

ENERGY CONSERVATION IN COAL CONVERSION

Case Study: The Thermodynamic Performance of Two
Combined Cycle Power Plants Integrated with
Two Coal Gasification Systems

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PREFACE

Improving power plant efficiencies is receiving ever-increasing attention today because of the realization that our fossil fuels are in finite and dwindling supply. Most experts agree that coal is plentiful enough to warrant its use on a much wider scale for power production in order to provide a near-term solution to the energy crisis. Coal gasification provides a relatively simple (and economical) way to remove the sulfur from the coal. Moreover, the combined-cycle concept may be used to help boost overall plant performance. This study shows how these two concepts may be integrated for the production of electrical energy. Indeed, seeking the optimal plant design results in energy conservation in its most basic form.

One of the key results pertains to the design constraints provided by the federal emission standards. Without consideration of the pollution criteria, a station efficiency of 41 percent may be expected; this is equivalent to a station heat rate of only 8300 Btu/kwhr. With consideration of the criteria, the station efficiency is reduced to about 37 percent or to a heat rate of 9200 Btu/kwhr. It is readily seen that meeting the pollution criteria requires an additional 900 Btu of energy for each kilowatt-hour of electrical energy produced.

Overall performance may be improved substantially by increasing the gas turbine inlet temperature from 2000 to 2400°F. A 400°F increase in this parameter improves the station efficiency by about

5 percentage points to nearly 42 percent or by about 1100 Btu/kwhr to a station heat rate of only 8100 Btu/kwhr, with consideration of the pollution criteria.

Clearly vast amounts of energy may be conserved by improving power plant performance. Although the pollution criteria take their toll on station efficiency, the next generation of gas turbines should make this integrated gasification and combine cycle concept very attractive from an energy utilization viewpoint.

The research reported in this document was conducted by F. L. Stasa as a PhD thesis in the Mechanical Engineering Department at Carnegie-Mellon University. J. F. Osterle was his thesis adviser. The work was partially supported by the subject DOE Contract.

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ABSTRACT

Thermodynamic models of both an adiabatic and an endothermic coal gasifier integrated with either a waste heat combined cycle or a supercharged boiler combined cycle are developed and incorporated into a Fortran computer program. The adiabatic gasification process requires air and steam, while the endothermic gasification process requires only steam. The former produces a low-Btu power gas, and the latter an intermediate-Btu power gas. Most of the sulfur in the coal is removed after the gasification step in the form of hydrogen sulfide. The resulting relatively clean power gas fires the combined cycle which is composed of an open Brayton cycle and a superheated regenerative Rankine cycle without reheat. Certain components are added to each configuration in an effort to improve thermodynamic performance, with the effect of each clearly noted. Each configuration is optimized with respect to certain key operating parameters, with and without consideration of the power plant emission standards established by the federal government through the EPA. Total consumable water requirements and steam cycle heat rejection requirements are also noted. Certain key parameters, like coal composition, are varied and the effect on performance is noted.

From the results, it appears that a minimum number of feedwater heaters should be used. Intercooled air compressors are not warranted. At least one regenerator is crucial to the success of the two configurations employing adiabatic gasifiers. Without consideration of the pollution criteria, the waste heat configurations are superior to the

supercharged boiler by more than 5 percentage points on station efficiency, with 41 percent for the former and only 36 percent for the latter. All station efficiencies include a 10 percent penalty for station loads. With consideration of the criteria, the station efficiencies for each configuration are within 1 percentage point of each other when flue gas recirculation is used as a means to control the amount of nitric oxide which enters the atmosphere. With a gas turbine inlet temperature of 2000°F and with consideration of the pollution criteria, the configuration employing an adiabatic gasifier and a waste heat system is marginally the best with a station efficiency of only 37 percent. The success of power generation schemes utilizing integrated gasification and combined cycles appears to be dependent on an increased gas turbine inlet temperature; for a 400°F increase, the station efficiency improves by 5 percentage points.

CHAPTER 1 OBJECTIVES

The primary objective of this dissertation is to provide a unified and consistent thermodynamic treatment of integrated coal gasification and combined cycle power plants. Two coal gasification processes and two combined cycle concepts will be integrated to produce four possible plant configurations. The best configuration will be sought with respect to thermodynamic performance which is defined qualitatively as usable energy output compared to energy input. Later it will be seen that the station efficiency will be used to quantitatively assess the cycle performance.

Beginning with the four basic cycle configurations, certain components will be added in an effort to improve the performance. It will be instructive to take each of these potential improvements in turn and to note the effect on each configuration. The purpose of this is to see more clearly the effect of adding a particular component. We shall see that performance is not always enhanced by adding equipment usually associated with improving overall efficiency.

Having done this preliminary "optimization" with respect to components, we shall then optimize each configuration in turn, trying to seek the best configuration. In order to see more clearly the effect of meeting the federal emission standards with respect to nitrogen oxides, this optimization will be done first without consideration of the applicable criterion. From the outset, however, the criterion on sulfur dioxide will be met since one of the primary reasons for coal gasification in the first place is to provide a relatively easy way to remove

most of the sulfur from the system well before the products of combustion enter the stack. The effect on cycle performance of meeting the nitrogen oxide emission criterion via flue gas recirculation will be clearly identified.

With each configuration optimized and designed to meet the federal emission standards, other important results will be given. Among these are the consumable water requirements and steam cycle heat rejection requirements. For completeness, typical compositions of the gas leaving the gasifier and the gas leaving the combustor will also be noted.

Finally, parametric studies on some key parameters will be presented. Included in these are coal composition, regenerator effectiveness, pressure drop and component efficiencies, boiler pinch point temperature difference, and gas turbine inlet temperature.

The relevant results are presented in Chapter 5 with the conclusions and recommendations for further study in Chapter 6. It should further be noted that, as much as is feasible, off-the-shelf equipment is to be used. For example, currently available gas turbines with a peak temperature of 2000°F are used instead of advanced technologies like air- or water-cooled turbines. Consequently, it is believed that the results to be presented later are indicative of the performance that can be expected with the technology of today.

It should be noted that economic considerations are outside the scope of this dissertation. This very important facet of the design problem is necessarily outside the realm of thermodynamics, since equipment would first have to be sized. Hopefully, this dissertation may provide the starting point for such an extension to this work.

