Development of Technologies and Analytical Capabilities for Vision 21 Energy Plants

FINAL SIMULATION RESULTS FOR DEMONSTRATION CASES 1 AND 2

Topical Report

Reporting Period Start Date: October 1, 2000
Reporting Period End Date: September 30, 2003

David Sloan, Ph.D.
Woodrow Fiveland, Ph.D.

October 15, 2003

DOE Cooperative Agreement No: DE-FC26-00NT40954

ALSTOM Power Inc.
US Power Plant Laboratories
P.O. Box 500, CEP 9005-1202
2000 Day Hill Road
Windsor, CT 06095

UNDER SUBCONTRACT TO
Fluent Inc.
10 Cavendish Court, Lebanon, NH 03766

DISCLAIMER

ACKNOWLEDGEMENT STATEMENT

This document was prepared with the support of the U.S. Department of Energy, under Award No. DE-FC26-00NT40954. However, any opinions, findings, conclusions, or recommendations expressed herein are those of the author(s) and do not necessarily reflect the views of the DOE.

ACKNOWLEDGEMENTS

Financial support for this project was provided by DOE National Energy Technology Laboratory (Cooperative Agreement No. DE-FC26-00NT46954) and ALSTOM Power Inc. Appreciation is expressed to John G. Wimer as the DOE Project Manager. The contributions of the many Vision 21 project team members from Fluent Inc., CERC, and Aspen Technology Inc. are also greatly appreciated. Fluent Inc. is particularly acknowledged for its leadership role as the prime contractor under Madhava Syamlal. Gratitude is expressed to Maxwell Osawe at Fluent Inc. for his diligence in striving to deliver quality software.

Within the ALSTOM Power divisions, appreciation is expressed to a number of individuals. John L. Marion, the ALSTOM Power Program Manager, and Woodrow A. Fiveland, the ALSTOM Power Project Manager, contributed to the success of this project. Appreciation is also expressed to ALSTOM Power business unit managers Richard C. LaFlesh, for provision of the experimental data and blueprints relative to Demonstration Case 1, and Thomas P. Mastronarde, for release of the HRSGPS code/runs and data pertaining to Demonstration Case 2.

The efforts of various individuals from ALSTOM Power who were instrumental in completing subtasks are also recognized: Paul L. Hansen, Lorraine S. Miemiec, Galen H. Richards, Eric A. Johnson, John C. Pedersen, and Oleg Kukar.

ABSTRACT

The goal of this DOE Vision-21 project work scope was to develop an integrated suite of software tools that could be used to simulate and visualize advanced plant concepts. Existing process simulation software did not meet the DOE's objective of "virtual simulation" which was needed to evaluate complex cycles. The overall intent of the DOE was to improve predictive tools for cycle analysis, and to improve the component models that are used in turn to simulate equipment in the cycle. Advanced component models are available; however, a generic coupling capability that would link the advanced component models to the cycle simulation software remained to be developed. In the current project, the coupling of the cycle analysis and cycle component simulation software was based on an existing suite of programs. The challenge was to develop a general-purpose software and communications link between the cycle analysis software Aspen Plus® (marketed by Aspen Technology, Inc.), and specialized component modeling packages, as exemplified by industrial proprietary codes (utilized by ALSTOM Power Inc.) and the FLUENT® computational fluid dynamics (CFD) code (provided by Fluent Inc). A software interface and controller, based on an open CAPE-OPEN standard, has been developed and extensively tested. Various test runs and demonstration cases have been utilized to confirm the viability and reliability of the software.

ALSTOM Power was tasked with the responsibility to select and run two demonstration cases to test the software – (1) a conventional steam cycle (designated as Demonstration Case 1), and (2) a combined cycle test case (designated as Demonstration Case 2). Demonstration Case 1 is a 30 MWe coal-fired power plant for municipal electricity generation, while Demonstration Case 2 is a 270 MWe, natural gas-fired, combined cycle power plant. Sufficient data was available from the operation of both power plants to complete the cycle configurations.

Three runs were completed for each Demonstration Case – (1) an initial baseline run using the existing component libraries in Aspen Plus®, (2) a second run where one of the library components was replaced with an ALSTOM Power proprietary code, and (3) a third run where a cycle component was replaced with a FLUENT® CFD simulation. Each of the three runs was successfully completed over a range of loads. This report documents the case runs and discusses the viability and capabilities of the linkage/interface software.

TABLE OF CONTENTS

LIST OF FIGURES

LIST OF TABLES

1.0 BACKGROUND ON VISION 21 PROGRAM

The goal of the overall program work scope was to develop an integrated suite of software tools that could be used to simulate and visualize advanced plant concepts that are being developed as part of DOE's Vision 21 program. Advanced simulation tools will be needed to evaluate new power plant concepts that could minimize costly laboratory and field trials.

The typical process simulation software that is commercially available to industry does not meet the DOE's objective of "virtual simulation" that is needed to evaluate complex cycles. The intent of the DOE has been to improve predictive tools for cycle analysis, and to improve the component models that are used in turn to simulate the cycle. Generally, the modeled performance of various components, e.g., a boiler, is derived from a simple set of rules and are used by the cycle simulation software primarily as a black box. These simple component models are not sufficient for component design and the evaluation of the impact of the component on cycle performance. To meet DOE's goal of predicting and visualizing the performance of these complex systems, there has been a need to upgrade the component models and their interaction protocols with cycle software, thus providing "hooks" for industrial design methodologies, CFD codes (like FLUENT®), and spreadsheets. The focus of the present Vision 21 project has been to provide the software interface that permits third-party codes to exchange information and run in conjunction with process simulation packages.

The simulation software has been based on an existing suite of programs being marketed by Aspen Technology, Inc. (AT), Intergraph Corp. and Fluent Inc. AT has developed a number of advanced process simulation tools, like Aspen Plus® and Zyqad®, that have many of the characteristics needed to evaluate Vision 21 concepts. Intergraph Corp., in partnership with AT, has developed elements of the visualization software. Fluent Inc. has developed a multi-dimensional flow and combustion code (FLUENT®) used by many segments of the power generation industry. The specific challenge of this project was to develop a general-purpose software and communications link between Aspen Plus® and other modeling software, such as ALSTOM's proprietary design codes and CFD codes like FLUENT®.

2.0 INTRODUCTION

The feasibility of using various models in concert with a process model like Aspen Plus® has been a focus of the Vision 21 project. The role of ALSTOM Power (AP) has been to assist the project team in helping to develop and demonstrate the capabilities of the advanced Vision 21 simulation and visualization tool. The primary AP responsibilities and tasks have included:

- providing its expertise and experience base in the utilization of both CFD and cycle analysis for the power generation industry,
- selecting and running two cases to test and demonstrate the feasibility of the concept,
- providing the data links and executables for the proprietary (AP) industrial codes that will be coupled with the process simulation software,
- forming an advisory board to provide project review and feedback.

2.1 Case Selections

One of the tasks, as specified in the Project Management Plan (Ref. 1), was to select the AP Test and Demonstration Cases. The project team's philosophy of progressing in a step-by-step manner, from the relatively simple to the more complex, was adopted in the plan. Therefore, Case 1 was required to be a conventional and relatively modest power generation cycle, of sufficient simplicity that it could be used to test the initial feasibility of using CFD and other methods in concert with a process model like Aspen Plus®. Case 2 was stipulated to be a more advanced cycle. More specifically, the two cases are defined as:

- Demonstration Case 1 -- a conventional steam cycle, containing a wall-fired coal boiler and post combustion cleanup equipment, fuel handling equipment, steam turbine and generator, heat exchange equipment, and pumps. A 30 MWe coal-fired power plant for municipal electricity generation was selected for the cycle study.

- Demonstration Case 2 -- a natural gas combined cycle, consisting of a gas turbine, steam turbine, heat recovery steam generator, etc. A 270 MWe, natural gas-fired, combined cycle power plant was selected for the cycle study.

Although neither case constituted a Vision 21 concept, a number of the cycle components in the cases exist in a Vision 21 plant. The final selection of an appropriate unit was also to be based on the availability of the cycle conditions and component data. Both Demonstration Case 1 and Demonstration Case 2 were selected and documented in separate letter reports to the DOE (Ref. 2 and 3, respectively).

One of the milestones and deliverables, as stipulated in the Project Management Plan (Ref. 1), was to provide a final task report, which contained a description of the case simulations, the results, and an itemization of desired software modifications or future work. This report summarizes and documents the demonstration case simulations, and will complete the requirement for the stipulated (contractual) final task report.

2.2 Run Selections

As described in the letter reports for Demonstration Cases 1 and 2 (Ref. 2 and 3, respectively), three (3) separate "runs" were planned and executed for each of the demonstration cases to demonstrate the viability of the software interfaces.

- <u>Run 1</u>: An initial (baseline) run was completed using the existing component libraries in Aspen Plus® to determine the overall cycle performance and characteristics.
- <u>Run 2</u>: The second run consisted of replacing one or more components or pieces of equipment with an AP proprietary design code.
- <u>Run 3</u>: The third run consisted of replacing a cycle component with a FLUENT® CFD code simulation.

Each of the three stipulated runs was performed over a range of loads. AP simulated the steam cycle at various loads (e.g., to simulate power demand changes from 100% to 50% in a pseudo-steady state fashion), using plant data for the initial calibration and subsequent predictive comparisons. Insofar as possible, for both Demonstration Cases 1 and 2, plant data was used to first calibrate the AP proprietary design codes over the load range, and then the computations of the design codes were used subsequently to calibrate and align portions of the cycle flowsheets.

The separate runs for each of the cases are tabulated below:

Table 1: Runs Pertaining to Each Demonstration Case

Demonstration Case	Run 1 (Baseline)	Run 2 (AP Design Codes)	Run 3 (CFD)	Component(s) Replaced
1	Library Modules	BPS	FLUENT®	Boiler “island”
2	Library Modules	HRSGPS	FLUENT®	HRSG “island”

It should be noted that the AP proprietary design codes utilized in Run 2 may encompass multiple pieces of equipment. For example, the boiler performance simulation (BPS) code encompasses the pulverizers or mills, the air preheater, the drum, and the boiler or industrial steam generator unit. The “boiler” unit calculated by the BPS code consists of the combustion chamber (connected to the gas-side of the cycle), as well as multiple heat exchanger tube banks (connected to the steam-side). In like manner, the heat recovery steam generator performance simulation (HRSGPS) code encompasses not only the heat recovery steam generator (HRSG), but also auxiliary pieces of equipment such as drums, separators, pumps, and desuperheaters. Therefore, when the user implements or instantiates a third-party code as a separate module on the flowsheet, that code may not simply replace a single analogous module, but may, in fact, replace several modules on the flowsheet, thus potentially necessitating additional cycle reconstructions and solution strategy modifications.

Unlike the proprietary design codes, the FLUENT® CFD simulations, associated with the Run 3 computations, are typically utilized to simulate only one piece of equipment at a time. However, that one piece of equipment may encapsulate the interaction or energy exchange between two or more independent streams. For example, the FLUENT® simulation for the boiler or HRSG will include not only the flow paths for the gas flow, but also the coupling of the gas-side convective and radiative heat transfer with the steam/water flowing through the various heat exchanger surfaces and tube banks inside of the unit.

Early in the project, it was recognized that the calculation of the boiler and HRSG islands in the demonstration cases could be approached in a couple of different ways. For example, one potential option was to break up a boiler or HRSG unit into its separate heat exchanger banks or surface types and treat each bank as a separate module on a flowsheet. However, in that type of treatment, the gas flow is passed to each heat exchanger bank as a single (bulk-integrated) material stream, and all of the 3-dimensional velocity, species, and temperature information is lost, thus effectively nullifying the reason for which the CFD model is being used in the first place. Furthermore, the simulation of energy transfer through complex, multi-dimensional processes, such as radiation transfer, becomes nearly impossible in a flowsheet environment. Consequently, it was decided that the FLUENT®

code should be able to treat, in coupled fashion, all of the gas-side flow, steam-side flow, and heat-exchanger processes that occur within a boiler or HRSG module, within a single CFD simulation of that module. Accordingly, AP worked with Fluent Inc. to enhance the prevailing heat exchanger model in FLUENT®, along with the corresponding AP proprietary subroutines (at no cost to DOE).

With this new tube bank model, the user can denote specific volumes within the computational domain as “tube banks” or heat exchanger “groups”, as well as connect them to each other in sequence, so that the output from one tube bank is automatically fed as the input to a “downstream” tube bank. The exterior (evaporative) boiler walls are handled with one of the available FLUENT® heat transfer boundary conditions (e.g., wall resistance plus a backside fluid temperature). The tube bank model has not been extended to superheat surfaces that are part of the external boiler walls or that hang down as isolated panels (i.e., the tube bank model is presently limited to volumes rather than surfaces). Customized correlations for heat transfer through the circular tubes of the tube bank are provided in AP user-defined functions (UDFs) or subroutines. The AP user-defined subroutines access steam-water properties through interpolative property tables.

All of the runs were performed with Aspen Plus® as the executive software. The “sequential-modular” solution approach was used in all cases, as opposed to the “equation-oriented” solution capability, since AT has not yet extended the CAPE-OPEN interface capability to the latter. Modules from the Aspen Plus® library were used without modification for all of the cycle components, with the exception of those components that were replaced by third-party software (as described above).

At one point in time, AT developed an advanced power plant cycle analysis package, as an add-on for Aspen Plus®, that was called STEAMSYS™. The STEAMSYS™ package provided sophisticated modules for power plant cycles, and utilized the “equation-oriented” or simultaneous solution technique to solve the set of governing equations. The equation-oriented methodology was required because the advanced modules forced much of the information flow to be in the “reverse” (upstream) direction, which made the governing equation set more stiff and precluded the use of the default “sequential modular” solution approach. However, AT has ceased to develop or support the STEAMSYS™ package and is considering whether the market will support the incorporation of the more advanced STEAMSYS™-type modules into Aspen Plus®. Consequently, the modules from the current Aspen Plus® library for power plant cycles are relatively simplistic and are not necessarily adequate in all cases for practical power plant analysis or “off-design” calculations. Oftentimes, engines and power equipment are typically designed to operate optimally at a single load point (denoted the “design” point). If it is assumed that the “design” point is near the maximum rating of the unit, then all lower loads are referred to as “off-design” points. In cycle analysis studies, the library modules may be calibrated so that they serve well at the design point, but that does not mean that they can properly simulate behavior at lower load or off-design points. It is presumed that companies that use Aspen Plus® for routine, practical power plant cycle analysis have enhanced the cycle modules through user-defined subroutines and performance mapping techniques and have validated the modules through repeated comparisons with plant data.

For the present project, the primary intent and focus was to demonstrate the viability of the controller interface and the linkage between Aspen Plus®, FLUENT®, and third-party codes. This project did not attempt to investigate the suitability of the library modules available in Aspen Plus®

to perform practical or rigorous power plant cycle analysis over the load range. In fact, neither the Aspen Plus® modules, nor the FLUENT® CFD cases, should ever be viewed as being wholly adequate for any rigorous design or cycle analysis without the requisite development and extensive validation and calibration exercises. While acknowledging that more could be done to enhance the reliability and accuracy of the demonstration case cycles and its components, this project used the Aspen Plus® library modules in their default form, with the primary purpose of demonstrating the integrity of the Vision 21 controller interface for cycle analyses of two existing power plants.

3.0 EXECUTIVE SUMMARY

The goal of this DOE Vision-21 project work scope was to develop an integrated suite of software tools that could be used to simulate and visualize advanced plant concepts. Existing process simulation software did not meet the DOE's objective of "virtual simulation" which was needed to evaluate complex cycles. The overall intent of the DOE was to improve predictive tools for cycle analysis, and to improve the component models that are used in turn to simulate equipment in the cycle. Advanced component models are available; however, a generic coupling capability that would link the advanced component models to the cycle simulation software remained to be developed. In the current project, the coupling of the cycle analysis and cycle component simulation software was based on an existing suite of programs. The challenge was to develop a general-purpose software and communications link between the cycle analysis software Aspen Plus® (marketed by Aspen Technology, Inc.), and specialized component modeling packages, as exemplified by industrial proprietary codes (utilized by ALSTOM Power Inc.) and the FLUENT® computational fluid dynamics (CFD) code (provided by Fluent Inc). A software interface and controller, based on an open CAPE-OPEN standard, has been developed and extensively tested. Various test runs and demonstration cases have been utilized to confirm the viability and reliability of the software.

ALSTOM Power was tasked with the responsibility to select and run two demonstration cases to test the software – (1) a conventional steam cycle (designated as Demonstration Case 1), and (2) a combined cycle test case (designated as Demonstration Case 2). Demonstration Case 1 is a 30 MWe coal-fired power plant for municipal electricity generation, while Demonstration Case 2 is a 270 MWe, natural gas-fired, combined cycle power plant. Sufficient data was available from the operation of both power plants to complete the cycle configurations.

Three runs were completed for each Demonstration Case – (1) an initial baseline run using the existing component libraries in Aspen Plus®, (2) a second run where one of the library components was replaced with an ALSTOM Power proprietary code, and (3) a third run where a cycle component was replaced with a FLUENT® CFD simulation. Each of the three runs was successfully completed over a range of loads.

For the two industrial proprietary codes (BPS and HRSGPS), the linkage with Aspen Plus® was based on a simple exchange of information through the CO parameter collection. The legacy codes functioned well in the CO environment, as might be expected, since the CO environment may be viewed as an enhanced extension of the Aspen Plus® custom UDF interface. In this project, no attempt was made to enhance the proprietary codes in any significant way, provide port connections, or automate them for this type of application, although much more work could be done in that area. In general, industrial proprietary codes have been validated through many years of use and are used routinely in the design process. Therefore, tremendous potential exists to utilize such codes synergistically within the framework of a process model environment, which may serve to motivate industry to move quickly to utilize proprietary codes in this manner. The only cost to industry will be the effort required to make the wrapper and the proprietary codes more automated and amenable to rapid cycle configuration changes.

The linkage between the FLUENT® code and Aspen Plus® has also been shown to be fairly well developed and straightforward. For the demonstration cases, the decision was made to provide a CFD boiler module for Case 1 and a CFD HRSG module for Case 2. Each of the CFD case grids were constructed with approximately 40,000 cells. These two modules involve coupling complexities that the typical FLUENT® module does not require, because not only was the 3-D computational domain linked up to the process flowsheet, but linkages also had to be provided for the 1-D tube bank model in the FLUENT® code. Because port connections were not available for the 1-D tube bank model, a large number (20 to 60) of additional stream and informational parameters had to be included in the CO collection.

Overall, the replacement of Aspen Plus® library modules with more detailed and versatile (third-party) software modules (e.g., proprietary industrial codes and CFD) enables the designer to operate the cycle in a much more realistic fashion over the load range. Furthermore, with the additional capabilities often times embodied within the third-party software, the designer can potentially interrogate the code or post-process the computational domain to obtain additional design information that is not normally available in library modules, such as emissions, particle distributions or pattern factors, etc..

4.0 EXPERIMENTAL WORK

There is no experimental work under this project.

5.0 RESULTS AND DISCUSSION

5.1 Demonstration Case 1 – Facility and Cycle Description

A municipal power station, which provides electricity to a city in the United States, was selected for the Case 1 conventional steam cycle. Facility details are also provided in Ref. 2. The reasons for selecting this particular cycle included:

- The quantity and quality of the available data from the unit was deemed to be sufficient for constructing a cycle and the component boiler models.
- In conjunction with a calibration effort, it was believed that appropriate assumptions and adaptations could be made that would permit the unit to be simulated successfully with an AP design package, as well as with other component software packages (e.g., CFD).

- Relative to other candidate units or cycle configurations, the unit offers the advantage of a potentially smaller mesh size, fewer heat exchanger sections in the boiler, and a simpler cycle connectivity.

5.1.1 Power Plant Facility

A municipal power station, which provides electricity to a city in the United States, was selected as the Demonstration Case 1 conventional steam cycle. The unit is shown in Figure 1. Two units (Units 1 and 2) share a common stack equipped with continuous emission monitoring (CEM) equipment. Unit 1 will be the focus of the computations.

Figure 1: Photograph of the Demonstration Case 1 Unit and Site.

In general, the steam generator for Demonstration Case 1 is a 1950s vintage front wall-fired, balanced draft, natural circulation steam generator with a nominal superheated steam flow of approximately 41 kg/s (325,000 lb/hr) at 755.4 K (900°F) and 6.2 MPa (900 psig). (The steam-generator or boiler was not designed or built by AP.) The six burners are arranged in two elevations of three burners each, and are supplied pulverized coal by a total of three Raymond #533 bowl mills. A single Ljungstrom® air preheater is used to heat the secondary air from ambient conditions to a windbox temperature of 599.8 K (620°F) at full load. Nominally rated at 33 MWe, the unit is equipped with a General Electric Turbine Generator, Westinghouse closed heaters, and a Worthington condenser. It is also equipped with an electrostatic precipitator. Other flue-gas cleanup equipment is available at the site, but is not presently used. The unit fires a midwestern bituminous coal.

In 1996, the original burners in unit were replaced with the ALSTOM Power Services' coal-fired, low NOx, RSFC™ (Radially Stratified Flame Core) burners. The RSFC™ burner has three air register zones to supply three different air annuli at the burner exit. The combustion flow field is controlled by means of individualized flow splits and swirl numbers for each air annulus. The swirl in the primary and tertiary air streams are generated through the use of moveable vane swirlers; an axial fixed vane swirler is utilized in the secondary air annulus.

The furnace width across the front wall (on which the burners are located) is 7.2 m (23' 7-1/2"), while the furnace depth (to the rear wall at the burner elevation) is 6.4 m (21' 1-1/8"). The approximate height of the furnace, to a mid-point on the slanted roof, is on the order of 19.8 m (65'). A sectional side view drawing of the boiler is shown in Figure 2.

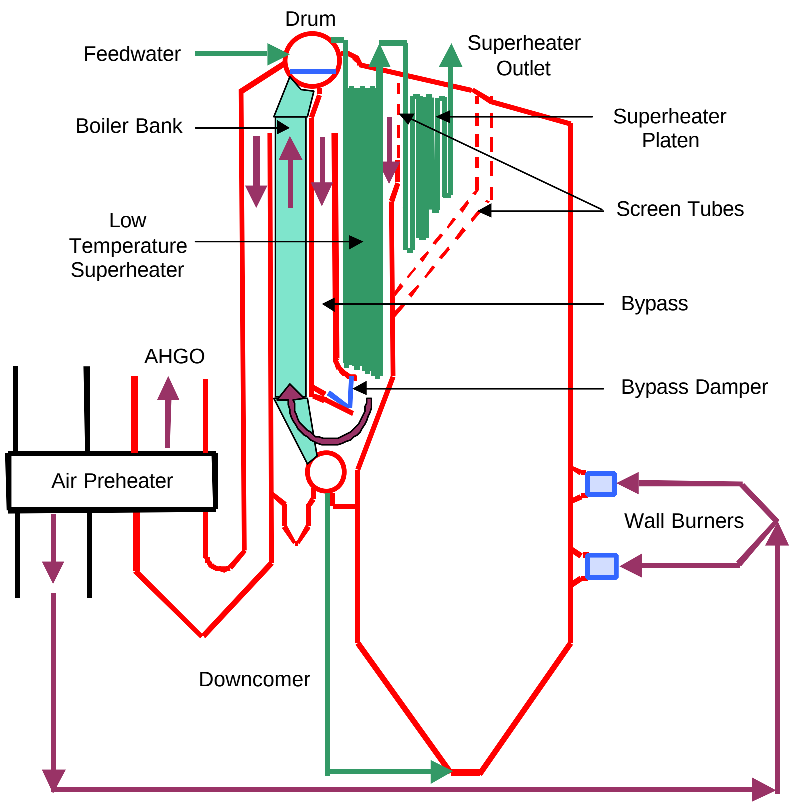

Figure 2: Sectional Side View of the Boiler Island for Demonstration Case 1.

Hot gases from the firing zone region flow upward through some "screen" tubes and then through the superheater platen section. After passing through an additional row of screen tubes, the flue gas then flows vertically downward through a low temperature superheater (LTSH) section and a bypass cavity, which are configured to be in parallel with each other. The extent to which the flue gas flows preferentially through either the bypass cavity or the LTSH section is determined by the backpressure supplied by the bypass damper. The flue gas then flows vertically upward through a "boiler bank" and then vertically downward through a final exhaust cavity or duct. The flue gas passes through an air preheater, heating the air to the secondary air temperature required by the burners. The flue gas exiting from the air preheater at the air heater gas outlet (AHGO) is then passed through an electrostatic precipitator and (possibly) other cleanup equipment, before it is exhausted to the stack.

On the steam side, subcooled feedwater is fed to the drum, where it is heated to saturated conditions. The saturated water flows down to a second holding drum (containing saturated water only), and from there, it flows through various "downcomers" to manifolds that feed the waterwall "riser" tubes that constitute the walls of the furnace. The combustion processes inside the furnace provide the heat flux to the walls that heat up the water inside of the riser tubes, producing steam. The waterwall tube circuits return the steam/water mixture to the drum. Connecting the upper and lower drum is a large number of single-pass tubes that are collectively referred to as a "boiler bank."

Only two types of heat exchanger sections are utilized in the Case 1 power plant – evaporative sections and superheat sections. The waterwall tube circuits, boiler banks, and screen tubes constitute the evaporative heat exchanger surfaces. The low-temperature superheat (LTSH) and platen sections constitute the superheat sections. Saturated vapor leaves the drum through the overhead steam line and travels through the (LTSH) section, followed by a higher temperature superheat platen section, where the steam is superheated to the temperature required by the turbine. The relative amount of the total absorption that is allocated to superheating versus the relative amount of the total absorption that is allocated to evaporative heating is controlled by the operator. The amount of superheat absorption is controlled primarily by factors such as bypass damper position and excess air. For example, if the bypass damper is closed, then the bypass cavity is back-pressured, causing most of the flue gas to pass through the low temperature superheater, thereby preferentially giving most of the remaining energy to the superheat section, at the expense of the boiler bank.

5.1.2 Steam Cycle

A schematic of the industrial steam cycle for Demonstration Case 1 is shown in Figure 3. Only evaporative and superheat sections prevail in the boiler. The boiler does not have any reheat or economizer sections. In addition, the steam cycle does not have any superheat (or reheat) desuperheater spray.

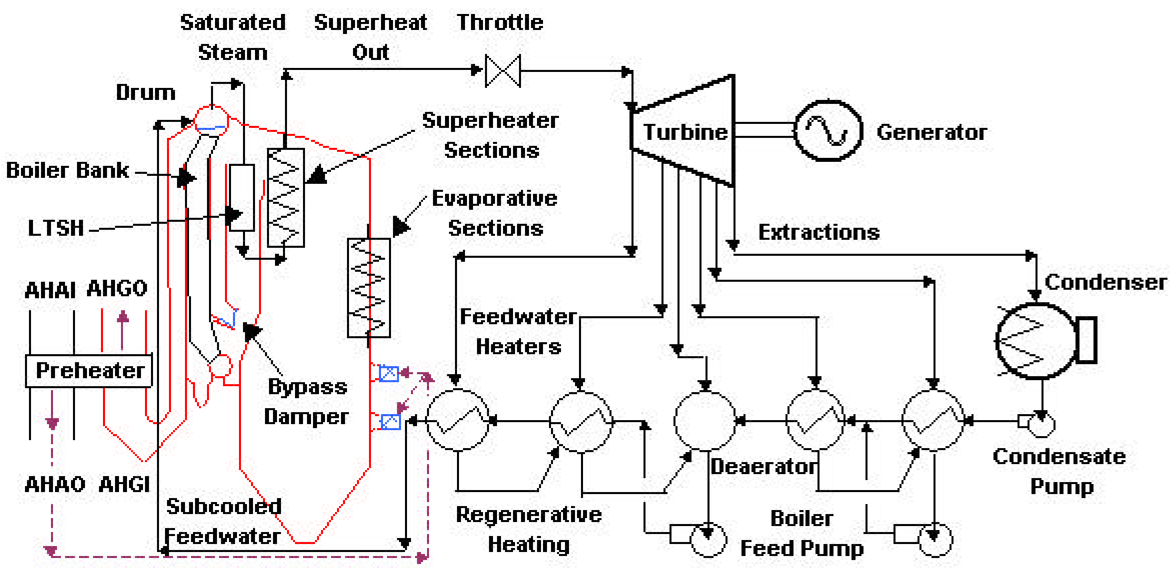

Figure 3: Steam Cycle Schematic for Demonstration Case 1.

As mentioned previously, the bypass damper is used to control the relative amounts of evaporative heat absorption versus superheat absorption. Superheated steam at the “superheat-out” location is passed through a throttle, which reduces the steam pressure to a value required by the turbine. The superheat outlet temperature is dictated by turbine material considerations and is maintained at a constant value over a range of loads, from the load at the maximum continuous rating (MCR) to the “Control” load (e.g., 67% of MCR), below which the boiler cannot achieve the required turbine inlet temperatures. At MCR, the boiler unit is designed to provide a superheat outlet steam flow of approximately 41 kg/s (325,000 lb/hr) at 755.4 K (900°F) and 6.2 MPa (900 psig).

Five “feedwater heaters” for regenerative heating are fed by a corresponding number of extractions from the turbine. The subcooled feedwater is heated by passing the condensate from a Worthington condenser, via two circulating water pumps, through the Westinghouse (closed) feedwater heaters and a deaerator. The subcooled feedwater is then routed to the boiler drum.

5.2 Case 1 : Run 1 – Aspen PlusÒ With Library Modules Alone

A rendition of the Demonstration Case 1 industrial steam cycle, as constructed by AP for use with Aspen Plus® library modules, is shown in Figure 4.

