DEVELOPMENT OF TECHNOLOGIES AND ANALYTICAL CAPABILITIES FOR VISION 21 ENERGY PLANTS

COOPERATIVE AGREEMENT NO DE-FC26-00NT40954

QUARTERLY REPORT FOR APRIL-JUNE 2002

FOR

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DISCLAIMER

1. Executive Summary

A software design review meeting was held May 2-3 in Lebanon, NH. The work on integrating a reformer model based on CFD with a fuel cell flow sheet was completed (Task 2.0). The CFD database design was completed and the database API's finalized. A file-based CFD database was implemented and tested (Task 2.8). The task COM-CORBA Bridge-I was completed. The bridge now has CO interfaces for transferring reaction kinetics information from Aspen Plus to Fluent (Task 2.11). The capability for transferring temperature-dependent physical properties from Aspen Plus to Fluent was implemented (Task 2.12). Work on "Model Selection" GUI was completed. This GUI allows the process analyst to select models from the CFD database. Work on "Model Edit" GUI was started (Task 2.13). A version of Aspen Plus with the capability for using CO parameters in "design spec" analysis has become available. With this version being available, work on adding CO wrapper to INDVU code has been started (Task 2.15). A preliminary design for the Solution Strategy class was developed (Task 2.16). The requirements for transferring pressure data between Aspen Plus and Fluent were defined. The ability to include two CFD models in a flow sheet was successfully tested. The capability to handle multiple inlets and outlets in a CO block was tested (Task 2.17). A preliminary version of the Configuration Wizard, which helps a user to make any Fluent model readable from a process simulator, was developed and tested (Task 2.18). Work on constructing a flow sheet model for Demo Case 2 was started. The work on documenting Demo Case 2 is nearing completion (Task 3.2). A Fluent heat exchanger model was installed and tested. Work on calibrating the heat exchanger model was started (Task 4.1). An advisory board meeting was held in conjunction with the Fluent Users Group Meeting on Monday, June 10, 2002. The meeting minutes and presentations for the advisory board meeting have been posted on the project website (Task 5.0). A paper entitled "Integrated Process Simulation and CFD for Improved Process Engineering" was presented at the European Symposium on Computer Aided Process Engineering-12, May 26-29, 2002, The Hague, The Netherlands (Task 7.0).

2. Technical Accomplishments

Task 2.0 Software Integration

A software design review meeting was held May 2-3 in Lebanon, NH. The agenda included:

- ?? Review current status of the development
- ?? Review/develop the design of subsystems
- ?? Finalize demo for Advisory Board meeting on June 10, 2002
- ?? Review the areas to focus on until June 10

<u>Task 2.8 CFD database</u>

CFD Database API was finalized. UML class diagrams for the new API were created. Information on the XML schema for Aspen Plus model classification was used as a guide. Documentation for Database API in Doxygen format, UML diagrams, and Database API usage code snippets were prepared. The SDD was revised to include information on the database design.

A draft version of the database with full functionality, as defined in the finalized database API, was developed. MagicDraw CASE tool was used to generate initial framework of C++ classes from the UML diagrams, which ensured compliance of the C++ code with the database API.

A V21Preference class, which is used in Model Selection GUI for persisting a list of libraries, was designed and implemented. The currently implemented functionality allows using the class in Model Selection GUI for test and demos. The Global Configuration dialog was created in QT Designer for demonstration of expected functionality for Global Configuration dialog.

The database design was reviewed in a team meeting and the need for a capability to handle pre-computed results was identified. A number of requirements for this capability were defined during the discussion and were later documented.

Task 2.11 COM-CORBA Bridge – 1

The work on implementing CO reaction kinetics interfaces in COM-CORBA Bridge was completed. The implementation was tested with the CSTR and the fuel cell test cases. The code was used for a demonstration of Aspen Plus – Fluent integration at the Advisory Board meeting.