CHAPTER 2
INTRODUCTION

2.1 Combined Cycles

Before describing two primary types of combined cycles, let us motivate the reason for considering combined cycles in the first place. Consider the thermodynamic cycle of a simple heat engine whose schematic is shown in Figure 2.1-1. Let us take Q_1 units of heat from a high temperature reservoir, let it be the heat source for a heat engine that operates in a cycle, and extract W_{12} net units of work. The second law of thermodynamics requires that heat be expelled from the cycle to the low temperature reservoir. Let the amount of rejected heat be Q_2 . The first law of thermodynamics requires that

$$Q_1 = W_{12} + Q_2 \quad (2.1-1)$$

The cycle efficiency η is defined to be the ratio of the net work W_{12} to the heat input Q_1 , or

$$\eta = \frac{W_{12}}{Q_1} \quad (2.1-2)$$

Now consider two such cycles in series, as shown in Figure 2.1-2. We shall refer to this arrangement as a combined cycle. The heat Q_1 from the high temperature reservoir drives the first heat engine which produces net work W_{12} . The amount of heat rejected to the second cycle is Q_2 . In this cycle, W_{23} net units of work are produced. The second cycle then expels Q_3 units of heat to the low temperature reservoir. To make our discussion more general and closer to our observations of the real world, let us further assume that Q_2 units of heat are transferred directly to

the low temperature reservoir from the first engine; thus, Q_L represents a heat loss. This is shown by the dashed line in Figure 2.1-2. The thermodynamic efficiencies for the first heat engine alone, the second heat engine alone, and for the two engines combined become respectively

$$\eta_1 = \frac{W_{12}}{Q_1}, \quad (2.1-3)$$

$$\eta_2 = \frac{W_{23}}{Q_2}, \quad (2.1-4)$$

and

$$\eta_{cc} = \frac{W_{12} + W_{23}}{Q_1} \quad (2.1-5)$$

If β is defined to be the ratio of the heat loss Q_L to the heat input to the second cycle Q_2 , we may write

$$\beta = \frac{Q_L}{Q_2}. \quad (2.1-6)$$

Then using Equations (2.1-3) and (2.1-4) in Equation (2.1-5), the following expression results for the combined cycle efficiency in terms of only η_1 , η_2 , and β :

$$\eta_{cc} = \eta_1 + \left[\frac{1-\eta_1}{1+\beta} \right] \eta_2 \quad (2.1-7)$$

From the definition of β , note that $\beta=0$ corresponds to no heat loss from the first heat engine. If β is infinite, then no heat is transferred to the second heat engine and the combined efficiency η_{cc} should be equal to η_1 . This last observation is consistent with Equation (2.1-7).

Let us examine the implications of Equation (2.1-7). Considering the abscissa to be η_2 and the ordinate η_{cc} , Equation (2.1-7) represents a straight line with η_1 as the y-intercept and the quantity $(1-\eta_1)/(1+\beta)$ as

the slope. Clearly, the presence of β in the denominator of the expression for the slope serves to reduce η_{CC} . The best combined cycle efficiency is obtained when β is zero. When β is one, half of the heat "rejected" from the first heat engine is lost and half drives the second heat engine. Let us plot η_{CC} versus η_2 with η_1 as a parameter for these two values of β , as shown in Figure 2.1-3. In this figure, the solid lines correspond to $\beta=0$ and the dashed lines to $\beta=1$.

Consider first the case of no heat loss ($\beta=0$). From Figure 2.1-3 it may be seen that η_{CC} is always greater than both η_1 and η_2 . For example, if $\eta_1=0.25$ and $\eta_2=0.25$, then $\eta_{CC}=0.44$ which represents a significant increase. A considerable amount of additional work, therefore, may be obtained by connecting two cycles in series thermodynamically. Let us now see how the presence of a heat loss affects the combined cycle efficiency.

Consider the case of a heat loss from the first heat engine to the low temperature reservoir such that $Q_L=Q_2$ or $\beta=1$. From Figure 2.1-3 it is seen that for the example above now $\eta_{CC}=0.34$, instead of 0.44 as before. This clearly indicates that the efficiency of a combined cycle may be improved significantly over that of both the individual cycles by reducing the heat loss from the first cycle. This assumes, however, that η_1 and η_2 remain unchanged, which is unlikely. From the definition of β , it is seen that β may be decreased by reducing Q_L or by increasing Q_2 . Making Q_2 larger with β fixed, however, necessarily lowers η_1 . Let us derive an alternate expression for η_{CC} that will prove to be more useful than Equation (2.1-7) in explaining some of the results to be shown later in Chapter 5.

An equivalent expression for η_{cc} is given by

$$\eta_{cc} = 1 - \frac{Q_L + Q_3}{Q_1} \quad (2.1-8)$$

and for η_2 by

$$\eta_2 = 1 - \frac{Q_3}{Q_2} \quad (2.1-9)$$

Solving Equation (2.1-9) for Q_3 and substituting this result into Equation (2.1-8) gives

$$\eta_{cc} = 1 - \left(\frac{Q_L + Q_2}{Q_1} \right) + \frac{Q_2}{Q_1} \eta_2 \quad (2.1-10)$$

As we shall soon see, a practical application for this combined cycle concept is the gas turbine cycle combined with a steam cycle. Reducing the heat loss Q_L from the first or gas cycle will be tantamount to reducing the heat transfer to the environment, including stack gas losses. Changing the heat input Q_2 to the second cycle will be equivalent to changing the heat transfer in the boiler from the gas cycle to the steam cycle.

It can be easily shown that the above combined cycle concept is superior to an ordinary gas cycle with regeneration. Let us assume that again the gas cycle efficiency (or η_1 above) is 25 percent. In addition, we conservatively assume that as much as 50 percent of the rejected heat is used to help provide the heat input to the cycle by regeneration. This last assumption will put an upper bound on the gas cycle efficiency with regeneration, since it is unlikely that 50 percent of the heat source could be provided by this method. Let us arbitrarily normalize this brief calculation on 2 units of work. As shown in Figure 2.1-4, this implies 8 units of heat into the cycle with 3 coming from the

regenerated rejected heat and 5 coming from the high temperature reservoir. Only 3 units of heat are actually rejected to the low temperature reservoir. Again we see that the engine by itself is only 25 percent efficient, but the entire system taken together is 40 percent efficient. The combined cycle above was shown to have an efficiency as high as 44 percent under consistent assumptions. Clearly, the combined cycle concept has a higher potential to boost overall plant performance.

In summarizing, application of the combined cycle concept could result in a significant increase in thermodynamic efficiency. Better overall performance can be expected for the combined cycle than for the simple gas turbine cycle with regeneration. Two feasible gas-steam combined cycle concepts will now be discussed: the waste heat system and the supercharged boiler system.