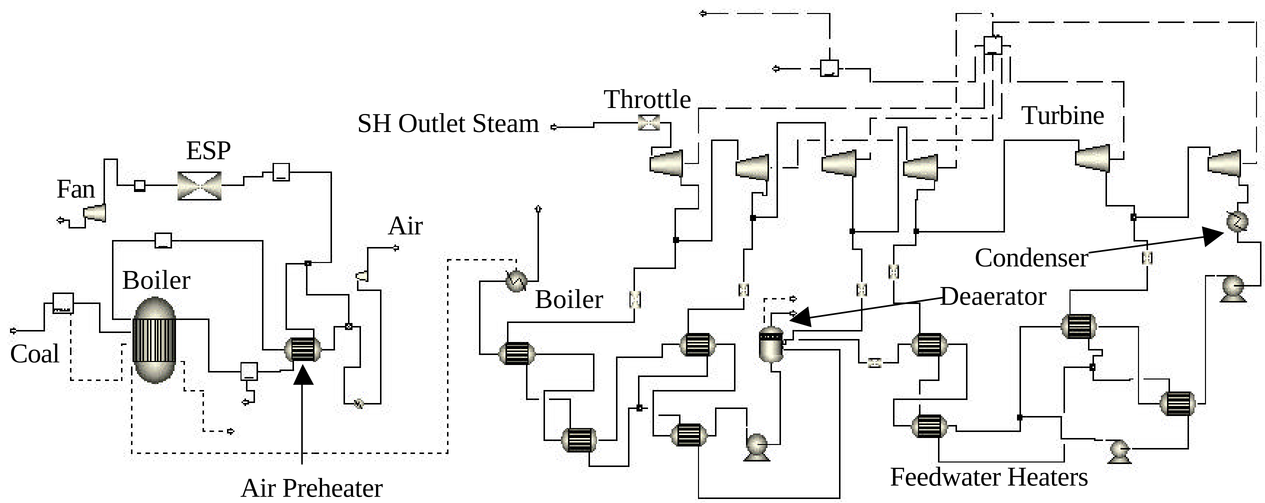

Figure 4: Aspen PlusÒ Steam Cycle Model for Demonstration Case 1.

In order to construct and calibrate the cycle, limited experimental (board) data at 33, 30, and 22 MWe was available from the 1950s. Additional boiler-related board data at those same load points (plus 14 MWe) was also available from more recent tests conducted during nozzle retrofits. The 33 MWe condition will be referred to as the maximum continuous rating (MCR) point for the unit. The 22 MWe condition is the “control” load (CL), and the 14 to 12 MWe load points are close to the minimum (flame) stability condition. It should not be assumed that industrial power stations operate “continuously” over a wide range of loads; rather, they will typically operate at their maximum possible load and perhaps one or two other “idle” or “start-up” loads. Since only a limited amount of data from the selected unit was available to perform the calibration, a number of assumptions were made about the operational characteristics of the equipment.

The cycle may be viewed as having a gas side and a steam side. On the gas side, air is heated in an air preheater and then sent to the boiler, where it is mixed with coal and combusted. Sufficient air is added to produce 20% excess air (over all loads). The boiler is represented by a chemical equilibrium reaction block from the Aspen Plus® library. The flue gases are exhausted from the boiler, through the air preheater, to an electrostatic precipitator (ESP).

The interface between the gas-side and steam-side portions of the cycle occurs in the boiler tube banks. This interface is represented by the chemical equilibrium reactor on the gas side and a single heat exchanger icon in the steam loop, representing the boiler tube sections. On the steam side, the overall enthalpy difference between the feedwater flowing into the heat exchanger block (from the feedwater heaters), and the enthalpy of the superheat outlet stream flowing to the turbine, is equal to the desired boiler duty. A knowledge of this calculated boiler duty is transferred from the heat exchanger block (on the steam side of the cycle) to the chemical equilibrium reactor (on the gas side) via an energy transfer stream (a dashed line). An Aspen Plus® design specification is used to manipulate or vary the coal feed rate until the objective function for the reactor or boiler heat duty is equal to that dictated by the heat exchanger block on the steam-side of the cycle. Over most of the load range, the boiler island simply produces the superheated steam at the pressure and temperature dictated by the steam cycle specifications and the turbine material considerations.

For the steam-side of the cycle, no performance maps were available for the components. Insofar as possible, the component performance was matched or fit to the available data as a function of the steam flow rate (normalized to the steam flow rate at the design point). The superheat outlet steam from the superheat platen tube bank in the boiler is throttled to the desired pressure, after which it is fed to the turbine. The turbine and feedwater heaters have been artificially split or multiplied in order to meet the various material stream mass and energy constraints for the feedwater extractions imposed by the Aspen Plus® solution methodology. The discharge pressures for the throttle and the turbine extraction points were fit from the data. The variation in discharge pressures as a function of load was related to the superheat outlet steam flow rate. The isentropic efficiencies of each turbine component were calibrated to provide the correct steam temperature at each turbine discharge.

The turbine extractions are fed to four regenerative feedwater heaters, configured in a countercurrent arrangement, as well as to a deaerator. Each feedwater heater is split into two blocks to accommodate a mixing junction positioned between the two blocks, the purpose of which is to accept an output stream from an adjacent feedwater heater bank. For the first of the two aforementioned blocks (which collectively represent a reheater), the hot stream outlet vapor fraction is set equal to zero (i.e., at a saturated liquid condition). In addition, an Aspen Plus® design specification is used to manipulate or vary the split fraction from the turbine extraction until the objective function for the terminal difference is satisfied. The terminal temperature differences for the feedwater heaters range from 5 to 1.7 K (9 to 3 °F). For the second reheater block, a hot stream outlet temperature approach (or drip approach) is specified with values that range between 7.8 and 1.1 K (14 and 2 °F).

The purpose of the deaerator or contact heater is to remove dissolved oxygen from the feedwater in order to minimize the formation of pre-boiler corrosion products. The deaerator block was solved in a manner similar to the feedwater heaters -- the vapor fraction was set to zero and the split fraction from the turbine extraction was varied in a design specification until the heat duty of the deaerator was zero (i.e., adiabatic conditions). All of the design “specs” were solved with the default secant method in Aspen Plus®.

Results from the Aspen Plus® run are shown in Figures 5 and 6. For these runs, the target superheat outlet temperature was about 755.4 K (900 F) and the superheat outlet pressure was 6.0 MPa (873.7 psi).

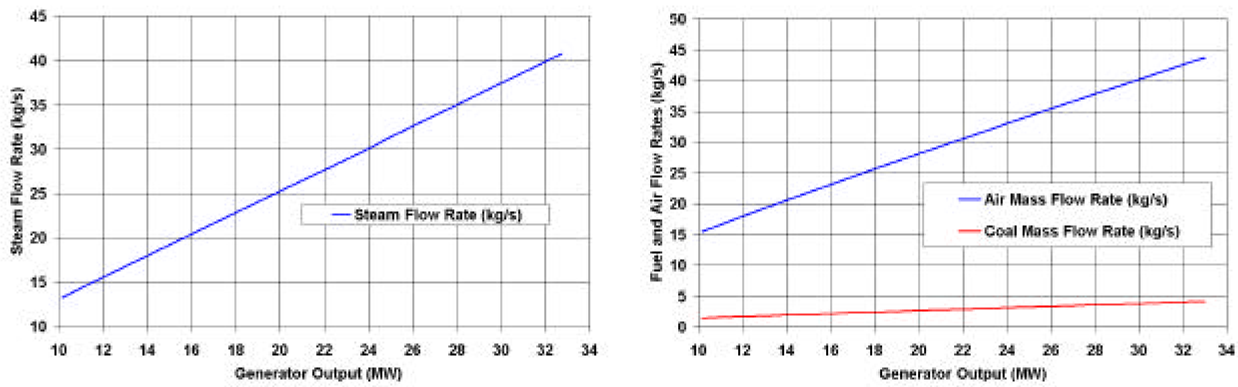

Figure 5: Case 1 : Run 1 Results – Steam, Fuel, and Air Flow Rates.

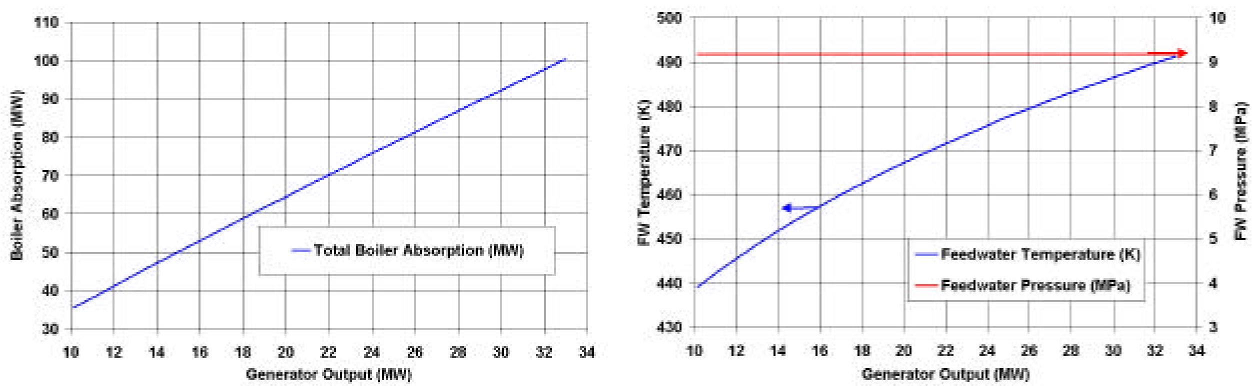

Figure 6: Case 1 : Run 1 Results – Boiler Absorption and Feedwater Conditions.

The results are representative of the experimental data (not shown), and were deemed adequate for demonstration purposes.

5.3 Case 1 : Run 2 – Aspen PlusÒ Coupled With BPS

Run 2 consists of the coupling of an AP proprietary code with Aspen Plus®. The AP proprietary design package selected for use was an industrial-boiler performance simulation (BPS) code. The BPS package is a legacy design code that was built upon proprietary empiricisms, refined over time through experiments and accrued experience, and effectively recalibrated with each completed contract. As is typical of many such codes in industry, it was constructed with old FORTRAN, fixed format inputs (left over from the card-input era), and batch output files. Certainly, the Vision 21 Virtual Simulation environment must have the ability to accept the valuable information contained in such legacy codes.

The BPS package had been coded and validated for ALSTOM industrial boiler designs only. The application of the design package to non-ALSTOM units posed some challenges. For example, modern ALSTOM industrial boilers do not have a bypass baffle for steam temperature control and consequently the BPS package did not have this capability. However, the performance simulation package did have the capability to accommodate a split backpass design, and following some minor code and input changes, this approach was used as a “work around” to simulate the baffle functionality. The BPS package also could not easily accommodate the geometric and design features (e.g., the serpentine backpass arrangement, the height of the boiler bank, etc.) associated with Demonstration Case 1. Nevertheless, with the appropriate assumptions, adaptations, and approximations, the calibration procedure did allow the (non-ALSTOM) boiler unit to be simulated successfully with an AP design package. Since the current project required a demonstration of proof of concept and viability of the overall approach, rather than a demonstration of a specified level of quantitative predictive accuracy, the code modifications were deemed adequate.

The BPS package contains a series of software modules that simulate various pieces of equipment in the boiler island. The air preheater module and the mill or pulverizer module were regarded by their division managers to be highly proprietary, and they were removed from the design code before the executable could be granted permission to be moved from its original server to a local computer and utilized in the present project. Simple models of the air preheater and mill operational characteristics were inserted into the BPS code to take the place of the modules.

5.3.1 Software Linkage

As shown in Figure 7, when the BPS code is “instantiated” (i.e., placed) as a CAPE-OPEN block upon the Aspen Plus® flowsheet from the Aspen Plus® CAPE-OPEN module template, it essentially replaces the entire gas-side of the cycle. The BPS code contains all of the required information about the gas-side components, including the air preheater, the pulverizers, etc. Components like the ESP could have been retained on the flowsheet, but were omitted for convenience. In the present case, the BPS code constitutes a single block icon on the gas-side of the flowsheet that must interact with and exchange information with the steam-side of the cycle. The BPS package has not been coded with material stream or port connections; that is, no provision has been made for the material or energy streams, which typically connect the flowsheet blocks in Aspen Plus®, to connect directly with the BPS block. Consequently, all of the information exchange between Aspen Plus® and the BPS code must occur through a transfer of shared variable or parameter values. The controller and software interfaces between the BPS code and Aspen Plus® package, constructed by the Vision 21 project team programmers, assists in the transfer of this information.

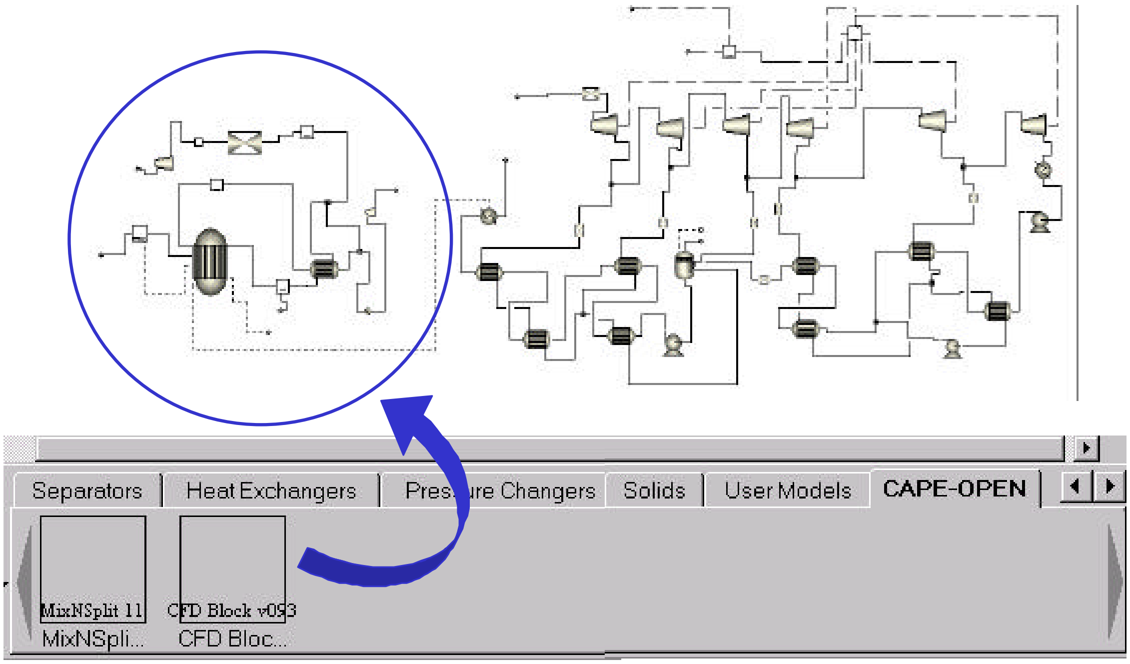

Figure 7: Instantiation of CAPE-OPEN Block Representing the BPS Code.

An extensive description of the interface software and utilities has been provided in the users' manual (Ref. 4) and other documentation provided by Fluent Inc. However, a sufficient description will be provided in the remainder of this section to orient the reader to those features and details that are germane to legacy, third-party codes.

A schematic showing the *V21 Controller* interface and "COM-CORBA" bridge configuration for proprietary legacy codes is shown in Figure 8. Aspen Plus®, the controller and the proprietary code wrapper all utilize the CAPE-OPEN standard as the basis for the exchange of information. The Global CAPE-OPEN (Computer Aided Process Engineering – Open Simulation Environment) standard consists of definitions for exchanging information with process simulation software (e.g., www.colan.org; Ref. 5). The CO interfaces were developed by a consortium of chemical companies, software vendors and universities under funding from the European Union. CO interfaces are well suited for the communication between plant-level and equipment-level models and are the *de facto* standard in process simulation technology. By using open (non-proprietary) and standard CO interfaces, developers are ensured that their models will be able to exchange information seamlessly with any other model in the *Virtual Simulation* environment. CAPE-OPEN Version 1.0 was used in all of the case interface constructions.

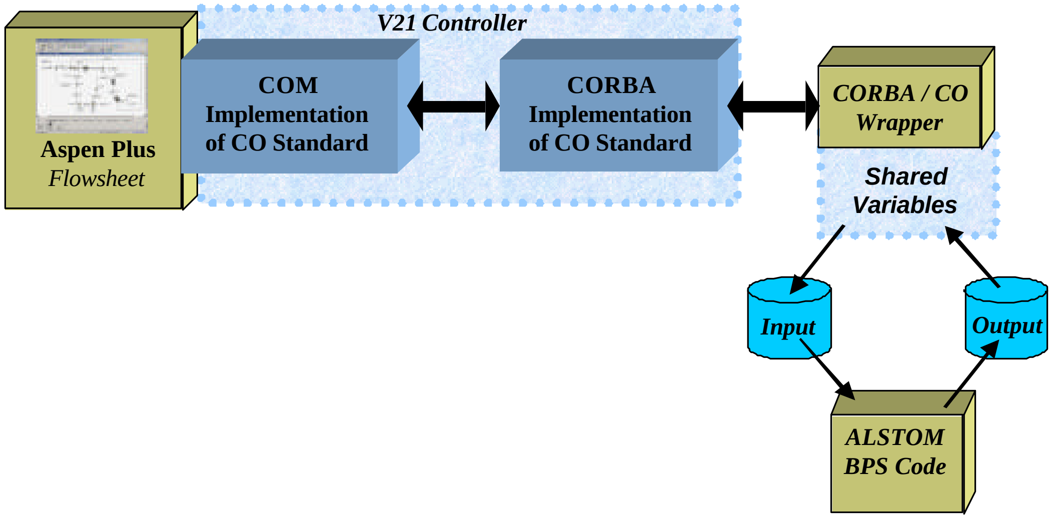

Figure 8: Software Controller Interface Configuration for the Proprietary BPS Code.

The "COM-CORBA Bridge" enables communication between models running under different operating systems. COM (Component Object Model) refers to both a specification and implementation developed by Microsoft Corporation that provides a framework for integrating software components running under the Windows operating system. CORBA (Common Object Request Broker Architecture) is a specification of a standard architecture for object request brokers (ORBs), which 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). The COM-CORBA Bridge enables, for example, Aspen Plus® running under Windows 2000 to communicate with a third-party code running under LINUX.

The V21 Controller exchanges information with the *CORBA/CO Wrapper*. For third-party codes, such as the BPS code, the CORBA/CO interface capability may be incorporated into the wrapper in at least two ways:

(1) Tightly integrated approach, where the third-party code "stays alive" during each of the flowsheet iterations, and the parameters are held in memory and transferred directly through the CO interface. In this approach, additional programming modifications to the third-party code are required to ensure that initialization routines are bypassed. The FLUENT® CFD code is an example of this approach.

(2) File I/O approach, where the third-party code is sequentially re-initialized and re-executed as a batch run with each flowsheet iteration. If the time associated with file I/O is small, then this approach becomes attractive, because modifications are made only to the input and output files, and access to the third-party source code is not required.

For the sake of simplicity and convenience, the latter approach was adopted. Fluent Inc. provided a template for the CO-compliant wrapper (written in C++), and appropriate modifications and additions were made to the wrapper to accommodate the BPS code requirements. Since the BPS code functioned in a file I/O mode, only a few of the interface routines from the CO library had to be modified (e.g., methods/functions such as getParameters, initialize, and calculate). The compiled wrapper was implemented as a dynamic link library (.dll). Approximately 3 man-weeks were required to complete the coding for the wrapper and debug it.

In order for the BPS code to execute properly and provide meaningful results, it must receive updated information from the Aspen Plus® cycle. A CO variable has been defined for each informational item or parameter that must be passed from Aspen Plus® through the V21 Controller to the BPS wrapper. The wrapper receives the updated CO parameter values and overwrites the BPS input file to reflect the current state of the shared variables. The wrapper then spawns the execution of the BPS code. It subsequently reads the BPS output file, extracts the specific parameters required by the Aspen Plus® cycle, and updates the state of the shared parameters. As with the input, a CO variable has also been defined for each informational item or parameter that must be passed from the BPS wrapper back to the Aspen Plus® cycle.

Both the V21 Controller and the CORBA/CO Wrapper must have a collection of CO parameters, and there should be one-to-one correspondence between those two collections. The CO collections and their relationship to the interfaces is shown in Figure 9.

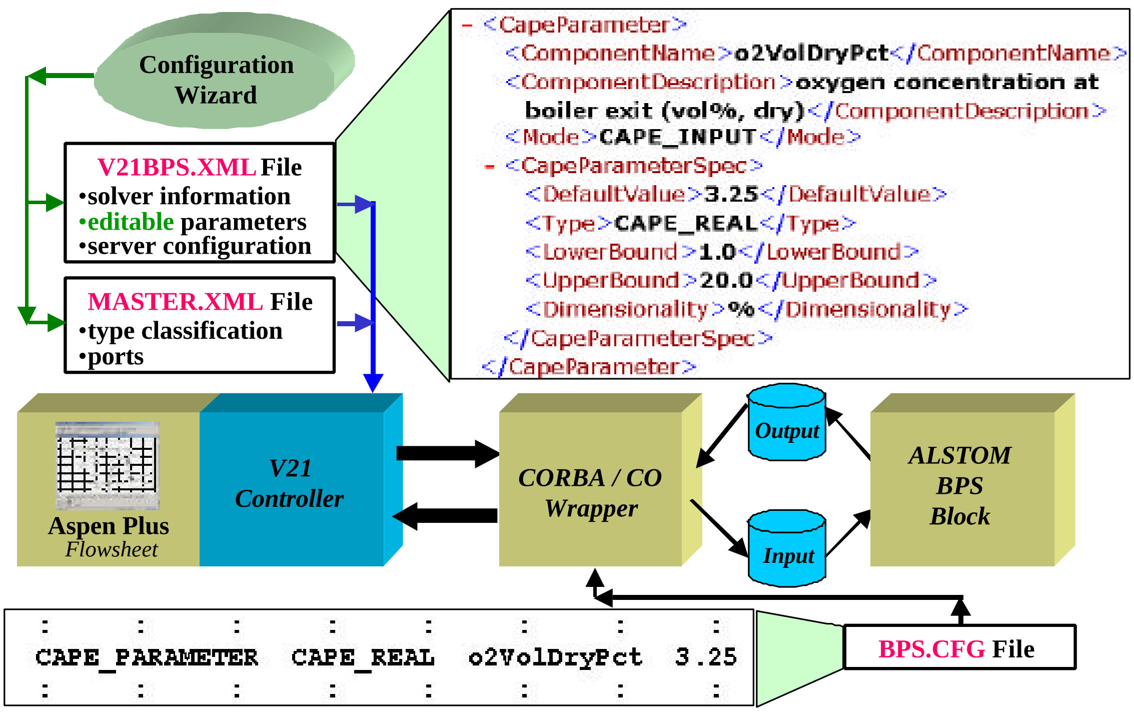

Figure 9: CO Parameter Collections for Both the Controller and the Wrapper.

The reason for the necessity of two "equivalent" CO collections is that the controller scrolls through its CO collection and looks for a parameter match in the wrapper's CO collection; only when it finds a match, does it update the value of the CO parameter on the wrapper side. On the controller side, the collection is created by reading in two XML files (created by running the *Configuration*

Wizard). On the wrapper side, for the BPS code, the CO collection is created by reading in a separate parameter listing in a configuration file (e.g., BPS.cfg), although the wrapper could also be made to read in the XML files as well.

5.3.2 Creation and Modification of the CO Collection for Legacy Codes

The *Configuration Wizard* (CW) is the utility used to create the two XML files that are read by the V21 Controller. For a legacy code, like the BPS code, the CW is launched by typing the word "cowizard" in an MS-DOS window (see Figure 10). The solver name is equivalent to the compiled dynamic link library name (e.g., prefix of V21BPS.dll). The V21 Controller automatically looks for the pertinent files in the default database directory "ModelDataBase." Drilling down to successive levels under the database directory tree, the model "category" directory was arbitrarily denoted as Reactors and the model "type" directory was designated "Boilers." The Aspen Plus® (.bkp) files, as well as the XML files, were placed in the "Industrial-Boilers.model" directory (under the Boilers directory). The suffix (.model) is a required feature in the directory name. The legacy code executable and I/O files, as well as the parameter configuration files for the wrapper, were put into a directory named V21BPS one additional level down (although this particular directory configuration may be restructured in the future).

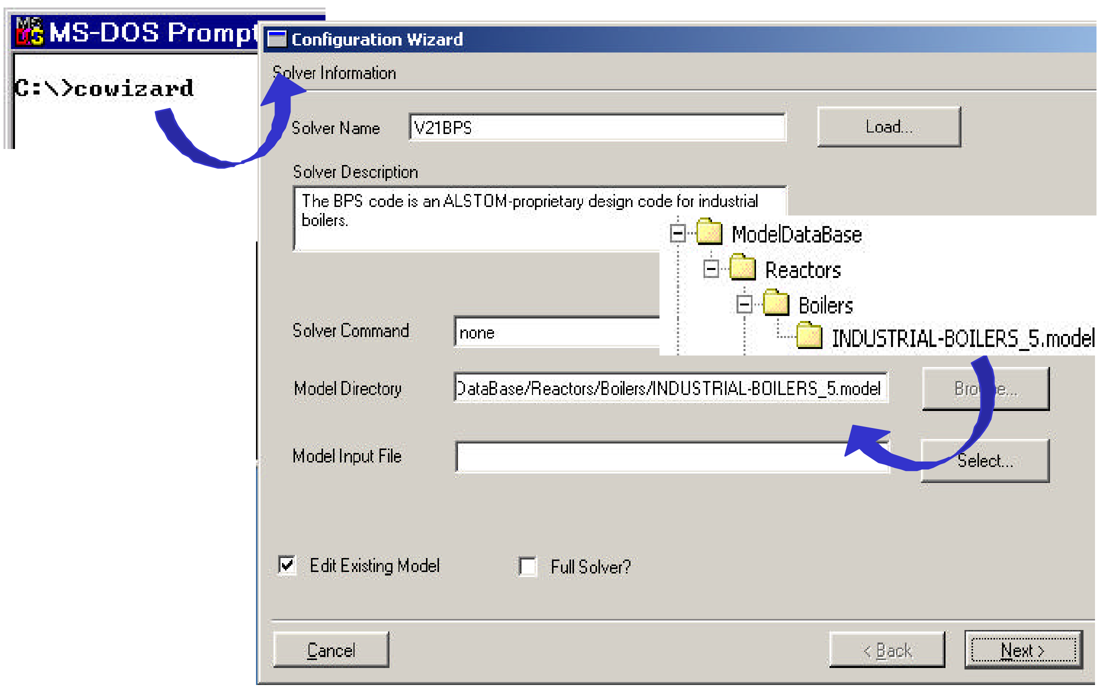

Figure 10: Configuration Wizard Panel for the BPS Code.

On the second panel (not shown) of the CW utility, specific model information is provided, as well as the aforementioned model "category" and "type" information. The third panel (not shown) deals with material stream ports, of which there are none in the BPS block. The fourth panel (not shown) is associated with the definition of basic CO parameters, and the fifth panel is associated with advanced CO parameters, as shown below in Figure 11. A total of 19 CO variables were defined in the "advanced parameters" panel, with type designated as "real" (as opposed to e.g., integer or boolean), and with their corresponding default values, units, and lower and upper limits. All of the variables were given Read-Write access (as opposed to Read-Only or Write-Only), which means that the user is permitted to access and modify the variables as desired through the Aspen Plus® graphical user interfaces (GUIs). Of those 19 CO parameters, 12 were used to modify the input file, and 10 were extracted from the output file to pass back to the Aspen Plus® cycle (with some overlap between the two sets). After all of the CO parameters have been entered on the Advanced Parameters panel (Panel 5), the CW writes the V21BPS.xml and Master.xml files to the model directory, as well as a file called Collection.dat, which contains a tabulation of all of the CO parameters.

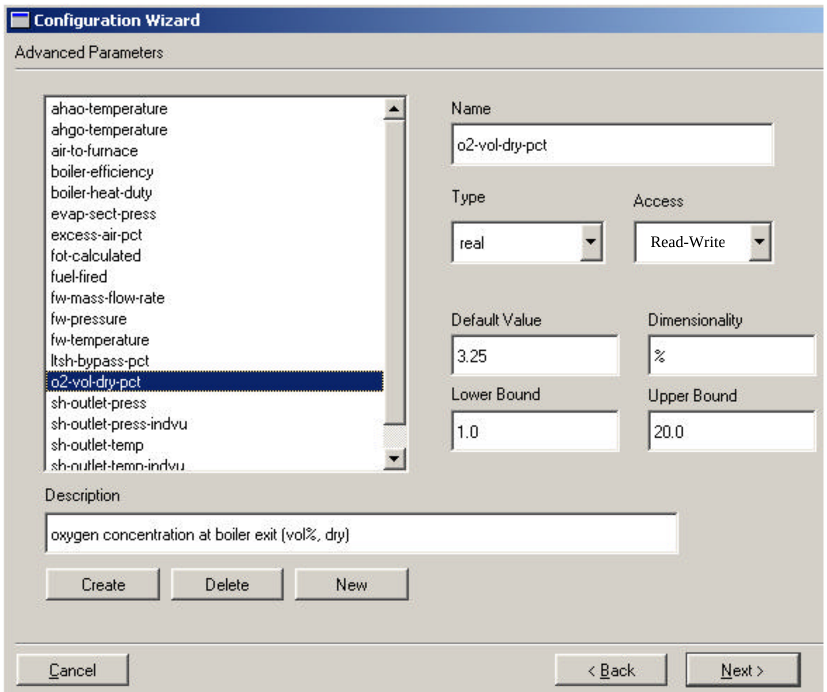

Figure 11: Advanced CO Parameters Panel for the BPS Code.

Once the XML files have been generated by the CW, one is poised to launch the coupled Aspen Plus® / BPS run. When the Aspen Plus® run is launched, the Model Selection panel (not shown) pops up with tabs for ports, parameters, and solver information. The user is expected to drill down to the appropriate directory in the model database, which, when completed, instantaneously populates the tabs in the GUI with the contents of the XML files. The Model Edit panel (not shown) then pops up, which contains additional tabs for solution strategy, basic parameters, and advanced parameters. At this juncture, the user can peruse the contents of the tabs and ensure that the case is set up as expected. When the user exits that panel, the Aspen Plus® cycle is launched and initialized, as well as the BPS wrapper.

The initial default values of the CO parameters can be modified in two ways: (1) by right-clicking on the BPS block and selecting Edit Model from the pop-up menu (see Figure 12), or (2) by accessing the Blocks section in the Aspen Plus® Data Browser, and selecting the CO block (denoted B1), and then subsequently selecting Parameters (see Figure 13). Both of these methodologies can be used to provide access to editable fields for the CO variables.