Task 2.12 Transfer physical properties

The capability for transferring temperature-dependent physical properties (specific heat, viscosity, thermal conductivity, and standard state enthalpy and entropy) from Aspen Plus to Fluent was implemented in the Fluent Cape-Open wrapper. This new functionality employs the Aspen Plus properties database in obtaining the inputs required for computing the pure-component physical properties. (The mixture properties are calculated by Fluent using one of the mixing rules). Polynomial coefficients characterizing the physical properties are generated dynamically using a least-squares fit of the data extracted from Aspen Plus database. The polynomial coefficients can be computed for an arbitrary range of stream temperature, which may be specified by a CFD expert or a process analyst. The current implementation uses a default stream temperature range of 298K – 3000K.

Task 2.13 GUI

A test-harness for the database API was developed to help GUI development. Prototype dialogs for browsing the database were demonstrated at the design review meeting on May 2 – 3, 2002. The GUI was refined based on the comments from the design review meeting. The integration of Database API with the Model Selection GUI was completed.

A number of bugs in the V21 Controller, including the non-display of Cape-Open parameters in the Aspen Plus GUI grid, were fixed. Parameter-display related problems, including the display of all the parameters as being of type “double” and the non-display of units of measurements for some of the real parameters were reported to Aspen Technology. KKT had a meeting with PEF, Andrea W. Felix and MOO to agree on an initial design of the V21 Controller model edit GUI. Some prototype GUIs based on a typical set of model and solver parameters were presented. The prototypes were reviewed and modifications were proposed for an initial implementation. Work on implementing the required model edit functionality was started.

Task 2.15 Proprietary Model

The work on the including CO interfaces in the INDVU was delayed because CO parameters could not be used in the Aspen Plus “design spec” analysis. Aspen Plus 12.1, Kit 52, delivered in June, contains the required feature, and the work on adding a CO wrapper to INDVU code has been started.

Task 2.16 Session Management

Worked on a design for the Solution Strategy class so as to comply with several requirements such as flexibility, seamless support for several solvers, and ability to support inner and possibly external (independent of COSE) optimization. Studied *Strategy* and *Interpolator* software design patterns for potential use in the design of solution strategy class. A preliminary class diagram based on *Strategy* and *Interpolator* GOF software design patterns and a top-level domain diagram were created.

Work on integrating the various V21 Controller subsystems was started. This includes the coupling of the database API and the GUI code to the existing COM-CORBA Bridge functionality. Two utility classes (SessionManager and SolverManager) were added to the V21 Controller. With these classes in place, there is no need to hard-wire Fluent case file name in the V21 Controller code. The process analyst can now browse the database of pre-configured models, and select an appropriate external model and its solver to describe a unit operation.

Task 2.17 COM-CORBA Bridge – 2

SEZ reviewed V1.0 of the Global CAPE-OPEN (CO) Thermodynamic and Reaction Kinetics Specifications and provided feedback to Michael Halloran (Aspen Tech CO interfaces developer) regarding the CO v1.0 functionality in Aspen Plus 12.1. The CO v1.0 Type Library will be available in Aspen Plus 12.1 at the end of July 2002. The CO v1.0 Reaction Kinetics will be available in Aspen Plus 12.1 at the end of August 2002. This will give us adequate time to meet the planned completion date of 9/30/2002 for this task.

Task 2.18 Configuration Wizard

Much progress was made in developing a Configuration Wizard, which helps the CFD analyst to make the CFD model readable by the process simulator (or make the CFD model CO-compliant). When the wizard is invoked from Fluent, it guides the user through the various steps such as selecting a model category, providing a model description, and selecting model and solver parameters that needs to be exposed to the process analyst. A Fluent CFD model consists of a *case* and a *data* file. Upon running the configuration wizard a configuration file (in XML) containing user-supplied information is also generated. The three files (case, data, and configuration) constitute a CO compliant CFD model. The Configuration Wizard was demonstrated at the Advisory Board meeting.

