

**DEVELOPMENT OF TECHNOLOGIES AND ANALYTICAL
CAPABILITIES FOR VISION 21 ENERGY PLANTS**

COOPERATIVE AGREEMENT NO DE-FC26-00NT40954

QUARTERLY REPORT FOR OCTOBER-DECEMBER 2000

FOR

Diane Madden
U.S. Department of Energy
National Energy Technology Laboratory
P.O. Box 10940, MS 920-L
626 Cocharans Mill Road
Pittsburgh, PA 15236-0940

BY

Madhava Syamlal, Ph.D.
Fluent Inc.
Primary Recipient
10 Cavendish Court, Lebanon, NH 03766
Point of Contact: Kristi C. Fenner (Business and Financial)
Point of Contact: Dr. Madhava Syamlal (Technical)

ALSTOM Power
US Power Plant Laboratories, 2000 Day Hill Road, Windsor, CT 06095

Aspen Technology, Inc.
Ten Canal Park, Cambridge, Massachusetts 02141-2200

Intergraph Corporation
One Madison Industrial Estate, Huntsville, AL 35894

Concurrent Engineering Research Center, West Virginia University
886 Chestnut Ridge Rd., Morgantown, WV 26506

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1. Executive Summary

To complete project planning, various project groups conducted several meetings and teleconferences. As a result a draft project management plan was written and circulated. The plan will be finalized in a project kick off meeting to be held on January 16, 2001 in Lebanon, NH, which will be attended by all project participants (Task 1.0). Various project personnel have been trained in the use of Fluent and Aspen Plus, which completes all the training tasks except for Aspen Plus and IDL training for Alstom Power (Task 2.1). A preliminary version of User Requirements Document (preURD) was written. This document will be sent to key users of Aspen Plus and FLUENT and their responses will be collected in January (Task 2.3). A prototype of Fluent integration with Aspen Plus was constructed for understanding the required software design. The development of a general architecture for the integrated software suite has been started (Task 2.6). Invitation letters for participation in an Advisory Board were sent out to several Vision 21 contractors. Their responses will be used to form an Advisory Board in January (Task 5.0). Fluent has awarded subcontracts to Alstom Power, CERC, and Aspen Tech and negotiations with Intergraph are underway. Aspen Plus and FLUENT were installed on a computer at CERC. The design of a project web site was completed, and the site setup was started (Task 7.0).

2. Technical Accomplishments

Task 1.0 Project planning:

Task 1.1 Project Planning

The project officially started on Oct 1 2000. Several planning meetings were conducted:

- A planning meeting between CERC (KJC, IBL) and Fluent (PEF, MXS) development personnel was held on September 27, 2000 in Morgantown, WV. The division of development tasks between CERC and Fluent was determined, and preliminary discussions about the proposed software architecture were conducted.
- A planning meeting was held in Morgantown, WV on October 18th with ALSTOM (WAF, DGS, JLM), CERC (IBL), and Fluent (MXS) personnel in attendance. The basic work-scope and schedule for the ALSTOM portion of the work was agreed upon.
- Three teleconferences attended by personnel from AspenTech (SEZ), CERC (IBL) and Fluent (RLC, OSH, PEF, MXS) were held to discuss the development tasks.
- MXS participated in a teleconference with Intergraph personnel to clarify Intergraph's work scope.
- The project plans and status were reviewed in a teleconference attended by AspenTech (SEZ, HB, RF), CERC (IBL), and Fluent (RLC, BJH, AH) personnel on December 6, 2000.
- The development tasks were discussed in a meeting held at Lebanon, NH and attended by AspenTech (SEZ), CERC (IBL) and Fluent (RLC, PEF, MXS) personnel.

A draft project plan was written and circulated among the project participants. The plan will be finalized after the kick off meeting on Jan 16, 2001 and submitted to DOE.

Task 2.0 Software Integration

Task 2.1 Training

IBL got a demo of FLUENT from the Mechanical Engineering Department of WVU. CERC personnel (IBL, KJC) were trained in the use FLUENT at the Fluent, Morgantown office on November 17, 2000.

OSH (Fluent) gave a preliminary presentation of Aspen Plus and the integration of Aspen Plus and Fluent to CERC (IBL) and Fluent (RLC, PEF, MXS) personnel. IBL (CERC) and MXS (Fluent) attended Aspen Plus training in Boston, MA. on December 5-7, 2000.

SEZ (AspenTech) attended Fluent training on December 4-7, 2000.

Task 2.2 User survey

To collect information from the users a pre-user-requirements-document (preURD) was written by Fluent. Fluent and AspenTech personnel reviewed the document. A list of nearly forty users of FLUENT and Aspen Plus that have an interest in the integration of CFD and process simulation was developed. The survey will be sent out to those users, and their responses will be collected in January 2001.