A simple gas turbine cycle is shown schematically in Figure 2.1-5. Note that this is an open cycle, since the air and fuel, presumably in a different chemical form, are eventually expelled to the atmosphere. Air is compressed by a compressor to an elevated pressure, mixed with fuel, and burned in the combustor. The hot product gas then expands in the gas turbine where useful work is done by the fluid before being expelled to the atmosphere. This cycle is known as an open Brayton cycle. The purpose of the cycle, of course, is to produce net work. We shall see in Chapter 5 that this cycle by itself is not very efficient, but its use in combined cycles significantly enhances the overall cycle performance. Typical gas turbine exit temperatures are in excess

of 1000°F. There is enough sensible heat in this exhaust gas to generate a significant amount of superheated steam in a steam cycle.

A simple schematic of a closed steam cycle is shown in Figure 2.1-6. In fact, this particular cycle is known as a Rankine steam cycle. Steam which is generated in the boiler from an external heat source is expanded in a steam turbine to a very low pressure. The fluid is then condensed in a condenser before it is pumped back into the boiler to continue the cycle. As mentioned above, there is sufficient sensible heat in the gas turbine exhaust to supply the heat necessary in the boiler to raise about 1000°F superheated steam. The efficiency for this steam cycle can be quite good when improvements to the cycle are made, such as regenerative feedwater heating. Let us now expound on the concept of the waste heat system

It has already been agreed that it is feasible to use the gas turbine exhaust to provide the heat needed in the boiler. Because the waste heat from the gas cycle is being used in this boiler, it is referred to as a waste heat boiler. The resulting combined gas and steam cycle, or combined cycle for short, will be referred to as a waste heat boiler system or even a waste heat system. As discussed in more detail in the next chapter, the waste heat boiler is composed of three sections: the superheater (SH), the evaporator (EV), and the economizer (EC). Suffice it to say now that the exhaust gas passes through the gas-side of the waste heat boiler in the order of superheater, evaporator, and economizer and leaves the system through the stack. In Figure 2.1-7 the path of the gas from the combustor to the stack is summarized. Because of metallurgical considerations, the gas turbine inlet temperature for land-based

operation may not exceed 2000°F based on present technology. Because the adiabatic flame temperature of the gas is much higher than this, the gas will have to be burned with a great amount of excess air. The excess air serves as a diluent, of course, since it will enter the combustor at a temperature significantly below the adiabatic flame temperature.

A second feasible way in which the Brayton and Rankine cycles may be incorporated into a combined cycle will now be discussed. Instead of expanding the gas in the gas turbine before allowing it to enter the boiler, let us try to do the reverse; that is, let us try to burn the gas in the combustor, generate steam in the boiler, and then expand the gas in the gas turbine. First it should be noted that if the economizer is before the gas turbine, the gas turbine inlet temperature will be necessarily too low to produce a significant amount of work. As a minimum, the gas turbine will have to be located upstream of the economizer. Second it should be noted that the highest possible turbine inlet temperature, 2000°F, should be used to get the best cycle efficiency. In order to have 2000°F gas after the superheater and evaporator, a gas temperature much higher than this is needed at the inlet to the evaporator and superheater sections of the boiler; that is, the gas should be burned with a minimum of excess air in order to obtain a gas temperature near the adiabatic flame temperature. Finally, because of the extremely high combustor exhaust temperature, the evaporator section must be placed upstream of the superheater section with respect to the gas-side flow. The reason for this, of course, is that the boiling in the evaporator section results in much higher heat transfer coefficients than the

single-phase heat transfer which occurs in the superheater. The high heat transfer coefficients due to boiling in the evaporator can better accommodate the high heat flux associated with the very hot combustor exit gas. The path of gas from the combustor to the stack is summarized in Figure 2.1-8.

This arrangement of gas cycle and boiler components will be referred to as a supercharged boiler, and a combined cycle which uses this type of boiler will be referred to as a supercharged boiler system. Note that the distinguishing feature between the two combined cycle concepts that have been discussed is the path of the gas through the combined cycle along with the resulting implications. In the waste heat system, the gas proceeds from the combustor to the gas turbine followed by the waste heat boiler. In the supercharged boiler system, the gas proceeds from the combustor to part of the supercharged boiler before going to the gas turbine and finally the economizer. The implications are that the gas for the former must be burned with a large amount of excess air and that for the latter with a minimum of excess air.

As we shall see in the next chapter, this difference between the two combined cycle concepts results in two different modes of operation for the combustor model. For the waste heat system, we shall want to specify the turbine inlet temperature (which is the same as the combustor outlet temperature) with the amount of excess air to be calculated. For the supercharged boiler system, it will be convenient to be able to specify the amount of excess air to be supplied to the combustor with the combustor exit temperature

to be calculated. These modes are easily accommodated in our model as we shall see in Section 3.2.

Next, coal gasification is examined as a means of providing a clean gaseous fuel source for the two combined cycles that have just been discussed.

2.2 Coal Gasification

Let us define coal gasification as a process which converts coal into a gas which contains combustible chemical species. We shall see shortly some of the ways in which coal gasification may be accomplished. Also, we shall examine how the various processes affect the heating value of the gas which is produced, eventually limiting these alternatives to only two: adiabatic gasification of coal with air and steam and endothermic gasification with steam only. Let us initially limit the discussion to pure solid carbon (C) instead of the more problematic coal to establish the distinguishing features of the various coal gasification processes. Of course, in the final analysis the carbon will be replaced by coal, which will significantly increase the complexity of the analysis.

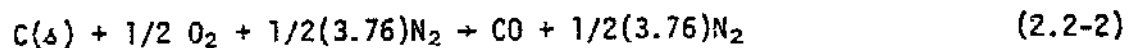
Let us try to put coal gasification into perspective by considering first the basic combustion reaction of pure solid carbon (C) with stoichiometric air. For added simplicity, let us assume only nitrogen (N₂) and oxygen (O₂) are present in the air. The reaction equation is



where (s) denotes the solid phase and where it has been assumed that there are 3.76 moles of N₂ per mole of O₂ for the air for these simplified calculations only. Let us now consider a hypothetical experiment in which the

reactants enter a combustion chamber in a steady-flow process at ambient conditions and the products leave at the same conditions. Approximately 14,100 Btu of heat per pound of carbon will be given up to the environment during the process and the product gas will have no heating value; that is, the carbon dioxide (CO₂) is not capable of further combustion in air. In this somewhat simplified discussion the distinction between high and low heating values will not be made.