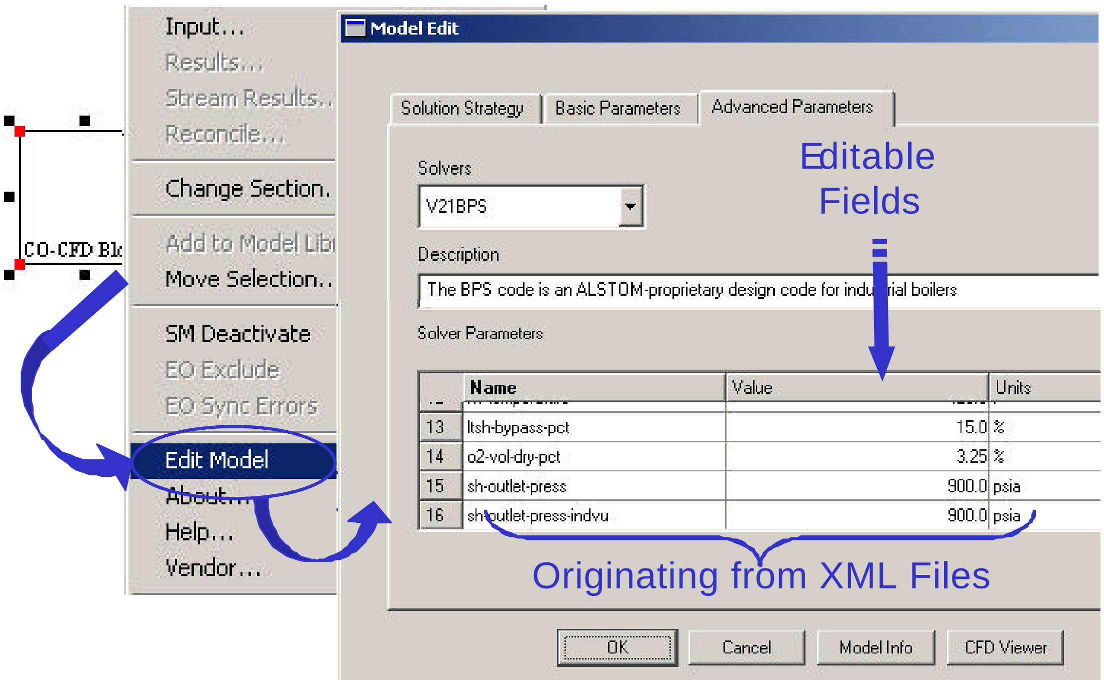

Figure 12: Model Edit Panel for Editing CO Variable Fields.

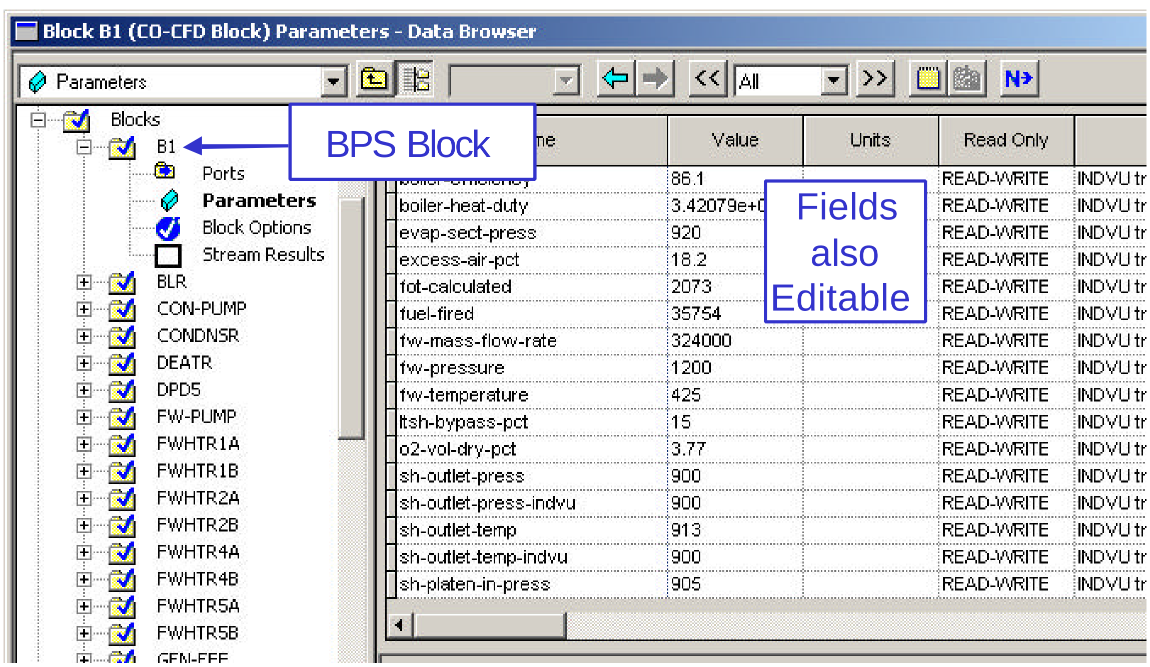

Figure 13: Block Parameters Panel for Editing CO Variable Fields.

5.3.3 Association of the CO Collection With Aspen Variables

Aspen Plus®, as the executive software, controls and manipulates execution of the BPS block through its internal utilities, including "design specs", "calculator blocks", and "sensitivity functions." For Aspen Plus® to be able to control and manipulate the BPS block, it must have access to the collection of CO parameters that the BPS wrapper and, in turn, the V21 Controller, have exposed to Aspen Plus®. As shown in Figure 14, the parameter or variable names that Aspen Plus® uses must be linked manually to the corresponding parameters in the CO collections maintained by the wrapper (or controller). These manual associations are performed in the Aspen Plus® utilities mentioned previously (i.e., design specs, calculator blocks, and sensitivity functions).

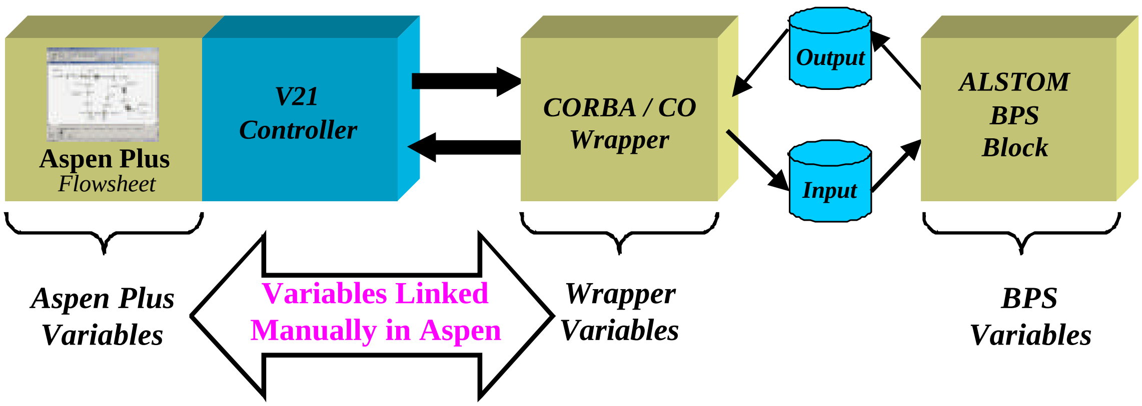

Figure 14: Accessing the CO Collection with Manual Associations in Aspen PlusÒ.

As an example of making such manual associations is provided in Figures 15 through 17. In the Design Spec DS-SHTEM, accessed from the Data Browser, the user may define a new variable within Aspen Plus® denoted O2DRY (see Figure 15). These new variable names must follow the Aspen Plus® naming conventions (e.g., maximum of 8 letters).

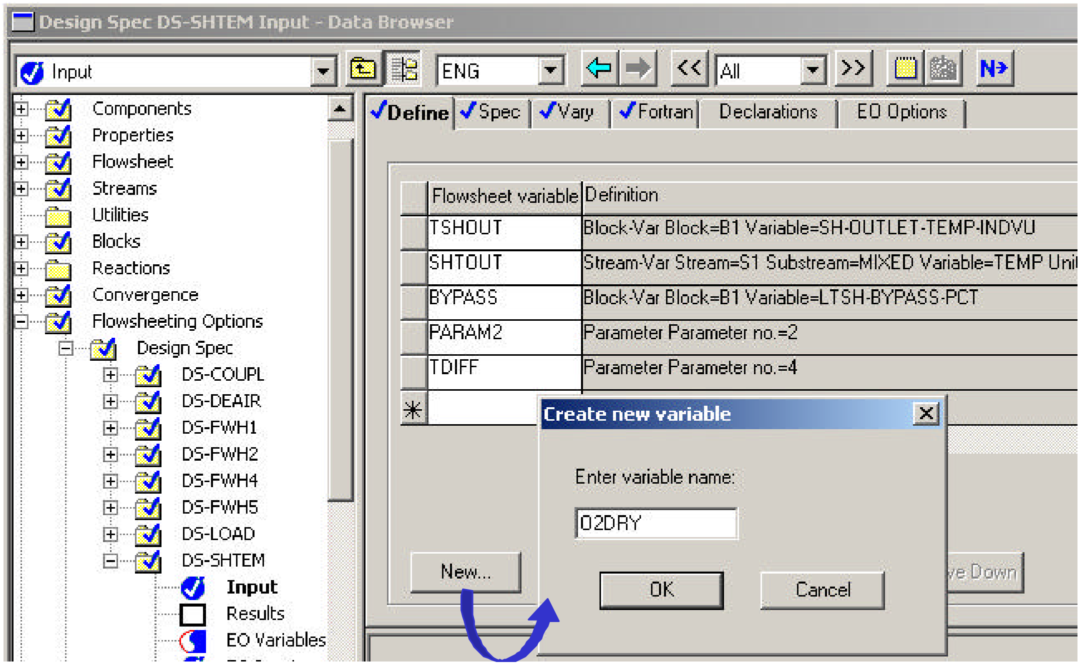

Figure 15: Creation of New Variable in BPS Design Spec.

When a new variable is defined, then the Variable Definition panel pops up, and the user is expected to associate a reference definition with the variable (e.g., a particular stream or block parameter). In this particular case (see Figure 16), the BPS block (Block B1) was selected, and for the Variable entry, a window pops open which exposes the tabulated collection of CO parameters and allows the user to select the corresponding CO variable. It should be noted that the variable names in the collection of CO parameters, which are read into the BPS wrapper (from a configuration file) or the V21 Controller (from the XML files), must not contain any upper-case letters (although Aspen Plus® will ultimately echo them as upper case).

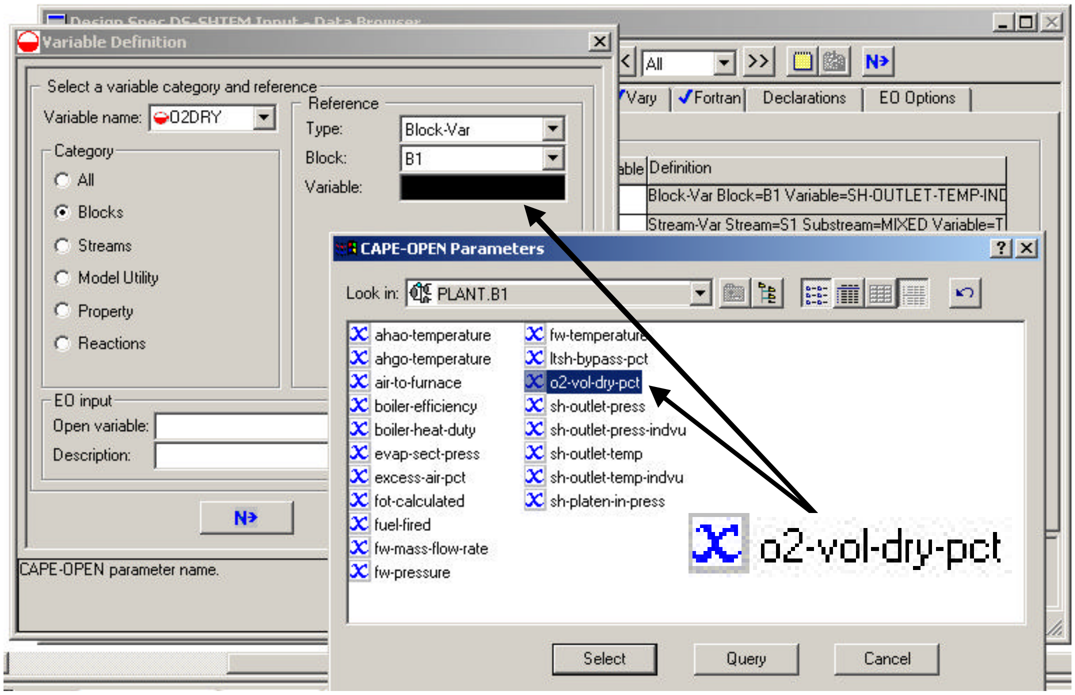

Figure 16: Selection of CO Parameter to Associate with Block Variable Definition.

The final associativity is reflected in the flowsheet variable definition field, with the Aspen Plus® parameter on the left-hand side, and the wrapper parameter on the right-hand side (as shown in Figure 17). With the associativity completed, the "Fortran" tab can be used to manipulate or make assignments to the Aspen parameter, and those alterations will be propagated to the corresponding CO variable pertaining to the BPS wrapper and block.

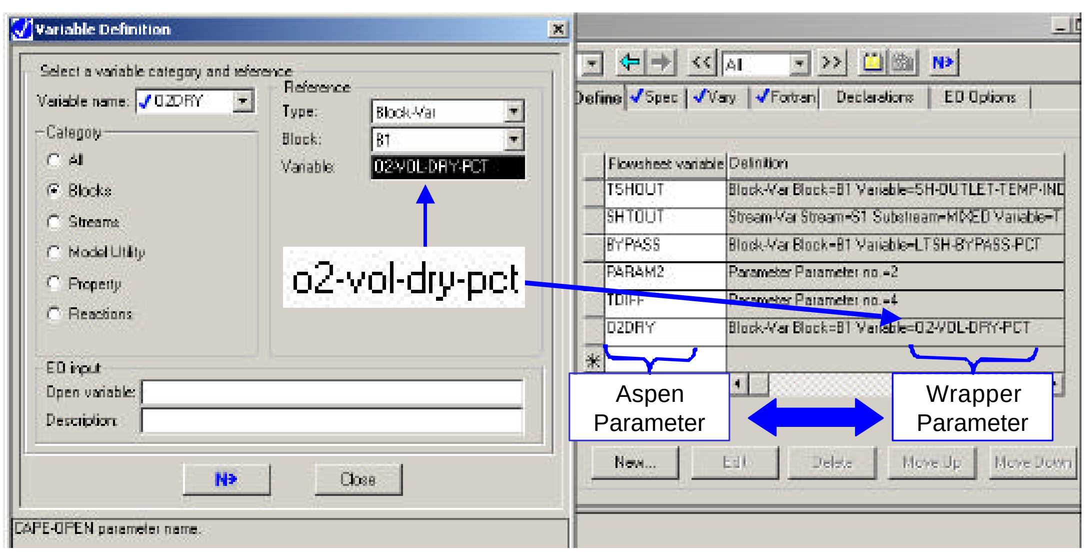

Figure 17: Association of CO Parameter with Block Variable Definition.

5.3.4 Solution Strategy and Results

The BPS code executes very quickly (on the order of several seconds). Given a feedwater flow rate and temperature, as well as a drum pressure, the convergence procedure typically involves varying parameters, such as the nozzle tilt, bypass damper, excess air, or desuperheater spray, until the requisite superheat and reheat outlet temperatures and total heat duty are achieved. At each of the parameter values, the code iterates internally on the air heater gas outlet (AHGO) temperature (which impacts the boiler efficiency and coal mass flow rate calculation), until the AHGO temperature is satisfied to within some tolerance.

In general, depending upon the size of the unit and customer needs, the boiler operator may potentially employ any number of sequential control strategies over the range of loads. Three potential strategies are illustrated in Figure 18, on a plot of the superheat outlet temperature as a function of steam flow rate (or load).

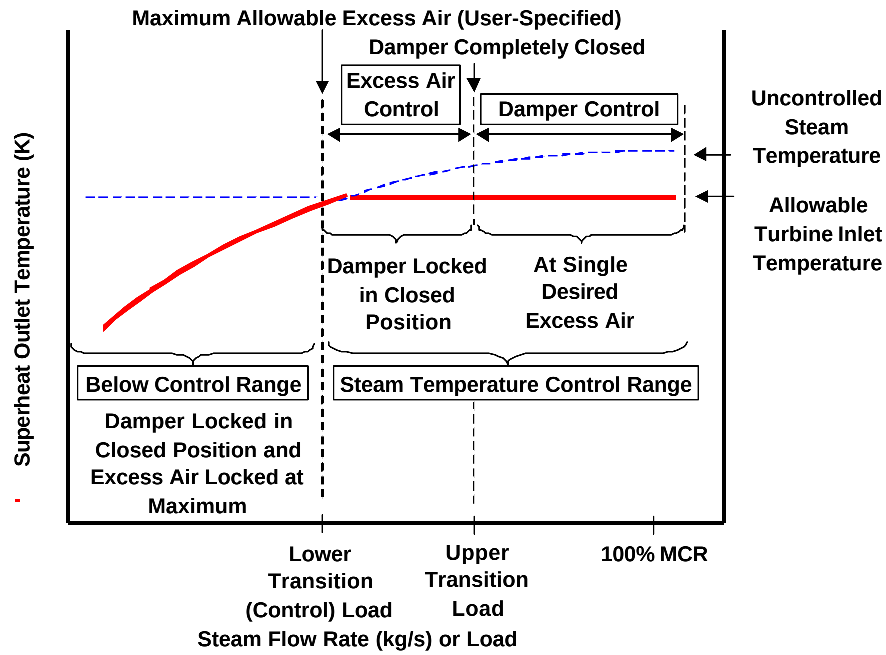

Figure 18: Hierarchy of Manipulated Variables.

At high loads, the damper control strategy (or nozzle tilt control on some units) is employed. For a single excess air, the damper is moved from the open position (at maximum load) to a closed position. At moderate loads, the excess air control strategy is used. The excess air is increased to a maximum value (e.g., 35% excess air) with the damper locked in the closed position. The high and moderate load range is denoted as the "steam temperature control range". Over this control range, the boiler is able to make the steam temperature dictated by the turbine. In essence, the cycle dictates both the feedwater flow rate and enthalpy, as well as the superheat outlet temperature, and the boiler is able to accommodate both the desired outlet steam temperature and the total heat duty, by adjusting its internal control mechanisms. Over the "steam temperature control range," the coupling of the boiler component with the rest of the cycle is relegated to "one-way" coupling and the BPS computations assume a post-processing functionality.

At low loads, designated as the "below control range" loads, the damper is locked in its closed position, and the excess air is locked at its allowable maximum. (In practice, the total air flow rate may be locked instead, to prevent fan stall and to permit purging.) At such loads, the boiler is simply not capable of making the desired steam temperature and the turbine must accept the prevailing boiler superheat outlet temperature. In this instance, rather than matching the "desired steam temperature", the boiler itself dictates what the turbine inlet temperature will be, thus providing feedback to the steam cycle in the form of "two-way" coupling. However, even with the feedback, the coupling is weak. The throttle, upstream of the turbine, tends to desensitize the steam cycle to the boiler perturbations and deviations.

The actual operational characteristics of the Demonstration Case 1 utility are not completely known. However, a reasonable, control strategy can be postulated and applied to the demonstration case in order to produce cycle results over the entire load range. The results are shown in Figure 19.

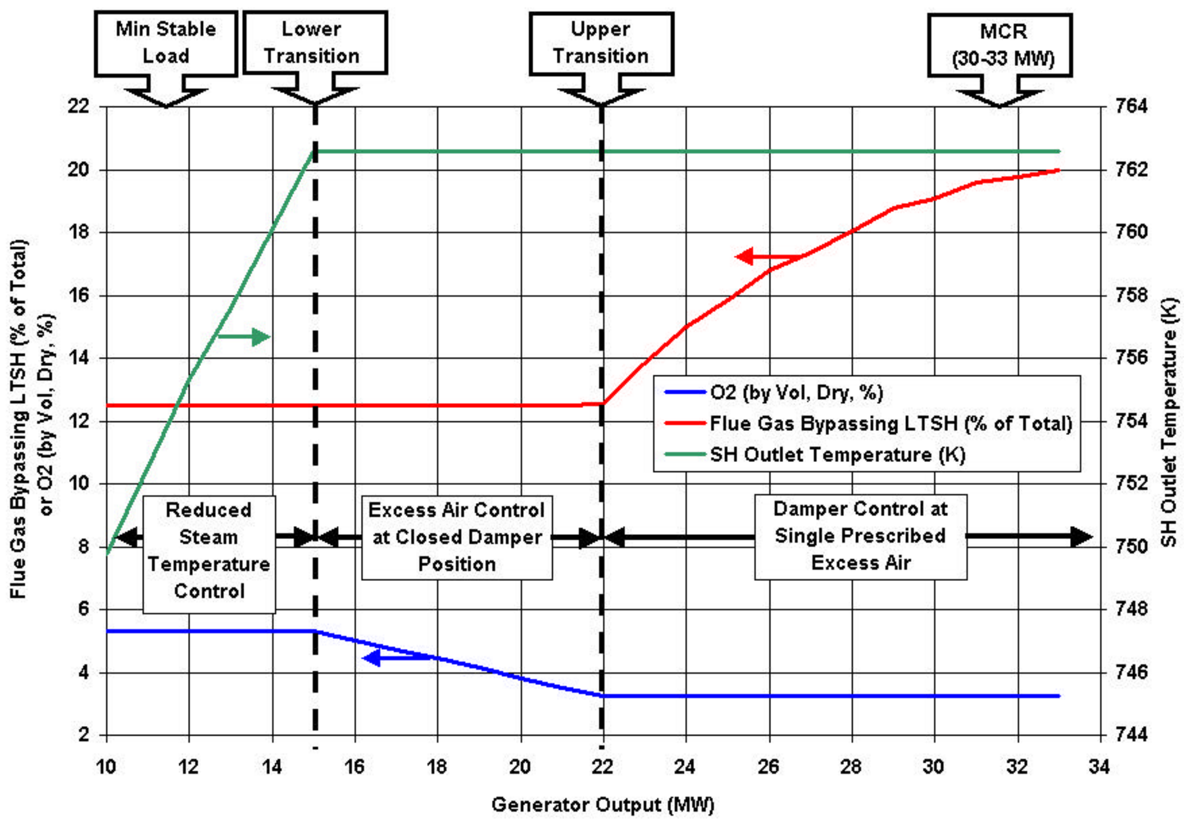

Figure 19: Control Parameters and Results for Case 1 with BPS-Aspen Coupling.

In the above figure, the three control regimes are shown, along with the behavior exhibited by the outlet oxygen concentration (equivalent to an excess air), the percent of the total flue gas that bypasses the LTSH, and the superheat outlet temperature. Over the upper load range, the percent bypass decreases at constant excess air as the bypass damper is closed. As the load is decreased over the range of intermediate loads, the outlet oxygen concentration (i.e., excess air) increases to an arbitrary maximum. Over the intermediate and upper load ranges, the boiler is able to sustain the desired superheat outlet temperature. Below the steam control range, the bypass gas and excess air are held constant, and the superheat outlet temperature decreases monotonically.

Additional results are shown in Figures 20 and 21 for the boiler absorption, feedwater conditions, and mass flow rates of various streams. In Figure 20, the steam flow rate is essentially linear with the generator output. The fuel and air flow rates also decrease monotonically with load, although the slopes of the lines may change, depending on the operational characteristics of the excess air. In Figure 21, the total absorption decreases as the generator output is reduced (as expected). The boiler efficiency, defined as the heat absorbed divided by the heat available from the fuel fired, fluctuates less than a percentage point over the range of loads. As the generator output decreases, the feedwater temperature drops slightly, while the feedwater pressure increases.

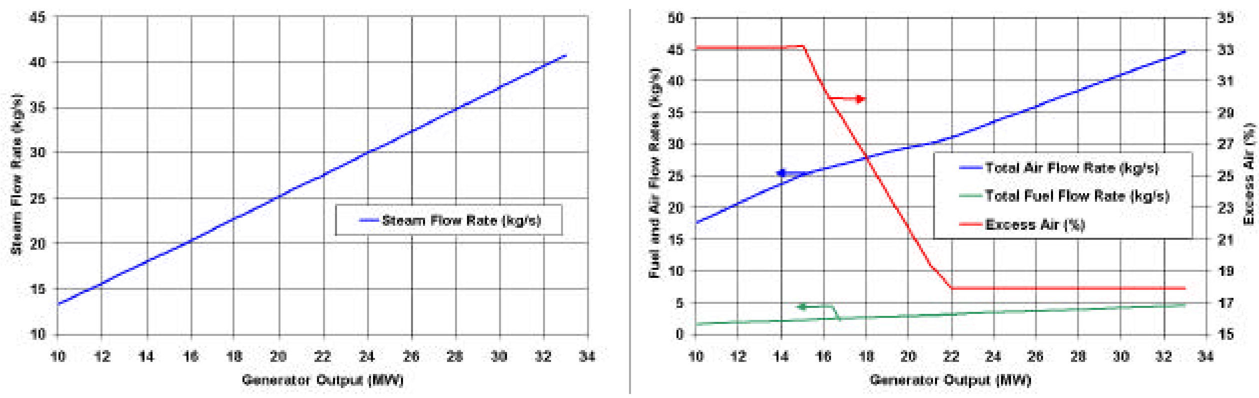

Figure 20: Case 1 : Run 2 Results – Steam, Fuel, and Air Flow Rates.

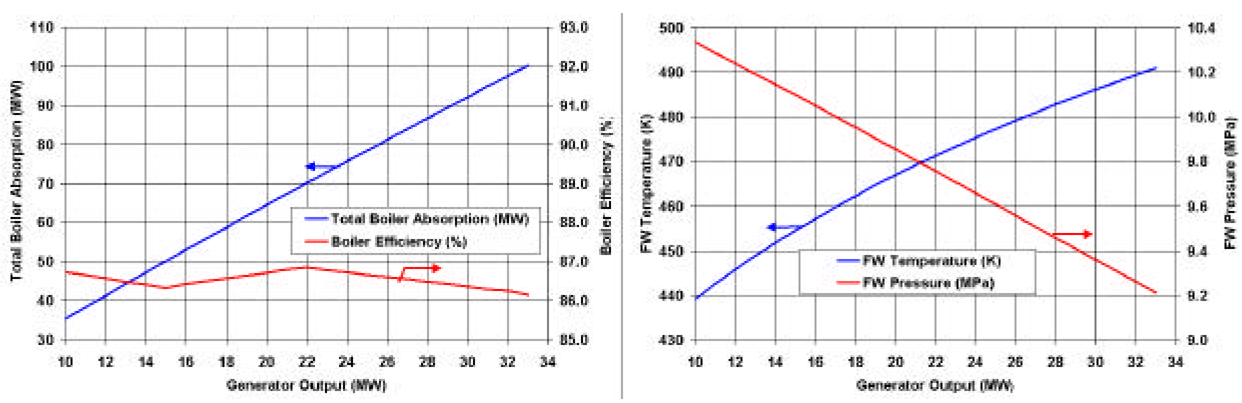

Figure 21: Case 1 : Run 2 Results – Absorption and Feedwater Conditions.

Any number of other parameters, of potential interest to the designer or operator, could be monitored and extracted from the Aspen Plus® computations. While more detailed equipment-level and operational strategy information would surely refine the above results, the predicted trends are sufficient to demonstrate and assess the viability of the coupling / connectivity between Aspen Plus® and an industrial legacy code, using the Vision 21 Controller and CAPE-OPEN interface.

The linkage of the BPS code to the Aspen Plus® package clearly demonstrates that a proprietary industrial legacy code can be effectively utilized as a module on a process model flowsheet. Legacy codes, relative to the library modules offered by Aspen Plus®, often have the advantage of many years of calibrated industrial design applications, and can bring a measure of accuracy and sophistication to the computation that would not otherwise be available.

5.4 Case 1 : Run 3 – Aspen PlusÒ Coupled With FLUENTÒ

Run 3 consists of the coupling of the Aspen Plus® package with the FLUENT® CFD code. FLUENT® Version 6.1.15 was used for all of the FLUENT® computations. The use of CFD in process modeling complements the use of industrial proprietary design software. Industrial legacy codes are typically pseudo 0-D or 1-D and are not usually very CPU intensive. They can be coupled with process models relatively easily, and with some additional coding to help with automation, they can be used in the design process on a routine basis. In fact, the coupling of industrial legacy codes with process models through the CO interface may be the first, low-risk applications that industry may venture towards in the near future.

CFD has the advantage that it is multi-dimensional, with computational sub-models that simulate, insofar as the “industrial” state-of-the-art permits, the actual physics of the component. In many applications, companies have invested heavily to enhance and validate CFD so that it can be used in the design process. In other (more-complex) applications, CFD has not been sufficiently validated and it has been relegated to a role of trend predictions and ”what-if” analyses. Nevertheless, CFD sub-models continue to be improved, and CFD is generally viewed as having the potential over the next decade(s) to substantially impact the design process in a wide variety of industrial and power-plant applications. One of the primary challenges in linking CFD with process models is the disparity in CPU usage. A CFD block, instantiated in a process flowsheet, would require “orders of magnitude” more CPU usage to converge than the process model itself. As a consequence, “reduced-order” models are being developed by the V21 team. Remote, parallel computations for the CFD block, combined with improvements in reduced-order model strategies and database management strategies, will conceivably help to pave the way to making CFD modules an integral part of the industrial process design system.

In the present project, development of remote computational capabilities over a local network was pursued (successfully) by V21 team members, but the full capability was not developed in time to allow the demonstration cases to be run on remote computer platforms. As a consequence, all of the demonstration case runs documented in this report were computed on a single-processor (500 MHz) PC. (Aspen Plus® only runs on a PC.) Because of the CPU-intensive nature of CFD runs, the CFD cases were understandably reduced in size and simplified considerably (relative to their industrial design counterparts) in order to make the computations feasible on a PC. It is not believed that the simplifications detract from the overall purpose of the contractual goals, that of demonstrating the feasibility and viability of the interface software.

5.4.1 Cycle Preparation

A CFD block is instantiated as a CO module on the flowsheet in much the same manner as a CO module for a third-party legacy code. The resultant cycle is shown in Figure 22. For the sake of convenience, auxiliary modules such as the ESP, fans, etc, were not included. The left-hand side of the figure represents the gas-side of the cycle, while the right-hand side represents the steam-side. The boiler, in essence, constitutes the interface between the gas-side and the steam-side. The boiler is represented as a simple heat-exchanger icon on the steam-side (to provide the required heat duty) and as a CFD block on the gas-side of the cycle.