Task 2.19 Low Order model

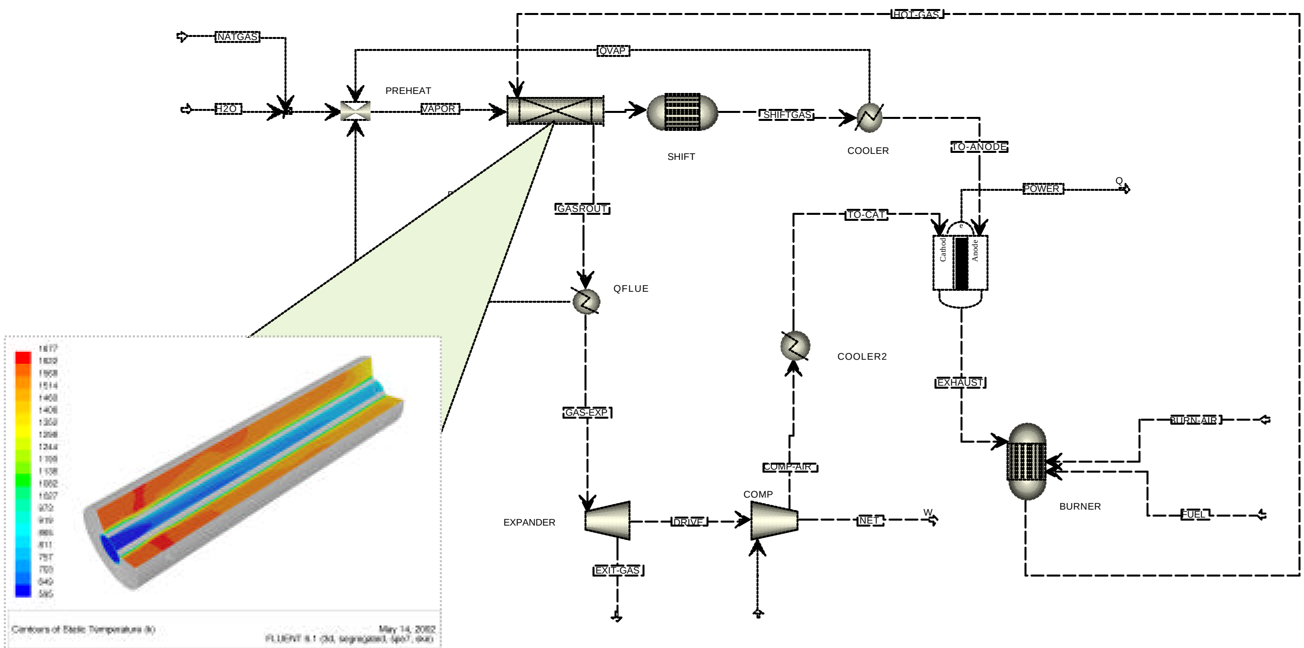
(No progress this quarter)

Task 2.20 Aspen Plus Analysis Tools

The accessing of CAPE-OPEN parameters from the Aspen Plus Case Study, Sensitivity Analysis, and Design Spec tools was successfully tested.

Task 2.21 Test Integrated Software

The work on integrating a reformer CFD model with a fuel cell flow sheet was completed. The process includes steam reforming of methane, shift conversion, fuel cell, anode exhaust combustor, a turbine, and a compressor. The reformer has a shell and tube configuration; the catalyst on the tube-side is heated with the products of the anode-exhaust combustion on the shell side. A Fluent CFD model was developed to describe the reformer. A converged solution was obtained with the integrated model.



Compared with the default model in Aspen Plus, the CFD model has the following advantages:

1) The heat transfer and pressure drop are calculated and need to be specified as an input.
2) 3D CFD model accounts for the radial variation in the reaction rate, which is larger near the tube wall than at the center.
3) The detailed temperature profile is useful for the process analyst to ensure that the catalyst temperature does not exceed the sintering temperature.

A list of defects and proposed enhancements for the Vision 21 Software was prepared and posted on the project web site. This list will be continually updated and used for tracking the resolution of defects and enhancements.

The requirements for properly handling the bi-directional transfer of pressure between Aspen Plus and Fluent were defined.

