

**SYSTEMS ANALYSES OF ADVANCED BRAYTON CYCLES  
FOR  
HIGH EFFICIENCY ZERO EMISSION PLANTS**

Task 1.1: Set Systems Study Methodology

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## INTRODUCTION

This document provides an explanation of the systems study procedure to be used to evolve the conceptual gasification based plant designs. It is the intent to adhere to the “Quality Guidelines for Energy System Studies” established by the DOE / NETL wherever possible.

This systems study procedure provides the following:

- site conditions and feedstock characteristics
- advanced Brayton cycle technology projections
- SOFC / GT design guidelines
- overall plant design criteria
- procedure for executing material and energy balances
- procedure for setting equipment specifications where required
- a procedure for third party validation of a detail or the entire study such that the documentation would minimize the study validation process by third parties.

## PROCESS DESIGN PROCEDURE

### Site Conditions and Feedstock Characteristics

Table 1 summarizes the site conditions to be used in this systems analysis study.

**Table 1: Site Conditions**

Dry Bulb Temperature	15° C <sup>1</sup>
Relative Humidity	60% <sup>1</sup>
Elevation	sea level <sup>1</sup>
Air Composition by Volume	
O <sub>2</sub>	20.74%
N <sub>2</sub>	77.338%
CO <sub>2</sub>	0.002%
H <sub>2</sub> O	0.99%
Ar	0.93%
Plant Make-up Water	Fresh Water
Plant Site	Level Greenfield without any Piling Requirement

<sup>1</sup> International Standards Organization (ISO) conditions.

## **Coal**

Pittsburgh No. 8 coal will be utilized for this study. Table 2 shows its ultimate, proximate, and sulfur analyses along with that of Illinois No. 6 coal for Sensitivity Analysis, taken from the “Quality Guidelines for Energy System Studies.”

## **Natural Gas**

The composition shown in Table 3 taken from the “Quality Guidelines for Energy System Studies,” which is based on the mean of over 6,800 samples of pipeline quality natural gas taken in 26 major metropolitan areas of the United States will be used.

## **Limestone**

Limestone if required (e.g., as a flux) having the composition shown in Table 4 (taken from the “Quality Guidelines for Energy System Studies”) will be utilized.

**Table 2: Coal Analysis**

<b>Rank</b>	<b>Medium-volatile Bituminous</b>		<b>High-volatile Bituminous</b>	
<b>Seam</b>	Pittsburgh No. 8		Illinois #6 (Herrin)	
<b>Sample Location</b>	PA		St. Clair Co., IL	
<b>PROXIMATE ANALYSIS</b>	As Received	Dry	As Received	Dry
<b>Moisture</b>	5.83	0	7.97	0
<b>Ash</b>	9.65	10.25	14.25	15.48
<b>Volatile Matter</b>	34.87	37.03	36.86	40.05
<b>Sulfur</b>	2.89	3.07	4.45	4.83
<b>Fixed Carbon (BD)</b>	46.76	49.65	36.47	39.64
<b>HHV</b>				
<b>kJ/kg</b>	28959	30806	25584	27798
<b>Btu/lb</b>	12450	13244	10999	11951
<b>ULTIMATE ANALYSIS</b>				
<b>Moisture</b>	5.83	0	7.97	0
<b>Carbon</b>	69.50	73.79	60.41	65.65
<b>Hydrogen</b>	4.53	4.81	3.89	4.23
<b>Nitrogen</b>	1.21	1.29	1.07	1.16
<b>Chlorine</b>	-	-	0.05	0.05
<b>Sulfur</b>	2.89	3.07	4.45	4.83
<b>Ash</b>	9.95	10.57	14.25	15.48
<b>Oxygen</b>	6.09	6.47	7.91	8.60
<b>SULFUR SPECIES</b>				
<b>Pyritic</b>	-	-	--	2.81
<b>Sulfate</b>	-	-	--	0.01
<b>Organic</b>	-	-	--	2.01

Notes: (1) Data reproduced/derived from Argonne National Laboratory, premium coal sample analytical data, (2) HHV (gross) measured experimentally; LHV (net) derived from the corresponding HHVs.

