

 Heat Recovery Systems & CHP Vol. 15, No. 2, pp. 105–113, 1995

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 0890_4332(94)00068_9
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 0890_95.000068_0
 0890-433205 \$9.50 + .00

SIMULATION OF COMBINED CYCLE POWER PLANTS USING THE ASPEN PLUS SHELL

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ABSTRACT

A computer simulation model in ASPEN PLUS shell has been developed to simulate the performance of IGCC and IGHAT cycle power plants. The model was used to study the effects of design and performance parameters on the efficiency and emissions from IGCC and IGHAT cycles. The simulation models are capable of performing mass, energy and exergy balances which may be used to trace system inefficiencies to their source component thereby providing insights into component interactions within the cycles and act as pointers to system optimization trade-offs.

INTRODUCTION

Concerns regarding the environmental impacts of power generation stimulated interest in energy efficient cycles. Amongst these, Integrated Gasification Combined Cycle (IGCC) shown in Figure 1 is considered to be one of the most attractive means for tapping the energy content of the abundant coal resources in an environmentally benign way. This technology can significantly reduce acid rain emissions (SO_x and NO_x) as well as the production of gases that are suspected to cause the greenhouse effect (CO₂). Means by which the efficiency of IGCC can be improved, and/or its capital cost requirements reduced, will strongly enhance the comparative advantages of IGCC and facilitate its adoption. Use of Integrated Gasification Humid Air Turbines (IGHAT) promises to achieve thermal efficiencies and emissions reductions comparable to conventional IGCC at significantly reduced costs.

The IGHAT cycle shown in Figure 2 is an intercooled, regenerative cycle with considerable addition of moisture to combustion air stream. Moisture addition is done in a saturator, where counter-current evaporation of water into combustion turbine air stream occurs. The saturator uses hot water, which can be produced by any low-level heat sources such as gasifier quench, compressor intercoolers and aftercoolers. Additional heat is extracted from the turbine exhaust in an economizer. This is in contrast to the IGCC where heat is recovered in the form of high pressure steam using relatively expensive syn-gas coolers. Major cost savings result from the fact that the IGHAT cycle needs no steam turbine, condensers, or associated cooling towers (Rao and Day, 1992).

Analysis of IGCC and IGHAT power plants is complicated due to the large number of units involved, interaction between the units and presence of streams of diverse compositions and properties. The efforts needed to evaluate the environmental impacts, performance and economic implication resulting for various options and a wide range of design and operating conditions for each piece of equipment require extensive computation of material and energy



Fig. 1: Schematic diagram of an IGCC power plant with a non-reheat Rankine bottoming cycle



Fig. 2: Schematic diagram of an IGHAT cycle

balances and economic parameters. There is evidently a need for a general tool that can be used to conduct fast, simply and with accuracy, technoeconomic assessment and optimization of these systems. Owing to the complexity of these systems and possibility of different equipment types and configurations thereof, a modular approach which allows independent development and testing of different sub-systems before integration is more suitable to model these systems. In this paper IGCC and IGHAT models developed within the ASPEN PLUS shell (ASPEN PLUS, 1988) and simulation results from these models are presented.

The model includes realistic representation of the various units used in commercial power plants reflecting pressure drops and characteristic temperature differences in heat transfer components. Mass and energy balances are constructed in ASPEN PLUS shell for each component using current practices and constraints. It should however be noted that IGCC technology has been demonstrated in various power plant projects throughout the world, whereas IGHAT technology is an emerging technology that has not seen actual application yet. One of the major concerns with HAT is the corrosion and associated turbine durability problems due to the high humidity gas in the turbine. However, as this and other studies indicate (Rao and Day, 1992), IGHAT is a promising technology that presents economic, efficiency and emission advantages.

SIMULATION IN ASPEN PLUS

ASPEN PLUS environment provides a flexible input language for describing IGCC plant components, connectivity, and computational sequences. Use of ASPEN PLUS leads to an easier way of model creation, maintenance and updating since small sections of complex and integrated systems can be created and tested as separate modules before they are integrated. It has an extensive physical property data base where the diverse stream properties required to model the material streams in an IGCC plant are all available with an allowance for addition of inhouse property data.

Additionally, ASPEN PLUS has many built-in model blocks (such as heaters, pumps, stream mixers, stream splitters, compressors etc.), some of which can directly be used in power plant simulation. Where more sophisticated block ability is required, additional information may be added to the block in the form of FORTRAN subroutines, or entirely new user blocks may be created. In this work, a number of new blocks (e.g. turbine, compressor, combustor, etc.) were developed as the built-in blocks were found not to be sufficiently detailed to conduct accurate simulations. Thus, ASPEN PLUS shell was mainly used to model the stream connectivity and to provide the material property data. For these purposes, ASPEN PLUS is an excellent modeling tool which is versatile and relatively easy to use in modelling of advanced power cycles.

