DEVELOPMENT OF TECHNOLOGIES AND ANALYTICAL CAPABILITIES FOR VISION 21 ENERGY PLANTS

COOPERATIVE AGREEMENT NO DE-FC26-00NT40954

QUARTERLY REPORT FOR JANUARY-MARCH 2002

FOR

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DISCLAIMER

1. Executive Summary

A software review meeting was held at Fluent Inc. in Lebanon, NH on January 31-February 1, 2002. The team reviewed the current status of the software and its compliance with the software requirements (Task 2). Work on a fuel cell based power-plant flow sheet that incorporates a reformer CFD model was started. This test case includes more features (multiple ports, temperature dependent properties) than the mixing tank test case developed earlier and will be used for the further testing of the software (Task 2). The software development plan was finalized (Task 2.7). The design and implementation of a CFD database was commenced. The CFD database would store various models that a process analyst can use in the flowsheet model (Task 2.8). The COM-CORBA Bridge was upgraded to use the recently published version 0.9.3 CAPE-OPEN specifications. Work on transferring reaction kinetics data from Aspen Plus to Fluent was started (Task 2.11). The requirements for extending CAPE-OPEN interfaces in Aspen Plus to transfer temperature dependent properties to Fluent was written and communicated to the Aspen Tech developer of CAPE-OPEN interfaces (Task 2.12). A prototype of low-order model based on the Multiple Regression technique was written. A low-order model is required to speed up the calculations with the integrated model (Task 2.19). The Berkshire Power (Agawam, MA) combined-cycle power plant was selected as the Demonstration Case 2 (Task 3.2). A CFD model of the furnace in Demonstration Case 1 was developed. The furnace model will be incorporated into the flowsheet model already developed for this case (Task 4.1). A new hire joined the Fluent development team for this project. The project management plan was revised based on the software development plan. A presentation on the project status was made at the Clearwater Conference, March 4-7, 2002. The final manuscript for ESCAPE-12 conference was submitted (Task 7.0).

2. Technical Accomplishments

Task 2.0 Software Integration

A software design review meeting was held at Fluent Inc. in Lebanon, NH on January 31-February 1, 2002. The software development team reviewed the current status of the CAPE-OPEN COM-Corba bridge version of the Vision 21 controller software, including the Configuration Wizard, Database, GUI, CFD Viewer, Lower-order Models, Proprietary Model Interfaces, and Physical Properties. The team also reviewed design compliance with the high-level use cases and discussed deliverables for the advisory board demonstrations at the Fluent UGM in June 2002.

Work was started on an integrated simulation of an Aspen Plus–Fluent fuel cell system (Figure 1). An existing Aspen Plus flowsheet for a solid oxide fuel cell (SOFC) system was modified in preparation for replacing the Aspen Plus reformer model (Rplug) by a Fluent CFD model. The fuel cell flowsheet includes fuel processing, hydrogen purification, fuel cell, and heat/water recovery, and is based on the Journal of Power Sources paper entitled “Effect of operating pressure on the system efficiency of a methane-fuelled solid polymer fuel cell power source” by Virji et al (1998). This test case includes more features (multiple ports, temperature dependent properties) than the mixing tank test case developed earlier and will be used for the further testing of the software