In a parallel effort a web based survey form is being developed. This form will be posted on the Vision 21 project web site and announced to a larger number of users through a write up in the Aspen eFlash, AspenTech's electronic newsletter. The user responses will be collected electronically for about three months.

CERC (KJC) started writing a draft version of the User Requirements Document.

Task 2.6 Software Design

Much work was done in prototyping software integration based on earlier work done by AspenTech and Fluent¹. SEZ has developed a working prototype using CAPE OPEN interfaces. SEZ reproduced the results of the coupled Aspen Plus/Fluent CFD simulation of the Continuous Stirred Tank Reactor (CSTR) described in that paper using CAPE OPEN interfaces. In the paper, the FLUENT CFD model is integrated into the process simulation via the Aspen Plus USER2 interface. SEZ is currently using this CSTR example to prototype the use of FLUENT CFD models in Aspen Plus via the Cape Open unit interface. The implementation is written in Visual Basic and uses the COM interface standard. A CFD block can be added to the Cape Open model library. The Cape Open CFD blocks can be placed on the Aspen Plus flowsheet. SEZ implemented the ICapeUnitEdit_Edit method to bring up the Fluent GUI when the user right clicks on the Cape Open CFD model on the Aspen Plus flow sheet and selects Edit Model. SEZ is currently focusing on implementing the ICapeUnit_Calculate method, which transfers data from Aspen Plus to FLUENT, spawns and executes the FLUENT CFD model, and gives the results back to Aspen Plus. The implementation is specific to the CSTR model discussed above in terms of the number of ports, number and types of chemical components, etc. Ultimately, this will need to be parameterized so that the user places a configurable model type onto the flowsheet instead of a fixed model instance. Several new Cape Open thermo calls were required in the ICapeUnit_Calculate implementation. SEZ provided PEF at Fluent with information on AspenTech's use of ActiveX automation in Aspen Plus and Aspen Custom Modeler.

IBL (CERC) has started working on running FLUENT and Aspen Plus jointly.

IBL (CERC) read some of the final documents for better understanding the CAPE-OPEN standard. Searched web for additional information on CAPE-OPEN: found a site with final documents on this standard: <http://www-i5.informatik.rwth->

¹ Oshinowo, L., Haidari, A., Kisala, T., and Field, R., "Improving Reactor Modeling In Sequential-Modular Process Simulation Using CFD," Chemical Reaction Engineering VII: Computational Fluid Dynamics, Québec City, Canada, August 6-11, 2000.

aachen.de/~koeller/COfinaldocs/COfinaldocs.html. Found several sites that have examples of use and additional discussions on application of CAPE-OPEN. IBL studied the CAPE-OPEN implementation in Aspen Plus.

IBL (CERC) studied COM, including writing of some samples. Reviewed general information on CORBA/Java/DCOM to make better choice of communication technology among modules. Prepared e-mail (for discussion) on proposed data exchange method (COM/OPEN-CAPE which is currently implemented in Aspen Plus). Since there is interest in implementing the Controller interface in CORBA, started studying CORBA (with C++/Java), including writing of some samples. Continued studying COM/CORBA, writing examples; and wrote a couple of simple Java examples (Java might be used in Controller V21)

KJC (CERC) Explored optimization methods, and read up on Design of Experiments optimization because of its relevance to the whole problem of FLUENT-Aspen Plus integration. Read up on iSight5 at Engineous.com with a view to its use as an integration technique. Talked to two persons at Engineous, Inc. about their University Software Program, with a view to getting their package iSIGHT for testing purposes.

CERC formulated requirement of an Exemplary Problem of FLUENT-Aspen Plus integration to be continually refined during this project.

Searched and reviewed visualization packages that can be used with the integrated software, as per a request made during a meeting between ALSTOM, CERC and Fluent.

Vision 21 Architecture: A general architecture design for hooking FLUENT up to Aspen Plus is taking shape. The basic approach will be presented at the Vision 21 kick-off meeting on January 16, 2001.

CFD Results Viewer: Investigation into using Java/Swing as a cross-platform GUI toolkit for the CFD results viewer has been completed (including a very simple GUI prototype). We have concluded that we cannot rely on the maturity and multiplatform robustness of client-side Java for the development of the CFD results viewer. We are considering a layered design that would allow us to develop the application GUI code using an interpreted language (e.g., Python), which is layered on top of a cross-platform C++ GUI toolkit, with the hope that the C++ GUI toolkit could be replaced by Java/Swing in the future, if desired.