A two-CSTR version of reaction-separation-recycle flowsheet was prepared, and the launching and simulation of multiple unit/reactor blocks in a given process flow sheet was successfully demonstrated. This capability was demonstrated by replacing the CSTR unit in Test Case 1 problem with a couple of CO CSTRs, i.e., by splitting the original stream into two halves. The results obtained in Aspen Plus using the two CO blocks were then compared with those of a single block. The comparisons show that an external solver program can be invoked from different model directories without introducing any errors in the results that are returned to Aspen Plus.

The Fluent wrapper code was modified so as to handle unit operations that have multiple inlets and outlets. The enhancements to the Fluent CO wrapper are now being tested using an Aspen Plus Fuel Cell flow sheet, which includes a Reformer unit operation model with two inlets and two outlets.

Task 3.0 Select Demonstration Cases

Task 3.2 Selection of Demo Case 2
Aspen Plus 11.1 was installed on Paul Hansen's (ALSTOM Power) machine so that he could begin to construct the cycle for Case 2. Through the initial construction of the cycle, Paul will ensure that sufficient information is available to run the cycle over the desired load range. He has constructed the gas turbine side and the HRSG side as separate cycles and is presently in the process of integrating them. Galen Richards (ALSTOM Power) is nearing completion of the documentation of the selected case.

Task 4.0 Run Integrated Simulations

Task 4.1 Simulations of Demo Case 1
An SGI version of the Fluent HEX model, provided by Fluent, was installed. An initial attempt was made to calibrate Case 1 with the new HEX model. The calibration procedure involves modifying the wall resistances and tube bank surface effectiveness factors until the computed furnace outlet temperatures match the results of the INDVU code over the load range. Fluent is currently addressing some bugs and requested refinements in the HEX code.

Task 5.0 Advisory Board Activities

An advisory board meeting was held in conjunction with the Fluent Users Group Meeting on Monday, June 10, 2002. The meeting minutes and presentations for the advisory board meeting have been distributed and posted on the project website.

The integrated Aspen Plus - Fluent fuel cell system simulation was demonstrated at the DOE Vision 21 Advisory Board Meeting and Fluent UGM CFD Pavilion. The demonstration highlighted the following Vision 21 components: Configuration Wizard, CFD Model Database, Model Selection GUI, V21 Controller, and CAPE-OPEN COM-Corba Bridge. The Fluent reformer model consists of a catalytic bed in a central tube heated from outside with combusted anode exhaust gas. The CFD model describes the fluid flow, heat transfer, and catalytic reactions in a 3D geometry. More specifically, it accounts for the heat transfer between the catalyst bed and the annular region, as well as the effect of the radial temperature profile on the rate of the catalytic reaction.

Intergraph had a meeting with the development team about managing the case data in SmartPlant (SP) Foundation. The following two items were considered:

?? Enhance the visualization based on queries from the Aspen runs
?? Manage the case data between the Aspen and Fluent tasks

Sample Fluent and Aspen Plus data files were given to Intergraph. The possibility of using SP Foundation for managing simulation data files is being investigated.

Task 7.0 Project Management

Presentations
An abstract entitled “An Integrated Process Simulation and CFD Environment Using the CAPE-OPEN Interface Specifications” was submitted by MOO, PEF, MXS, IBL, KJC, and SEZ for presentation at the AIChE 2002 Annual Meeting, November 3-8, in Indianapolis, IN.

SEZ presented the paper entitled “Integrated Process Simulation and CFD for Improved Process Engineering” at the European Symposium on Computer Aided Process Engineering-12, May 26-29, The Hague, The Netherlands (2002). The paper was co-authored with MXS. The presentation included a demonstration of a Fluent CSTR model running in an Aspen Plus reaction-separation-recycle flowsheet.

SEZ prepared and completed the AspenTech-internal RUP Elaboration Phase Review for the DOE Vision 21 project.