Next the carbon is reacted with only half of the stoichiometric air according to the following reaction



Instead of forming CO₂, the reaction produces carbon monoxide (CO), which has a non-zero heating value since CO can be burned further in air to form CO₂. If the same type of experiment described above is performed, now only 3960 Btu of heat are given off per pound of carbon. However, the heating value of the CO makes up the difference. The reaction has produced a gas, composed of CO and the diluent N₂, which has an effective heating value of about 110 Btu per standard cubic foot (Btu/SCF) of product gas. It is important to remember that heat is released for this reaction. To put this in perspective, let us compare this heating value to that of natural gas which is approximately 1000 Btu/SCF. It is readily seen that the gas which was produced has about only 10 percent of the heating value of natural gas.

In order to eliminate the diluent N₂ from the product gas, the carbon may be reacted with half a mole of pure O₂ according to



in which only CO is produced. Again this gives up about 3960 Btu of heat, but the heating value of the gas is now 310 Btu/SCF of product gas, or 30 percent of that of natural gas. However, the chief disadvantage of this process lies in the fact that pure O₂ is needed as a reactant. Let us now show how just about the same heating value may be obtained without the use of pure O₂.

Let us react the pure solid carbon with steam and, according to the following balanced chemical equation, produce CO and H₂ (hydrogen) gases.



This reaction is endothermic, however, and *requires* about 9400 Btu of heat if the same kind of experiment is performed. However, a gas has been produced that has a heating value of about 290 Btu/SCF without the use of pure O₂. It is important to keep in mind that heat is required to effect this reaction.

Let us follow the usual convention used in the literature and refer to a gas with a heating value in the range of 0 to 200 Btu/SCF as a low-Btu fuel gas, one in the range of 200 to 400 Btu/SCF as an intermediate-Btu fuel gas, and one above 400 Btu/SCF as a high-Btu fuel gas. Natural gas and synthetic natural gas, of course, are included in the last category. Several coal gasification processes exist which produce a high-Btu gas. These processes are considerably more complex than those described above and require much additional equipment. Also, it makes no sense to produce

a high-Btu gas to be burned and used in an electrical power generation scheme. We shall see in Chapter 5 that very high flame temperatures are possible with a low- or intermediate-Btu gas. Let us restrict our attention, therefore, to only these two types of power gases.

It is instructive to summarize the above gasification reactions. By reacting carbon with half stoichiometric air, a low-Btu fuel gas was obtained, but heat was *produced*. By reacting carbon with pure O_2 , an intermediate-Btu fuel gas resulted with heat again being produced. By reacting carbon with steam, an intermediate-Btu fuel gas was produced but heat was *required*. Let us now eliminate the process which requires pure O_2 from further consideration on the grounds that an expensive oxygen plant would be required and that an intermediate-Btu gas may be obtained by the endothermic reaction of carbon with steam anyway. It is rather easy to see that if the reaction in Equation (2.2-2) releases heat and the reaction in Equation (2.2-4) requires heat, then the two could be combined in such a way as to have no net heat transfer. We shall refer to this gasification process of carbon (and later coal) with steam and air with no net heat transfer as adiabatic gasification for short. In Chapter 5, it will be seen that this process produces a low-Btu fuel gas with a heating value of about 150 Btu/SCF, since the diluent N_2 is present in a significant amount from the air that is used. We shall refer to the gasification process of carbon with steam (and no air) and with heat transfer to the process as endothermic gasification for short. It will be seen that this process produces an intermediate-Btu fuel gas with a heating value of about 300 Btu/SCF.

It should be noted that later when the carbon is replaced by coal, compounds containing sulfur will be formed. Most of the sulfur fortunately

ends up as hydrogen sulfide (H_2S) and a much smaller amount as carbonyl sulfide (COS). In the next section the implications of this are discussed.

It is appropriate at this point to state some of the advantages of coal gasification to power an electrical power generation plant. The fact has been established that combined cycles have a high potential to increase overall power plant efficiency. It then followed that a gas and steam cycle could be combined in such a way to achieve this objective. Using natural gas or oil for this purpose may be ruled out because these sources are expected to be in short supply in the near future. Because of the high potential for blade erosion problems in gas turbines using the products of combustion from coal, a relatively clean fuel is needed in order that the working fluid in the gas cycle also be relatively clean. Coal gasification provides such a fuel because proven technology¹ is already available to clean the sulfur compounds (and particulates) out of the fuel if low temperature cleanup is accepted. In addition, it is more economical¹ to clean gas at elevated pressures (which we shall do) than at low pressures, and as we shall see in Chapter 5, there is a significant reduction in the amount of gas to be cleaned if it is cleaned before any combustion takes place. It is felt that these advantages provide enough incentive for looking for ways to utilize our most abundant, albeit dirty, domestic energy source. Coal gasification provides such a means.

It will be necessary, then, to operate the gasifier in two distinct modes: adiabatic gasification of coal with air and steam and endothermic gasification of coal with steam only. In the next section a possible source for the heat needed for the endothermic process will be identified. Also, it will be seen how these two gasification processes may be

integrated with the two combined cycle schemes to form four different electrical power generation plants.

2.3 Combined Cycle Power Plants Integrated with Coal Gasification Systems

In the last two sections, two practical combined cycles and two feasible coal gasification processes were discussed. This suggests four different possible cycle configurations: (1) an adiabatic gasifier integrated with a waste heat system, (2) an adiabatic gasifier integrated with a supercharged boiler system, (3) an endothermic gasifier integrated with a waste heat system, and (4) an endothermic gasifier integrated with a supercharged boiler system. Each of these basic configuration descriptions will now be used to put together the simplest possible cycle for each configuration. As will be seen shortly, each configuration will require the following components: a gasifier, air compressors, a steam generator, a gas throttle valve, a gas cooler, a combustor, a gas turbine, either a waste heat boiler or a supercharged boiler, steam throttle valves, steam turbines, pumps, and a condenser. In addition, a low temperature desulfurization process is needed in which unwanted species from the power gas are removed. Low temperature cleanup is used since proven technology already exists for it. It will be seen later that one such system could be the Benfield process. Let us now take each of these configurations in turn and lay out the simplest possible component arrangement.