**Table 3: Natural Gas Composition**

<b>Component</b>	<b>Volume Percentage</b>	
Methane, CH <sub>4</sub>	93.1	
Ethane, C <sub>2</sub> H <sub>6</sub>	3.2	
Propane, C <sub>3</sub> H <sub>8</sub>	0.7	
<i>n</i> -Butane, C <sub>4</sub> H <sub>10</sub>	0.4	
Carbon Dioxide, CO <sub>2</sub>	1.0	
Nitrogen, N <sub>2</sub>	1.6	
	<b>LHV</b>	<b>HHV</b>
MJ/scm	34.71	38.46
Btu/scf	932	1032

Notes:

1. The reference data reported the mean volume percentage of higher hydrocarbons (C<sub>4</sub> +) to be 0.4%. For simplicity, the above composition represents all the higher hydrocarbons as *n*-butane (C<sub>4</sub>H<sub>10</sub>).
2. The reference data reported the mean volume percentage of CO<sub>2</sub> and N<sub>2</sub> (combined) to be 2.6%. The above composition assumes that the mean volume percentage of CO<sub>2</sub> is 1.0%, with the balance (1.6%) being N<sub>2</sub>.
3. LHV = lower heating value; HHV = higher heating value

**Table 4: Greer Limestone Analysis**

<b>Component</b>	<b>Dry Basis %</b>
Calcium Carbonate, CaCO <sub>3</sub>	80.40
Magnesium Carbonate, MgCO <sub>3</sub>	3.50
Silica, SiO <sub>2</sub>	10.32
Aluminum Oxide, Al <sub>2</sub> O <sub>3</sub>	3.16
Iron Oxide, Fe <sub>2</sub> O <sub>3</sub>	1.24
Sodium Oxide, Na <sub>2</sub> O	0.23
Potassium Oxide, K <sub>2</sub> O	0.72
Balance	0.43

## ADVANCED BRAYTON CYCLE TECHNOLOGY PROJECTIONS

Some of the technological advances being made or being investigated to improve the Brayton cycle include the following:

- Rotor inlet temperature of 1700°C (3100°F) or higher which would require the development and use of advanced materials including advanced thermal barrier coatings and turbine cooling techniques including closed loop steam cooling.
- High blade metal temperature in the neighborhood of ~1040°C (1900°F) while limiting coolant amount would again require the development and use of the advanced materials including advanced thermal barrier coatings.
- Improvements to the aerodynamic and mechanical design such as pressure gain combustion, improved compressor and / or turbine isentropic efficiencies.
- Advanced gas turbine combustor concepts to limit the combustor diluent addition to a value which optimizes the overall plant thermal efficiency while minimizing the NO<sub>x</sub> emissions.
- High pressure ratio compressor (greater than 30 to take full advantage of higher firing temperature).
- Catalytic combustors (such as that being developed by PCI).
- Cycle changes such as air humidification and recuperation, inlet air fogging, in-situ reheating and intercooling.

The balance of plant configuration and technology will be selected in order to synergistically integrate with the particular Advanced Brayton cycle under investigation such that the overall plant performance is optimized. The effect of incorporating the various advanced technology concepts will be studied methodically such that any gain in performance realized can be associated with the particular change in cycle condition or configuration made.

A myriad of gas turbine based cycles have been proposed in the past but the majority of these cycles have been for natural gas applications. Thus, it is important to identify only those cycles that have a potential for success in coal based gasification plants also and the following lists the initial activities included in this task to select promising cycles for inclusion in the systems analysis:

- Based on a literature search, identify gas turbine based cycles that have a potential for high efficiency.