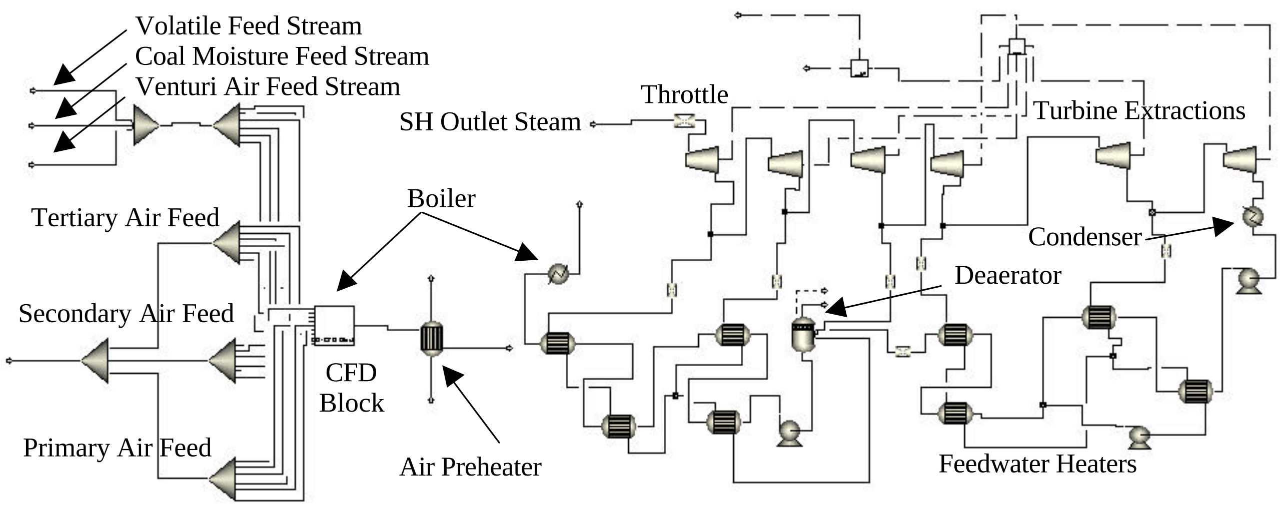

Figure 22: Coupled FLUENTÒ and Aspen PlusÒ Cycle for Demonstration Case 1.

As explained in an earlier section, the boiler has six burners, arranged in two elevations of three burners each. In each burner, coal and “venturi” air are fed through a coal injection system. In addition, each burner has three air register zones to supply three different air annuli at the burner exit. The combustion flow field is controlled by means of individualized flow splits and swirl numbers for each air annulus. The swirl in the primary and tertiary air streams are generated through the use of moveable vane swirlers; an axial fixed vane swirler is utilized in the secondary air annulus. Therefore, each burner contains 4 air inlets, for a total of 24 inlets for the overall boiler. On the flowsheet, the venturi, primary, secondary, and tertiary streams are each partitioned into 6 individual streams, one for each burner.

CFD calculations that include (coal) particle models are much more CPU intensive than gas-only models. Therefore, in order to eliminate the CPU penalty associated with particles, it was decided to approximate the coal fuel as a gaseous fuel. The coal was converted into an equivalent gaseous “volatile” species component and the coal moisture was added as a separate stream. The ash component was ignored. Both the coal moisture and venturi air flow rates were prescribed as functions of the volatile flow rate.

As discussed previously for Run 2, at a given load, Aspen Plus® externally manipulates the damper position and the excess air (or exit oxygen concentration) in order to achieve the specified steam superheat outlet temperature (or superheat absorption/duty). For any given fuel mass flow rate and excess air, the total air mass flow rate is calculated from stoichiometric reaction relationships.

In practice, the air preheater (AH) is connected to the boiler in the manner shown in Figure 23, where the incoming ambient air (AHAI) is heated by the flue gas (AHGI) and then fed to the boiler. The fuel flow rate is manipulated until the temperature of the AH gas outlet (AHGO) stream stops changing, or alternatively, until the total boiler absorption/duty matches the duty calculated from the enthalpy difference across the steam-side boiler (heat exchanger) icon. Consequently, for Demonstration Case 1, proper boiler operation at any given load involves manipulation of two sets of independent variables: (1) damper position or excess air (which primarily controls the superheat absorption), and (2) the total coal mass flow rate (which controls the total absorption).

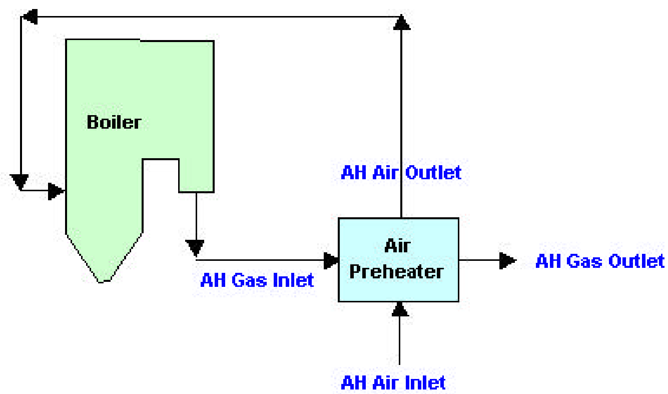

Figure 23: Air Preheater and Boiler Connectivity for Demonstration Case 1.

In the present project, converging the boiler within the Aspen Plus® environment as a function of two sets of manipulated variables for a range of loads was viewed as being rather CPU intensive on a PC. Consequently, the link between the boiler and the air preheater air outlet (AHAO) stream was broken, and the coal mass flow rate and the air temperatures to the boiler were hard-wired as a function of load. Aspen Plus® manipulated only the first set of independent variables (i.e., the damper position and excess air) in order to achieve the desired superheat outlet temperature. Time and money did not permit a more complete calculation of the problem (with both sets of independent variables).

5.4.2 FLUENT® Case and Interface Files Preparation

The FLUENT® case and data files were prepared and calibrated prior to coupling with Aspen Plus®. Typical industrial grids for boilers are (at least) on the order of 500,000 to a million cells. However, in order to decrease the CPU penalty associated with large cases, the grid was reduced to approximately 40,000 cells. The grid is shown in Figure 24. A non-conformal interface was used in the vicinity of the burner inlets in order to transition quickly from a small cell size to a larger one. Grid adaption was used to help resolve features in the vicinity of the inlets and the tube banks.

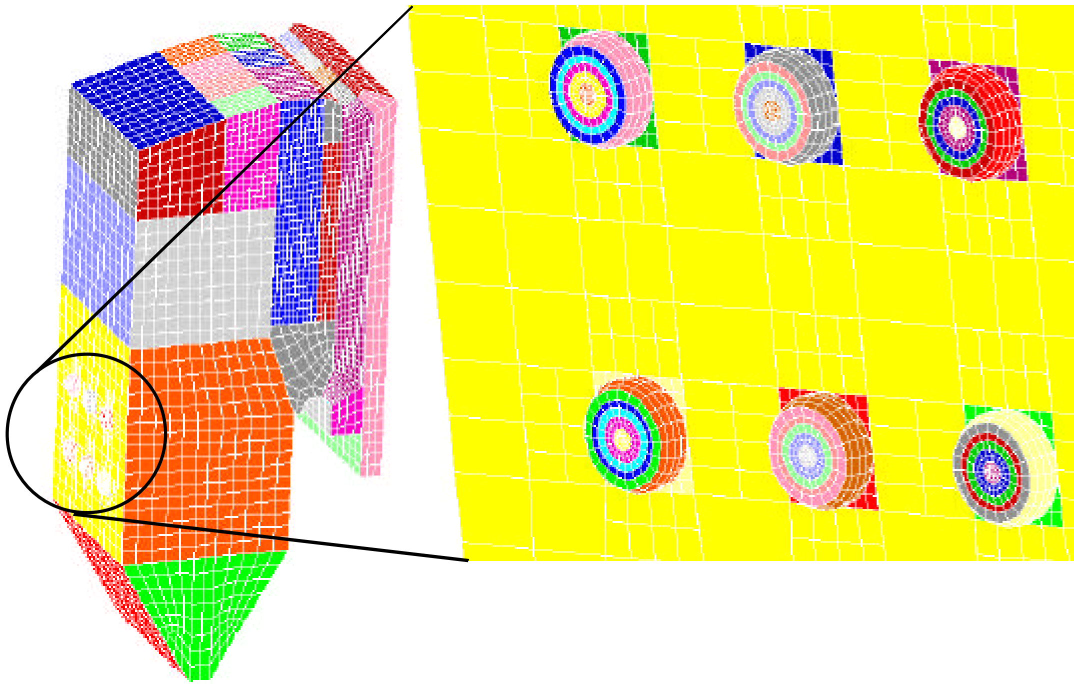

Figure 24: Exterior Grid for Demonstration Case 1.

Each burner has 4 concentric inlets, for a total of 24 inlets. The venturi air stream is not swirled. The fractional mass flow splits and the swirl numbers for the primary, secondary, and tertiary air streams were determined from experimental campaigns and were taken as constant over the load range. The swirl direction for the primary, secondary, and tertiary air streams is uniform for a given burner, but the swirl direction for adjacent burners is in a checkerboard swirl/counter-swirl arrangement. The exhaust plane is a pressure-outlet boundary condition. The heat transfer boundary condition for the walls is prescribed as being either adiabatic or a function of a wall heat transfer coefficient and a back-side "free-stream" fluid temperature. The wall internal emissivity was set equal to 0.75.

Three heat exchanger tube banks or sections were defined in the CFD case – a "boiler bank", a low-temperature superheater (LTSH), and a superheater platen (see Figure 25). The LTSH and the superheat platen are connected in series with each other, which the heat exchanger model in FLUENT® automatically accounts for. The boiler bank is part of the evaporative section (along with the external walls). Each of the tube banks was subdivided into 4 heat exchanger zones in the span-wise direction (i.e., across the width) of the boiler. Since the tube bank model in FLUENT® is a pseudo 1-D model, breaking up a tube bank into smaller span-wise zones may help the user (or designer) to assess whether a serious maldistribution or non-uniformity in the gas temperatures exists in the approach flow upstream of the tube banks. The porous media "inertial" resistances were determined from a knowledge of the tube bank geometry and ALSTOM design standards.

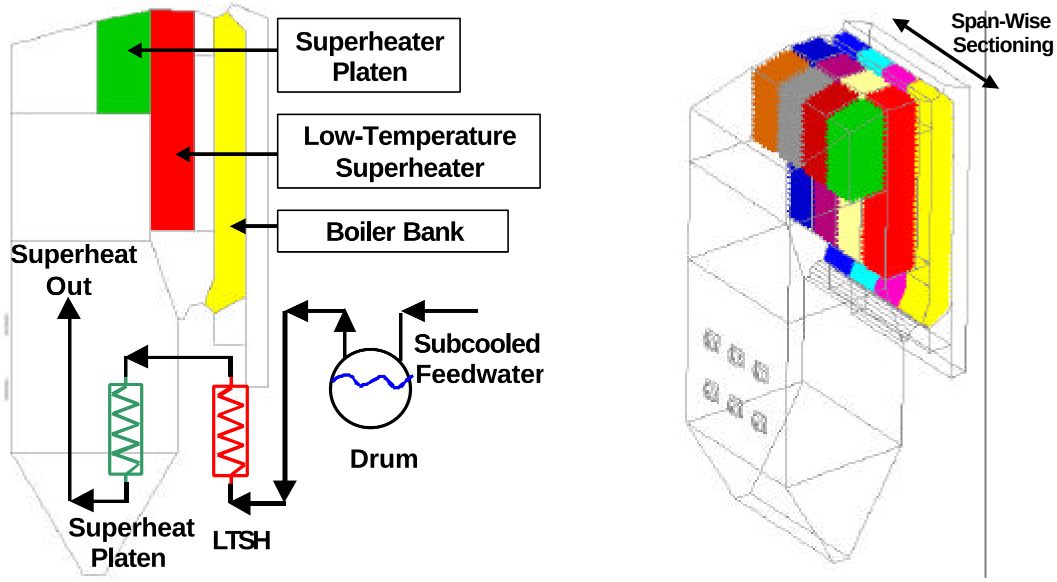

Figure 25: Tube Bank Configuration and Sectioning for the FLUENTÒ Block of Case 1.

The sub-models for the CFD runs consisted of the k-ε turbulence model with standard wall functions, the discrete ordinates radiation model, and the eddy-dissipation reaction model (without any finite kinetic rate) with a 2-step reaction formulation (fuel to CO and CO to CO_2) and 7 species. The turbulent intensity of the inlet streams was set equal to 10% and the inlet dissipation rates were made a function of the hydraulic diameter of each of the inlet ports. The inlet velocities for each burner were based on a local cylindrical coordinate system and a prescription of the axial, radial and circumferential velocities.

The gas- and steam-side connectivity between Aspen Plus® and the FLUENT® block is shown in Figure 26. The material streams in the Aspen Plus® flowsheet representing the gaseous inlet streams connect directly with the corresponding port connections that have been defined for the CFD block. (Such definitions are prescribed in the Configuration Wizard.) A single material stream was connected to the pressure-outlet boundary condition. The connectivity ports allow the direct and automatic transferral of stream information from Aspen Plus® to the CFD case, and vice-versa. For stream information, Aspen Plus® currently transfers the mass flow rate, pressure, temperature, species names, molecular weights, and mole fractions. The CO wrapper around FLUENT® itself then interrogates each boundary condition face for its type (e.g., mass flow rate, velocity normal to boundary, velocity components, etc.) and responds accordingly. The CO wrapper calculates the mixture density and area of the boundary condition face, calculates the average velocity, and then applies that velocity to the boundary condition. In the present case, a user-defined function (UDF) is utilized to calculate the tangential velocity for each of the inlet planes, based on a specified swirl number, inlet dimensions, and longitudinal (axial) velocity (presuming a local cylindrical coordinate system at each burner).

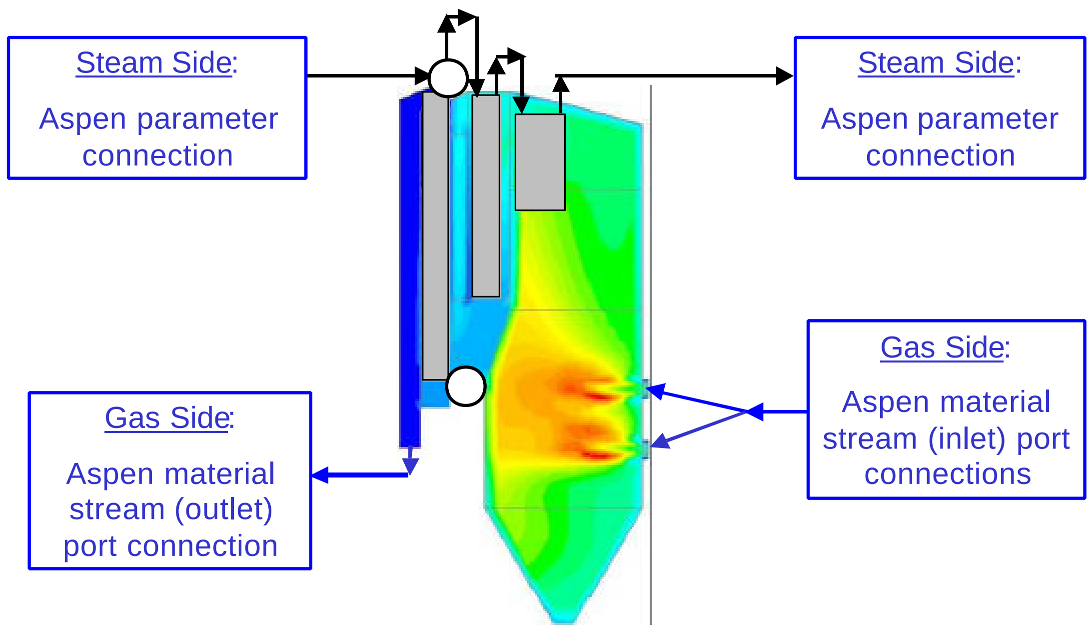

Figure 26: Gas- and Steam-Side Connectivities for the FLUENTÒ Block of Case 1.

Aspen Plus® also has the capability to transfer species properties to FLUENT®. The properties include specific heat, thermal conductivity, and viscosity, and they can be transferred as either constant-value or temperature-dependent properties. For temperature-dependent properties, the properties are transferred from the databases in Aspen Plus® as discrete points over a prescribed temperature range (specified by the user in the Configuration Wizard). Once the discrete tabulations have been transferred to the FLUENT® CO wrapper, the wrapper curve fits them as polynomials, in a form that is congruent with the standard FLUENT® usage. In this way, FLUENT® can avail itself of the extensive property packages in Aspen Plus®, and the risk of incompatibility or inconsistency in property calculations between the two codes is eliminated. In the present case, it was found that the specific heats of all of the species were essentially identical between Aspen Plus® and FLUENT®, except for oxygen. The divergence in the oxygen specific heat from the standard used in FLUENT® (and other databases) caused the CFD case to produce superheat outlet temperatures that were off by approximately 30 K. The reason for this disparity in specific heat values between the Aspen and Fluent databases for the oxygen species is unknown. To prevent having to recalibrate the CFD case to account for the disparity in specific heats, the transferral of properties from Aspen Plus® was turned off. (Property transferral was turned off for both Demonstration Cases 1 and 2.)

It should be noted that the controller and wrapper presume that there is a one-to-one correspondence between the species "names" in Aspen Plus® and the species "names" in the FLUENT® case. The user-specified name (limited to 8 letters) given to the "Component IDs" in the species selection panel of Aspen Plus®, must correspond in both literal sequence and spelling, to the "chemical formula" name listed for the "Selected Species" in the FLUENT® mixture material panel. It should further be noted that the user should typically provide both a "chemical formula" and a "name" for each of the species in FLUENT®, in which case, the "Selected Species" listing will preferentially display the chemical formula. This is somewhat problematic because it forces the user to exercise care when preparing both the Aspen Plus® and FLUENT® cases to ensure name conformity. If the cases were prepared without this issue in mind, then the materials definitions in either or both of the codes must be redone. It is hoped that this constraint will be eased via through continued development of the controller and wrapper in the future.

5.4.3 FLUENT® Calibration and Setup of the CO Collection

The FLUENT® heat exchanger (HX) model was calibrated to match the BPS design code results at the 30 MW condition. The calibration was performed by changing the resistances for the external evaporative walls and by adjusting the surface effectiveness factors of the tube banks. The calibration accounts for the unknown effects of fouling and slagging, radiation shadows, and various other heat transfer inefficiencies. The calculated temperature contours at the 30 MW condition are shown in Figure 27.

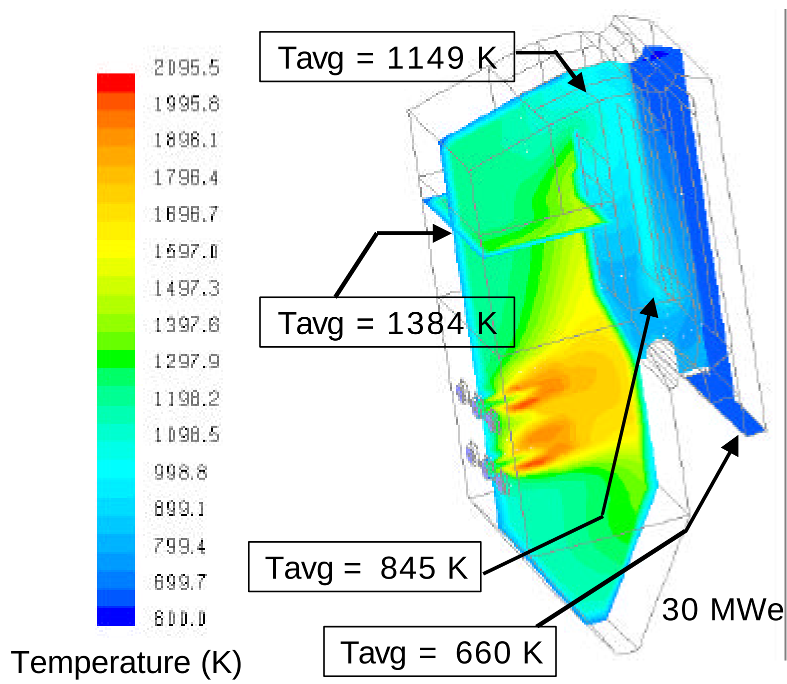

Figure 27: Contour Plots Following Calibration of FLUENTÒ HX Model for Case 1.

Once the calibration at the 30 MW condition was achieved, an investigation was made into how well the (stand-alone) FLUENT® results would align themselves to the BPS results over the rest of the load range by either changing the damper control or the excess air (as shown in Figures 28 and 29). The damper control in the bypass channel was computationally mimicked by changing the bypass channel into a porous medium, and then varying the amount of flow resistance assigned to that porous medium. An "inertial" resistance (with units of reciprocal meters) was defined for each coordinate direction, and the three component resistances were forced to be equal to each other at any particular load. The excess air was controlled (in the same design spec) by manipulating the flow rate of the inlet air (excluding the venturi air) required to produce a specified oxygen mole percent (dry) in the exhausted flue gas (assuming complete combustion of the fuel).

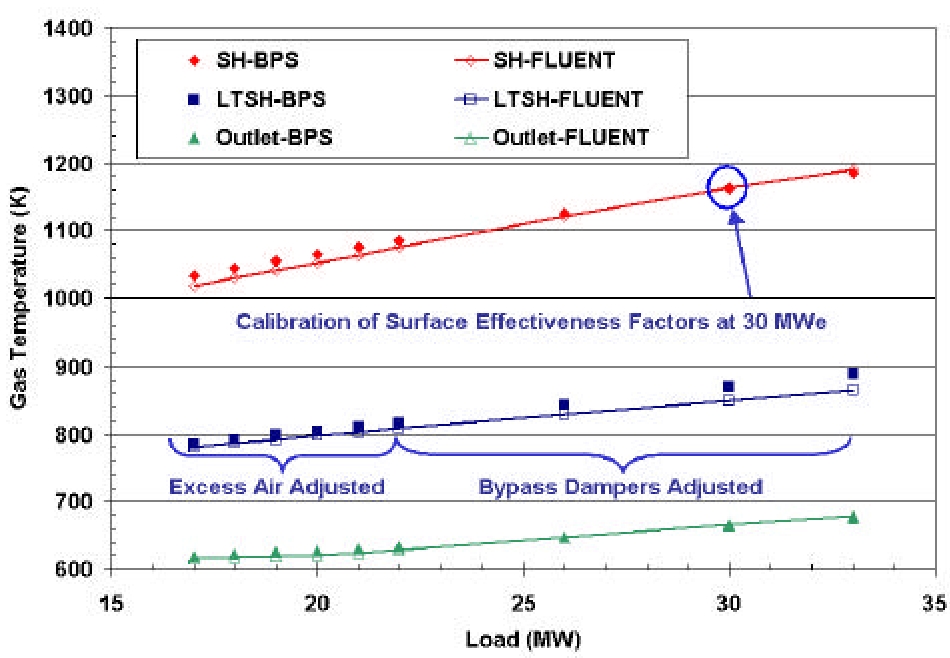

Figure 28: Calibration of Gas Temperatures Using FLUENTÒ HX Model for Case 1.

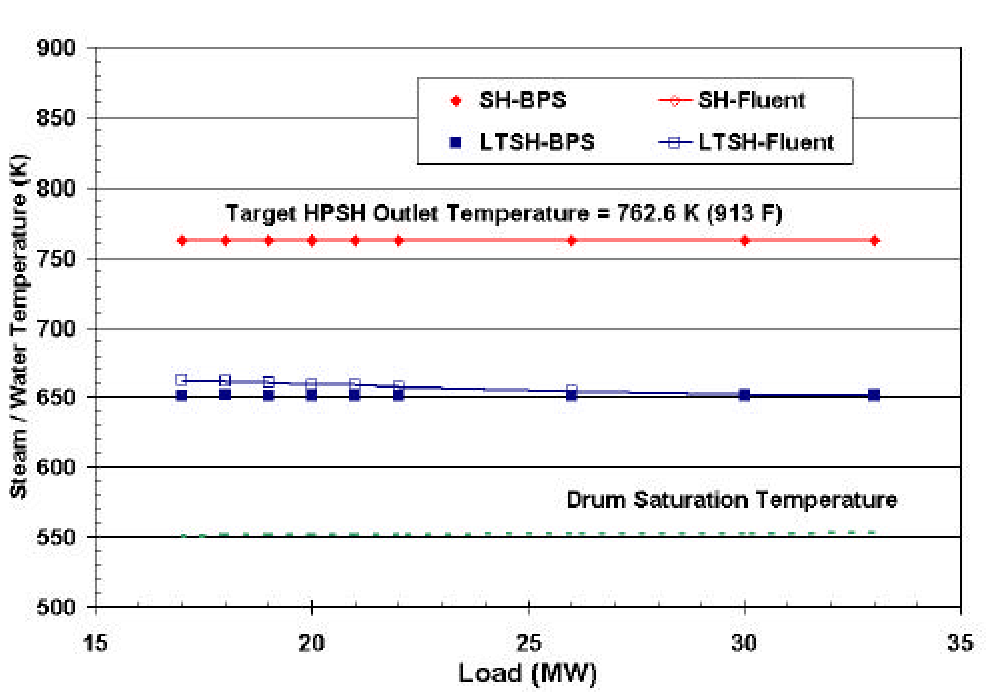

Figure 29: Calibration of Steam Temperatures Using FLUENTÒ HX Model for Case 1.

The superheat outlet steam temperature in the above figure is maintained at the requisite 762.6 K (913 °F). It can be seen from the above figures, that following the initial calibration exercise at 30 MW, the calculation of the desired exit gas and superheat steam temperatures over the load range is attainable, to within a reasonable degree of accuracy, by manipulating the damper and excess air control parameters. From the above calibration exercise, one can be reasonably assured that Aspen Plus®, via manipulation of those same control parameters, would be able to achieve the same task.

A total of 19 CO parameters were defined in order to exchange information between Aspen Plus® and FLUENT®. Among those CO parameters, 3 parameters specified the inertial resistance for the bypass channel, and 12 parameters specified the requisite pressure drop, inlet temperature, inlet pressure, inlet steam quality, and mass flow rates for each of the tube banks. The CO collection for the CFD wrapper was defined in the FLUENT® *Configuration Wizard* (CW). Details associated with the usage of the CW are fully explained in the FLUENT® User's Manual (Ref. 4). However, some comments will be made relative to the three ways in which FLUENT® variables for Demonstration Case 1 may be accessed, all of which are options within the CW.

The CW in launched by first launching FLUENT® and then typing the command (load "cowizard"). Following the input of model information and port information, the CO variables are defined in the "Advanced Parameters" panel. FLUENT® "accessible" parameters are denoted as "RP-VAR" parameters. If one opens up a FLUENT® case (.cas) file, then one can see a long tabulation of the RP-VARs that Fluent has made generally available to its users. Access to variables through RP-VARs is important in many instances, since the user does not have access to the Fluent source code.

If RP-VAR variables are accessible inside of FLUENT® as single values, then the use of the "rp-var" option is appropriate. The selection of this option is exemplified in Figure 30 for the superheat outlet temperature. In this particular case, since the superheat outlet temperature RP-VAR does not currently exist as part of the FLUENT® RP-VAR tabulation, it is created or defined within a Scheme file, and it is subsequently assigned a value within an ALSTOM user-defined function (UDF) for tube banks. Scheme is a dialect of LISP, and is a language that is heavily used by Fluent personnel to interact with and exchange information with the FLUENT® environment.

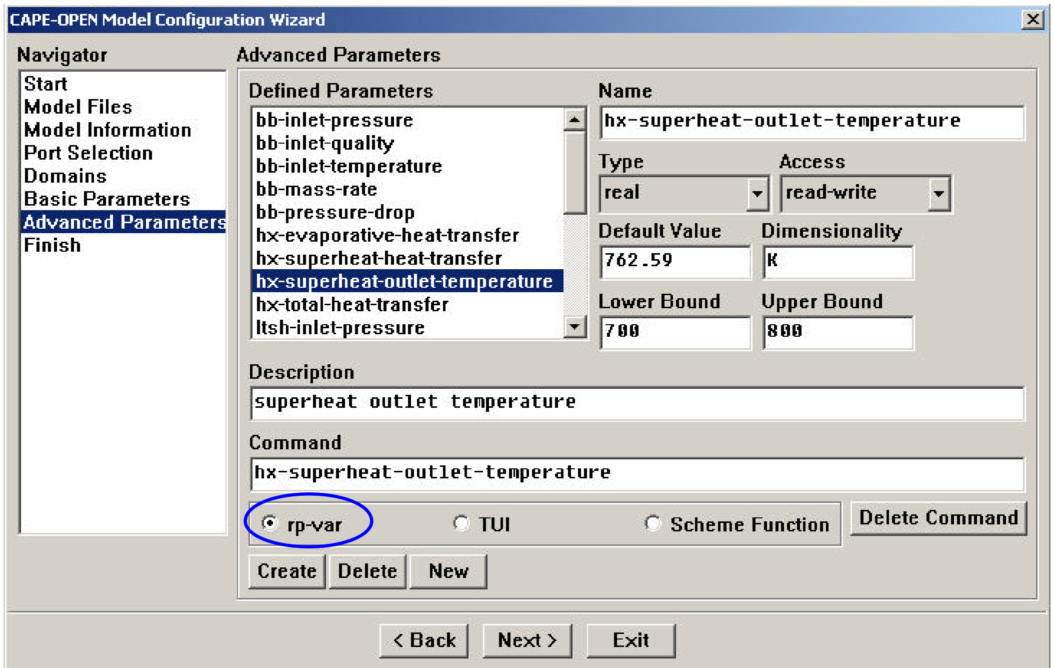

Figure 30: Accessing Variables in the Configuration Wizard with the RP-VAR Option.

Sometimes the pertinent RP-VAR is returned as a “list,” and the desired CO variable must be inserted into or extracted from this listing. In this case, Scheme functions are required. An example is shown in Figure 31 for the LTSH inlet pressure. Fluent personnel kindly provided the necessary Scheme function to be able to associate a CO parameter with a particular “element” in an RP-VAR listing.

