DEVELOPMENT OF TECHNOLOGIES AND ANALYTICAL CAPABILITIES FOR VISION 21 ENERGY PLANTS

COOPERATIVE AGREEMENT NO DE-FC26-00NT40954

QUARTERLY REPORT FOR JULY-SEPTEMBER 2002

FOR

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TABLE OF CONTENTS

DISCLAIMER

1. Executive Summary

The implementation and testing of a file-based CFD database was completed (Task 2.8). The capability for transferring temperature-dependent physical properties from Aspen Plus to Fluent was developed (Task 2.12). The GUI for enabling the process analyst to select models from the CFD database and edit certain CFD model parameters was developed and tested (Task 2.13). Work on developing a CO wrapper for the INDVU code was started (Task 2.15). A *solution strategy* capability for enabling the process analyst to switch between different models representing a unit operation block was developed and tested (Task 2.16). The development of the *Configuration Wizard* for converting a FLUENT CFD model into a CO UO model was completed (Task 2.18). A low-order model based on the multiple regression technique was developed and tested (Task 2.19). An installation kit for the *V21 Controller* was developed using the Installer Vise software (Task 2.24). A flow sheet model for Demo Case 2 was developed and tested for three loads (100%, 75%, and 50%). Documentation of Demo Case 2 was completed and submitted to DOE (Task 3.2). The debugging of the tube bank heat transfer model was completed. The model calibration for a range of loads was started. A problem of oscillating gas temperature was encountered. Work is underway to overcome this problem (Task 4.1).

2. Technical Accomplishments

Task 2.0 Software Integration

Task 2.8 CFD database

The documentation of the pre-computed results and interpolation data interfaces was updated based on development team discussions. The development of the pre-computed results dB API was completed. Thus the development and testing of a file-based CFD database system was completed.

Task 2.12 Transfer physical properties

The capability for transferring temperature-dependent physical properties from Aspen Plus to Fluent was developed. The problem encountered in transferring newly added species data from Aspen Plus to Fluent was fixed. The testing of the capability for units with multiple ports was completed. The capability for allowing the process analyst to specify whether or not to use temperature dependent physical properties was developed. This task has been completed.

Task 2.13 GUI

The GUI for selecting a CFD model from a model database and editing the model parameters was implemented. This GUI appears in the process simulator when the CFD block is double-clicked. The GUI was further enhanced to include a *solution strategy*, which enables the process analyst to specify a sequence of models (e.g., CFD and low-order) to be used during Aspen Plus iterations and the criteria for switching between the models. This task has been completed.

Task 2.15 Proprietary Model

Fluent developed a C++ template to be used to write a wrapper for integrating INDVU code via the *V21 Controller*. Alstom Power evaluated the template and identified the additional work required to adapt the C++ template for the INDVU code.

Task 2.16 Session Management

The *Solution Strategy*, *Solver Manager*, and *Session Management* classes were implemented. An instance of a *Solution Strategy* class is expected to define an analyst's choice of external solvers for resolving a given unit operation. The *Solver Manager* class has the primary task of launching

all the selected solvers for any given block on the flow sheet and to make the solver references available on demand. The *Session Manager* class handles the correct switching to any of the activated solvers.

The session management capability of the *V21 Controller* was demonstrated. It was shown that through a user-specified *Solution Strategy*, the *V21 Controller* could be made to switch from one unit model to another during Aspen Plus iterations. Currently, the iteration number is used as a switching criterion. Work on implementing more sophisticated switching criteria is underway.

Task 2.17 COM-CORBA Bridge – 2

A new version of the CO Fluent block that was not properly displaying all inlet ports when placed on the Aspen Plus flowsheet was debugged.

Task 2.18 Configuration Wizard

This task has been completed. A domain mapping functionality was added to the *Configuration Wizard* , to allow the CFD analyst to map the ports with a continuous fluid zone or region. The mapping functionality is required to check and enforce strict mass balance in the CFD results. Regression tests were conducted to verify the new functionality. The CSTR test case and the Fuel Cell reformer test cases have passed the designed regression test.

The temperature-dependent boolean parameter and the maximum and minimum real parameters were moved from the "Solver Parameters" page to the "Model Parameters" page of the *Configuration Wizard* GUI. Several bugs related to the event handling in the Configuration Wizard were fixed.

Task 2.19 Low Order model

The implementation and demonstration of a low-order model was completed. The model is based on the multiple regression technique. The input and out put data from several CFD simulations are stored in pre-computed results database. Then for a new set of input conditions, the output data are calculated using an interpolation technique. The coding required to connect this model via the *V21 Controller* with Aspen Plus material streams was implemented. A combination of CFD and the low order model was used to simulate the mixing tank reactor model in the reaction-separation-recycle flowsheet.

Task 2.20 Aspen Plus Analysis Tools

Using the Aspen Plus CO MixNSplit block, the defect encountered when using a CO parameter from a CO Fluent block in an Aspen Plus analysis tool was reproduced. This defect was submitted to the Aspen Plus 12.1 defect database.

Task 2.21 Test Integrated Software

Testing of the integrated software consisting of CFD model and low order model was conducted. The defects-enhancement list was updated with new defects and enhancements identified.

Task 2.24 Prepare release version

A copy of the Installer Vise software (www.MindVision.com) was obtained and an installation kit of the *V21 Controller* was developed. The kit automatically registers the controller DLL, places the program files in the appropriate directories and appends to the system wide PATH variable.