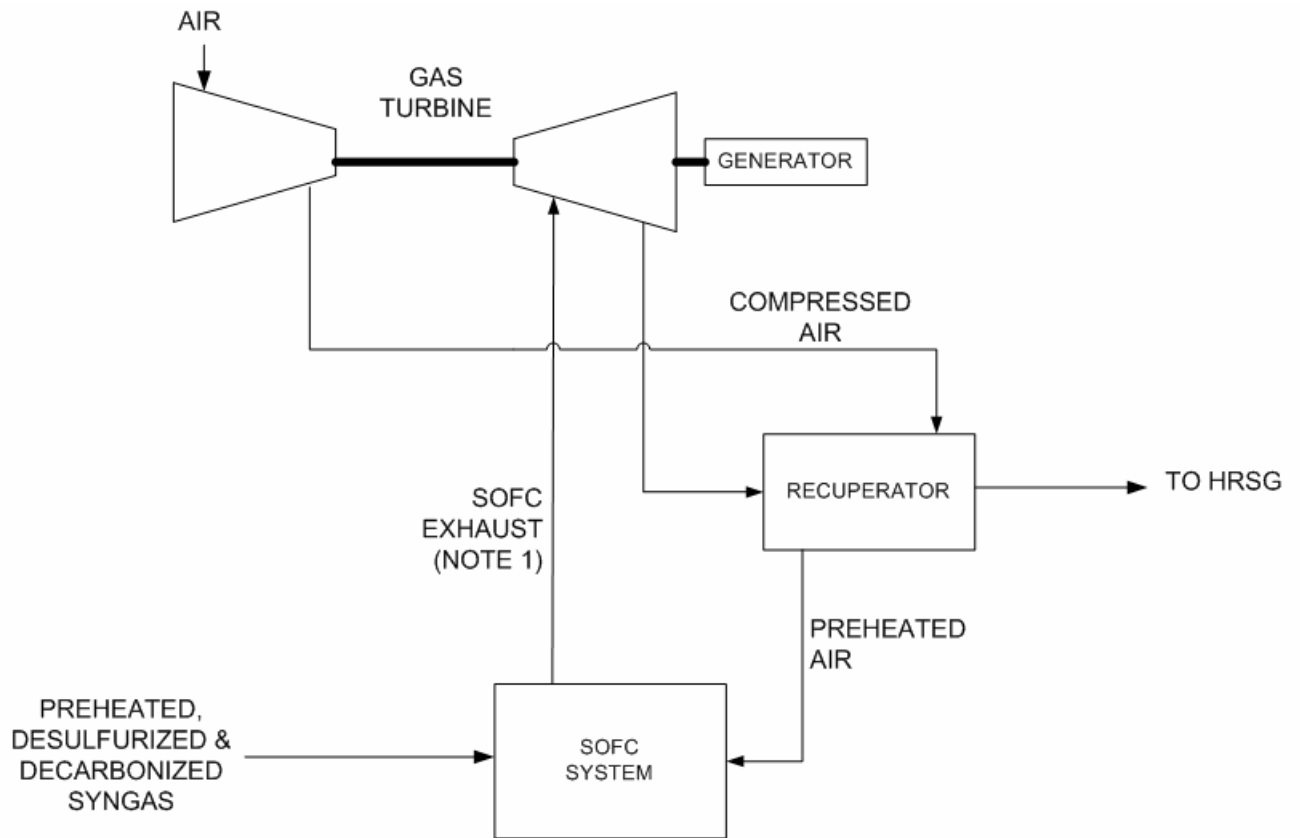
- Conduct brainstorming sessions in order to identify those gas turbine based cycles that have a potential to meet the objectives of this program. Improvements to these cycles as well as the evolution of new cycle configurations by synergistically combining aspects of other cycles will also be brainstormed.

After the selection of the advanced cycles, a narrative accompanying the recommended cycles as well as the integration scheme with the remainder of the plant for each of the cases will be made to the COR. Upon COR approval, UC Irvine will proceed with detailed systems analysis and design for these cases. Three or more systems studies will be conducted in the second year which integrate these advanced technologies upon mutual agreement of UC Irvine and COR (the exact number of cases dependent upon funding availability).