2.3.1 Adiabatic Gasifier Integrated with Waste Heat System

It should first be noted that it is necessary to operate the gasifier under pressure, since the power gas is to fuel the Brayton cycle. An air

compressor is needed in order to supply the air for the gasification process. Since adiabatic gasification requires steam, a steam generator is required to generate the steam under pressure with the water being supplied by a pump. Since it will be possible to produce a very hot power gas, some of the sensible heat in this gas may be used to generate the required steam. This is not only feasible but also desirable, since the gas must be cooled anyway for the low-temperature cleanup process. Obviously, high temperature cleanup would be more efficient, but it is not yet technologically nor economically proven. A throttle valve will be placed in the gas flow path to make the operating pressures in the gasification and combustion systems compatible.

Because the steam generator will not necessarily be able to lower the gas temperature to within the operating range of the desulfurization process (between 200 and 260°F), a gas cooler will be needed to accomplish this. After the "dirty" power gas is cleaned via the desulfurization process to a specified purity, the "clean" gas is then burned in a combustor under pressure with the air supplied by a second air compressor. The hot combustor product gas is expanded in a gas turbine. The turbine exhaust gas then is used to supply the heat to the waste heat boiler, where superheated steam is generated for the Rankine cycle. The steam is expanded in a steam turbine with the turbine exhaust being condensed in a condenser. A feed-water pump is used to supply the feedwater to the steam-side of the waste heat boiler which operates under pressure, of course.

This relatively simple basic arrangement and all modified versions of it are hereinafter referred to as Configuration 1. A simplified schematic of this configuration is shown in Figure 2.3-1. The schematic representation

of each component will be formally introduced in the next chapter, where each component model is described. To avoid ambiguity on the schematic of Configuration 1 and on the other three schematics later, each component is labeled explicitly. Simplified schematics for the steam generator and waste heat boiler are used at this point.

2.3.2 Adiabatic Gasifier Integrated with Supercharged Boiler System

As the description of this configuration suggests, a system similar to that of Configuration 1 is sought, but the waste heat boiler is to be replaced by a supercharged boiler. The portion of the system from the gasifier to the combustor and its air compressor remain unchanged. However, the product gas from the combustor now enters the evaporator and superheater sections of the supercharged boiler before the gas turbine. The exhaust gas from the turbine then passes through the economizer section of the boiler. The steam cycle is identical to that of Configuration 1 and will not be discussed again here.

This arrangement, hereinafter referred to as Configuration 2, is shown schematically in Figure 2.3-2. Note that again a simplified representation is used.

2.3.3 Endothermic Gasifier Integrated with Waste Heat Boiler

Recall that, for endothermic gasification, coal is gasified with steam only. It follows that the air compressor serving the gasifier must be removed from the systems shown thus far. In addition, a provision for heat transfer to the gasifier must be included since endothermic gasification is desired. Because the gasifier could conceivably operate at high

temperatures (presumably well above 1000°F), a high temperature heat source must be used. Clearly, the combustor provides such a source, and by using some heat transfer medium, heat can be removed in the combustor and transferred to the gasifier. The technical feasibility of accomplishing this in practice will be discussed in Chapter 5. From the combustor to the stack, the gas cycle and the steam cycle remain the same as in Configuration 1. This basic arrangement shall hereinafter be referred to as Configuration 3, which is shown schematically in Figure 2.3-3.

2.3.4 Endothermic Gasifier Integrated with Supercharged Boiler

Clearly for this configuration the gasification system of Configuration 3 must be integrated with the combined cycle arrangement of Configuration 2. Indeed, nothing is new at this point. This cycle arrangement represents the final configuration and is shown schematically in Figure 2.3-4. This basic arrangement shall hereinafter be referred to as Configuration 4.

2.3.5 Remarks

Four basic cycle configurations have been developed which incorporate two gasification processes and two combined cycle systems. For each of these configurations, the open Brayton cycle and Rankine steam cycle are used. The components have been arranged in the simplest possible manner under the constraints of each respective configuration.

These four configurations represent the starting point from which the cycles may be optimized and improved. Recall that one of our goals is to improve the performance of each cycle by setting optimum operating conditions

and by adding components where necessary. This objective as well as the others stated in Chapter 1 can only be met through very tedious calculations, since the cost of an experimental undertaking would be extremely prohibitive. The need for a mathematical model of each configuration is obvious. This aspect of the problem is approached by modeling each component separately, which is done in Chapter 3. Also obvious is the need for computer capability, since it will be necessary to calculate the performance for many different operating conditions. The component models developed in Chapter 3 are used in the computer program, which is fully described in Chapter 4. Finally, in Chapter 5, an attempt will be made to improve the basic cycle configurations shown in Figures 2.3-1 to 2.3-4 by adding components and by specifying optimum operating conditions.

2.4 Background

Much work has been done on the design of various types of coal gasifiers and gas cleanup systems and surprisingly little on the integration of these systems to combined cycle power plants for the production of electrical energy. It is instructive to summarize some of these gasification and cleanup systems to demonstrate the large degree of flexibility in designing an integrated system. In fact, both the gasification and cleanup systems seem to be so flexible that the results of this dissertation may be used as a basis for designing new systems. For example, one of the key results from Chapter 5 will be the optimum gasification temperature and pressure which fixes certain other parameters such as steam and, for the adiabatic case, air flow. This type of result may be helpful when one actually tries to design a coal gasifier capable of operation under conditions which are optimum with respect to overall performance.

It is a well-known fact today that some sort of coal gasification technology has been in existence for almost 150 years. In the early 1830's, Faur built a low-Btu gasifier for the production of a producer gas. In the 1920's, there were about 11,000 gasifiers of this type mostly used by the steel industry. Admittedly, these systems today are no longer feasible because of updated environmental constraints. In the mid 1870's, an intermediate-Btu fuel gas was made by the blue water gas process. More than fifty years later this was followed by the Lurgi process² which is now being used in at least fourteen industrial plants³. Clearly, processes for the production of low- and intermediate-Btu gas have been in existence for a long time.

The present state of affairs is summarized best by an ad hoc panel of the National Research Council which was established to assess the state of low- and intermediate-Btu coal gasification technology:

... there has been a long hiatus in the use of gas producers and in the development of new technology for making producer gas. Recent interest in the development of related technology stems from the hope that it will provide a means for producing a clean fuel from coal and, from the possibility of increasing the efficiency of coal conversion if the gas is generated under pressure and used in a combined cycle, helping to alleviate the shortage of scarce fuels.¹

Many processes have since been devised, thus demonstrating the inherent flexibility in gasifying coal¹. The coal and gas flows may be parallel-flow or counterflow. The gasifier may operate at atmospheric pressure or under pressurized conditions. Air or oxygen may be used in addition to steam. Heat may be added to the process, eliminating the need for pure oxygen⁴. Tar, soot, mercaptans, phenols, thiophenes, and so forth may be avoided by operating the gasifier at high temperatures. The ash may be removed in dry, slag, or agglomerated form. The gasifiers are typically

classified as fixed bed, fluidized bed, entrained flow, molten bath, and underground¹. Obviously the last two types are not applicable to the problem of interest and will not be discussed further.