3. Issues and Resolution:

- ?? Task 2.13 GUI: The completion date of this task has been postponed to 7-30-02. The “Model Select GUI” was completed and demonstrated at the Advisory Board meeting. The work on “Model Edit GUI” is mostly done, and testing and debugging are going on.
- ?? Task 2.18 Configuration Wizard: The completion date of this task has been postponed 9-15-02. The work is mostly done. But a new requirement was defined. The CFD analyst needs to identify flow domains and associate inlet and outlet ports with the flow domain. So the completion of this task will take more time than previously anticipated.
- ?? Task 4.1 Demonstration Case 1 Simulation: The completion date for this task has been postponed to 12-30-02. The delay was caused by two factors: 1. A version of Aspen Plus that can use CO parameters in "design spec" analysis, which is required for developing a CO wrapper for the INDVU code, became available only last month. DGS has contacted MOO and PEF and ideas have been generated regarding the best approach for CO/C++ wrapping of the INDVU code. MOO and PEF have suggested an approach based on developing a skeleton code by stripping out the CORTEX-related code from the Fluent wrapper. 2. Developing a heat exchanger or tube bank model for FLUENT is taking more time than anticipated. The heat exchanger model has been essentially completed, but some bugs and application issues were discovered when the model was run with Demonstration Case 1. When the heat exchanger model is fully operational, then the tube bank and external wall heat transfer parameters will be calibrated over the load range. Following the calibration effort, the Fluent boiler simulation of Demonstration Case 1 can be integrated with the Aspen Plus cycle. The delay in this deliverable is not expected to affect the completion of the project. ALSTOM Power is bringing additional resources to the project to finish up or accelerate various tasks.

4. Progress forecast for the next quarter

- ?? Task 2.8 CFD database
  - ?? Update V21 Database API with methods to access pre-computed results.

- ?? Task 2.12 Transfer physical properties
  - ?? Fix the current problem encountered in transferring newly added species data from Aspen Plus to Fluent, so that additional reaction(s) specified by the process analyst in Aspen Plus GUI involving this new species, do not result in warnings of mass imbalance in Fluent during the first cycle of iterations.

- ?? Complete the testing of transfer of temperature-dependent physical properties from Aspen Plus to Fluent and handling of units with multiple ports

- ?? Enhance the Fluent Cape-Open wrapper code to include a boolean parameter specification type, so that the process analyst can specify whether to use temperature dependent or constant physical properties

?? Task 2.13 GUI
- ?? Complete work on the development of a Model Edit GUI, which will permit the process analyst to edit some of the pre-configured solver/model parameters
- ?? Employ the Configuration Wizard generated XML file to display model information in the model selection GUI
- ?? Fix the existing time-out problem, which is related to the display of the model selection GUI.
- ?? Add persistence code so that the process analyst can save a given co-simulation and automatically re-run it when the Aspen Plus data file is re-loaded.

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

?? Task 2.16 Session Management
- ?? Finish Solution Strategy class diagrams and create C++ prototype of the class. Discuss with MOO possible modifications of existing classes and come to a mutually agreed solution to this problem.

?? Task 2.18 Configuration Wizard
- ?? Verify the validity of the configuration file
- ?? Include logic for defining flow domains and associating inlets and outlets for each flow domain.

?? Task 2.19 Low order model
- ?? Continue work on a Low-Order model

?? Task 3.2 Selection of Demo Case 2
- ?? Continue work to gather data for the advanced cycle case and complete documentation of selected case.

?? Task 4.1 Demonstration case 1 simulation
- ?? Complete debugging of the tube bank heat transfer model.
- ?? Subsequently calibrate tube bank parameters for the RP&L case over the range of loads.
- ?? After the calibration, integrate the Fluent case with Aspen Plus using the CO methodology.

?? Task 5.0 Advisory Board Activities
- ?? Solicit feedback from the Advisory Board attendees.

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	9-31-02		
2.10	Prototype with reaction kinetics data transfer	12-31-01		12-31-01
2.11	COM-CORBA bridge - 1	6-30-02		6-30-02
2.12	Transfer physical properties	12-30-02		
2.13	GUI	6-30-02	7-31-02	
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	9-15-02	
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	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		
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
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.
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.
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.
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.
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).