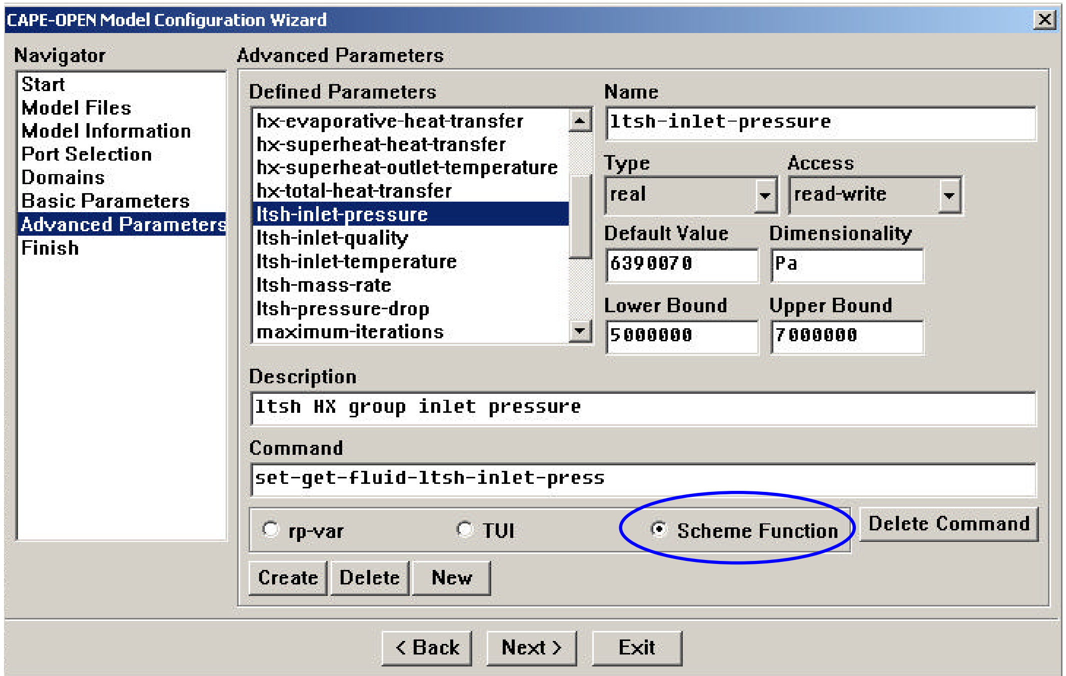

Figure 31: Accessing Variables in the Configuration Wizard with the Scheme Option.

FLUENT® has the ability to exchange information either through graphical user interfaces (GUIs) or through textual user interfaces (TUIs) in FLUENT®'s console window. An example of using the TUI option is shown in Figure 32 for the inertial resistance in the x-coordinate direction of the bypass channel porous medium. This CO parameter pipes a series of TUI commands and responses to the console. The series of 27 commas in the command line indicate an acceptance of the default values proposed for various characteristics of the porous media zone. Currently the TUI command is uni-directional. The TUI command is useful in sending single values from Aspen Plus® to FLUENT®. However, it cannot generally be used to extract values from FLUENT® and send them back to Aspen Plus®, which would be very useful, particularly for post-processing purposes. This is because the TUI response involves some wording as well as a value, and the controller has not yet been provided with a general parser than can extract the desired value. (This capability should be added at some point in the future.)

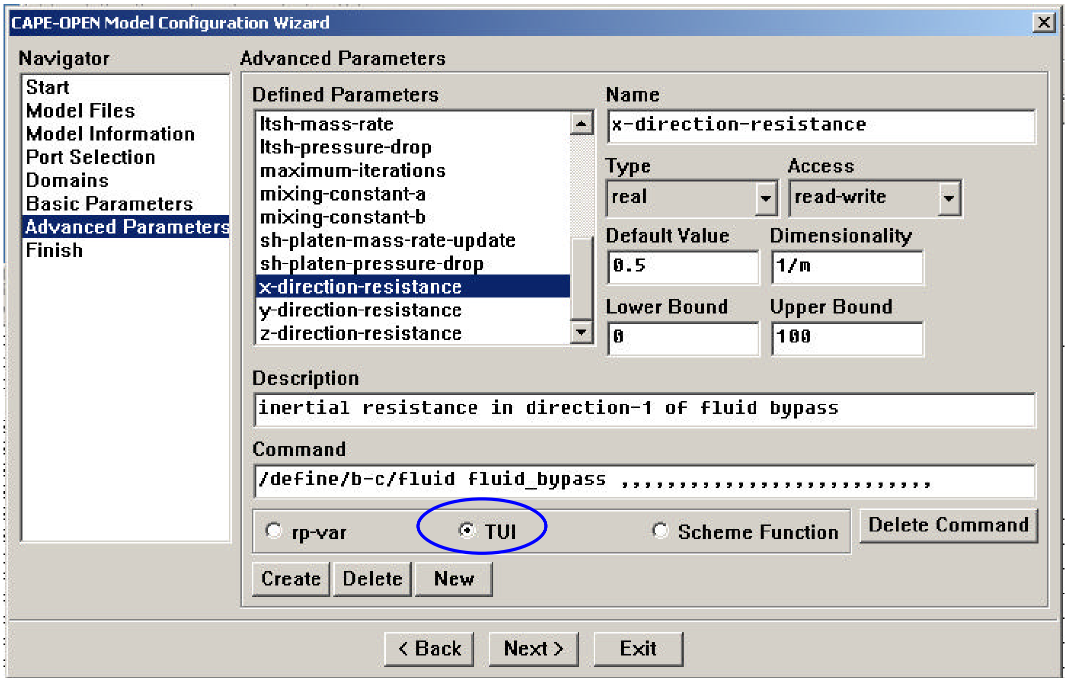

Figure 32: Accessing Variables in the Configuration Wizard with the TUI Option.

5.4.4 Convergence Characteristics and Results

The user must be sufficiently familiar with the convergence characteristics of his CFD case to be able to specify a reasonable limit on the maximum number of iterations that FLUENT® would be allowed to compute during any given execution of the CFD block. The specified convergence values for the residuals were set such that convergence could be achieved within that maximum number of iterations. A careful balance must often be struck. If the under-relaxation factors are too low, then FLUENT® will iterate to the maximum specified value each time and the convergence of Aspen Plus® will be time-consuming and inefficient. On the other hand, if FLUENT® has difficulty settling down and is not allowed to converge to a tight enough tolerance, then Aspen Plus® may be trying to compute search directions based on inaccurate results from FLUENT®, which is also a form of inefficiency. The number of iterations, the values for the under-relaxation factors, and the target tolerances in the overall design specs governing FLUENT® block execution are interrelated and must be adjusted accordingly.

Typically, for any given load point and steam conditions, Aspen Plus® (through a series of “design specs”) determines the steam mass flow rate required to produce a particular generator output (e.g., 30 MW). Subsequently, when the boiler or FLUENT® CFD block is reached in the cycle, Aspen Plus® typically executes another “design spec” which varies the bypass damper control (or excess air) until the superheat outlet temperature achieves the desired target temperature of 762.6 K (913 °F). Some representative convergence characteristics for Demonstration Case 1 are provided in Figure 33, where the superheat outlet temperature from the superheat platen is being tracked as a function of FLUENT® iterations. The maximum number of FLUENT® iterations allowed, within any given design spec iteration, was set at 600. Good initial conditions were provided in this instance so that convergence would occur within only a few Aspen Plus® iterations (and within a reasonable clock time). At the load points of both 26 and 24 MW, it can be seen that the FLUENT® block is executed 3 times, and on the third attempt, the convergence algorithm was able to estimate the bypass channel resistance that produced the desired superheat outlet temperature. The convergence tolerance arbitrarily prescribed for the superheat temperature is 0.28 K (0.5 °F). In each FLUENT® execution, the under-relaxation factors have been set such that convergence of FLUENT® is attained before the maximum iteration limit of 600 iterations is reached. The first iteration at each load required on the order of 500 iterations for the superheat outlet temperature to stabilize; successive iterations stabilized and converged much more quickly.

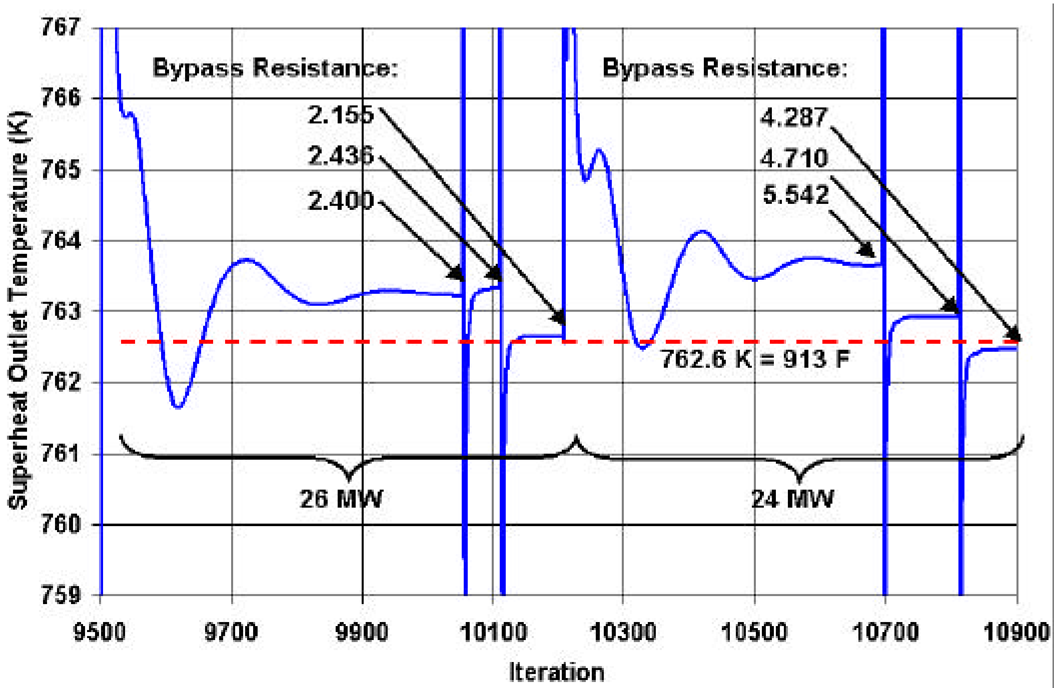

Figure 33: Convergence of Superheat Outlet Temperature for Case 1 at 26 and 24 MW.

It should be noted that each time that FLUENT® is newly executed, the steam temperatures in the tube bank model spike to unrealistic levels and then quickly recover in the form of a damped oscillation. The reason for this is presently unknown, particularly since FLUENT® "stays alive" from execution to execution and the flow field is supposedly not reinitialized. Since the tube bank model is an integral part of any power plant cycle, effort should be expended to make various aspects of the tube bank model more robust.

The residual history for turbulent kinetic energy, y-momentum, and z-momentum, over the same corresponding set of FLUENT® iterations, is shown in Figure 34. The residuals spike each time that FLUENT® is executed, but the residuals recover and approach convergence fairly quickly.

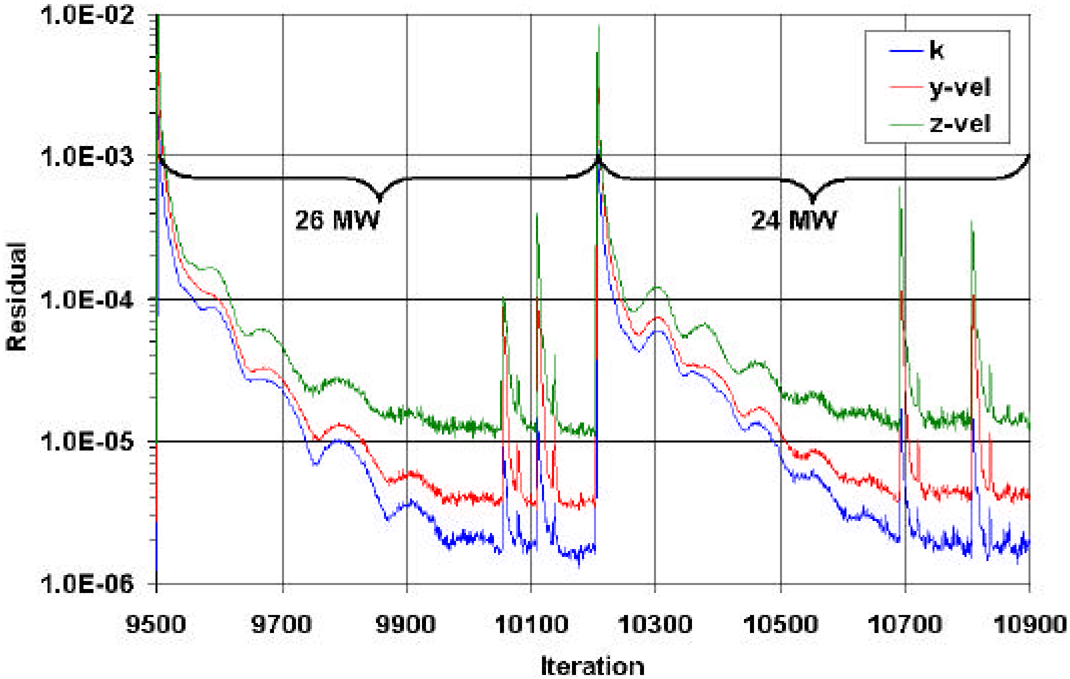

Figure 34: History of Various FLUENTÒ Residuals for Case 1 at 26 and 24 MW.

At lower loads, the residuals oscillate significantly more and convergence is not as easily attained. Figure 35 shows the convergence history at of the superheat outlet temperature at 19 and 17 MW, and the corresponding residual history is shown in Figure 36. The maximum number of FLUENT® iterations, within a given design spec iteration, was expanded to 800, but each execution of the FLUENT® block completed the entire 800 iterations and still did not attain convergence, because of the persisting oscillatory behavior. This illustrates the point that if FLUENT® performs a "sensitivity analysis" over a wide range of a parameter (e.g., load), FLUENT® may require different under-relaxation factors and convergence tolerances over different segments of that parameter range. There is currently no available means (that has been tested) to pause both Aspen Plus® and FLUENT® during a run and change their respective convergence criteria, and then continue the computations.

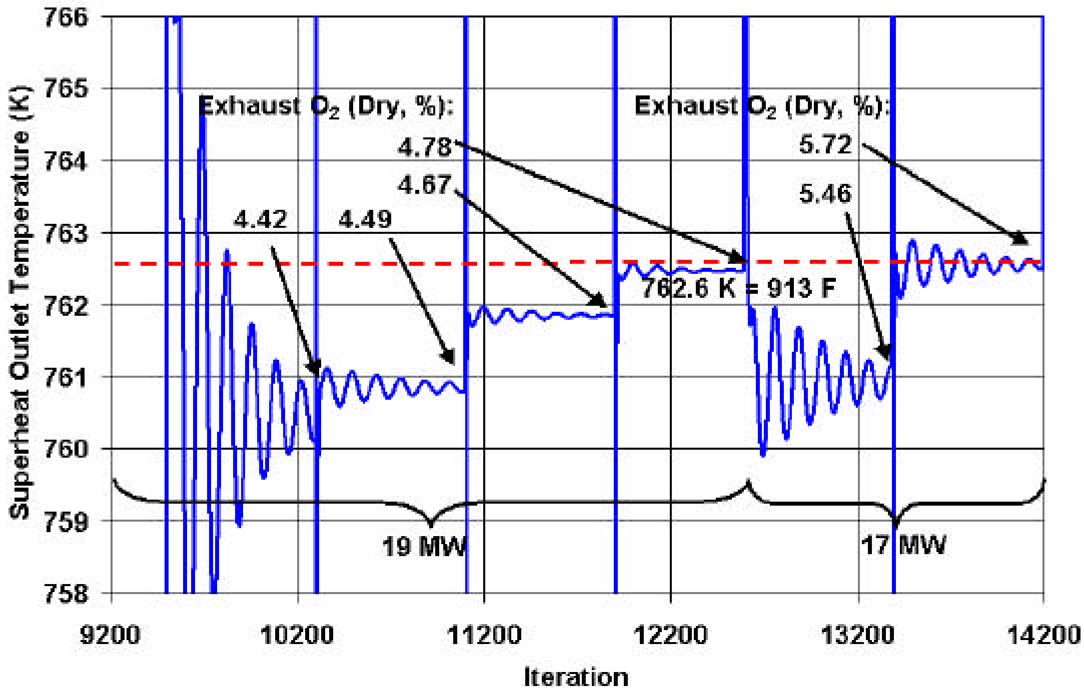

Figure 35: Convergence of Superheat Outlet Temperature for Case 1 at 19 and 17 MW.

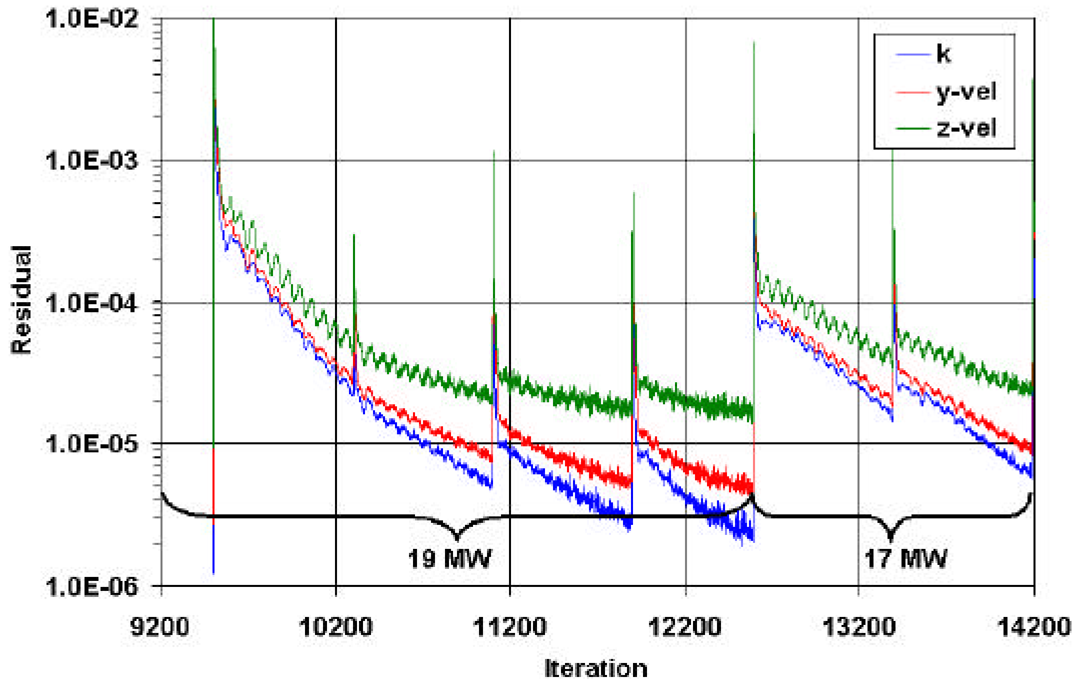

Figure 36: History of Various FLUENT® Residuals for Case 1 at 19 and 17 MW.

Results over the load range for the FLUENT®/Aspen Plus® coupling is shown in Figure 37. Aspen Plus®, as the executive software, was able to successfully manipulate the specific control parameters in order to produce the desired superheat outlet temperature. The porous media inertial resistance in the bypass channel was the controlling parameter at high loads and the exhaust oxygen concentration was the controlling parameter at moderate loads. With the CFD coupling, 11 of the load points were run over the range from 33 MW to 15 MW (beginning at the highest load). No attempt was made to run the CFD coupling at very low loads, in the reduced-steam-temperature-control range; the points that have been run are sufficient to demonstrate the viability of the interface. Running at very low loads is significantly more CPU intensive. When the capability exists to run the FLUENT® block remotely on parallel computers, then this case can be exercised more extensively, and the additional loop for the calculation of the coal flow rate and total absorption (as discussed previously) can be added as well.

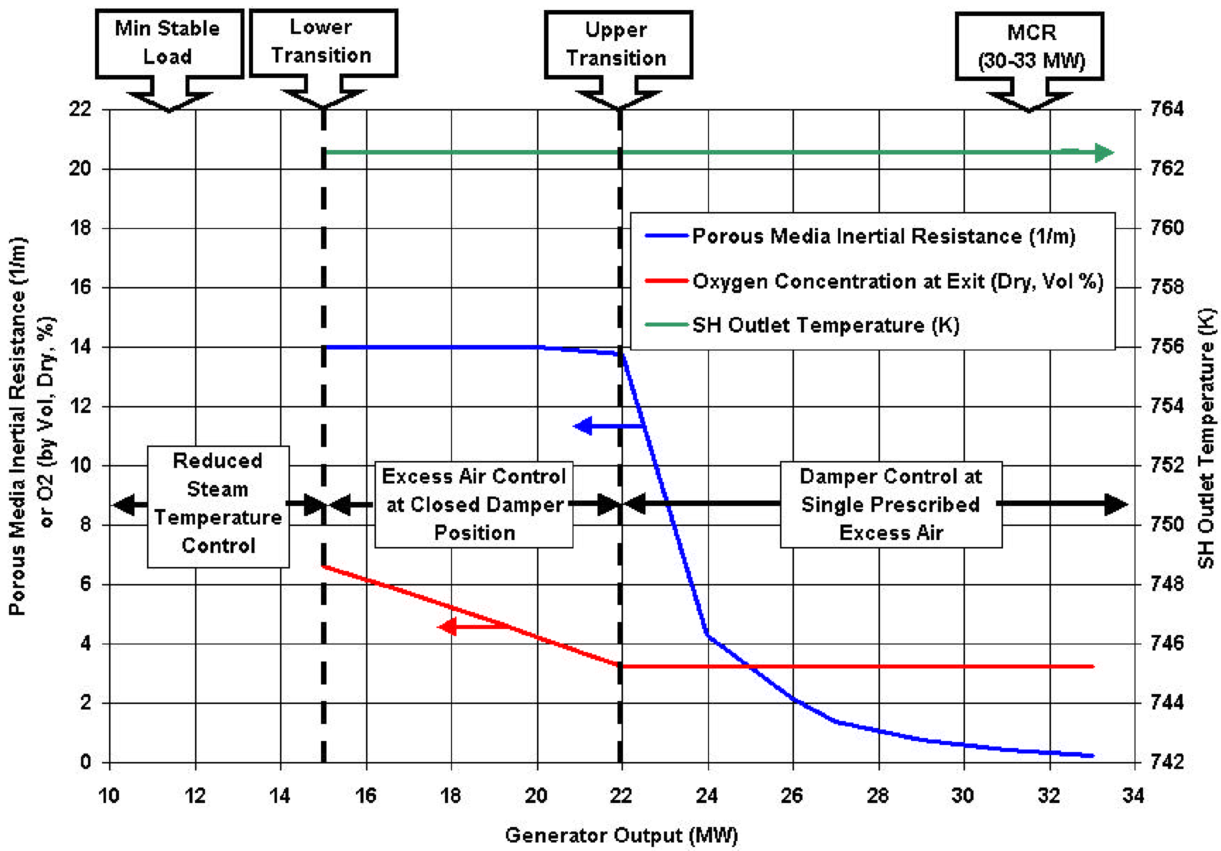

Figure 37: Control Parameter Results for Case 1 with FLUENTÒ-Aspen Plus® Coupling.

The present results with FLUENT® are somewhat different than the results from the BPS coupling (e.g., compare final exit oxygen concentrations at 15 MW of 6.6% versus 5.3%). However, upon reflection, there is no strong reason why the two sets of results should be identical, since the calibration for the BPS code is based upon a different set of tuneable equations or coupled submodels than that of the FLUENT® code. The bypass control in the BPS code was simply based upon specification of the flow rate through the bypass channel. The maximum flow rate allowed in the bypass channel was based loosely on the cross-sectional area in the bypass channel relative to the total cross-sectional area, which was a somewhat arbitrary assumption. The bypass control in FLUENT® was based upon the porous media resistances, not only for the bypass channel, but also for the LTSH. The flow must pass through the LTSH before it reaches the bypass channel, and the resistances assigned to the LTSH (which are different in each of the 3 coordinate directions) influence the flow through the channel. Such assumptions impact the subsequent external wall and tube bank calibrations. The fact that gaseous fuel was used rather than coal in the CFD case will also impact the heat transfer distribution in the boiler and the subsequent calibration. Calibration ensures that the desired metrics (e.g., gas temperatures at particular stations) are being achieved; it does not necessarily mean that the assumptions, control parameters, and equation sets within the two separate models have an equivalent range, response, and sensitivity.

Figure 38 shows the steam, fuel, and air flow rates over the load range. The feedwater and superheated steam flow rates/conditions for the cycle are essentially equivalent to those shown earlier for the BPS code, since the steam-side of the cycle does not change over the high and moderate load ranges. (The individual superheat and evaporative absorptions were not captured in the CFD runs because of a Scheme/UDF error.)

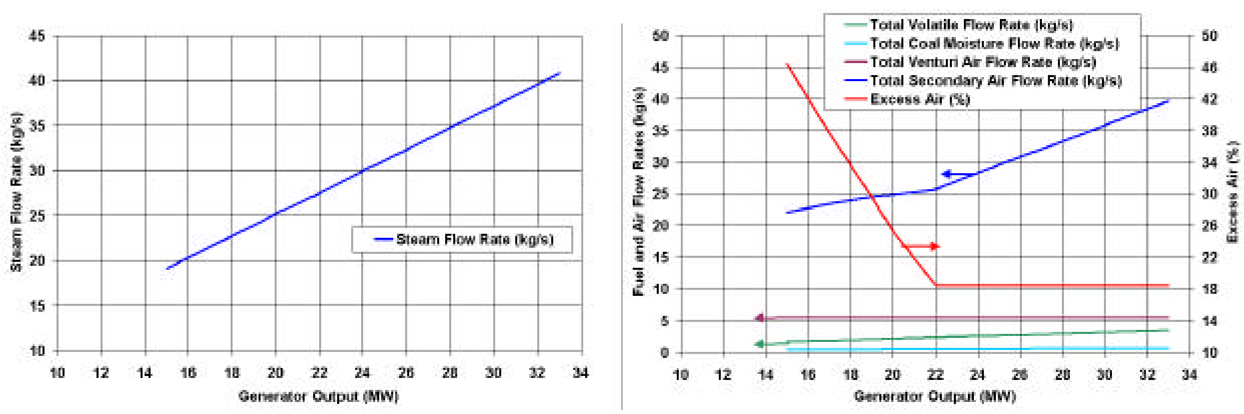

Figure 38: Case 1 : Run 3 Results – Steam, Fuel, and Air Flow Rates.

5.5 Demonstration Case 2 – Facility and Cycle Description

A natural gas combined cycle power plant was selected for the Case 2 advanced cycle. Additional facility details are provided in Ref. 3. The reasons for selecting this particular cycle included:

- The combined cycle unit selected offered significant quantities of relevant data on a high efficiency plant built with the "latest" in power generation technology.

- The quality of the available data from the selected unit was deemed to be sufficient for constructing a cycle and the component boiler models. Appropriate assumptions and adaptations could be made that would permit the unit to be simulated successfully both with an AP design package and with CFD.

5.5.1 Power Plant Facility

An aerial view of the combined cycle power plant is shown in Figure 39. The power plant consists of an advanced gas turbine, steam turbine, generator, and heat recovery steam generator (HRSG) all supplied by ALSTOM Power. Plant construction was completed in the late 1990s.

Figure 39: Photograph of the Combined Cycle Power Plant.

The gas turbine generates approximately 2/3 of the 270 MWe of electrical output from the combined cycle power plant. The gas turbine generator has an efficiency of 38.5% when firing natural gas fuel with an ambient air temperature of 288.15 K. The exhaust gas exits the gas turbine around 923 K where it enters an HRSG.

In combined cycle mode, the power plant operates at a net efficiency of 57.5%. The HRSG is a dual pressure reheat design. The HRSG combines a low pressure, natural circulation steam drum system with a high pressure once-through boiler. Saturated, low-pressure (LP) water from the LP drum is used to feed the “once-through” high pressure (HP) system. The HP system utilizes a novel “once-through” steam/water separator to maintain high steam quality while eliminating the need for a thick-walled, thermally sluggish HP steam drum. This allows the power plant to more rapidly cycle to adjust to variations in load.

5.5.2 Steam Cycle

A schematic of the combined cycle unit is shown in Figure 40. As illustrated in the figure, the gas and steam turbines are both on a single shaft. The HRSG contains both high and low pressure evaporative and superheat surface as well as HP reheat. Condensate from the condenser is mixed with a small quantity of hot water from the feed water economizer (FWECON) to control the water temperature into the FWECON. The main portion of the hot water from the FWECON is fed into the LP drum. Water flows through downcomers into evaporator tubes and the resulting saturated steam/water mixture is returned to the drum through risers by natural circulation. The saturated steam exits the top of the LP drum where it passes through a superheater section before entering the LP section of the steam turbine.

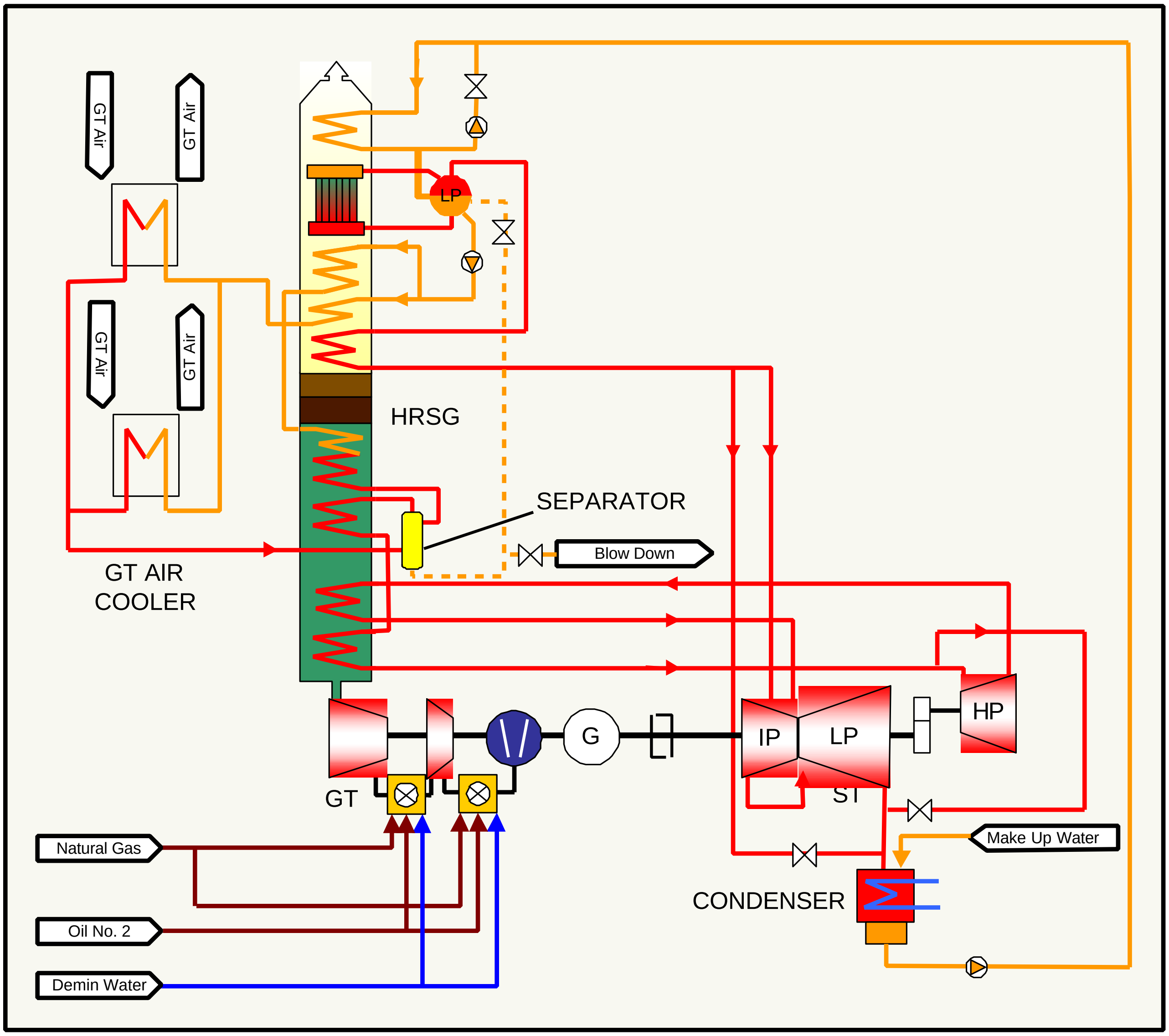

Figure 40: Steam Cycle Schematic for the Combined Cycle Power Plant.