The fixed bed gasifier designs are well developed. Coal and gas flows are countercurrent. This type of gasifier typically has long residence times which allows for essentially complete carbon conversion. Operation at elevated pressures could be problematic because of softening, sticking, and swelling of some bituminous coals¹. Gas exit temperatures are usually less than 1200°F which means a large amount of tars, phenols, and so forth are formed. Among the dry-ash pressurized processes are Lurgi², Gegas⁵, and MERC⁶. The present Lurgi process is capable of using air to produce a low-Btu gas or pure oxygen to produce an intermediate-Btu gas, which may then be used as a feed for the production of synthetic natural gas. The Gegas process has a much lower steam-to-air ratio than is typical of this type of gasifier. The MERC process produces about 3% tar, indicating a relatively low gasification temperature. The Wellman-Galusha³ and Kellogg⁷ systems use atmospheric dry-ash fixed-bed gasifiers. Among the slagging fixed-bed processes are the British Gas⁸, ERDA/GFERC⁶, and Thyssen-Galoczy⁵, the last of which gasifies coal at almost 3000°F, but at atmospheric pressure.

Fluidized-bed gasifiers⁹ are better suited for continuous gasification at high feed rates¹. This gasifier type is capable of using a wide-range of coals. Again the ash can be removed in two different forms: dry or agglomerated. One dry ash process, Winkler³, which has been commercial since 1926¹, has a gasification temperature in the range of 1500°F to 1850°F and pressure at about atmospheric. Even at this relatively low

temperature no tar or hydrocarbons are formed. This system uses a heat recovery system before the gas purification stages. Sixteen industrial plants are presently in operation. Similar to this type of gasification system are the CO₂-Acceptor³, Exxon⁷, Synthane³, and U-Gas³ processes. These are basically used to provide an intermediate-Btu gas as a feed to the methanation step in the production of synthetic natural gas. The CO₂-Acceptor is somewhat unique in that heat is provided for the carbon and steam reaction by reacting the carbon dioxide with dolomite. This represents another way to get an intermediate-Btu gas without the use of pure oxygen. Operation is pressurized from 150 to 300 psia and gasification takes place at 1600°F. Dolomite serves a secondary purpose also; it is used to remove the H₂S (and CO₂) from the product gas. In the U-Gas process, gasification takes place at about 350 psia and 1900°F³. Again heat recovery takes place before the gas is cleaned. Among the agglomerating ash processes are those by Union Carbide⁷ and by Westinghouse³. Although the Union Carbide system is designed for atmospheric pressure, plans for 100 psia operation are under way, for which higher feed rates are expected. A unique feature of this process is that heat for the carbon-steam reaction is provided by circulating hot ash. This process also has a heat recovery step before the purification system. Raw product gas leaves the gasifier at about 1800°F. The Westinghouse process incorporates high temperature (about 1400°F) desulfurization by using limestone or dolomite in the gasifier. Westinghouse plans to use this process in a combined cycle pilot plant.

Finally, there are gasifier designs which are of the entrained-flow type. Some of the advantages of this gasifier are little or no tar production, ease of adaptability to utilization of a wide range of coals, and

high reaction rates because of the high temperatures. Again, there are both dry-ash and slagging processes. Among the former are Bi-Gas¹⁰, Combustion Engineering⁷, and Foster-Wheeler⁶. The Bi-Gas process demonstrates that the gasification process itself is fairly insensitive to pressure since pressures from 500 to 1500 psia have been successfully tested. The Combustion Engineering process is presently designed for atmospheric operation, but operation at elevated pressures is contemplated, and apparently uses a heat exchanger before the gas cleanup stage. The slagging processes include Babcock and Wilcox⁷, Koppers-Totzek⁸, Ruhrgas¹¹, and Texaco⁵. Details of the Babcock and Wilcox process are largely unknown. Koppers-Totzek is presently designed for atmospheric pressure using pure O₂, but there are plans for pressurized operation. The gas exit temperature is extremely high (about 2750°F) and results in no tar, hydrocarbon, or phenol production. The Ruhrgas system apparently uses dirty power gas to raise steam for the gasification process. The Texaco gasifier is designed for operation at 2200 to 2500°F and 300 to 1200 psia¹. The process uses a slurry of coal and water injected into the gasifier. Progress is reported on materials problems associated with coal slag¹.

The gas purification systems may be divided into two broad classifications: hot cleanup and cold cleanup. Hot cleanup takes place within the temperature range from 1000 to 2500°F and cold cleanup from 100 to 250°F. While it is reported that hot cleanup can increase the thermal efficiency of a combined cycle by about three percent, the technology is not well-proven and is expensive. For this reason low-temperature cleanup is accepted as being more viable, and hot cleanup is not discussed any further. The Ad Hoc Panel also points out that

Most of the heat in the hot gases after gasification can be recovered by heat exchange so that the loss in thermal efficiency is minimized.¹

The Panel identifies at least six cold cleanup processes which are presently available or under development: (1) solid adsorbents, (2) membranes, (3) the Stretford process, (4) amine gas, (5) physical solvents, and (6) hot potassium carbonate. Reference 1 provides an excellent summary of these processes. Some of the characteristics of the hot potassium carbonate process, which is available commercially as the Benfield process, will be summarized since this type of cleanup system will be used in each configuration. Developed in the early 1950's, the Benfield process has been used for fourteen years. It is presently used on about 400 units for the removal of H₂S (and CO₂) from natural gas, ammonia synthesis gas, and hydrogen gas. The Panel points out further

Where the purification of low- and intermediate-Btu gases from coal is concerned, the use of the Benfield process fits well into the usual process conditions. The gasification pressure usually ranges from 100 to 400 psig. The preferred method of dedusting and cleaning the gas is by water quench, resulting in a water-saturated gas that is at a temperature of 200 to 260°F.¹

In addition, the Benfield process is compatible with a Claus plant, which may be used to convert the H₂S to elemental sulfur. At 90 to 95 percent H₂S removal, the cost of this process is estimated to be only \$18/kw, but at 99 percent, the cost slightly more than doubles¹. We shall see in Chapter 5 that 90 percent H₂S removal is more than sufficient to keep the SO₂ effluent in the stack well below the federal limit.