## **SOFC / GT DESIGN GUIDELINES**

The following lists the design guidelines that will be adhered to in developing the steady state and dynamic simulations of the SOFC / GT based system. The overall plant steady state simulation will be developed while the dynamic simulations will be limited to the SOFC / GT system as depicted in Figure 1.

1. Overall Plant:
  - a. General Design Basis same as Baseline IGCC case for the Advanced Brayton Cycle study [CO<sub>2</sub> Capture = 90% of Gasified Carbon (leaving gasifier as gaseous components)]
  - b. Size of each FC / GT Power Block or Train = 100 MW (plant will consist of multiple 100 MW trains to take advantage of a larger gasification plant)
  - c. HRSG pressure drop for the dynamic simulations will be estimated by assuming flow through a non-choked orifice.
2. SOFC:
  - a. Planar SOFC
  - b. Non Internal Reforming
  - c. Hydrocarbon Content of Syngas < 1%
  - d. Average Operating Temp = 750°C ( $\pm 25^\circ\text{C}$ )
  - e. Power Density = 500 mW/cm<sup>2</sup>
  - f. Fuel Utilization = 80%
  - g. Max Temp. Rise on Anode Side  $\leq 100^\circ\text{C}$
  - h. Max Temp. Rise on Cathode Side  $\leq 100^\circ\text{C}$
  - i. Air Preheat within Stack  $\leq 100^\circ\text{C}$  Temperature Rise
  - j. Fuel Preheat within Stack: Ratio Consistent with Air Preheat
3. Gas Turbine:
  - a. Ideal or Optimal Turbine to Accommodate the SOFC.



**NOTES:**  
 (1) AFTER ANODE EXHAUST GAS COMBUSTION WITH CATHODE EXHAUST GAS

**Figure 1: SOFC / GT System for Dynamic Simulations**

## OVERALL PLANT DESIGN CRITERIA

Table 5 summarizes the design criteria for the Cases 1.1 through 2.0 as defined in the following.

**Table 5: Overall Plant Design Criteria**

Location	Midwest U.S.
ASU-GT Integration	GT Air Extraction and N <sub>2</sub> Injection into GT
Hydrogen Export	None (only Qualitatively Discussion)
CO <sub>2</sub> Removal	90% of Carbon in Coal less Carbon in Slag
NO <sub>x</sub> Emission Limit	3 ppmVd (15% O <sub>2</sub> Basis)
Liquid Wastes	Treated Wastes (Non-Zero Discharge)
Plant Heat Rejection	Mechanical Draft Cooling Towers

## **MATERIAL AND ENERGY BALANCES**

The material and energy balances will be developed utilizing a predictive computer simulation technique. The following lists the tools that will be utilized:

- Advanced Power Systems Analysis Tool (APSAT)
- Aspen Plus®
- Thermoflex
- Matlab-Simulink(R)

The capabilities of APSAT, a simulation tool developed by UC Irvine are described later in this section and is useful for high level evaluations of alternative schemes while the primary heat and mass balance code will be the Aspen Plus® simulator. Thermoflex which is a Thermoflow Suite product will be utilized primarily in developing the performance for the steam cooled H technology gas turbine on syngas as well as the Advanced Brayton cycles identified for analysis in this project.