ASPEN PLUS also incorporates an integrated costing and economic evaluation system. Using this feature, equipment size and cost, as well as plant cost and profitability analyses can be made. Inclusive are the tools to help the user to override the default base cost of major process equipment and the ability to estimate certain important factors from historical cost data.

The next sections briefly discuss how ASPEN PLUS and the model blocks developed to simulate the performance of various key power plant components are used to simulate both IGCC and IGHAT cycles. The components common to IGCC and IGHAT are presented first.

COMPRESSORS, FANS AND TURBINES

Compressors, fans and turbines are simulated in ASPEN PLUS by a block called COMPR. COMPR models polytropic and positive displacement compressors, isentropic compressors/ turbines, and fans. COMPR calculates the power required (or produced) given the pressure ratio, isentropic, polytropic, and mechanical efficiencies, and (for positive displacement compressors) clearance volume. The accuracy of the results depend on the efficiencies specified.

A more elaborate procedure is required to model the compressors and turbines in the IGCC and IGHAT cycles as pressure and mass flow rate matches must be established in the cycles. Therefore, the COMPR block in ASPEN PLUS was extensively modified by incorporating new FORTRAN subroutines to model the compressors and turbines used in these cycles. The compressor subroutine utilizes the generalized maps developed by Johnson (1990) and Saravanamuttoo (1992). The turbine subroutine estimates the mass flow rate through the turbine using the choked nozzle approach by Erbes and Gay (1989). Turbine cooling is estimated using the method developed by El-Masri (1986). More detailed descriptions of these subroutines are given in Ong'iro et al. (1993). The performance of steam turbine is modeled using methods reported in Spencer et al (1963) and Baily et al (1967).

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COMBUSTOR

A combustor converts the chemical energy in the fuel to heat energy which is transferred to the working fluid. Combustors can be modeled as reactors in ASPEN PLUS. There are several different approaches for modeling of reactors. These include stoichiometric, equilibrium, kinetic, etc. The reactor model used here to model the syn-gas combustor is a Gibbs type reactor (RGIBBS) which calculates equilibrium by GIBBS free energy minimization with phase splitting subject to atom balance constraints. It is used when the entire system approaches equilibrium, and does not require reaction stoichiometry. The reaction stoichiometry does not need to be specified but a list of possible products may be specified. RGIBBS can also be used when the system does not reach complete equilibrium by specifying the extent of equilibrium. In a combustor, the reaction stoichiometry and kinetics are unknown but a list of possible products is known.

To improve the model's accuracy of simulating the combustion reactions in the different zones of the combustor, the combustion process was divided into three sections (Kauffman, 1980, Lefebvre, 1983 and Dunbar and Lior, 1991). Each section was represented by a separate RGIBBS block. In the first section, a stoichiometric amount of air is mixed with fuel and the reactor equilibrium calculation is done at adiabatic flame temperature to model the primary zone where rapid reaction between air and fuel occurs in a well insulated combustion chamber (approaching adiabatic reaction conditions). In the second section, the amount of additional air is regulated until the reactor temperature drops to 1800 K to model the intermediate zone where dissociation loss recovery and combustion of any carry over fuel from the primary zone combustion takes place. Finally in the third section, an amount of air is added until the reactor temperature required at turbine inlet. The cold and pressure loss allowances are based on the values reported in Lefebvre (1983). Steam or water injection for NO_x emission control, if any, is introduced into the primary zone to reduce the maximum flame temperature.

HEAT EXCHANGERS

Heat exchangers in the IGCC and IGHAT cycles, which are heat recovery steam generators (HRSG), condensers, intercoolers, syn-gas coolers etc., are simulated by the ASPEN PLUS HEATX block. HEATX allows the use of different heat transfer coefficients for different zones of the exchanger. The heat transfer coefficients for the different types of heat exchangers used in the simulations are calculated using typical design and operating values and methods given in Kays and London (1984), Patankar and Spalding (1978) and Zhang et al. (1993). More detailed models for HRSG's, condensers, etc. are currently being developed and will be published later.

GASIFIER

The performance data for the gasifier were taken from a design study conducted by Bechtel Canada Inc. for Nova Scotia Power Inc., Halifax, Canada. (Bechtel Canada Inc., 1992). The design used represents a commercial scale (290 MW) plant employing a Texaco entrained-bed gasifier, using Donkin coal. Syn-gas coolers are used for the IGCC plant, but quench type gasifier is used for IGHAT modeling. Generalized and more detailed models for entrained bed and fluidized bed gasifiers are currently being developed.