The concept of a combined cycle power plant is not new. Today it is receiving ever-increasing attention because of the growing awareness that conventional fuels are in finite and dwindling supply. Boosting cycle

efficiency helps to get more usable energy from the same amount of fuel. The most comprehensive study to date is the Energy Conversion Alternatives Study, known as ECAS. Actually, ECAS has examined about ten coal conversion power generation systems in Phase I of the study and seven in Phase II. One of these conversion concepts is the combined cycle integrated with a low-Btu gasifier. This study was essentially done in parallel by Westinghouse and General Electric and has culminated in several volumes of reports^{12,13}. In this work, no attempt has been made to determine optimum conditions or plant configurations. They have both used advanced equipment, such as air- and water-cooled gas turbines. The NASA Lewis Research Center has evaluated these studies and has summarized its findings in a lengthy report¹⁴.

It is difficult to compare the Westinghouse results with those of General Electric, since different operating conditions and plant layouts were used sometimes with different assumptions. However, the Westinghouse design appears to be 46.8 percent efficient compared to 39.6 percent for that of General Electric. Part of this difference is due to Westinghouse's using hot gas cleanup while General Electric elected to use cold. In any event, the thermodynamics of the integrated systems are obscured in many, many details. It is not clear how the systems evolved from a basic plant layout.

Ahner, et al.¹⁵ have developed a design for an integrated gasification combined cycle plant without actually optimizing with respect to plant performance. However, the authors do provide a relatively simple equation which may be used to find the "first cost incentive" from some specified

base case. As mentioned in Chapter 1, however, an economic study is outside the scope of this dissertation.

Osterle¹⁶ provided the basis for this dissertation by scoping the basic gasification reactions in a manner similar to that of Section 2.2. Intrigued by the many new degrees of freedom that a coal gasifier adds to the otherwise routine thermodynamic design process of a fossil-fueled power plant, Osterle incorporated his early work into a power cycle and performed many of the tedious hand calculations which were a necessary prelude to a computerized study. To help in this effort, Impink developed a large number of gas table property subprograms, processing codes, and the steam table processor subprogram (see subroutine FINDER in Section 4.5.2), many of which are used in this dissertation. Look developed the first computer model of an adiabatic model following Osterle's analytical model. Impink extended this model and developed the endothermic model, in which rather crude numerical methods were employed. Impink also developed many of the preliminary computerized component models, again following Osterle's analytical development. Impink and Osterle then demonstrated the feasibility of modeling integrated coal gasification processes and combined cycle systems and introduced the initial elements of pollutant emission calculations. Finally, in addition to augmenting the gas table library, Candris developed a preliminary flue gas recirculation model following Osterle's derivation. Their work culminated in a report¹⁷ to the Pennsylvania Science and Engineering Foundation, who supported some of their effort. Clearly, the present work is in a sense a culmination of several years of prior effort.