The SOFC/GT dynamic simulations will utilize the Matlab-Simulink(R) framework. This effort will include modifying and applying verified dynamic simulation techniques and models to the system design(s) of interest. These existing dynamic models that have been developed in the Matlab-Simulink(R) framework take into account the dynamic physical, chemical and electrochemical equations that govern fuel cell, gas turbine, and other component technology performance. Some degree of geometric resolution is captured in each of the significant component models (e.g., fuel cell, compressor, heat exchanger), albeit in a simplified (usually one- or two-dimensional) manner. Since the performance of fuel cells, reformers and even simple heat exchangers depends upon local conditions and properties (temperature, pressure, species concentrations) it is important to capture some of the geometrical features of major system components for accurate predictions and insight. However, full three-dimensional and dynamic resolution of the concurrent processes (e.g., chemistry and electrochemistry, heat transfer, mass transfer, momentum) that apply to each of the components in a complex system model is too computationally intensive. The current approach captures essential geometrical features in a simplified manner allowing solution of the dynamic equations that govern heat and mass transfer, momentum and energy conservation, chemistry and electrochemistry in

complex fuel cell systems. The current effort leverages earlier work funded by the California Energy Commission, the U.S. Department of Energy, and the U.S. Department of Defense Fuel Cell Program that supported the development of generic dynamic SOFC and other system component models. The capabilities of these dynamic simulation tools have been demonstrated many publications [e.g., Gemmen et al., 2000; Roberts, et al., 2004; Roberts and Brouwer, 2005; Mueller, Brouwer, and Samuelsen, 2005; Freeh, Pratt, and Brouwer, 2004; Yuan, Brouwer, and Samuelsen, 2004].

The following specific modeling guidelines will be applied to the overall energy system:

- Process models will generate sufficient information to generate a complete process flow diagram and a stream property table.
- Heat loss, blowdown amount, pressure drop, mechanical efficiency, auxiliary and miscellaneous power and cooling water requirements will be taken into account for each piece of equipment or plant section.
- All major streams appearing in the flow diagram will be labeled with an accompanying table that will provide stream compositions, flowrates and conditions of pressure and temperature.
- Overall performance summaries will be developed showing the power generation by each equipment and the power consumed by the plant. The “plant” will include all necessary facilities for a stand alone operation and will include the coal and limestone receiving and processing, raw water and boiler feed water treating, condensate handling, general facilities such as waste water treating, cooling water system and instrument air.

### **Advanced Power Systems Analysis Tool (APSAT)**

Existing models for analysis of systems such as power plants may be divided into two types (1) those developed for simulating chemical process plants (e.g. commercially available Hysis, Aspen, Pro II) and (2) those developed for simulating power plants (e.g. commercially available Thermoflex and GATE/Cycle). Models in the first category have the capability for predicting the performance of typical process equipment and the thermodynamic properties of non-ideal systems but do not include the proper models for power cycle equipment such as gas turbines, steam turbines and fuel cells. The models in the second category have the capability of modeling gas and steam turbines in detail but do not handle rigorously the modeling of process equipment such as gasifiers or partial oxidation units, shift reactors and humidifiers which are playing an important role in IGCC plant designs, nor the properties of non-ideal gases except for pure steam.

Non-ideal gas behavior is quite important in thermodynamic analyses, as there are many processes where such behavior is critical. Two examples of where non-ideal properties for a gas stream need to be accounted for are: (1) predicting the Joule-Thompson cooling

of natural gas when its pressure is reduced from typical pipeline pressure to the pressure required by say a heavy frame gas turbine which typically operates at a pressure-ratio in the neighborhood of 15, and (2) the recovery and compression of the carbon dioxide to supercritical pressures (which is typically required for sequestration with greenhouse gas emissions becoming a more global concern). Predicting the saturated vapor content of water vapor in a gas stream at high pressure, which is important in determining the correct heat release curve for syngas cooling, also requires the proper accounting of the non-ideal behavior of the vapor phase.

After years of piecing together the chemical process models with the power plant models, it was obvious that an overall fuel-in to kW-out simulation capability was needed especially in complex multi working fluid/multi power generating component cycles that are becoming more attractive. Beginning in 1997 development began on Advanced Power Systems Analysis Tool (APSAT). This modeling system is based on more than 30 years of process industry and power plant experience with gasification licensors and process/power plant engineering firms. APSAT is a C-based (C++) simulation tool that runs on a PC. Components are described in a series of modules (e.g., see below) and the thermodynamic and flow properties from one module feeds into the following module(s). A series of balances are calculated and convergence obtained. Molar properties are tracked for each stream. APSAT has been successfully used in a number of studies for the DOE and other energy industry members. It is an organic modeling capability and additional modules are added as new technology requires.