The HP feed pump also takes water from the LP steam drum, a small part of which is sent to the gas turbine cooler. Most of the HP feedwater flows through the HP economizer and then into the once-through evaporator section where it exits as slightly superheated steam. The steam is then sent to the HP separator where it is mixed with superheated steam from the gas turbine (GT) cooler. The steam is then superheated and conditioned in the HP desuperheater and sent to the HP steam turbine. From the steam turbine outlet, the steam passes through a reheat (RH) section and then into the RH desuperheater.

At the maximum continuous rating (MCR), the HRSG is designed to provide a superheat outlet steam flow of approximately 60 kg/s at 838.15 K and 16.5 MPa. The design reheat steam flow is approximately 59 kg/s at 836.15 K and 3.6 MPa, while the low pressure steam flow is approximately 12 kg/s at 595.15 K and 0.7 MPa. The HRSG component and "island" will be the focus of Runs 2 and 3. The HRSG geometry is represented in Figure 41.

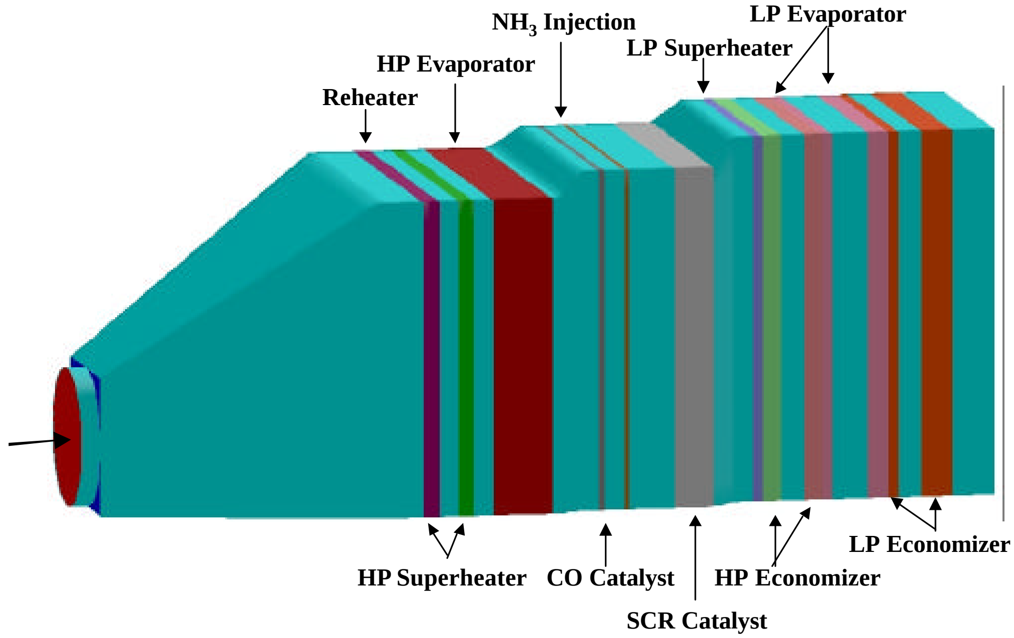

Figure 41: HRSG Geometry for Demonstration Case 2.

As the combined cycle power plant selected for this study is recent technology, the quantity of available plant data is quite large. The plant was well instrumented and the current control and data acquisition systems allow for much of the plant data to be monitored by personnel online through proprietary Internet technology. The requisite heat and mass balance information was available and such data was accessed as required to calibrate the flowsheet simulation.

5.6 Case 2 : Run 1 – Aspen PlusÒ With Library Modules Alone

A rendition of the Demonstration Case 2 natural gas combined cycle, as constructed by AP for use with Aspen Plus® library modules, is shown in Figure 42. The left-hand side of the figure may be viewed as being the gas-turbine (GT) side of the cycle, and the right-hand side may be regarded as the steam-turbine side of the cycle.

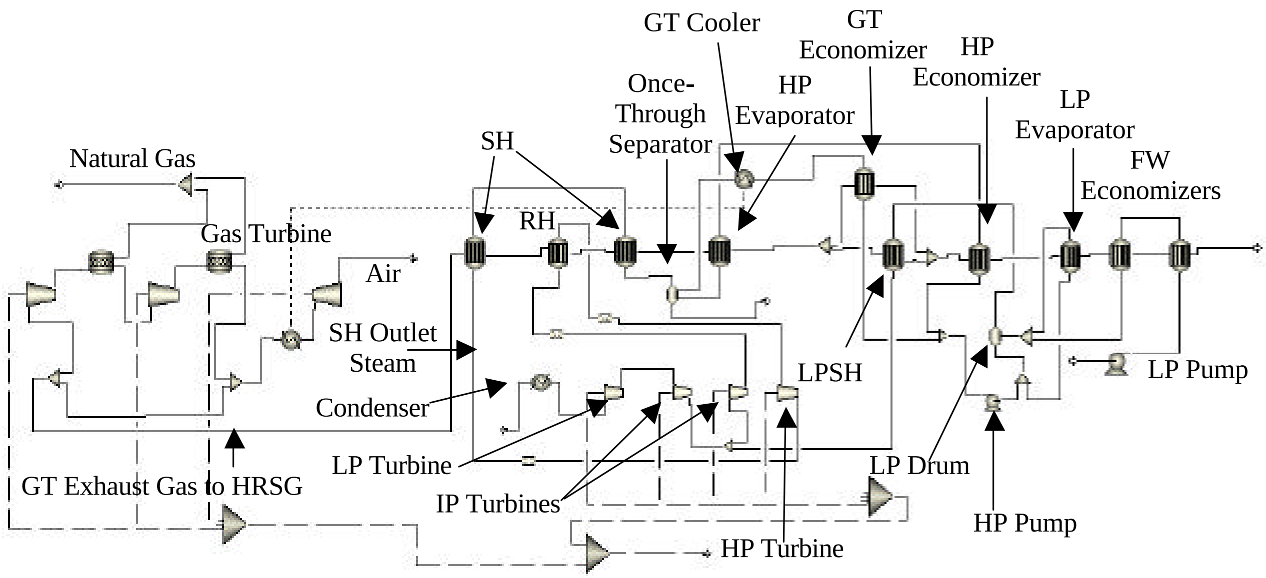

Figure 42: Aspen PlusÒ Steam Cycle Model for Demonstration Case 2.

A proprietary internal design code, denoted the HRSGPS code, had been used to study this cycle in detail at various loads. Heat and mass balance information was extracted from the HRSGPS runs, as well as from available experimental data, and was used to construct and calibrate the cycle.

For the gas-turbine side of the cycle, two design specs were used, in conjunction with the Broyden convergence algorithm, to produce the desired GT exhaust gas temperature. In the first design spec, the air flow rate was varied until the gas turbine produced the target generated power output (in MW). In the second design spec, the natural gas flow rate was varied until the gas turbine exhaust reached its target value of 923.15 K (1202 °F). The maximum continuous rating (MCR) for the gas turbine was denoted as the 100% GT load, and a sensitivity function was set up which varied the GT load from 100% MCR to 50% MCR. The gas turbine contains two combustors -- a combustor upstream of the HP turbine, as well as a “reheat” combustor downstream of the turbine.

On the steam-turbine side of the cycle, the heat exchanger modules, pumps, separator, and drum are part of an HRSG “island” (see Figure 43). A single design spec was used to solve for the superheat outlet temperature of the HP steam exiting the HRSG system, i.e., the flow rate of feedwater to the LP pump was varied until a target superheat outlet steam temperature of 838.15 K (1049 °F) was achieved. The feedwater flows from the LP pump into the feedwater economizer banks. Some of the FW economizer outlet flow is typically recycled from the downstream economizer to the upstream economizer in order to raise the outlet water temperature to a specified temperature (to prevent cold-water corrosion). However, the recycle stream was omitted in this cycle for the sake of simplicity.

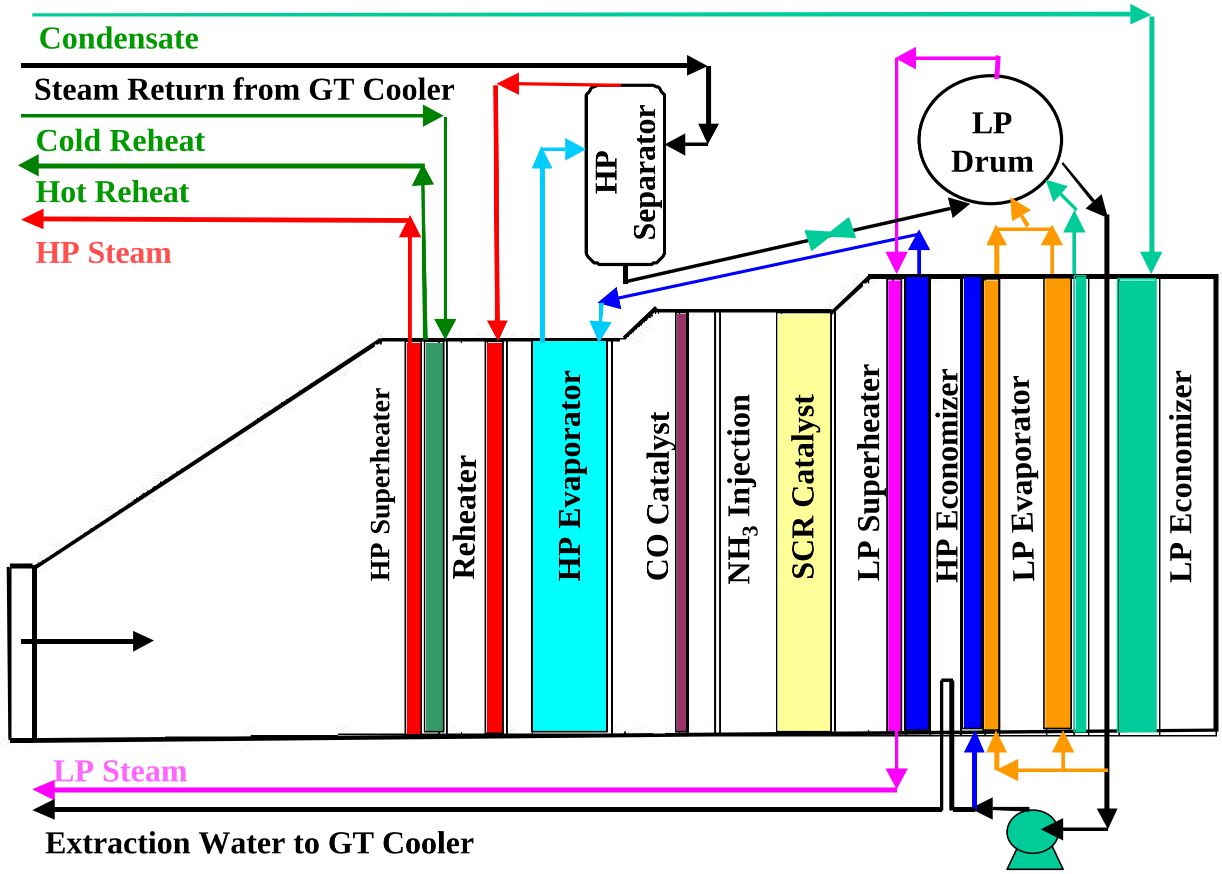

Figure 43: Schematic of HRSG Island for Demonstration Case 2.

The LP control system monitors the LP (saturated) steam flow (coming off of the drum), the feedwater flow, and the drum level. For example, if the drum level starts to decrease, the feedwater increases to compensate. The circulation flow rate through the LP evaporator is by natural circulation. Because of the height of the downcomer, static pressure changes associated with drum level changes have a negligible effect on the flow rate through the LP evaporator, and the flow through the LP evaporator remains relatively independent of other changes in the system. Consequently, as a simplification to the cycle, the natural circulation flow rate of saturated water flowing through the LP evaporator was maintained at a constant (and relatively high) circulation rate for all loads. The LP outlet pressure slides over the range of 100% to 80% (of steam load) after which it is fixed. Similarly, the HP outlet pressure slides over the range of 100% to 40% (of steam load) after which it is fixed.

The flow through the HP section is forced circulation (as implied by the presence of the HP pump). An overall mass balance over the HRSG island leads to the expression:

mass flow rate of the LP feedwater = HP-section feed (equivalent to the SH outlet flow rate) + mass flow rate of the LP (saturated) steam leaving the drum (equivalent to the LPSH outlet flow rate).

The control system attached to the LP pump simply modulates the incoming feedwater flow rate in order to balance the two outlet streams.

The majority of the HP feed is routed to the HP economizer, and subsequently, to the HP evaporator section and the once-through separator. The once-through separator is used to separate out any saturated water and return it to the LP drum. However, in typical steady-state operation, the stream entering the separator is always slightly superheated, which is then fed to the SH tube banks. About 10% of the HP feed is routed to the GT economizer, and subsequently to the GT air cooler. The heated GT return steam is then fed directly to the once-through separator. Design standards for the GT steam return flow rate, pressure, and temperature, are referenced to the % GT load.

The superheated steam leaving the "once-through" separator is fed to two sequential superheat tube banks. Under some conditions, if the superheat outlet steam temperature is too high, HP desuperheat is added to the superheat outlet stream to reduce the temperature to the desired setpoint. However, the HP desuperheat is never used at the design (MCR) condition; it is only required at low loads and for transient lags. At low loads, a comfortable margin of (e.g., 15 K to 40 K) superheat may be desired for the once-through (OT) separator, in which case, the overall HP steam flow may be reduced, and HP desuperheat may be required to reduce the temperature of the superheat outlet stream. After the superheat outlet steam flows through the HP turbine, it is fed to the reheat (RH) tube bank, and subsequently, to the intermediate pressure turbines. A RH desuperheat spray may also be used at the lower loads. In the present Aspen Plus® runs, an HP desuperheat was added at one point to the cycle, but desuperheat sprays constitute a discontinuity in the set of equations being solved and Aspen Plus® converged with difficulty. Consequently, the desuperheat mass addition, which represented e.g., less than 1% of the HP steam flow at low loads, was ignored in the present computations.

Since no performance maps were available for the cycle components, the component pressure drops and discharge pressures were simply curve fit as a function of the load from the HRSGPS code results and experimental results. Tube bank effective heat transfer areas, as well as component efficiencies, were calibrated as necessary to produce the desired output results at the design (MCR) condition. For the tube banks, a power-law expression for the gas-side (hot-side) overall heat transfer coefficients was used, with an exponent of 0.75.

In actuality, all of the tube banks in the HRSG are finned tubes, the heat transfer correlations for which are available from the vendor/manufacturer. The actual heat transfer coefficient expressions are a complex function of Reynolds number (and hence blockage) and various finned-tube design parameters, specific to HRSG-type heat exchangers, that are not available in an Aspen Plus® library module. One of the challenges that process modelers face is the availability of validated equipment modules. Generally, the library components in Aspen Plus® are relatively simplistic and have not been customized with the appropriate performance maps or manufacturer's correlations required to make accurate predictions. For this reason, it is not surprising that the Aspen Plus® runs, calibrated for the MCR condition, begin to deviate from the HRSGPS results at off-design conditions. Nevertheless, the results from the Aspen Plus® runs remain representative of the experimental data, despite the apparent limitations.

Results from the Aspen Plus® run are shown in Figures 44 through 46. For these runs, the target setpoint for the superheat outlet temperature was about 838.15 K (1049 °F), with a sliding superheat outlet pressure, starting at MCR, of about 16.6 MPa (2413 psi).

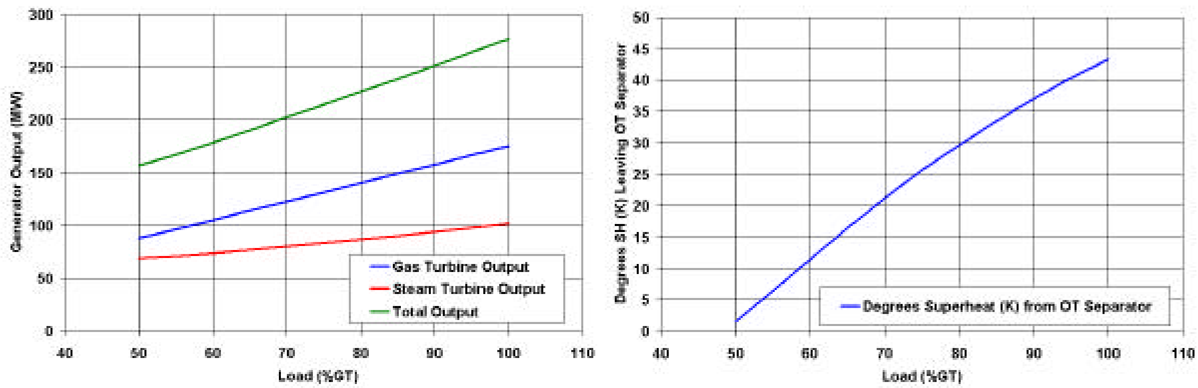

Figure 44: Case 2 : Run 1 Results – Generator Output and Degrees SH at OT Separator.

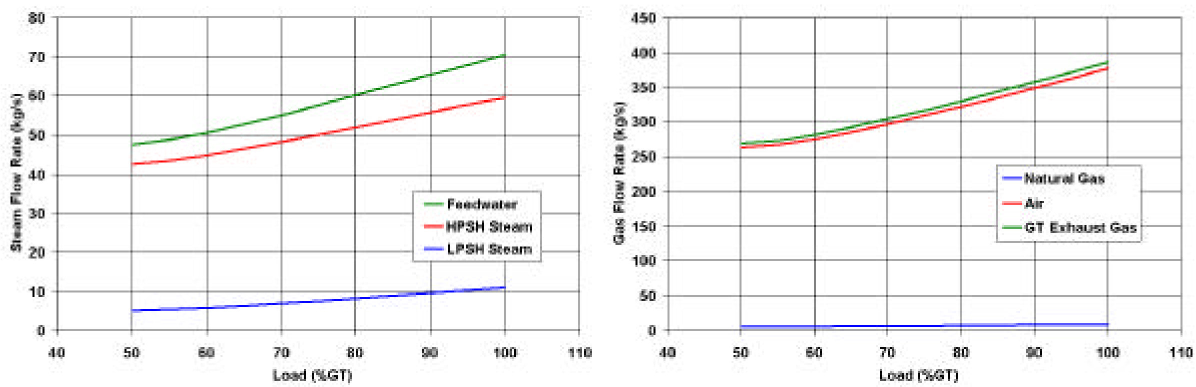

Figure 45: Case 2 : Run 1 Results – Steam, Fuel, and Air Flow Rates.

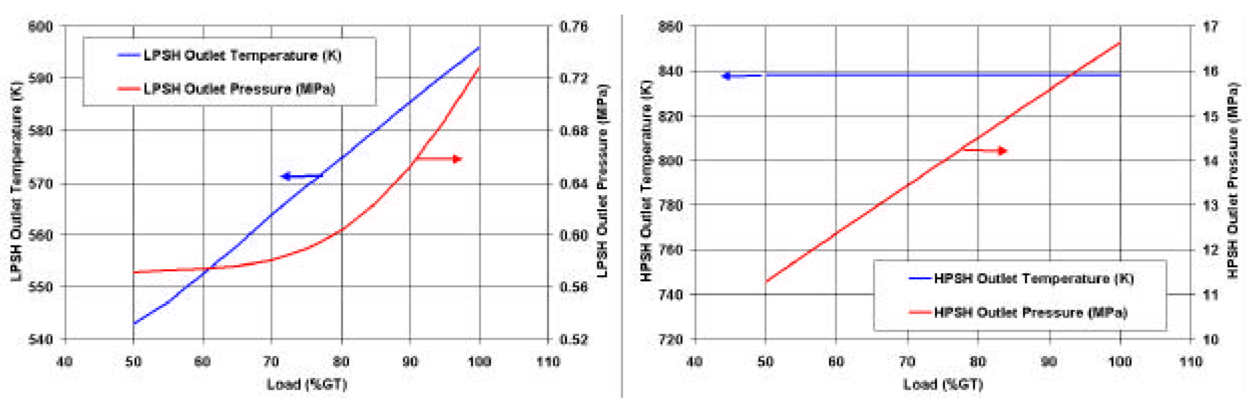

Figure 46: Case 2 : Run 1 Results – LPSH and HPSH Temperature and Pressure.

The results are representative of the experimental data (not shown), and were deemed adequate for demonstration purposes.

5.7 Case 2 : Run 2 – Aspen Plus® Coupled With HRSGPS

Run 2 consists of the coupling of an AP proprietary code with Aspen Plus®. The AP proprietary design package selected for use was a heat recovery steam generator performance simulation (HRSGPS) code. The performance-modeling package is a proprietary (0-D) design code that reflects ALSTOM's design standards and experience. It was constructed with Visual Basic and permits user interaction through GUIs. The HRSGPS is another example of an industrial design code, with which the Vision 21 Virtual Simulation environment must interface.

5.7.1 Software Linkage

As shown in Figure 47, the HRSGPS code essentially represents the entire HRSG island, and it replaces a large segment of the cycle. When the performance simulation code is instantiated as a CAPE-OPEN block upon the Aspen Plus® flowsheet from the Aspen Plus® CO module template, it essentially replaces ten of the tube bank modules, in addition to pumps and drums/separators. The HRSGPS code contains all of the required information about the GT exhaust gas and water/steam flow rates, and automatically incorporates desuperheater sprays. In the present case, the HRSGPS code constitutes a single block icon on the steam-turbine side of the flowsheet that must interact with and exchange information with the gas turbine portion of the cycle, as well as the remainder of the steam-side of the cycle.

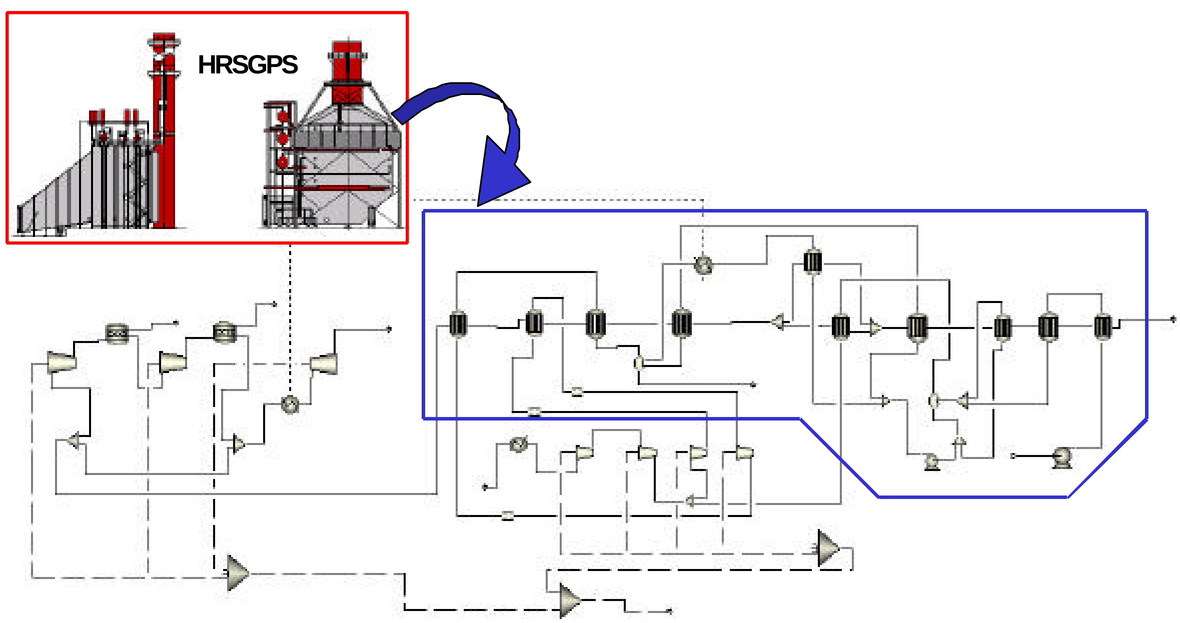

Figure 47: Portion of Cycle Replaced by the HRSGPS Code.

The HRSGPS package has not been coded with material stream or port connections. Consequently, all of the information exchange between Aspen Plus® and the design code must occur through a transfer of CAPE-OPEN parameters. From the gas turbine side of the cycle, information such as

GT exhaust mass flow rate, temperature, pressure, and species concentrations must be passed to the HRSGPS code. On the steam-turbine side of the cycle, all of the stream information that would have been transferred had ports been provided (e.g., where the blue line in Figure 45 intersects with each of the cycle streams) must also be exchanged. Some of the stream information, such as the steam mass flow rate, pressure, temperature, and quality, must be passed from the performance design code to Aspen Plus®, and some of it must be passed in the opposite direction, depending upon whether the stream's directional flow is "into" or "out of" the HRSGPS code. Besides the obvious stream connectivity information, the HRSGPS solution procedure requires that additional stream parameters and HRSG-related inputs also be provided; and Aspen Plus®, as the executive software, is responsible for providing this information as well. The controller and software wrapper that act as an interface between the HRSGPS code and Aspen Plus® package, assists in the transfer of this information.

In stand-alone mode, the user interfaces with the HRSGPS code and provides input through GUI panels. The execution of the code is prompted by the user and is interactive, rather than batch. Although the user inputs information via GUIs, that information is ultimately pushed to an input data file, which is then read in immediately prior to execution. The input data file typically contains a series of "cases" or "runs". The first case is always the design (or MCR) load. Subsequent cases are cases at different loads or different operating conditions, and HRSGPS runs each of them in series. However, all of the subsequent cases rely upon the execution of the first (i.e., design load) case, since pressure drops and other parameters at lower loads are calculated by reference to those corresponding values computed previously at the design load. When the HRSGPS code is run in conjunction with Aspen Plus®, the first design case was preserved in the input data file in its original form, and then a second case was added, which the Aspen Plus® code would overwrite as appropriate to reflect the load condition that it is currently solving.

For the sake of simplicity and convenience, it was decided to couple the performance simulation code with Aspen Plus® in much the same manner as the BPS code. A template for the CO-compliant wrapper (written in C++) was provided by Fluent Inc., and appropriate modifications and additions were made to the wrapper by an AP programmer to accommodate the HRSGPS code. Access was granted to the HRSGPS "source" code, so that modifications could be made directly to the Visual Basic coding. This permitted the wrapper interface to function in a somewhat more sophisticated manner than was possible with the BPS code. Only a few of the interface routines from the CO library had to be modified (e.g., methods/functions such as getParameters, initialize, and calculate). The compiled wrapper was implemented as a dynamic link library (.dll). Approximately 3 man-weeks were required for the programmer to complete the wrapper coding and debug it.

Since access to the HRSGPS source code was available, the performance simulation package was converted into a batch execution code that Aspen Plus® could launch each time that the CO block was encountered in the cycle. In order for the HRSGPS code to execute properly and provide meaningful results, updated information must be received from the Aspen Plus® cycle (see Figure 48) prior to each execution. A CO variable was defined for each informational item or parameter that is passed from Aspen Plus® through the V21 Controller to the HRSGPS wrapper. In general terms, the wrapper receives the updated CO/CORBA parameter values and creates a single-columned "list file" that contains those values. The wrapper then spawns the execution of the

HRSGPS code, which displays the iterative solution results on the screen so that the user can monitor its progress. The HRSGPS code reads in its entire (primary) input file, and then subsequently reads in the list file, which overwrites the designated CO parameters (of the second case only) in memory to reflect the current state of the shared variables. When the HRSGPS code completes its (serial) execution (of the two cases), it then writes its normal output file, as well as another “list file”, which contains the CO parameters which need to be transferred back to the Aspen Plus® cycle. As with the input, a CO variable was also defined for each informational item or parameter that is passed from the HRSGPS wrapper back to the Aspen Plus® cycle. The wrapper reads the output list file and passes the values to the CO collection in the V21 Controller, and from thence, to Aspen Plus®.

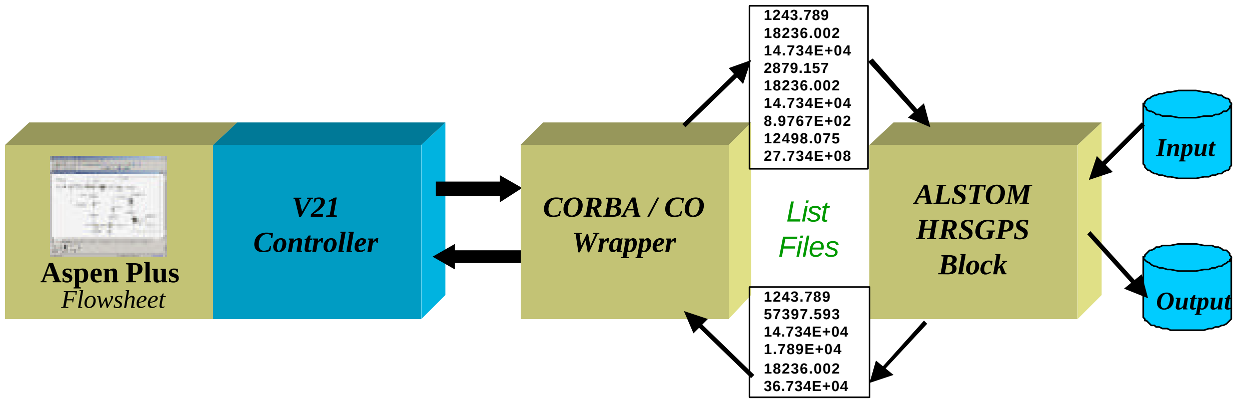

Figure 48: CO Parameter Exchanges Between the HRSGPS Code and the Wrapper.