SATURATORS, SCRUBBERS AND COOLING TOWERS

These are counter-current heat and mass transfer devices. The saturator, which is used to heat and humidify the combustor inlet air for the IGHAT cycle, consists of a multistage tower in which hot water flows from top to bottom, and the cooler air rises from the bottom and bubbles up through the water flowing across the trays. If air and water were thoroughly mixed and allowed to stay in contact for an infinite period, equilibrium would be established with exiting air saturated with moisture. In an actual saturator, because area of contact between air bubbles and water is not infinite and time of contact cannot be infinite, equilibrium state is not achieved, and the air leaving the saturator is not quite saturated. The saturator is modeled in ASPEN PLUS by using the RADFRAC block which is an equilibrium rigorous tool for modeling ordinary distillation, absorption, reboiled absorption, stripping, reboiled stripping and equilibrium as well as rate controlled reactive distillation, and as such is a complex block. The performance of RADFRAC block was corrected for non-equilibrium operation by specifying either Murphree or vaporization efficiencies, or by using subroutines written in FORTRAN to introduce factors such as those developed by Treybal (1980) for predicting non ideal saturator performance.

A wet cooling tower is used to cool hot water from the water cooled condenser by contacting it with air at a lower temperature. In the scrubbers such as those used to clean syn-gas, the syngas mixture is contacted with a liquid for the purposes of preferentially dissolving one or more of its components and to provide a solution of them in liquid. Both wet cooling towers and scrubbers are modeled in a similar manner to the saturator.

RESULTS AND DISCUSSION

The results of a series of IGCC and IGHAT simulations focusing on effects of ambient conditions and adjustable design parameters are presented and discussed. These analyses are also useful in illustrating the capabilities of the models. The design point values of the parameters employed in the simulations are given in Table 1. No exergy or economic analysis results from the model are presented in this paper.

Figure 3 shows that the thermal efficiency of the IGCC increases as the steam throttle pressure increases in the bottoming Rankine cycle. The thermal efficiency increases to a maximum, and levels off with any further pressure increase. The initial rapid rise of efficiency is because of the increase in specific work with expansion pressure ratio of the steam turbine offsetting the effect of reduced steam flow rate (HRSG duty is fixed by the topping cycle). For higher pressure ratios, these two effects cancel out and the efficiency levels off. Thermal efficiency of the IGCC also increases with adding reheat to the bottoming Rankine cycle as shown in Figure 3. The efficiency of the IGCC with reheat Rankine cycle also initially increases with pressure and then levels off. The reasons for this variation are similar to those in the non-reheat case. The higher efficiency in reheat cycle is because more heat is fed to the bottoming cycle at higher temperature than in the non-reheat cycle. Reheating improves the efficiency of Rankine cycle (hence that of IGCC) by improving the ability of heat extraction at the upper temperature end in the HRSG. Further increases in Rankine cycle efficiency may be obtained by improving heat

Net power	250 MW
Syn-gas composition (% molar basis)	TEXACO gasifier with Donkin coal $31.67 H_2$, $42.27 CO$, $9.512 CO_2$, $0.084 CH_4$, $0.763 N_2$, $0.987 Ar$, $3E-4 H_2S$, $1.24E-3 COS$, $15.21 H_2O$
Ambient air conditions	
pressure	1.01325 bar
relative humidity	60%
temperature	15 C
Air compressor	
isentropic efficiency	0.9
mechanical efficiency	0.99
pressure ratio	14:1
mass flow rate	360 kg/s
Gas turbine	
polytropic efficiency	0.92
mechanical efficiency	0.99
inlet temperature	1260 C
Heat exchangers	
pinch temperature difference	16 C
Steam turbine	
isentropic efficiency	0.92
hp stage pressure	101 bar
hp stage temperature	538 C
ip stage pressure	18 bar
ip stage temperature	538 C
lp stage pressure	4 bar
condenser pressure	25.4 mmHg
water available at	20 C

Table 1: Design point parameters



extraction at the lower temperature end of the HRSG. This can be done by adding a second steam circuit operating at a lower pressure (secondary) than the main steam circuit (primary).

Figure 4 shows that there is an optimal secondary circuit pressure for every value of main steam pressure. This is because the presence of the secondary circuit will control the position of pinch point and hence the amount of heat transfer in the HRSG.

Figure 5 shows that thermal efficiency of the IGCC increases with steam temperature at turbine inlet. At each steam turbine inlet temperature, there is an optimal value of steam pressure beyond which no further increase in thermal efficiency occurs. The reduction in work output due to reduced mass flow rate of steam (at constant HRSG duty) balances the increase in work output due to increase in specific work with steam temperature.

Figure 6 shows that the temperature difference between water and the combustion gases varies over a large range because the transition to steam is a constant temperature process. This increases the amount of irreversibility and result in a lower exergetic efficiency of the HRSG.