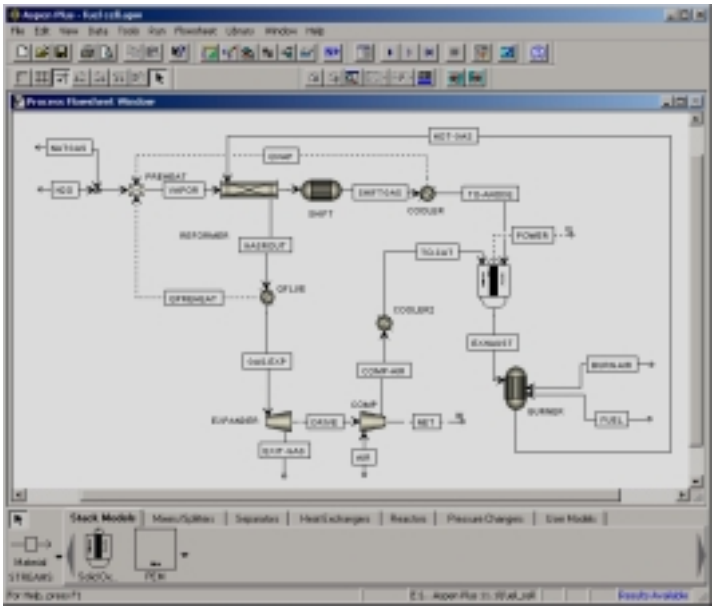

Figure 1. Methane fuelled SOFC power source

Task 2.7 Software Development Plan

The software development plan (SDP) was discussed during development team weekly meetings and the plan was finalized on January 21, 2002. Although several tasks were progressing even before the SDP was finalized, the SDP helps to formalize the plans and to track the future progress. Beginning with this quarterly report the new task names will be used to describe the project progress.

Task 2.8 CFD database

A list of V21 Database features and major requirements was prepared. Feedback was collected from the development team members, and the list was updated with the results of the discussion.

Searched information and studied available documentation on XML and object database design to be used in the V21 Controller. Installed an evaluation version of XML Spy 4.2 development suite and created a draft XML structure for a V21 Controller Model in XML Spy development suite. Added mapping information to map parameters and ports in XML V21 model structure. Discussed with the development team and refined draft XML structure of V21 Controller Model.

Created two draft versions of database APIs (UML diagrams and Sequence diagram of use for the first API). The first version emphasized more general approach to traverse model directory. The second version emphasized specialization of access classes for use by V21 controller.

Task 2.11 COM-CORBA Bridge – 1

COM/CORBA Bridge and the Fluent CORBA wrapper were upgraded to v0.9.3 of the CAPE-OPEN specifications. The version was verified to be accurately working using the Aspen Plus 12.1 beta version.

Work on further upgrading the COM/CORBA Bridge to permit automatic transfer of reaction kinetics data from Aspen Plus to Fluent was started. The implementation is now in its final stages, and it involves writing Scheme code that will update the Fluent case file prior to each CFD solution per Aspen Plus iteration.

Task 2.12 Transfer physical properties
SEZ outlined requirements for extending the CAPE-OPEN thermodynamic interfaces in Aspen Plus to provide Fluent with temperature-dependent pure component physical property data for density, heat capacity, thermal conductivity, and viscosity. SEZ provided the requirements to Michael Halloran (AspenTech UK, CAPE-OPEN expert) for review.

Task 2.19 Low Order model
MOO has prototyped a low-order model based on the Multiple Regression paradigm. The proposed model can correlate CFD model output with model input parameters such as feed mass flowrates, composition and temperature. A low-order model is required to speed up the calculations with the integrated model.

Task 3.0 Select Demonstration Cases

Task 3.2 Selection of Demo Case 2
John Holmes and Wes Bauver of Alstom Power agreed to provide data for the Berkshire Power (Agawam, MA) combined-cycle power plant. The Case Selection Report will be prepared when this data has been gathered and reviewed.

Task 4.1 Simulations of Case 1
A grid for the Richmond Power & Light, Whitewater Valley, Unit 1 case was prepared. The grid was made as coarse as possible in order to run it on a PC in conjunction with Aspen Plus. A base grid of 14,000 hexahedral cells was prepared, with non-conformal interfaces between the nozzles and the body of the furnace. Certain regions of the furnace were later adapted in order to more fully resolve the nozzle regions and the tube bank regions, bringing the total cell count up to around 45,000 cells.

Although the RP&L furnace burns coal, gaseous fuel is being combusted in the CFD case for the sake of expediency. A volatile species, with a composition and heating value equivalent to that of the coal, was utilized as fuel. A porous media with the appropriate pressure drop coefficients represents the tube banks. An initial case was run and convergence was deemed acceptable.

Task 5.0 Advisory Board Activities
Feedback from attendees at the second advisory board meeting has been requested.

Task 7.0 Project Management
A new hire Krishna Thotapalli joined the Fluent development group. Krishna has an M.S. in computer science from Loyola University. He will initially focus on the GUI and configuration wizard tasks.

The project management plan was revised based on the revised SDP. The revised plan was submitted to DOE for approval. The tasks and completion dates given in this quarterly report are based on the revised project management plan.

Presentations

- A paper entitled "Software Integration for Power Plant Simulations" was submitted and accepted for presentation at The 27th International Technical Conference on Coal Utilization & Fuel Systems, March 4-7, Clearwater, Florida (2002). WAF gave a presentation on the project progress to date at the conference.