Table 6 lists the major modules available in APSAT along with brief descriptions. Note that each of these modules consist of a number of subroutines that calculate the thermodynamic and flow system parameters that are then sent along to the next module.

## **Gas Turbine**

Two types of gas turbine models are included, one that may be configured by the user to include multiple compression stages with intercooling between the stages and multiple expansion stages with reheat (with combustors) between the stages, and the second consisting of a fixed geometry simple cycle (or conventional Brayton cycle) with no intercooling of the compressor or reheat during expansion.

In the user-defined gas turbine model, the efficiency of the compressor and expander and the air required for cooling the blades of the turbine as well as its purge air requirements are calculated by first calibrating a simple cycle engine based on data published by the gas turbine manufacturer, and then applying adjustments to the values determined for the "base-line engine." The program determines internally the necessary parameters for the base-line engine and for use with the user-defined model (as well as with the "fixed geometry" model).

The fixed geometry model assumes that the gas turbine has the same geometry as the gas turbine used for calibrating the engine. The firing temperature and pressure-ratio of the gas turbine are adjusted for variations in flow rate and composition of the working fluid. The firing temperature is adjusted in order to maintain the same metal temperature of the

first-stage blades as that for the base-line engine since the turbine cooling flows are not controlled in an engine. A correlation derived from published performance data for the Nuovo Pignone gas turbine (Model PGT 5B/1) which has an output of 5.4 MW at ISO conditions is utilized to adjust the polytropic efficiency of the compressor for changes in the pressure-ratio. The small Nuovo Pignone gas turbine is utilized since it is in the size range being considered by industry for fuel cell based hybrid applications.

The performance curves generated by the model for a large industrial gas turbine (General Electric MS 7001EA model with output of 85 MW at ISO conditions) are presented along with data published by General Electric in Figure 2. As can be seen, the agreement between the model predictions and published data are in excellent agreement despite the more than an order of magnitude scale-up in the size of the gas turbine.

A comparison of the combustor outlet temperature as developed by APSAT for a syngas fuel is compared to that calculated by ASPEN in Table 7. As can be seen, the outlet temperatures are in close agreement validating the thermodynamic basis used.

### **Humidifier Model**

The humidifier is modeled rigorously by accounting for the simultaneous heat and mass transfer rate-controlled processes occurring within this contact device rather than modeling it simplistically as a series of equilibrium stages.

### **Compressor and Steam Turbine Models**

APSAT has the advantage of predicting the isentropic efficiency using relationships that take into account the capacity of the unit in the case of a compressor (Gas Research Institute Report, 1993), while in the case of steam turbines, correlations developed by Spencer et. al. (1974) may be utilized to predict the isentropic efficiency for each of the sections (high pressure, intermediate pressure and condensing). A comparison of the compressor outlet temperature as predicted by APSAT is compared to that calculated by ASPEN in Table 7 while utilizing the isentropic efficiency as predicted by APSAT in ASPEN. As can be seen, the outlet temperatures are in close agreement validating the thermodynamic basis used.