FLUENT/V21 Controller Middleware: We have started to investigate various middleware technologies for communication between the V21 controller and FLUENT. Currently, we are looking at CORBA and XML technologies.

Task 5.0 Advisory Board Activities

Larry Ruth of the DOE provided a list of Vision 21 contractors. From that list, a letter was drafted and sent to prospective advisory board members, which invited a representative from their company to be a panel participant. A number of responses to the letter have been received. Final replies to the letter are to be received by January 15, 2001.

Task 7.0 Project management

Subcontract negotiations between Fluent and ALSTOM, AspenTech, CERC, and Intergraph were conducted. Fluent awarded subcontracts to ALSTOM, CERC, and AspenTech. Negotiations with Intergraph are continuing. All subcontracts incorporate the FAR clauses 52.227-13 (Patent Rights) and 52.227-14 (Rights in Data), suitably modified to identify the parties.

CERC investigated various options for online project collaboration and wrote report on choice of a collaboration tool: Eroom was the tool of choice. However, because of security concerns Fluent decided to set up a simpler project web site for collaboration. A web site design was completed. The site is being set up.

Several applicants were interviewed for a new hire identified for this project. One interview was conducted. Two more has been scheduled.

Software license agreements for the Aspen Plus software for one simultaneous user that expires on Sept 30, 2003 were signed by ALSTOM, CERC, and Fluent. Software license agreement for Fluent was signed by CERC.

Options for CERC hardware configuration were discussed. Decided to build from purchased parts, rather than buy ready-made to economize on the budget. Finalized order for parts for machine for project work. Changed to better graphics card (GeForce), got a CD Writer drive, and a switch to enable monitor, mouse, and KB to be switched between an existing CERC computer and the new machine. Assembled and installed a computer from purchased components. Installed Windows 2000, Office 2000, and all updates and verified proper working. Fluent and AspenPlus licenses installed on the machine at CERC

3. Issues and Resolution:

None.

4. Progress forecast for the next quarter

- Task 1.1
 - Conduct project kick off meeting on January 16, 2001
 - Submit Project Management Plan to DOE
- Task 2.2
 - Complete User survey
 - Write User Requirements Document
- Task 2.3
 - Write Software Requirements Specifications
- Task 2.6:
 - Continue to work on prototype of a Fluent CFD model running in Aspen Plus via the Cape Open unit interface.
 - Complete the investigation of middleware technologies for FLUENT/V21 controller communications

- Task 3.1:
 - Initialize selection of Demonstration Case 1.
- Task 5.0:
 - Form Advisory Board
- Task 7.0:
 - Complete subcontracts to AspenTech and Intergraph
 - Complete project web site

5. Project Milestones

Task Number	Milestone/Deliverables	Completion Date		
		Original	Revised	Actual
1.0	Project Management Plan	1-30-01		
2.2	User Requirements Document (URD)	3-15-01		
2.3	Software Requirements Specifications (SRS)	4-15-01		
2.6	Software Design Documentation	5-15-01		
2.7	Software Development Plan	6-30-01		
2.7	Working Test Case 1	6-30-01		
2.10	Working Test Case 2	9-30-01		
2.12	Working Test Case 3	1-15-02		
2.13	Working Test Case 4	3-30-02		
2.14	Working Test Case 5	1-1-02		
2.15	Working Test Case 6	6-15-02		
2.17	Working Test Case 7	9-15-02		
2.17	Beta version of Controller	9-15-02		
2.18	User documentation for Controller	12-30-02		
2.20	Integrated Software suite and demonstration	6-30-03		
3.1	Demonstration Case 1 selection	1-31-01		
3.2	Demonstration Case 2 selection	8-30-01		
4.1	Demonstration Case 1 simulation completed	6-30-02		
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		
5.2	Advisory Board Meeting	9-30-01		
5.3	Advisory Board Meeting	3-31-02		
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		
7.0	Final project report	12-31-03		

6. Personnel initials, List of Abbreviations and Glossary

<u>Personnel Name</u>	<u>Affiliation</u>	<u>Initials</u>
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
Lanre Oshinowo	Fluent	OSH
Madhava Syamlal	Fluent	MXS
Bob Fisher	Intergraph	RJF

<u>Name</u>	<u>Description</u>
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.
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.quantisci.co.uk/Cape-Open).
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)
DCOM	Distributed Component Object Model – An extension of COM that allows software components to be distributed over a network.
GUI	Graphical User Interface
IDL	Interface definition language, which is used for defining the communications between software components linked through a middleware.
Java	Java programming language.
Middleware	Connectivity software that consists of a set of enabling services that allow 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
Swing	A Java GUI tool kit.
Visual Basic	Visual Basic programming language
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).