A total of 44 CO variables were defined in the “advanced parameters” panel of the Configuration Wizard, with type designated as “real,” and with their corresponding default values, units, and lower and upper limits. Of those 44 CO parameters, 27 were used to modify the inputs, and 21 were extracted from HRSGPS to pass back to the Aspen Plus® cycle (with some overlap between the two sets).

5.7.2 Solution Strategy and Results

Each execution of the proprietary performance design code requires about 80 seconds (on the 500 MHz PC). A screen capture of the flowsheet, with the instantiated HRSGPS block, is shown in Figure 49. The blue and red circles (indicating the flow leaving and entering the block, respectively) represent some of the connection points where stream information must be exchanged with the HRSGPS block.

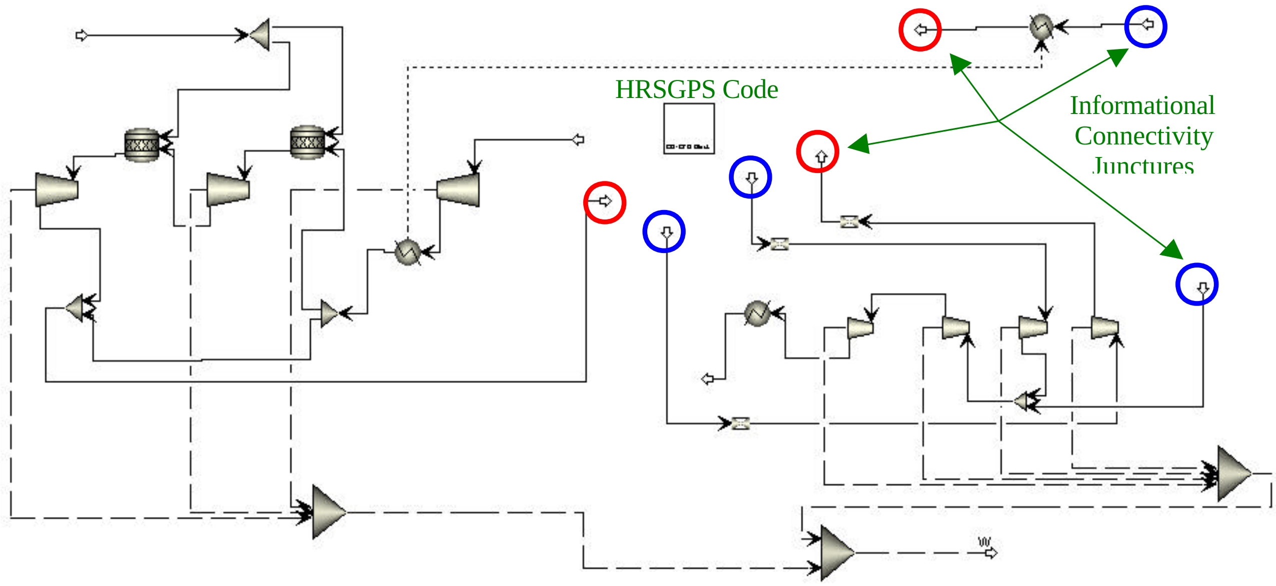

Figure 49: The Instantiated CO Block for the HRSGPS Code on the Aspen Flowsheet.

Essentially, the HRSGPS code internally varies the superheat outlet flow rate until the desired superheat outlet temperature is achieved. The superheat outlet flow rate essentially determines what the upstream HP steam flows will be, and the feedwater flow rate is adjusted to provide the requisite mass balance around the LP drum.

Additional results are shown in Figures 50 through 52 for the mass flow rates of the various streams, as well as the LPSH and HPSH conditions.

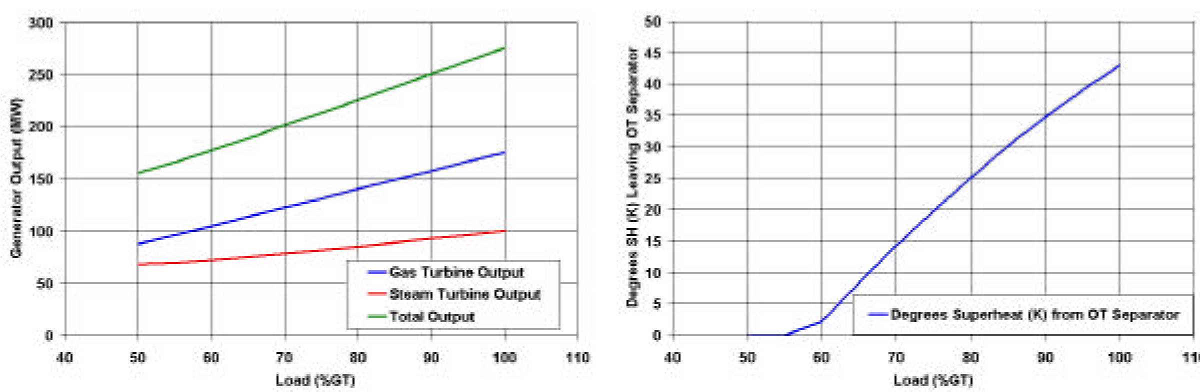

Figure 50: Case 2 : Run 2 Results – Generator Output and Degrees SH at OT Separator.

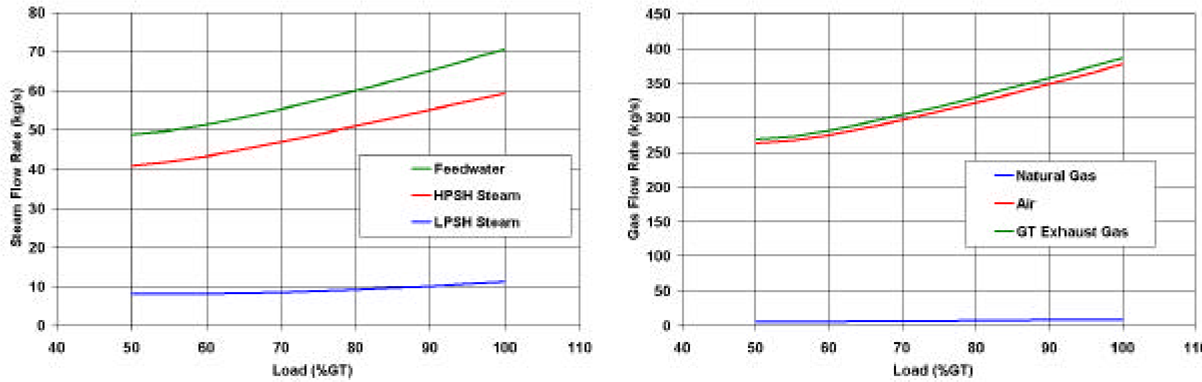

Figure 51: Case 2 : Run 2 Results – Steam, Fuel, and Air Flow Rates.

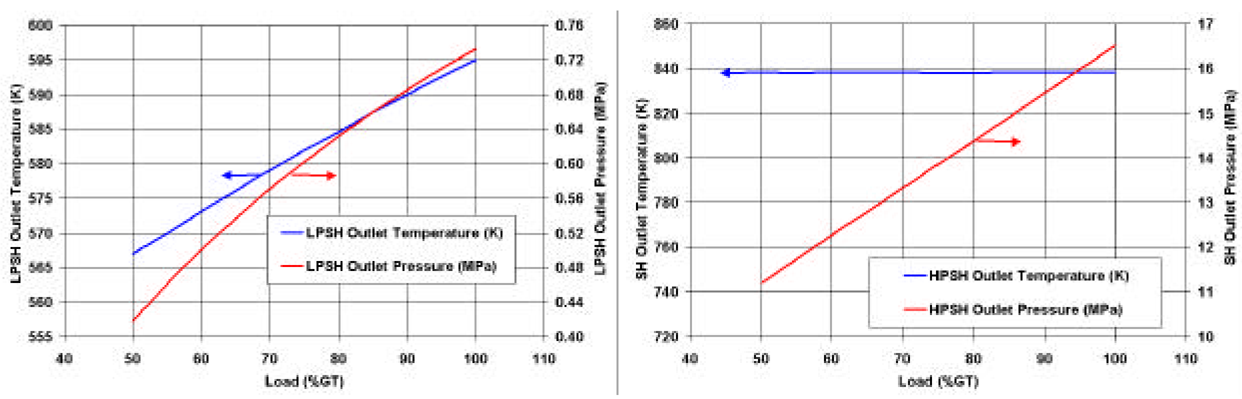

Figure 52: Case 2 : Run 2 Results – LPSH and HPSH Temperature and Pressure.

In this run, the HP desuperheat spray was not allowed, since as Aspen Plus® was using that value as a target temperature. The resultant degrees superheat from the OT separator has decreased to zero (i.e., saturation), which would not be permitted in practice. The typical response would be to decrease steam mass flow rate and then to apply desuperheat spray to bring the superheat outlet temperature down to the desired setpoint. While the inclusion of desuperheat or more detailed equipment-level and operational strategy information would surely refine the above results, the predicted trends are sufficient to demonstrate and assess the viability of the coupling / connectivity between Aspen Plus® and an industrial legacy code, using the Vision 21 Controller and CAPE-OPEN interface.

5.8 Case 2 : Run 3 – Aspen PlusÒ Coupled With FLUENTÒ

Run 3 consists of the coupling of the Aspen Plus® package with the FLUENT® CFD code. FLUENT® Version 6.1.15 was used for all of the FLUENT® computations and the demonstration case was run computed on a single-processor (500 MHz) PC. Because of the CPU-intensive nature of CFD runs, the CFD cases were understandably reduced in size and simplified considerably (relative to their industrial design counterparts) in order to make the computations feasible on a PC. It is not believed that the simplifications detract from the overall purpose of the project goals, that of demonstrating the feasibility and viability of linking advanced computational models with flowsheet software.

5.8.1 Cycle Preparation

The CFD block was constructed to collectively represent only the tube bank components within the HRSG. It does not encapsulate or embrace as many flowsheet components as the HRSGPS code does. As shown in Figure 53, when the CFD block is instantiated on the flowsheet, it essentially replaces that portion of the cycle that is encapsulated by the blue box. (The gas-turbine side of the cycle has been omitted for illustrative purposes.)

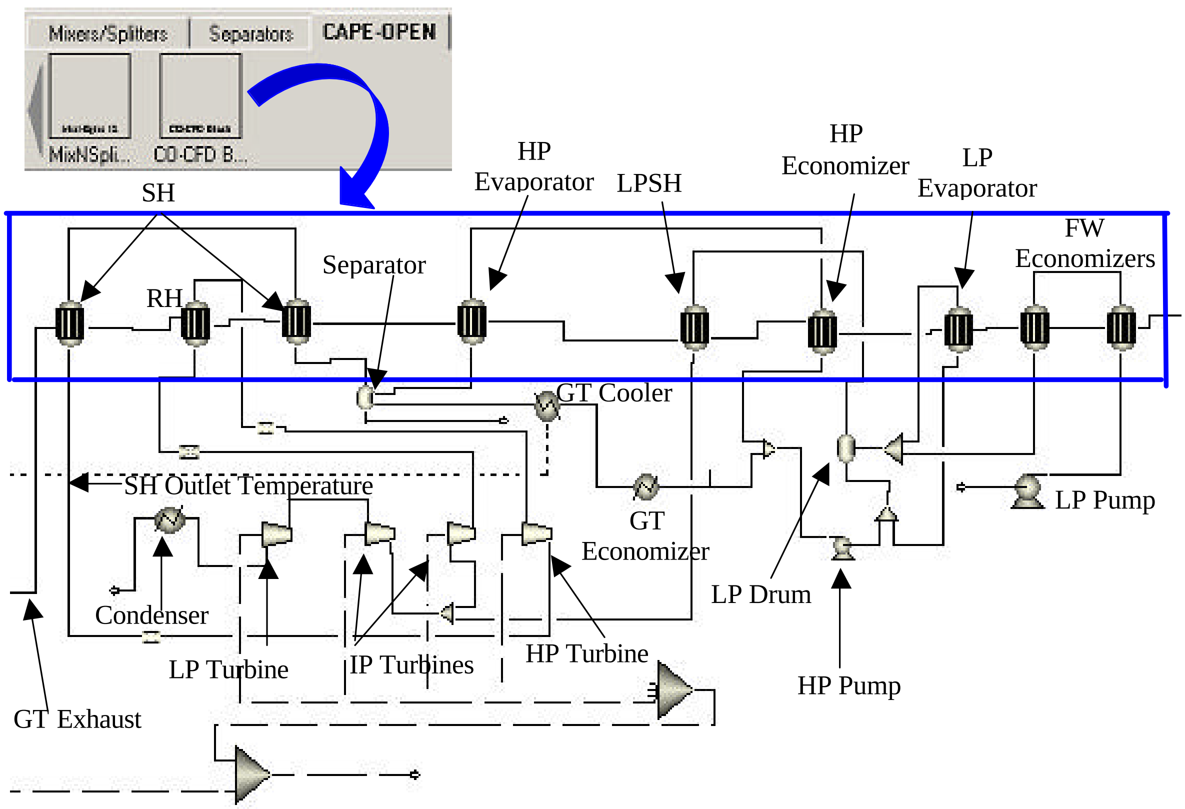

Figure 53: Flowsheet Modification Strategy Prior to Instantiation of HRSG CFD Block.

It should be noted that the GT economizer tube bank, which was originally positioned in parallel with the LPSH component, was re-routed and hard-wired as a simple heat exchanger. This modification was made for the sake of simplifying the CFD grid. The GT economizer bank typically occupies only a small portion of the total span across the width of the HRSG. Since the HRSG grid was anticipated to be rather coarse, and since the GT economizer receives less than 10% of the HP steam flow anyway, it was decided not to resolve the GT economizer section within the CFD mesh. Consequently, the GT economizer was taken out of the GT exhaust path, trusting that such an alteration would not have a significant impact on the rest of the components (at least for the purposes of the present study).

Connectivity junctures, at which information must be exchanged between the instantiated CFD block and the Aspen Plus® cycle, occur wherever the blue line (in the preceding figure) intersects and cuts a stream. As shown in Figure 54, two of the stream junctures, involving the GT exhaust stream, are material stream port connections. Information, such as the stream mass flow rate, temperature, pressure, and quality, must be transferred at the junctures of the other 10 streams (5 of which are entering, and 5 of which are leaving the encapsulated area).

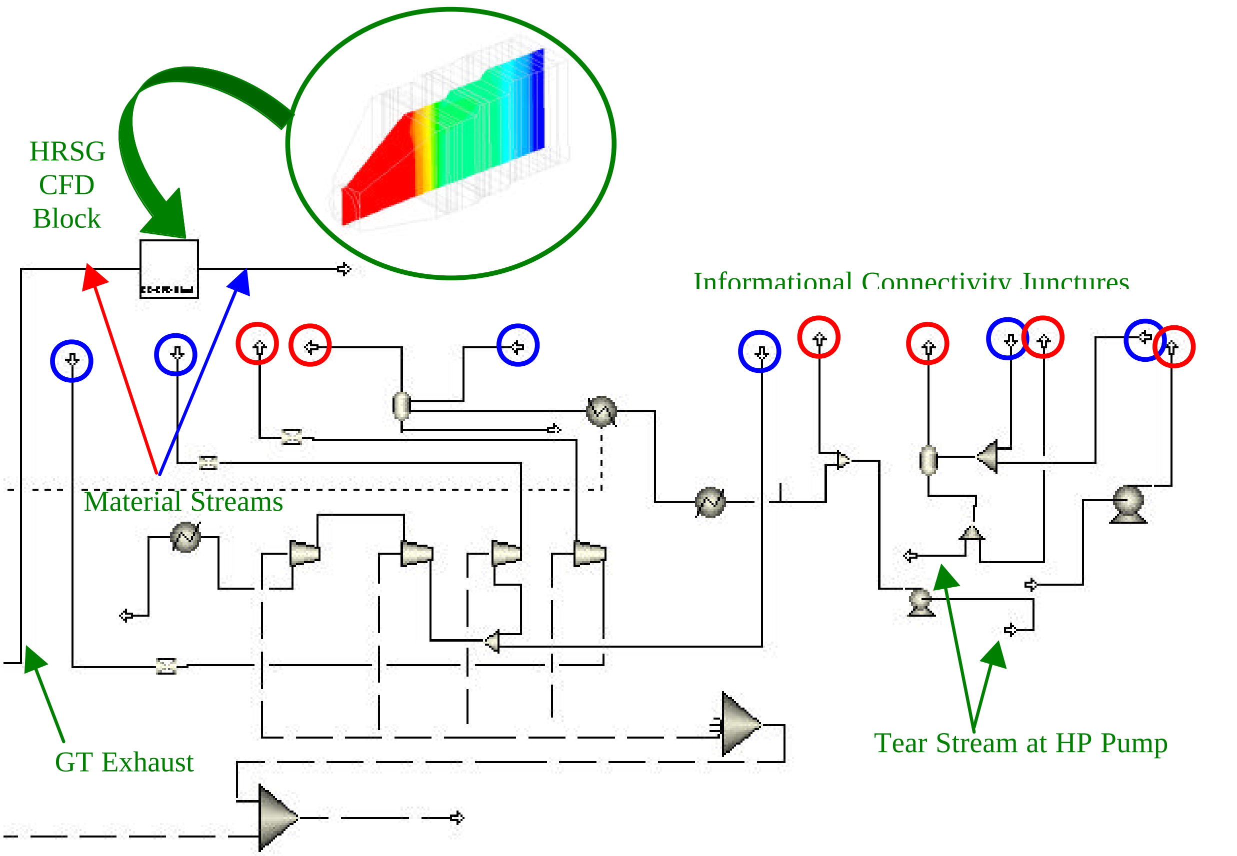

Figure 54: Coupled FLUENTÒ and Aspen PlusÒ Cycle for Demonstration Case 2.

Since the solution method for the HRSGPS code is based upon iterative estimates of the HP stream mass flow, a similar approach was followed here. A tear stream was torn immediately prior to the HP pump. The design spec for the steam-turbine side of the cycle consisted of manipulation of the mass flow rate into the HP pump until the desired superheat outlet steam temperature was achieved. (Allowing the design spec to manipulate the LP pump feedwater flow rate would probably also have been successful.) However, it can be seen that all of the discrete, unconnected segments within the cycle can be problematic. For example, if the design spec specifies a new value of the mass flow rate at the HP pump, the tube bank model within the CFD code is aware of the new mass flow rate only at the corresponding juncture which feeds the HP economizer and the HP evaporator. The HPSH and RH sections are still using the previous/old value of the mass flow rate, and will not be aware of the new flow rate until FLUENT® completes its execution and subsequently provides the new mass flow rate as an output to the HP (once-through) separator. Therefore, it can be seen that, with the current approach, the mass flow rates in the HPSH and RH sections will always lag the mass flow rates in the HP evaporator section. Accordingly, the design spec will not be able to accurately establish a new search direction and magnitude until the mass flow rates, temperatures, etc. have propagated fully throughout the cycle and an effectual mass and energy balance have been accomplished.

In order to overcome this problem, the convergence procedure was manually sequenced within the steam-turbine design spec. For purposes of discussion, the convergence of the CFD block, followed immediately by the solution of the remainder of the components in the steam-turbine cycle, may be viewed as a single solution "pass" of a "couplet." In principle, this "couplet" (the alternating solution of the CFD block followed by the steam-turbine cycle) is solved a sufficient number of times within a single design spec iteration, until the mass and energy balances stop changing. Once the stream information has propagated sufficiently from one end of the HRSG to the other, and the flow rates and temperatures, etc. have stopped changing and are considered to be in balance, then the calculated superheat outlet temperature may be considered to be reliable, and the design spec can then establish a new search direction and magnitude for the manipulated variable(s).

The preceding discussion dealt principally with the HP section of the cycle. The LP section was solved with a "direct substitution" type method. For each calculation pass of the "couplet," the mass flow rate into the LP pump was manually updated and adjusted to be equal to the sum of the HP pump mass flow rate plus the prevailing LPSH flow rate. (This direct substitution approach was thought by Aspen Plus® personnel to be similar to utilizing the "balance block" method in Aspen Plus®, which was not attempted.)

In the current method, the successive "couplets" were manually sequenced multiple times within a single iteration of a design spec. Additional discussions with Aspen Plus® personnel, after the runs were completed, have indicated that it is possible to replace the manual sequencing with automatic sequencing that is controlled by the Aspen Plus® solution algorithms. This may be done by adding composite heater blocks to the cycle to essentially replicate those that are in the CFD block. For example, a single composite FW economizer heater block could be added to the cycle to represent the two FW economizer banks in the CFD block (see Figure 55). Similarly, other composite heater blocks could be added to represent the LP evaporator, the composite HP economizer/evaporator, the dual superheaters and the single reheater. After the FLUENT® block has been converged, the appropriate outlet mass flow rate, temperature, pressure, and quality calculated for each of the tube banks inside of the CFD block (or alternatively, the heat duty) could be passed via the CO parameters to the replicated heater blocks. In this way, full connectivity throughout the steam loop would be maintained, which would allow the mass and energy balances information to be propagated throughout the steam-turbine portion of the cycle. This doesn't mean that the CFD block would only be executed once within a single design spec iteration, because the CFD block would still have to exchange information multiple times with the Aspen Plus® cycle before the "couplet" converges to a stable solution. It does mean however, that Aspen Plus® would automatically control the number of couplet passes according to some convergence tolerance, which would, in principle, be more efficient than the previous manual sequencing procedure.

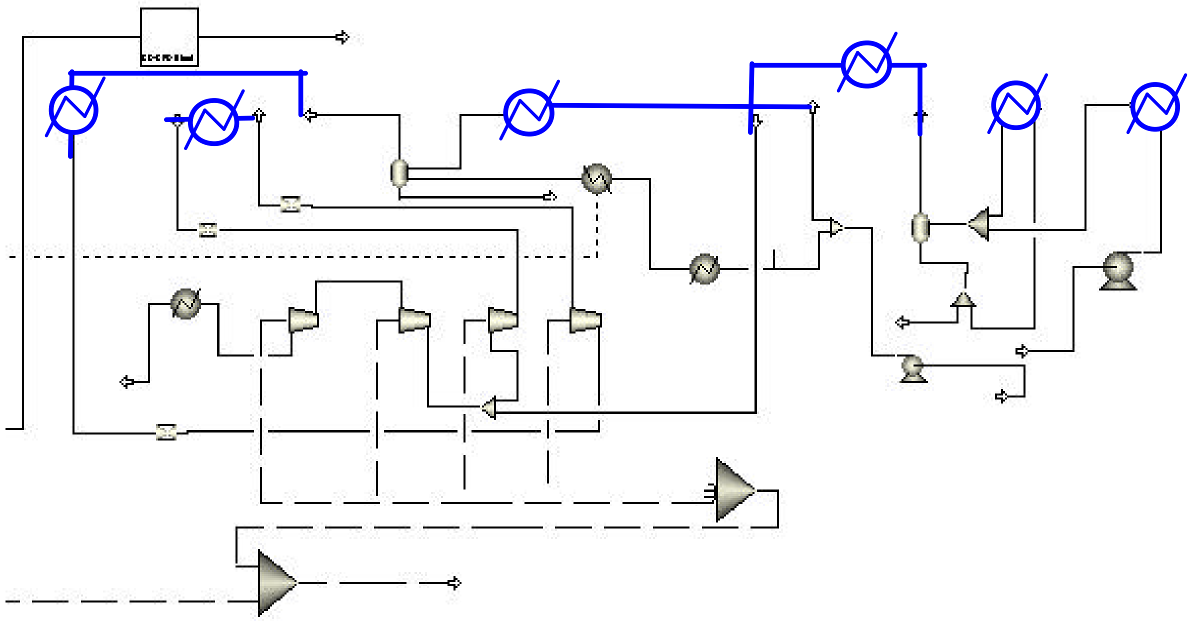

Figure 55: Alternative Sequencing Methodology for Demonstration Case 2.

5.8.2 FLUENT® Case and Interface Files Preparation

The FLUENT® case and data files were prepared and calibrated prior to coupling with Aspen Plus®. Typical industrial grids may be on the order of 500,000 to one million cells. However, in order to decrease the CPU penalty associated with large cases, the grid was reduced to approximately 40,000 cells. The external grid structure is shown in Figure 56. A non-conformal interface was used in the vicinity of the inlets in order to transition quickly from a small-celled paved mesh to a larger-celled square mesh.

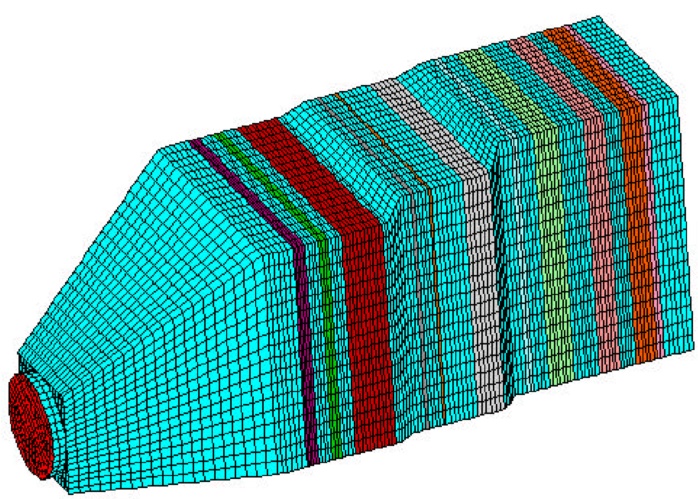

Figure 56: Exterior Grid for HRSG in Demonstration Case 2.

The blueprints indicate that some of the tube banks in the HRSG were split into two separate sections with a slight amount of longitudinal space between them. However, for purposes of the computation, where only empty space separated two sections belonging to the same tube bank, the two sections were collapsed into a single composite section. (In actuality, a heat exchanger model bug, which has since been fixed, prevented, at the time, 3 or more heat exchanger groups to be connected to each other.) The tube banks are finned and significant pressure drop exists through the banks. The flow is effectively straightened after the first or second tube bank, and therefore, the tube banks were retained as single zones (without any subdivisions in the span-wise direction). The porous media inertial resistances for the finned tube banks were determined by calibration to the overall pressure drops reported in the HRSGPS output.

The exterior walls were made adiabatic. Heat loss occurred only through the tube banks. The inlet boundary condition was rectilinear flow with a mass flow rate boundary condition. The inlet turbulence intensity was set to 10%, and the inlet dissipation rate was a function of the inlet hydraulic diameter. The outlet boundary was defined as a pressure-outlet boundary condition. There was no supplemental fuel injection or reaction near the inlet of the HRSG. Deactivation of the radiation model was viewed as an acceptable simplification.

The sub-models for the CFD runs consisted of the k-ε turbulence model with standard wall functions and species transport for 5 species (CH_4, O_2, CO_2, H_2O, and N_2). Although the inlet methane concentration was identically zero, it had to be included in the species list in order for the Aspen Plus® and FLUENT® species list to correspond precisely in formula name and sequence.

The material stream in the Aspen Plus® flowsheet representing the gas turbine exhaust connects directly with the corresponding inlet port connection that was defined for the CFD block (through the Configuration Wizard). A single material stream representing the HRSG exhaust was connected to the pressure-outlet boundary condition. The connectivity ports allow the direct and automatic transferral of stream information from Aspen Plus® to the CFD case, and vice-versa. For stream information, Aspen Plus® currently transfers the mass flow rate, pressure, temperature, species names, molecular weights, and mole fractions. Again, as with Demonstration Case 1, the disparity in the oxygen specific heat between Aspen Plus® and FLUENT® was a concern, and the option to transfer properties “curve fits” (specific heat, thermal conductivity, and viscosity) from Aspen Plus® to FLUENT® was turned off.

5.8.3 FLUENT® Calibration and Setup of the CO Collection

The FLUENT® heat exchanger (HX) model was calibrated to match the HRSG design code results at the MCR condition. In the calibration exercise, the FLUENT® case was run in a stand-alone mode, using the flow rates and conditions reported in the HRSGPS code at 100% GT load. The calibration was performed by adjusting the surface effectiveness factors for the tube banks. It should be noted that the tube bank model and associated ALSTOM UDFs in the FLUENT® model did not contain any finned-tube heat transfer correlations. Therefore, the calibration not only accounts for the unknown effects of fouling and various heat transfer inefficiencies, but also for the completely artificial application of bare-tube correlations to finned tubes. An example of the calculated temperature contours at the MCR condition is shown in Figure 57, where mass-averaged temperatures are provided at the outlet (i.e., "Tout") of selected tube banks. Calculated inlet steam temperatures (i.e., steam/water entering the tube banks) and the corresponding tube bank absorptions at the 100% GT load condition (i.e., MCR) are provided in Figure 58.

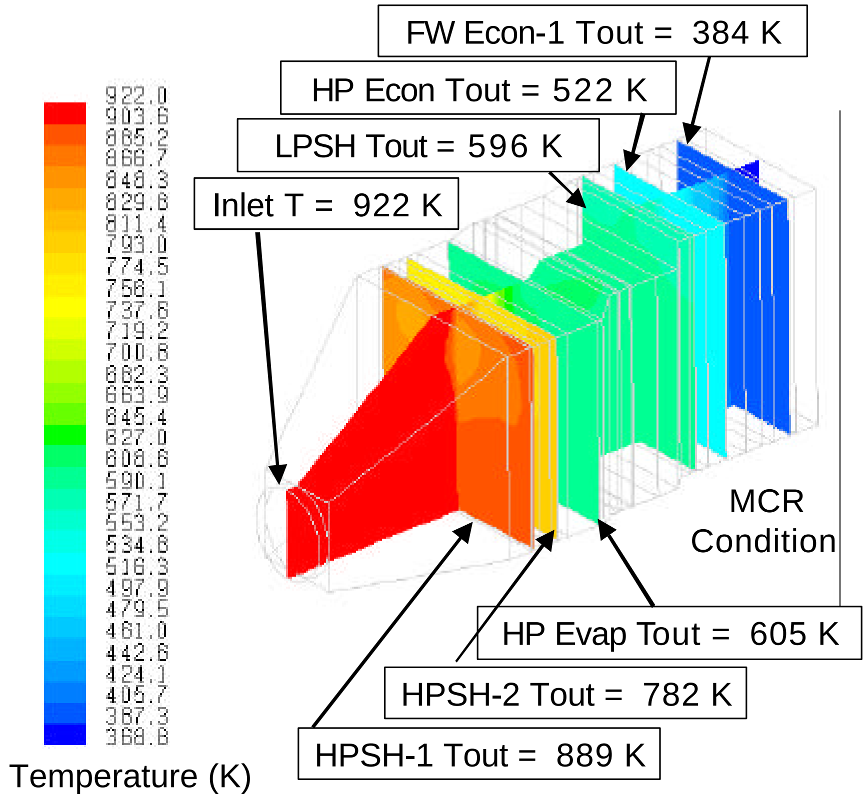

Figure 57: Contour Plots Following Calibration of FLUENTÒ HX Model for Case 2.