**Table 6: List of Modules in APSAT**

<b>Module Name</b>	<b>Description</b>
Combine	Combines two streams adiabatically to give the mixture temperature at pressure equal to the lower of the two streams being combined
Combust	Calculates effluent composition & conditions for a combustor with specified gloss and pressure drop
CombustT	Calculates effluent composition & conditions & heat release for a combustor with given outlet temperature and pressure drop
Compress	Calculates the power and outlet temperature of a compressor for a given outlet pressure (the isentropic efficiency may either be specified or can be calculated by module)
Controller	Adjusts variable upstream to make desired variable match target value (while simulating a flowsheet with iterations to satisfy a specified design criteria)
COSHyd	Adiabatic COS hydrolysis reactor to calculate effluent composition and conditions
Deaer	Calculates the effluent conditions from & heat required by a boiler feed water deaerator
Decant	Decanter to separate a solid from water for a specified moisture content in separated solid
ExchQ	Calculates outlet temperature for a specified heat duty and pressure drop
ExchT	Calculates heat duty for a specified outlet temperature and pressure drop
Expand	Calculates the power and outlet temperature of a gas expander for a given outlet pressure (the isentropic efficiency may either be specified or can be calculated by module)
GTcalib	Calibrates gas turbine (for use in below Gas Turbine modules)
GasTurb	Gas turbine of geometry same as that specified in GTcalib
GTcombEXP	Combustor/Expander of a gas turbine consistent with GTcalib (used in configuring a new cycle)
GTcomp	Compressor of a gas turbine consistent with GTcalib (used in configuring a new cycle)
GTsplit	Splits for cooling air of gas turbine consistent with that specified in Gtcalib. Cooling air is taken just upstream of combustor specified in GTcombEXP. (used in configuring a new cycle)

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HPstmTurb	Calculates the power and outlet temperature of a steam turbine – HP section (the isentropic efficiency may either be specified or as a default, it is calculated using the Spencer-Cotton Correlations)
Humid	Calculates gas & water streams leaving a Humidifier or Dehumidifier (composition of gas as well as flowrate, temperature & pressure) by solving simultaneous heat and mass transfer equations using nodal analysis.
IPstmTurb	Calculates the power and outlet temperature of a steam turbine – IP section (the isentropic efficiency may either be specified or as a default, it is calculated using the Spencer-Cotton Correlations)
LPstmTurb	Calculates the power and outlet temperature of a steam turbine – condensing section (the isentropic efficiency may either be specified or as a default, it is calculated using the Spencer-Cotton Correlations)
Membrane	Calculates the outlet streams while taking into account the partial pressure gradients
Pipe	Calculates outlet conditions for specified pressure and temperature drops
Pox	Calculates adiabatic POX effluent composition and conditions
PoxH2	Calculates adiabatic H2 POX effluent composition and conditions
PoxH2Temp	Calculates H2 POX effluent composition and conditions & qloss for a given outlet temperature
PoxTemp	Calculates POX effluent composition and conditions & heat loss for a given outlet temperature
Pump	Calculates power required and outlet temperature for a pump for a given discharge pressure and isentropic efficiency
Recycler	Iterates till two streams match or their temperatures maintain a specified delta T
Reform	Calculates reformer effluent composition and conditions and absorbed duty
Results	Shows results with stream composition, temperature and pressure, elemental flow rates (for quick check of the elemental balance), energy and exergy contents (for cycle analysis), physical properties (for equipment specs), overall plant thermal efficiency.
SatStmHP	Calculates energy (enthalpy above 60 deg F) of saturated steam/BFW mixture for given pressure
SatStmHT	Calculates energy (enthalpy above 60 deg F) of saturated steam/BFW mixture for given temperature
Separate	Separates water condensate & liquid/solid from a stream