The irreversibility in a heat exchanger can be reduced by using an ideal cold fluid with thermodynamic and transport properties such that the differential temperature between the hot fluid and the cold fluid is uniform throughout the heat exchanger. An ideal heat exchanger will therefore have uniform and infinitesimal temperature differential between the hot and cold fluids. However, since this is not possible, some irreversibility is inevitable in the HRSG.

In the IGHAT cycle the HRSG is replaced with a moist air recuperator and an economizer as shown in Figure 2. Since moist air behaves like a fluid with variable boiling point, and only liquid water is heated in the economizer, the temperature profiles in the IGHAT cycle economizer and recuperator can be made to approach to that in an ideal heat exchanger as shown in Figure 7. This will result in a heat exchanger with higher exergetic efficiency than that of HRSG of a similar duty. Figure 8 shows the variation of efficiency in an IGHAT cycle with the temperature of water in the saturator for different gas turbine pressure ratios. Thermal efficiency increases with an increase in pressure ratio, due to the increased expansion work. Thermal efficiency decreases with saturator temperature at a fixed pressure ratio. Despite the increase in specific work with saturator temperature as shown in Figure 9, more fuel must be burnt to keep the turbine inlet temperature constant as the moisture fraction of combustion air increases with saturator temperature as shown in Figure 10. As the temperature of the saturator is decreased further, thermal efficiency peaks and then drops to levels similar to that in a steam injected cycle (STIG) which is less than that in either IGHAT cycle or in IGCC.

From Figures 8 and 3, it can be seen that the IGHAT has a higher thermal efficiency than the IGCC power plant. This is due to the following factors:

- i) More energy is recovered from the gasifier by generation of hot water in IGHAT compared to that recoverable in the form of high pressure steam in IGCC.
- ii) Air compressor work is decreased since excess amount of air is used in the gas turbine to limit turbine inlet temperature in the conventional Brayton cycle of IGCC. This absorbs substantial amount of work from the turbine, whereas in IGHAT cycle because of introduction of moisture, the amount of excess air required is reduced, reducing air compressor work.
- iii) Using air with high content of moisture instead of low humidity air as in IGCC results in increased mass flow rate through the cycle. Since combustion products with the highly humidified air have higher specific heat capacities, more expansion work is generated for the same expansion ratio.

Carbon dioxide emissions per unit of electric power generated is inversely proportional to the plant thermal efficiency, therefore the IGHAT cycle has an advantage over IGCC with respect to CO_2 emissions.

Figure 11 shows that the adiabatic flame temperature in the primary zone of the combustor decreases with the air saturator temperature. This is because the air moisture content increases as shown in Figure 10. The specific heat capacity of air-water vapor mixture increases with the mass fraction of water vapor. As a consequence of the reduction in the maximum flame temperature, the NO_x emission decreases with increase in saturator temperature as shown in Figure 12. It is predicted that the relative NO_x emission for the IGHAT cycle is less than 30-40% of that from IGCC depending on such parameters as saturator temperature in IGHAT, steam pressure in IGCC, etc.

Figure 13 shows that the IGHAT cycle performance is less sensitive to ambient temperature than IGCC. The water vapor absorbed in the saturator balances out the changes in air flow rate through the compressor, limiting the departure of operating point from the design point. In the IGCC, the increase in ambient temperature results in reduced air mass flow rate and



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the compression ratio of the compressor drops for the turbine to cope with decreased mass flow rate. Thus, from thermodynamics of expansion in the turbine, reduced pressure ratio with constant turbine inlet temperature leads to an increase in gas exhaust temperature. The work output of the topping Brayton cycle therefore decreases, but more steam is generated in the HRSG leading to an increase in the bottoming Rankine cycle work output. The increase in work output from the Rankine cycle offsets the decrease in work output from the Brayton cycle and reduced flow rate (as a result of decreased air mass flow rate) leads to an increase in thermal efficiency. This finding is in agreement with that presented by Kehlhofer (1991).

CONCLUSION

Computer simulation models of IGCC and IGHAT cycle were developed in ASPEN PLUS shell. These models are capable of carrying out mass, energy and exergy balances. They can be used to study the effects of changes in design and performance parameters on the efficiencies, emissions and economics of IGCC and IGHAT cycles. The models are flexible and can easily accommodate any desired changes in cycle configurations, input, and component performance data. The results given in this study, although specific to inputs and the design parameters used in the calculations, predict patterns and quantities which conform with those observed in practice.

ACKNOWLEDGMENT

The authors gratefully acknowledge the financial support provided by the Natural Sciences and Engineering Research Council of Canada (Operating Grant OGPOO41739), and Canadian Commonwealth Scholarship and Fellowship Plan.

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