class stores a map of the user-specified solution steps or strategy for each CO block. Each block strategy encapsulates the criteria for switching from one solver to another.

The design for Solution Strategy classes and API was completed. API and class diagrams for Solution Strategy were modified to reflect discussions at the October 2002 Design Review meeting. The inner design of classes was changed by adding new private attributes and functions. All global solution strategy logic and conditional switching was developed and debugged (classes SolutionStrategy, SequenceEngine, SolutionStep, StrategyCondition, StrategyAction). The Solution Strategy class and its associated GUI were integrated with the V21-Controller subsystem, and the new functionality was tested.

A MassBalanceCondition class was developed and partly debugged, without integration to the Controller, however. The class declarations were modified to support changes in strategy's core classes and correct execution logic.

Task 2.21 Test Integrated Software

Various simplified runs of Demonstration Case 1 (with 4 mass inlet boundary conditions, no swirl, etc.) were constructed, along with an Aspen Plus gas-only cycle, to assist Maxwell Osawe in debugging the Configuration Wizard and V21 Controller, in order to accommodate the Demonstration Case 1 species list and reaction scheme.

The Configuration Wizard was enhanced to accommodate the requirements identified by ALSTOM Power while conducting Demonstration Case 1 (Richmond Power & Light) simulation. The new enhancements allow the CFD expert to specify CFD parameters that may be modified during an integrated simulation. With these enhancements a parameter can be modified by invoking the "rpsetvar" commands in FLUENT, or through a set of Scheme functions (written by the CFD expert), or by specifying Text User Interface (TUI) commands. The implemented Scheme functions are stored in a file and automatically loaded when a FLUENT process is launched.

Two enhancements to the Fluent Cape-Open wrapper, as required by ALSTOM Power, were implemented:

- The automatic conversion of inlet mass flow rates into velocity boundary conditions.
- The capability for sending pressure inlet data type to FLUENT

Task 2.24 Prepare release version

Version 0.3 of the V21 Controller was released. The new kit automatically registers the Controller DLL, places the program files in the appropriate directories and appends to the system wide PATH variable.

An option was added in the GUI, to indicate whether the V21 Controller should write the pre-computed Fluent results to a file or not.

A Global Configuration Dialog was implemented, to allow the analyst to add or remove a Model Database at run-time. The Global Configuration dialog is launched from the Model Selection GUI.

The database API was updated to reflect requirements elicited at the October 2002 Design Review meeting. A pre-computed results database API was developed. The Model Database was ported to use Xerces 2.1 parser. The new parser library conforms to current XML standards and provides bug fixes and additional functionality, which are useful in the V21 Controller (writing XML files, additional functions).

A code review process was initiated. A methodology for code review was discussed and adopted at Design Review meeting in October 2002. The criteria for a quick review and a checklist were developed. Approximately half the modules in the CFD database code (6 modules) have been circulated for review and preliminary feedback was obtained. So far much of the code review dealt with the coding style only. Reviews of the logic, maintainability, and bug-proneness of the code may be taken up in the future.

Task 4.0 Run Integrated Simulations

Task 4.1 Simulations of Demo Case 1

Several development requirements were identified and communicated to the developers:

- V21 Controller and Configuration Wizard must be ported to FLUENT V6.1
- The capability to turn off the transfer of temperature dependent properties from Aspen Plus
- A more robust way to associate the species in Aspen Plus with the species list in FLUENT
- Two-way data exchange capabilities between Aspen Plus and FLUENT using scheme, rpvar, or tui commands/files in the configuration wizard
- Multithreading, to allow the analyst to gain control over a FLUENT simulation launched by Aspen Plus
- The capability to accommodate velocity boundary conditions

The calibration of the tube bank parameters for the RP&L case was completed. At low loads the temperature may oscillate from 5-10 K, however. This could be resolved through the usage of a better grid or a better solution strategy. It could also be a real physical feature (no steady-state solution). The resolution of this issue is beyond the scope of the current project. We anticipate only running cases for a high and medium load range.

Task 4.2 Simulations of Demo Case 2

Galen Richards has gathered the requisite information to build the points file (in preparation for using Gambit) prior to constructing the Case 2 HRSG grid. Galen Richards prepared an initial grid for the HRSG component.

Task 5.0 Advisory Board Activities

An advisory board meeting was held on December 18th. The PlaceWare service was used for a web-based presentation. Minutes of the meeting have been prepared and were distributed. The Vision 21 web-page was updated with this information.

Intergraph designed and built a data model and loaded the data from Aspen Plus output into SmartPlant Foundation to demonstrate a system for managing simulation datasets generated over a period of time. Intergraph made a presentation of the prototype system at the Vision 21 Simulation meeting, Iowa State University, November 18/19, 2002, Ames, Iowa.