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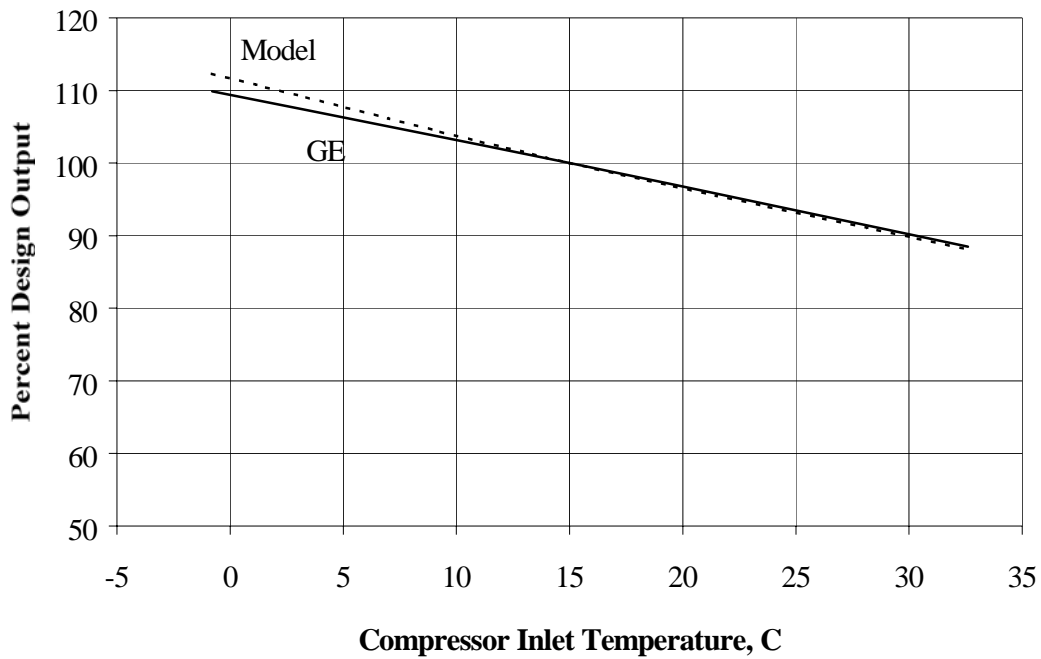
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SepComp	Removes a specific vapor component (by %) from a stream
Shift	Adiabatic shift reactor to calculate effluent composition and conditions
ShiftTemp	Non-adiabatic shift reactor to calculate effluent composition and conditions & duty in shift reaction for a specified outlet temperature
SOFC	Performance (depleted fuel and oxidant composition and conditions and power) and sizing of Solid Oxide Fuel Cell
SplitFlo	Splits a stream into two streams for a given kg/s (or lb/s)
SplitPer	Splits a stream into two streams for a given % Split
SteamGenM	Steam generator (calculates steam produced, blowdown, heat duty for a specified steam pressure and BFW flowrate)
SteamGenQ	Steam generator (calculates steam generated, blowdown, BFW required for a specified heat duty and pressure)
SteamCon	Steam consumer (calculates steam required, condensate produced for specified heat duty and pressure)
Substitute	Substitutes or duplicates a stream
Valve	Calculates outlet conditions including any phase change for a specified pressure drop

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**Table 7: Comparison between APSAT and ASPEN**

Syngas Combustor	Air Compressor
Inlet Air Conditions = 404 °C, 15.85 atm	Inlet Conditions = 15 °C, 1 atm
Inlet Syngas Composition = 38.4% H <sub>2</sub> , 1.2% CO, 0.06% CH <sub>4</sub> , 1.63% CO <sub>2</sub> , 31.1% H <sub>2</sub> O, 26.76% N <sub>2</sub> , 0.81% Ar, 0.04% H <sub>2</sub> S	Outlet Pressure = 15.85 atm
Outlet Pressure = 15.29 atm	Isentropic Efficiency = 85.7%
Calculated Outlet Temperature:	Calculated Outlet Temperature:
ASPEN = 1233 °C	ASPEN = 404.4 °C
APSAT = 1235 °C	APSAT = 404.2 °C



**Figure 2: Variation of Power Output with Compressor Inlet Temperature**

## **SPECIFICATIONS FOR UNIQUE EQUIPMENT AND PLANT UNITS**

Duty / functional specifications will be developed where necessary for unique equipment and plant units.

## **THIRD PARTY VALIDATION**

The flow diagrams and stream summaries along with the overall performance summaries as described previously will form the basis for a third party validation if the DOE so chooses. The plant cost estimates will be broken down by major process units so that a third party may be able to assess the reasonableness of the cost estimate while the study basis and assumptions will be clearly identified.

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