- The final manuscript entitled "Integrated Process Simulation and CFD for Improved Process Engineering" was submitted for presentation at the ESCAPE-12 Conference to be held in The Hague on May 26-29, 2002. This will be published in a special edition of the journal *Computers and Chemical Engineering*.

3. Issues and Resolution:

- The revised completion date (3-30-02) for AP Case 2 documentation milestone has not been met. The site for Case 2 has been selected: Berkshire Power's 270 Mwe combined-cycle power plant in Agawam, Massachusetts. Initial meetings with ALSTOM personnel were held in January to discuss the availability of the data. Since ALSTOM currently manages the site, access to most of the raw data should not be a problem. A magazine article on the plant was published, and therefore an overview of the plant is already in the public domain. Because aspects of the technology of the plant are considered sensitive for a variety of reasons, the plant data will be used in the form of an "idealized" test case, and references to the plant name/location/etc. will be deleted in any future presentations (just as they have been in recent presentations of the RP&L boiler). One of the important concerns was the extent to which foreign divisions of ALSTOM (e.g., Sweden and Switzerland) should be involved in preparing the Aspen Plus flow sheet for the plant, since those divisions are better able to incorporate representative performance curves (which are considered proprietary) for the gas and stream turbines. Since project funding cannot be used to fund their activities an alternative arrangement needs to be sought. DGS is currently pursuing this issue. Further delay should not impede contractual scheduling and commitments since the second case does not need to be done until 5-30-03. However, the preparatory work does need to start now so that an Aspen Plus model can be built. The documentation for Case 2 will be written up by the end of June and the Aspen Plus modeling should be underway by that time.

4. Progress forecast for the next quarter

- Task 2.0 Software Integration
  - Continue work on fuel cell flowsheet and reformer CFD model

- Task 2.8 CFD database
  - Complete coding for initial implementation of CFD database and APIs for the Third Advisory Board demo

- Task 2.11 COM-CORBA bridge – 1
  - Enhance the existing reactions transfer capability so that additional reactions, involving new material species can be specified in Aspen Plus GUI, and be correctly transferred to Fluent
  - Enhance the Fluent Wrapper code implementation, so that multiple Unit Operation ports can be handled

- Task 2.12 Transfer physical properties
  - Commence work in implementing the automatic transfer of temperature dependent material properties from Aspen Plus to Fluent

- Task 2.13 GUI
  - Review documentation on the QT software used for developing GUI
  - Create prototypes of GUI
  - Implement GUI for model selection and editing for the Third Advisory Board demo

- Task 3.2 Selection of Demo Case 2
  - Document Demo case 2 selection

- Task 4.1
  - Calibrate the tube bank heat transfer model, recently upgraded by Fluent Inc. to provide the appropriate level of heat extraction over a range of loads
  - Integrate the tube bank heat transfer model with Aspen Plus

- Task 5.0 Advisory Board Activities
  - Plan the Third advisory board meeting
  - Conduct the Third advisory board meeting

5. Project Milestones

Note that the project milestone chart in this quarterly has been revised based on the revised project management plan submitted to DOE for approval.

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	8-10-2001
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	9-31-02		
2.10	Prototype with reaction kinetics data transfer	12-31-01		12-31-01
2.11	COM-CORBA bridge - 1	6-30-02		
2.12	Transfer physical properties	12-30-02		
2.13	GUI	6-30-02		
2.14	CFD Viewer	9-30-02		
2.15	Proprietary model template	12-30-02		
2.16	Session Management	12-30-02		
2.17	COM-CORBA bridge - 2	9-30-02		
2.18	Configuration Wizard	6-30-02		
2.19	Low Order model	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	
4.1	Demonstration Case 1 simulation completed	6-30-02		

		Completion Date		
4.2	Demonstration Case 2 simulation completed	6-30-03		
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	
5.4	Advisory Board Meeting	9-30-02		
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
7.0	Final project report	12-31-03		

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.
GCO	Global CAPE-OPEN, an extension of the CAPE-OPEN project. (www.global-cape-open.org)
GUI	Graphical User Interface.
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.
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.
RP&L	Richmond Power and Light power plant.
Scheme	Programming language used in CORTEX
SDD	Software Design Document.
SRD	Software Requirements Document.
SDP	Software development plan
Swing	A Java GUI tool kit.
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).