Task 3.0 Select Demonstration Cases

Task 3.2 Selection of Demo Case 2
The cycle was converged for 100%, 75%, and 50% load cases, although additional effort will be required to fully replace the EO mode with the SM mode, and implement an automated loop over the entire load range. Additional calibration may also be required since the Aspen cycle results diverge from the (industrial proprietary) HRSGSYM results at the lower loads. The Case 2 documentation was completed and submitted to NETL.

Task 4.0 Run Integrated Simulations

Task 4.1 Simulations of Demo Case 1
The RP&L model was calibrated over the upper load range (associated with changes to the bypass damper position), and over most of the moderate load range (associated with excess air changes). Apparently, more iterations are required to converge to a stable and non-oscillating Tsh,out value (within a fraction of a degree) at the lower loads than at the higher loads. Differences in submodel capability between the FLUENT and INDVU codes have surfaced, as manifested in the different calibration and operational factors required to achieve the same Tsh,out.

In calibrating the RP&L CFD model over the moderate to low load ranges, an oscillatory temperature behavior (which does not exist at the higher loads) was encountered. The gas temperatures may oscillate +/- 5 K with a period of a couple of hundred iterations. This oscillatory behavior causes a corresponding oscillation in the Tsh,out. Such behavior may cause convergence difficulties when the CFD case is implemented as a flowsheet block in Aspen Plus. Means are being sought to overcome this problem.

Task 5.0 Advisory Board Activities
Work on designing and building a data model from Aspen Plus output and loading the data into Intergraph's database system. The concept will be demonstrated at the November Vision 21 Simulation meeting at Iowa State University.

Task 7.0 Project Management

Presentations
An initial set of slides was prepared for the presentation "An Integrated Process Simulation and CFD Environment Using the CAPE-OPEN Interface Specifications" to be given at the AIChE 2002 Annual Meeting.

An abstract was entitled "Application of an Integrated Process Simulation and CFD Environment to Model Fuel Cell Systems" was submitted to the 2003 AIChE Spring National Meeting and Process Industries Exposition, March 30 - April 3, 2003, New Orleans, Louisiana.

3. Issues and Resolution:
Task 2.14 CFD Viewer The completion date for this task was postponed to 12-30-02 to allow time for developing other higher priority features required for demos (e.g., Task 2-12 was completed before the planned completion date).

Task 2.15 Proprietary Model Developing a wrapper for INDVU code has become a more challenging task than initially expected. Additional personnel with experience in C++ and CORBA need to be allocated to the task of preparing the CO wrapper, prior to the integration of the INDVU code (and later the industrial code for Demonstration Case 2). One possibility being

considered is to bring on board an ALSTOM employee with the requisite skills background (C++, CORBA, and mixed programming) to help with the coding.

Task 2.17 COM-CORBA Bridge – 2 The completion date for this task was postponed to 12-30-02 to allow time for developing other features required for demos (e.g., Task 2-12 was completed before the planned completion date).

Task 4.1 Demo Case 1 The tube bank heat exchanger model that ALSTOM is using for Demonstration Case 1 is in FLUENT V6.1. The *V21 Controller* and *Configuration Wizard* have only been supplied for V6.0. In order to complete Demonstration Case 1, they must be migrated to V6.1 (which will be released as a production version in November) in the near time frame. Fluent Inc. is investigating the work and schedule requirements for this task.

Task 5.0 Advisory Board Activities: Because DOE is not planning to conduct a Vision 21 program review meeting this November, a face-to-face advisory board meeting cannot be conducted. As an alternative a web-based advisory board meeting was proposed to DOE and permission was obtained.

4. Progress forecast for the next quarter

- Task 2.14 CFD Viewer
  - Commence work on the CFD Viewer

- Task 2.15 Proprietary model
  - Continue work on developing a CO wrapper for the INDVU code.

- Task 2.16 Session Management
  - Complete the session management implementation.

- Task 2.17 COM-CORBA bridge 2
  - Commence work on COM-CORBA bridge 2 task.

- 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 and develop a demo for the Aspen World conference

- Task 2.24 Prepare release version
  - Make changes in database to have separate directories for multiple models and multiple CO blocks in one simulation run.
  - Conduct code reviews

- Task 4.1 Demonstration case 1 simulation
  - Complete the calibration of the tube bank parameters for the RP&L case over the range of loads and overcome the temperature oscillation issue.
  - After the calibration, integrate the Fluent case with Aspen Plus using the CO methodology.

- Task 5.0 Advisory Board Activities
  - Organize web-based advisory board meeting

- Task 7.0 Project management
  - Conduct a project review meeting
  - Conduct a demo of the integrated simulation at the Aspen World Conference, October 28-30, Washington, DC.
  - Make a presentation at the AIChE annual meeting, Indianapolis, IN, November 8, 2002.
  - Attend the Vision 21 Simulation Meeting to be held at Iowa State University, November 19-20, 2002 and make a presentation on project status.

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	
2.15	Proprietary model template	12-30-02		
2.16	Session Management	12-30-02		
2.17	COM-CORBA bridge - 2	9-30-02	12-30-02	
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		
2.21	Test integrated software	12-30-02		
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	12-30-02	
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	

		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
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.
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).