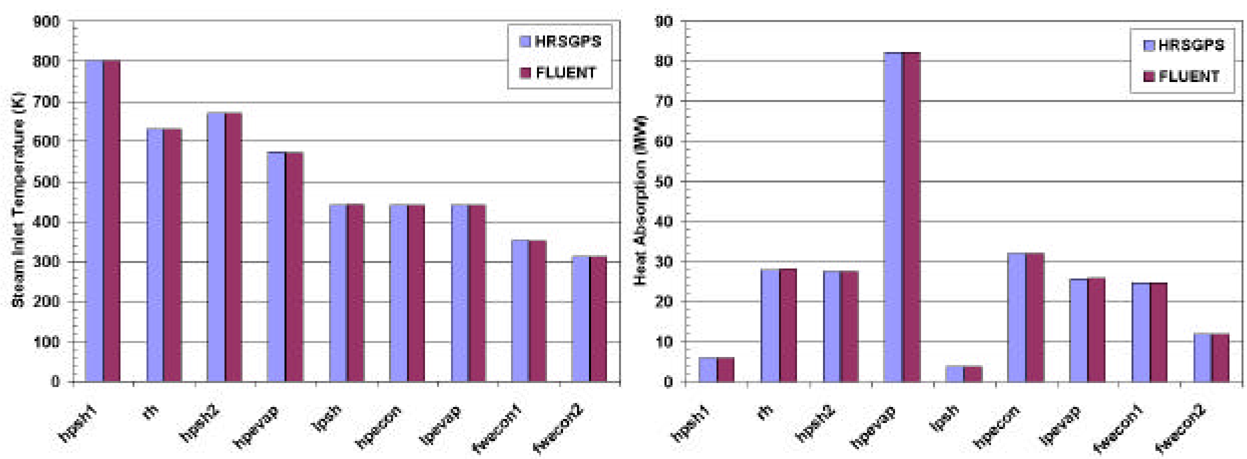

Figure 58: Calibrated Results Using FLUENTÒ HX Model for Case 2 at 100% GT Load.

Once the calibration at the MCR condition was achieved, the alignment of the FLUENT® results at the 75% GT load condition was investigated. Again, FLUENT® was run using the mass flow rates and conditions from the corresponding HRSGPS case. As can be seen, the 75% GT load case continued to show good agreement, even though the calibration was done at the 100% GT load condition. To the degree that the Aspen Plus® cycle mimics the internals of the HRSGPS code, the run, in which Aspen Plus® is coupled with FLUENT®, should produce comparable results.

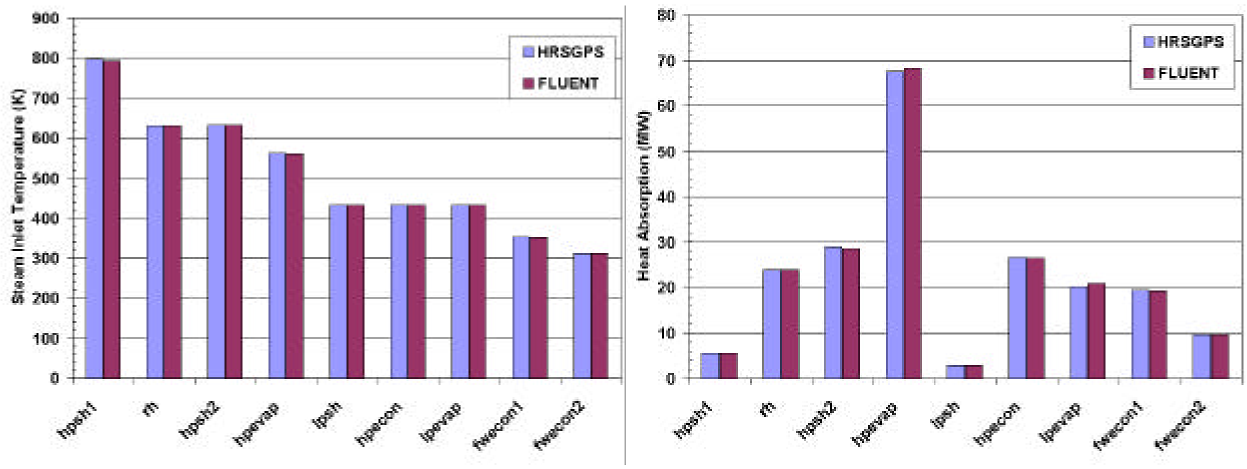

Figure 59: FLUENTÒ HX Model Results for Case 2 at 75% GT Load.

A total of 60 CO parameters were defined in order to exchange information between Aspen Plus® and FLUENT®. Of those CO parameters, 36 variables were defined via Scheme functions to pass the requisite tube bank pressure drop, inlet temperature, inlet pressure, inlet steam quality, and mass flow rates (as required) from Aspen Plus® into FLUENT®. An additional 24 variables were defined as RP-VARs to pass tube bank outlet quantities (temperature, pressure, mass flow rate, and quality) from FLUENT® to Aspen Plus®. The CO collection for the CFD wrapper was defined in the “Advanced Parameters” panel of the FLUENT® *Configuration Wizard.*

5.8.4 Convergence Characteristics and Results

In Demonstration Case 2, the cycle is more difficult to solve since the CFD block has multiple points at which information is exchanged with several different sections of the steam-turbine side of the cycle. As mentioned previously, in order to overcome this problem, the convergence procedure was manually sequenced within the (steam-turbine) design spec. In principle, the alternating solution of the CFD block followed by the solution of the remainder of the steam-turbine cycle (termed a “couplet”) is solved successively a pre-determined number of times within a single design spec iteration. The hope is that the “couplet” will have been solved a sufficient number of times for the overall mass and energy balances to converge to within some tolerance. Once the stream information has propagated sufficiently from one end of the HRSG to the other, and the flow rates and temperatures, etc. have stopped changing and are considered to be in balance, then the calculated superheat outlet temperature may be considered to be reliable, and the design spec can then establish a new search direction and magnitude for the manipulated variable(s). Through some experimentation, it was found that the “couplet” must be solved on the order of (at least) 15 to 20 times before the design spec would be able to reliably converge to a solution. In the current approach, FLUENT® was allowed to perform a maximum of 50 iterations during each of the 16 passes (for a maximum of 800 FLUENT® iterations per design spec iteration). As will be seen, this number of iterations and passes is considered to be "barely adequate," but provides sufficient accuracy for the design spec to ultimately converge on the target superheat outlet temperature to within a coarse tolerance. A more refined convergence is possible, but the HRSG CFD block converges relatively slowly, since any small perturbation to one of the tube banks impacts other tube banks in the HRSG, both upstream and downstream from its position. Multi-processor compute resources will be required to adequately solve this demonstration case to the desired accuracy.

The design spec for the steam-turbine side of the cycle manipulates the HP steam flow rate fed to the HP pump until the superheat outlet steam temperature achieves the desired target temperature of 838.15 K (1049 °F) to within a tolerance of 1.1 K (2 °F). Some representative convergence characteristics for Demonstration Case 2 are provided in Figure 60 for the 70% GT load point, where the superheat outlet temperature is being tracked as a function of FLUENT® iterations. Good initial conditions were provided in this instance so that convergence would occur within only a few Aspen Plus® design spec iterations (and within a reasonable clock time). At the 70% GT load point, it can be seen that the design spec iterates 3 times. Within each design spec, the CFD block and the cycle are solved in alternating fashion a total of 16 times. Each time that the CFD block executes, FLUENT® is permitted to iterate a maximum of 50 times. Two of the CFD block executions are shown in the expanded "blowup." The superheat outlet temperature spikes and oscillates rapidly when it is first executed, after which it quickly settles down and becomes well behaved.

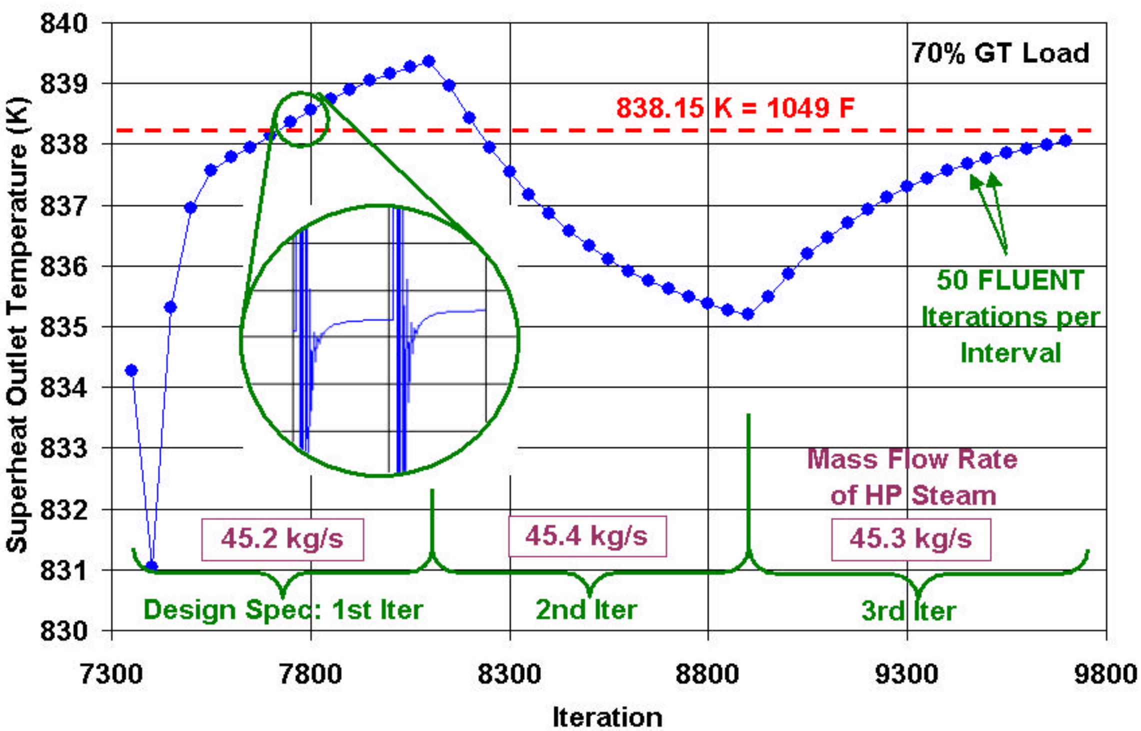

Figure 60: Convergence of Superheat Outlet Temperature for Case 2 at 70% GT Load.

It is apparent that the 16 successive solutions of the “couplet” within each design spec is somewhat insufficient, since the superheat outlet temperature has not leveled off to its “asymptote.” However, it is probably within a degree Kelvin of its asymptote, which is also the design spec tolerance. Ideally, one might continue to solve the couplet with additional iterative passes until the superheat temperature has leveled out more before pronouncing the design spec completed. However, one must consider the computational cost of making the additional passes versus the cost of having to do additional design spec iterations because of inadequately converged solutions. The safe and sure route, of course, is to ensure that the couplet has been solved with a sufficient number of passes, so that the design spec always has fairly accurate and reliable solution with which to establish the next search direction and step size; otherwise, the design spec may “bounce around” inordinately, or even fail.

The manual sequencing utilized here should be replaced by a methodology discussed earlier (with the additional heater blocks) which gives Aspen Plus® the control over the number of iterative passes and the extent of convergence based on a user-specified tolerance.

Results over the load range for the FLUENT®/Aspen coupling are shown in Figures 61 through 63. Aspen Plus®, as the executive software, was able to successfully manipulate the control parameters in order to produce the desired superheat outlet temperature. With the CFD coupling, 6 of the load points were run over the range from 100% GT load to 50% GT load.

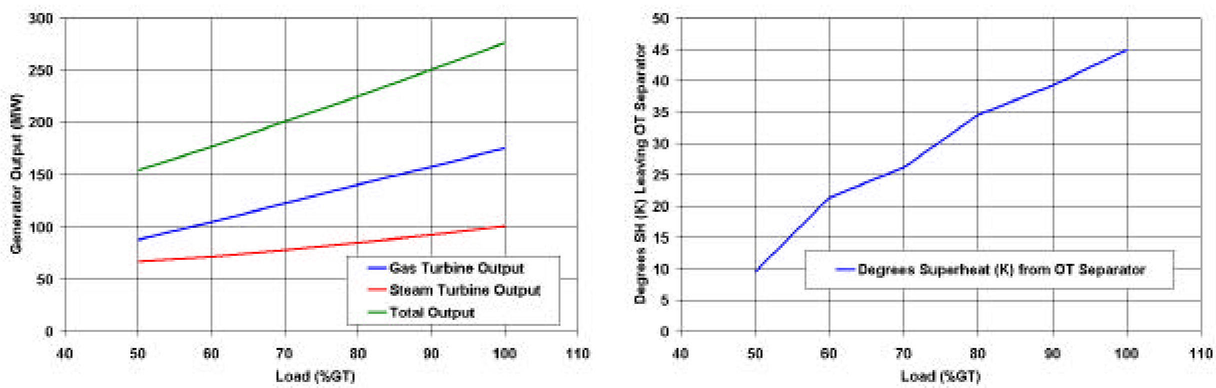

Figure 61: Case 2 : Run 3 Results – Generator Output and Degrees SH at OT Separator.

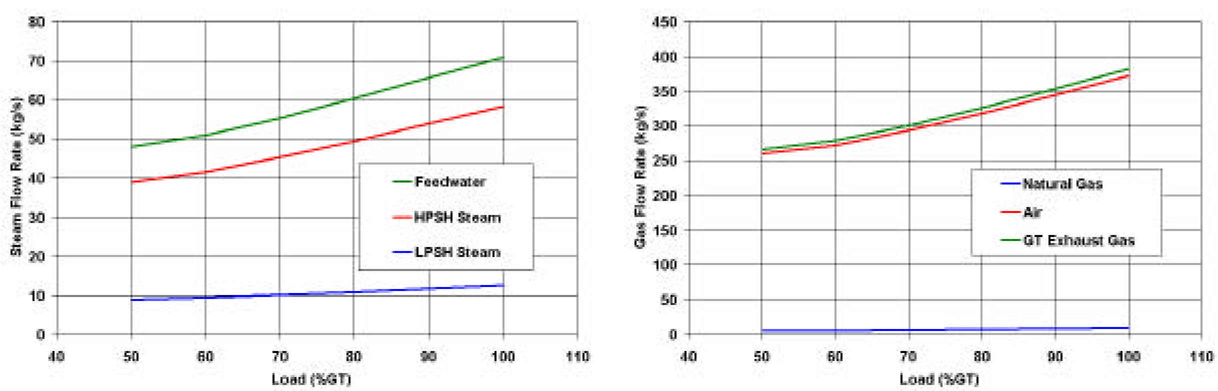

Figure 62: Case 2 : Run 3 Results – Steam, Fuel, and Air Flow Rates.

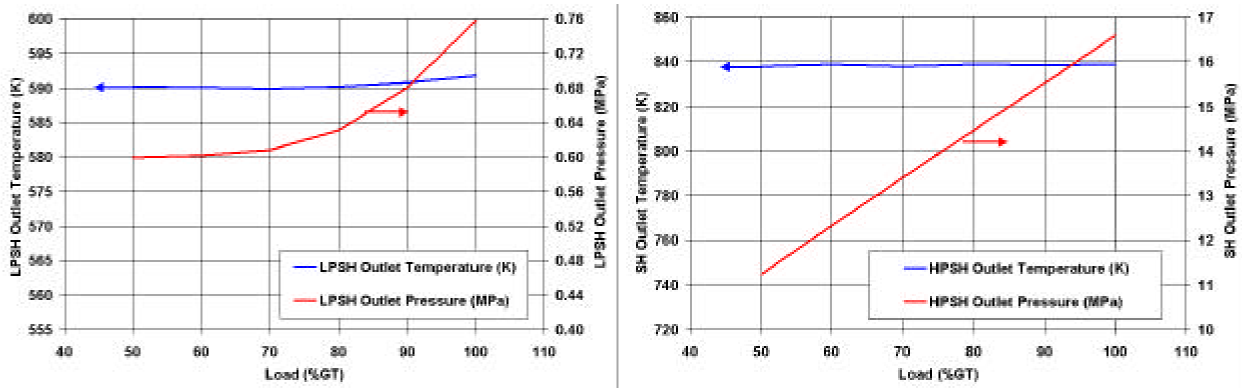

Figure 63: Case 2 : Run 3 Results – LPSH and HPSH Temperature and Pressure.

In comparing the above figures to those corresponding to the HRSGPS code (Run 2) and the Aspen library module (Run 1), it can be seen that the results are fairly similar. There are some minor differences, indicating that complete congruency between the adaptions of the software packages to the cycle was not necessarily maintained in every case. In addition, the behavior and interaction of some of the software packages relative to each other and the library modules, particularly at the off-design conditions, should be expected. In the CFD runs, the tolerance on the superheat outlet temperature was not as tight as the other runs, and this is reflected in the slight “waviness” of the lines. Overall, however, all of the runs were successfully completed and demonstrate reasonable trends.

6.0 CONCLUSIONS AND RECOMMENDATIONS

The demonstrated results from this Vision 21 project represent a novel and unique advancement in the field of process modeling and design. A V21 Controller and wrapper interface, based on the CAPE-OPEN standard, have been constructed, which allow third-party software to be instantiated on the Aspen Plus® flowsheet as surrogate equipment modules. One of ALSTOM Power’s objectives, as a member of the V21 team, was to demonstrate the feasibility and viability of the controller and wrapper interfaces by completing two demonstration cases. These two demonstration cases required (a) the selection of a conventional steam cycle (Case 1) and a natural gas combined cycle (Case 2), (b) the construction of those cycles using Aspen Plus® library modules, and (c) a demonstration that third-party software could be linked to Aspen Plus® and run in conjunction with it. The third-party software consisted of two industrial proprietary codes (the BPS and HRSGPS codes), as well as the FLUENT® CFD code. All of the runs were completed successfully.

For the two industrial proprietary codes, the linkage with Aspen Plus® was based on a simple exchange of information through the CO parameter collection. The legacy codes functioned well in the CO environment, as might be expected, since the CO environment may be viewed as an enhanced extension of the Aspen Plus® custom UDF interface that Aspen Technology has provided for many years. In this project, no attempt was made to enhance the proprietary codes in any significant way, provide port connections, or automate them for this type of application, although much more work could be done in that area. In general, industrial proprietary codes have been validated through many years of use and are used routinely in the design process. Therefore, there is tremendous potential to utilize such codes synergistically within the framework of a process model environment. Since industry may move quickly to utilize proprietary codes in conjunction with CO-compatible process models, significant effort needs to be put into making the wrapper and the proprietary codes more automated and "black-boxed", so that the skills of a programmer are not required each time that the cycle is modified.

The linkage between the FLUENT® code and Aspen Plus® has also been shown to be fairly well developed and straightforward. For Demonstration Cases 1 and 2, the decision was made to provide a CFD boiler module (for Case 1) and an HRSG module (for Case 2). These two modules involve coupling complexities that the typical FLUENT® module does not require, because not only was the 3-D computational domain linked up to the process flowsheet, but linkages also had to be provided for the 1-D tube bank model in the FLUENT® code. Because port connections were not available to the 1-D tube bank model, a large number of additional stream and informational parameters had to be included in the CO collection.

Overall, the replacement of Aspen Plus® library modules with more detailed and versatile (third-party) software modules (e.g., proprietary industrial codes and CFD) enables the designer to operate the cycle in a much more realistic fashion over the load range. Furthermore, with the additional capabilities often times embodied within the third-party software, the designer can potentially interrogate the code or post-process the computational domain to obtain additional design information that is not normally available in library modules, such as emissions, particle distributions or pattern factors, etc..

Observations and conclusions, along with the corresponding recommendations, are enumerated below:

(1) <u>Conclusion</u>: In the demonstration cases, no attempt was made to provide component performance maps or to encumber the calculations with additional complexity, given the already strenuous challenges involved. However, there is some concern that the library modules available in Aspen Plus® have not been constructed with sufficient sophistication for advanced power plant design and cycle analysis, particularly for off-design conditions. While the modules are certainly adequate for many applications, they are not as sophisticated or complex as those used previously in Aspen Technology's previous power plant analysis code, i.e., the STEAMSYS™ code, which required the Equation-Oriented (EO) solution methodology.

[1-A] <u>Recommendation</u>: Effort should be expended to evaluate the modules and to determine if additional improvements to the library modules are warranted, particularly for Vision-21 applications and advanced components.

[1-B] <u>Recommendation</u>: More sophisticated (steady-state) power plant cycles and modules may prove to be more stiff and may require the use of the "equation oriented" (EO) solution methodology, as opposed to the "sequential modular" (SM) solution approach. In this project, the CO interface was developed only for the SM approach, and not for the EO approach. Additional work should be done to extend the interface to incorporate the EO solution method. (Progress toward transient simulations will also require practical experience with EO.)

(2) Conclusion: CFD enjoys wide appeal because of the tremendous potential that it has to impact design. However, relative to typical Aspen Plus® run times, orders of magnitude more CPU time will be required to compute CFD modules within the process modeling environment. The CFD cases computed in this project only had 40,000 cells, and were at least an order of magnitude smaller in grid size than typical industrial cases. Furthermore, if a Lagrangian particle model or more detailed chemistry is required, the required CPU burden may increase by another order of magnitude (or more). Reduced-order model development will reduce the required CPU time somewhat, but the CPU burden will still require access to parallel computing clusters through a network connection.

[2-A] Recommendation: Fluent Inc. has already, to some degree, developed some remote computing capability. This capability should be fully extended and tested at industrial sites, thus demonstrating that Aspen Plus® can be run on a PC, while the FLUENT® code runs remotely over a local area network (e.g., in parallel on multi-node clusters). This remote-running capability can then be extended to embrace Web deployment technologies, where runs are conducted over the Internet, with the attendant security protocols.

[2-B] Recommendation: To ease the CPU burden associated with repeated executions of a FLUENT® block, reduced-order models should be more fully developed. Archived databases of previous CFD runs can be accessed and selected parameters can be extracted from which the appropriate "curve-fits" can be made. The Aspen Plus® cycle can then rely on the curve fits to arrive at an approximate solution, running the full CFD case only when the cycle is operating in a sparse-valued region, or in the limit of near convergence to "fine-tune" the final cycle solution.

(3) Conclusion: The utilization of CFD modules for routine optimization of process modeling implicitly presumes that CFD is used in the design process for a particular application. CFD may often be used for "what if" studies, qualitative analyses, or trend predictions for many applications within a corporation, but that does not mean that the CFD has been validated to the extent that it can be used in the design process itself. The designer uses only those tools for which guarantees, with minimal liability risk, can be reliably made. While CFD is certainly used within the design process for "some" industrial applications, additional time may be required before CFD has been sufficiently validated by equipment vendors/manufacturers for all of the modules in a power plant. If a user replaces a module in Aspen Plus® with a CFD block, and if the cycle is being used for design optimization, then, at the very least, the user should be aware of any limitations in the predictive accuracy of that block.

[3] Recommendation: The DOE, in a consortium effort with industry, should select those Vision 21 cycle components for which a CFD model may be used as a surrogate predictor, and ensure that a CFD model is reasonably validated for those applications.

(4) Conclusion: When Aspen Plus® executes a cycle with library modules, the design specs and sensitivity functions may allow initial conditions, control parameters, or step sizes to vary over a fairly wide range. Aspen Plus® is generally versatile and forgiving, achieving eventual convergence, even though it may temporarily compute unrealistic transients. When a third-party code or CFD is used as an instantiated module on the flowsheet, care must often be taken to ensure that stream conditions are within the realm of convergence for that module. FLUENT® or its submodels may not have been originally designed to be as robust as the Aspen Plus® algorithms demand.
For example, the tube bank model may fail if large changes are made relative to a given baseline solution. Many times the ALSTOM steam properties predictor proved to be inadequate, because it was asked to provide solutions beyond its tabulated bounds. Such examples may be indicative of a larger problem, i.e., additional work may be required for a particular application to make the FLUENT® submodels or properties more robust and reliable over a broad range.

[4-A] Recommendation: Presently, the tube bank model in FLUENT® should be made more robust, at least in the context of repeated Aspen Plus® runs at varying flow rates. When the mass flow rate changes and the tube bank parameters change, the steam temperatures may spike and reach unrealistic extremes, before they begin to settle down. Usually this is in the form of a damped oscillation and the flow field recovers, but this convergence characteristic should be investigated to see if certain variables are not stored or "kept alive" between the individual executions of FLUENT®, or whether other bounds/limits can be applied which will help the tube bank models be more stable.

[4-B] Recommendation: ALSTOM's steam property tables contribute to this problem. These property tables are interpolative tables constructed from the standard steam property correlations solely to interact with the FLUENT® tube bank model. During the calculations, the tube bank models may request a table lookup that is beyond the bounds of the tables or that is in a region that is not well resolved by linear interpolation (e.g., near the two-phase envelope). Either a more reliable steam-property predictor should be added to FLUENT®, or FLUENT® should be adapted to access the steam-property predictor in Aspen Plus®.

(5) Conclusion: During a combined FLUENT®/ Aspen Plus® run, particularly when Aspen Plus® is utilizing a sensitivity function to loop over multiple values of a parameter (e.g., load), the FLUENT® CFD case may exhibit somewhat different convergence characteristics over different regimes of that parameter. For example, FLUENT® may be somewhat more difficult to converge at a lower load, thus necessitating a change in under-relaxation factors or the maximum number of FLUENT® iterations allowed within a design spec iteration. The user may also wish to interrogate the current status of the CFD run by accessing the post-processing functions.

[5] Recommendation: During a combined FLUENT®/ Aspen Plus® run, the user should ideally be able to pause the run, interrogate the results via post-processing, and change

any convergence parameters "on the fly" in either FLUENT® or Aspen Plus®. This feature should be developed. Care should also be taken to ensure that the "reinitialize" feature in Aspen Plus® also works properly when third-party codes are involved.

(6) Conclusion: The tube bank model in FLUENT® is pseudo 1-D and does not have any port connection capability. All information exchanges between Aspen Plus® and the tube bank model must be made manually in Aspen Plus® functions (e.g., calculator blocks, etc.).

[6] Recommendation: Since heat exchangers and tube banks are so prevalent in power plant cycles, port connection capability should be added to the tube bank model in FLUENT®. Port connection capability might also provide an avenue for the steam-property predictor in Aspen Plus® to be more easily transferred to FLUENT®.

(7) Conclusion: The user often has a need to extract post-processed quantities (e.g., surface or plane integrals) from the CFD simulation that can be passed automatically to Aspen Plus® as part of the solution output. While FLUENT® itself provides such capabilities in the form of text user interface (TUI) commands or Scheme commands, the controller cannot currently extract the desired numerical values, because the result of the command contains both text and numbers.

[7] Recommendation: The controller or FLUENT® wrapper should be modified so that the desired post-processed quantities (e.g., planar integrals at selected planes) can be easily parsed and extracted for automatic transferral to Aspen Plus®.

(8) Conclusion: Species naming conventions in FLUENT® and Aspen Plus® must presently be identical to each other (both in sequence and spelling) in order to ensure the proper transfer of properties and mole fractions between the two codes. This means that property definitions must usually be redone in one or both of the codes. This will be particularly problematic when reduced-order models and existing archives of CFD runs are used. In general, it is difficult for the individuals running FLUENT® or Aspen Plus® to know *a priori* what the species list and sequence is going to be in the "other" code, because the corresponding cases may be created by different individuals at different times of the year, with initially unrelated intents/goals.

[8] Recommendation: The user needs the capability to survey the species list in the FLUENT® and Aspen Plus® runs and, by assignment, associate the names in one list with the names in the other. If there is an unequal number of species, then the user should be able to form composite species or renormalize the mass fraction distributions.

(9) Conclusion: Presently, whenever a FLUENT® block completes its execution, it writes pre-set post-processed graphical files. If Aspen Plus® is looping over a series of values in a sensitivity function, then those post-processed files are overwritten.

[9] Recommendation: Post-processed results at the conclusion of a sensitivity loop, whether in graphical or text form, should be sequenced and stored for later access (rather than be overwritten).

7.0 REFERENCES

1. "Project Management Plan, Development of Technologies and Analytical Capabilities for Vision 21 Energy Plants, Cooperative Agreement No. DE-FC26-00NT40954", for Diane Madden USDOE-NETL, compiled by M. Syamlal, representing team entities: Fluent Inc., ALSTOM Power, Aspen Technology Inc., Intergraph Corporation, and Concurrent Engineering Research Center (West Virginia University), January 23, 2001.

2. Sloan, D., and Fiveland, W., "Discussion on Test and Demonstration Case 1," for Diane Madden, U.S. DOE (NETL), under Cooperative Agreement No. DE-FC26-00NT40954, Development of Technologies and Analytical Capabilities for Vision 21 Energy Plants, April 30, 2001.

3. Richards, G., Sloan, D., and Fiveland, W., "Discussion on Test and Demonstration Case 2," for John Wimer, U.S. DOE (NETL), under Cooperative Agreement No. DE-FC26-00NT40954, Development of Technologies and Analytical Capabilities for Vision 21 Energy Plants, August 15, 2002.

4. Software Integration Tool Kit for Advanced Process Simulation, Users' Manual Version 1.0, Fluent Inc. (September 18, 2003).

5. Braunschweig, B. L., C. C. Pantelides, H. I. Britt, and S. Sama, September 2000, Process Modeling: The Promise of Open Software Architectures, Chem. Eng. Progress, 96(9), 65-76.