Task 7.0 Project Management

Aspen Tech has designated Dr. Richard Brogan (Aspen Tech, UK) as their new project representative and Dr. Sergi Sama (Aspen Tech, Spain) as the technical point of contact. The project team may continue to contact Michael Halloran (Aspen Tech, UK) regarding CAPE-OPEN issues. The previous AspenTech representative, Dr. Steve Zitney, has accepted a position with Fluent and will start work on February 3, 2003. So the Aspen Tech personnel change would not adversely affect the project.

Presentations

MXS and AH attended the Aspen World Conference, October 28-30, Washington, DC and demonstrated the integrated simulation capability at a Fluent booth.

MOO attended the AIChE Annual Meeting, Indianapolis, IN, November 8, 2002 and gave a presentation entitled, "An Integrated Process Simulation and CFD Environment Using the CAPE-OPEN Interface Specifications,"

WAF, MXS, FJ and PPS from the project team attended the Vision 21 Simulation Meeting held at Iowa State University, November 19-20, 2002. MXS gave a presentation on the project status and future plans. The project team members participated in “road-mapping” discussions. Paul Chapman (ALSTOM Power) provided a demonstration of CFD visualization using the commercial virtual reality software, Virtual Vantage.

3. Issues and Resolution:

Task 2.15 Proprietary model:

A model template has been developed and given to ALSTOM Power. ALSTOM Power has nearly completed the wrapping of INDVU code. The code remains to be debugged, which has delayed the completion of this task.

Task 2.16 Session Management:

Coding is nearly complete. The completion of this task has been postponed pending the completion of debugging.

Task 2.17 COM-CORBA bridge - 2:

The issue of upgrading the V21 Controller to CO version 1.0 is yet to be resolved. Aspen Plus 12.1 has a version of the CO 1.0 implemented, which still needs some revisions. We can upgrade V21 Controller to Version 1.0 only after Aspen Tech finalizes the CO version 1.0 implementation. A teleconference was held with Michael Halloran (Aspen Tech, UK) and Daniel Pinol (Aspen Tech, Spain) to discuss this issue. Michael agreed to give us a CO 1.0 IDL by end of January 2003.

Also this upgrade needs to be completed before a bug (the inability of Aspen Plus to recognize a CO parameter in calculator blocks, design specs, and optimization) can be fixed. The bug seems to exist only in integrated simulations. Two FLUENT licenses were given to Michael Halloran in preparation for debugging.

The completion of Task 2.20 (Aspen Plus analysis tools), Task 2.21 (Test integrated software), and Task 4.1 (Simulations of Demonstration Case 1) has been delayed pending completion of this task.

4. Progress forecast for the next quarter

- Task 2.15 Proprietary model
  - Complete the CO wrapper for the INDVU code and then implement that coding into the Aspen Plus code in place of the user-defined function capability.

- Task 2.16 Session Management
  - Complete the debugging of solution strategy
  - Complete debugging of multithreading

- Task 2.17 COM-CORBA bridge 2
  - Commence the upgrade work on COM-CORBA bridge 2 using Cape-Open version 1.0

- 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 2.24 Prepare release version
  - Conduct code reviews

- Task 4.1 Demonstration case 1 simulation
  - Work with Fluent Inc. as required to correct bugs and to provide additional enhancements to FLUENT V6.1 and the V21 Controller. Once that work is completed/debugged, ALSTOM can begin to integrate the Fluent case with Aspen Plus using the Cape Open methodology.

- Task 4.2 Demonstration case 2 simulation
  - Finalize the gridding of the HRSG for Case 2 and prepare the CFD case.
  - Initiate work on integrating the HRSGSIM code with Aspen Plus.

- Task 5.0 Advisory Board Activities
  - Continue to solicit feedback from the Advisory Board members.

- Task 7.0 Project management
  - Make a presentation at the AIChE 2003 Spring Meeting, March 30 - April 3, New Orleans, LA (2003).

5. 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	3-1-03	
2.16	Session Management	12-30-02	3-30-03	
2.17	COM-CORBA bridge - 2	9-30-02	3-1-03	
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	3-30-03	
2.21	Test integrated software	12-30-02	5-30-03	
2.22	Documentation	3-30-03		
2.24	Prepare release version	6-30-03		
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	3-30-03	
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
5.4	Advisory Board Meeting	9-30-02	12-30-02	12-18-02

		Completion Date		
5.5	Advisory Board Meeting	3-31-03		
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
7.0	Draft Final Technical Report	10-30-03		
7.0	Final Technical Report	12-30-03		

6. Personnel initials, List of Abbreviations and Glossary

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.
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.
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
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.
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).