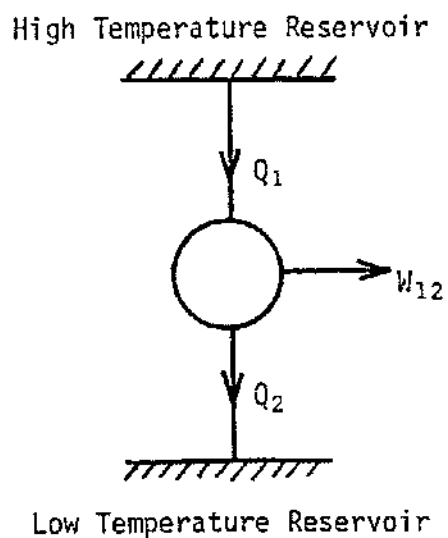


Figure 2.1-1 Schematic of Simple Heat Engine

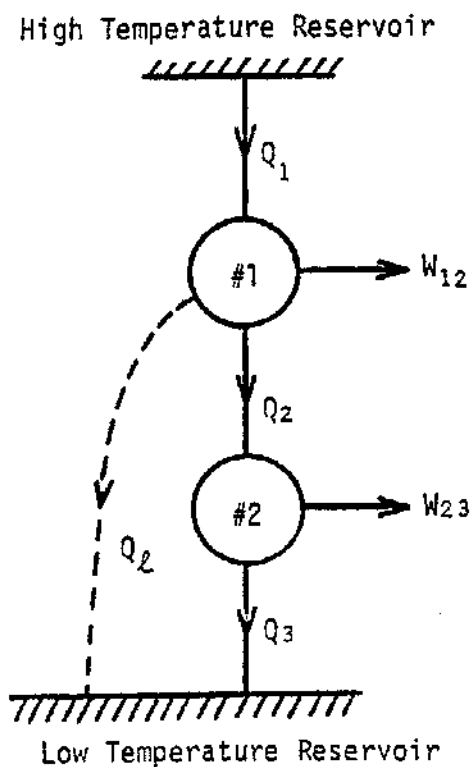


Figure 2.1-2 Schematic of Two Heat Engines Connected in Series with Loss

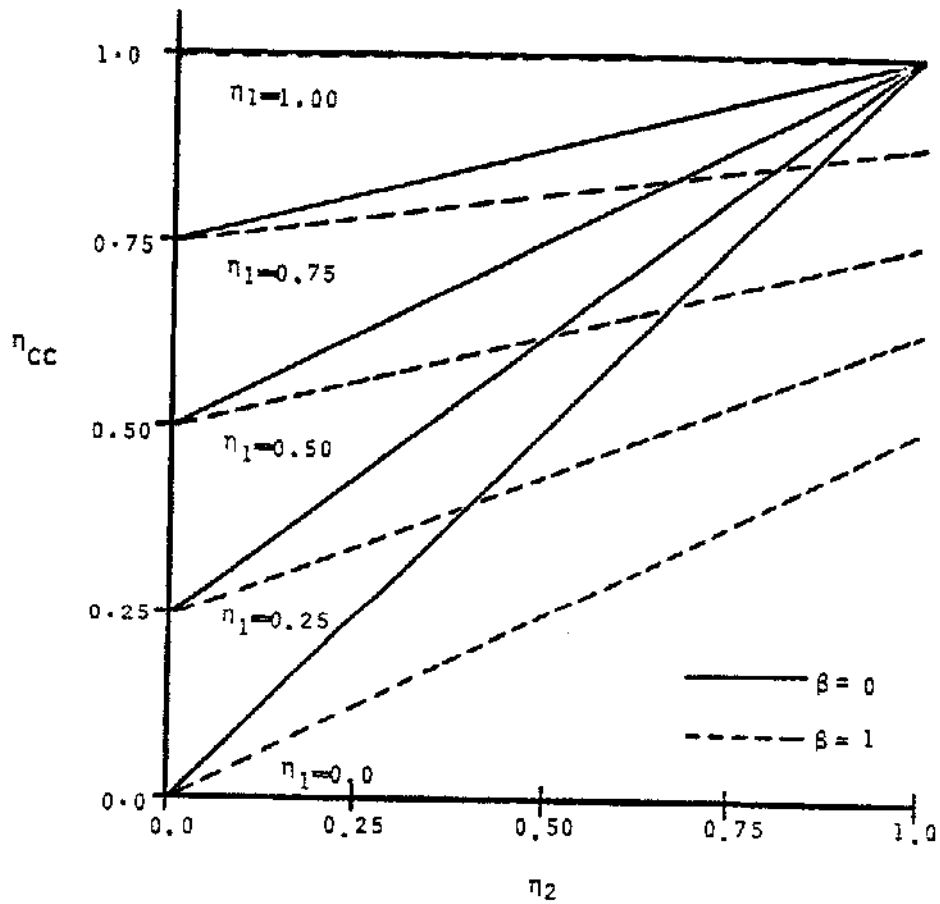


Figure 2.1-3 Combined Cycle Efficiency η_{cc} Versus Second Engine Efficiency η_2 with First Engine Efficiency η_1 as a Parameter for $\beta = 0$ and $\beta = 1$. (Refer to Eq. 2.1-7)

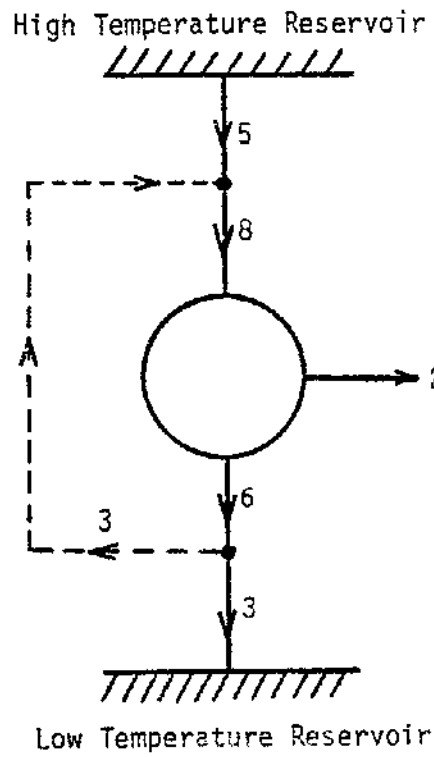


Figure 2.1-4 Schematic of Heat Engine with Efficiency of 25 Percent and with 50 Percent Regeneration Giving an Over-all Efficiency of 40 Percent

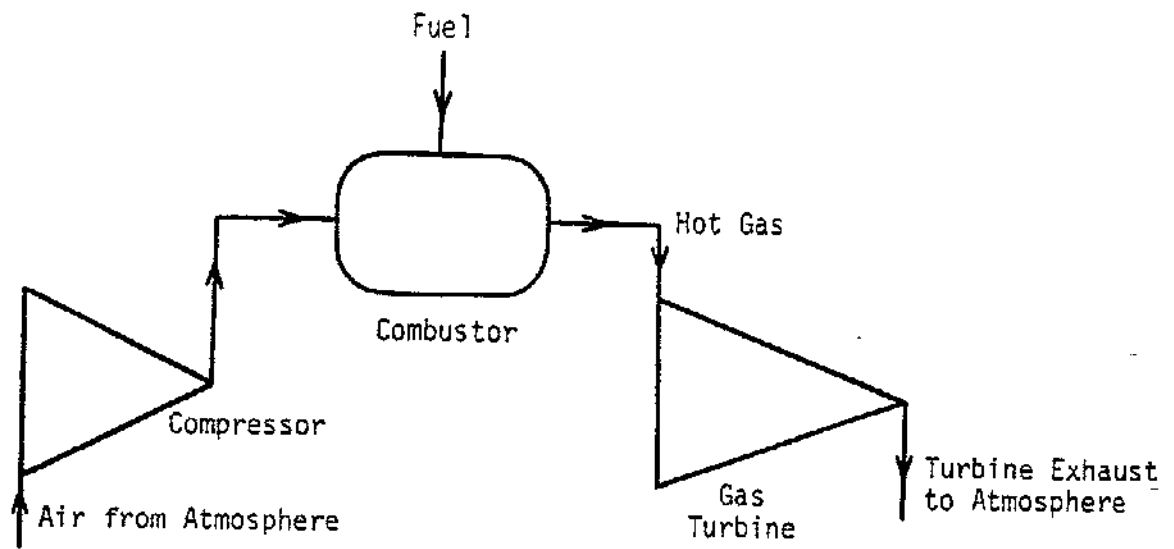


Figure 2.1-5 Simplified Schematic of Open Brayton Cycle

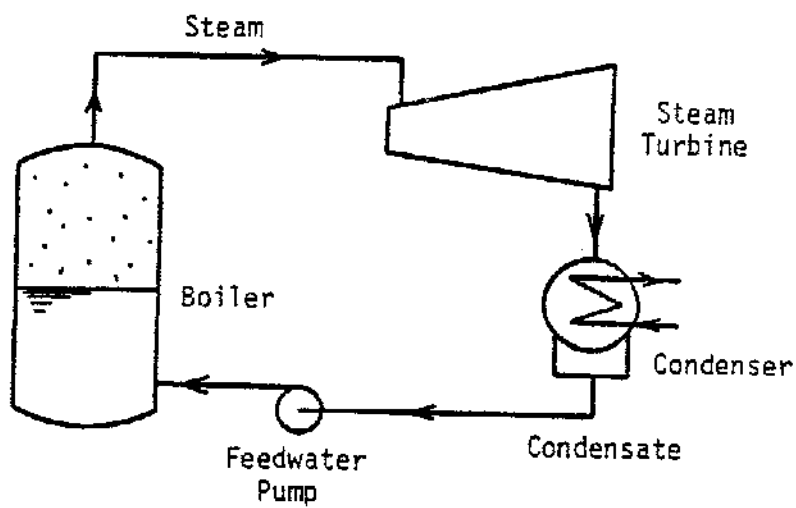


Figure 2.1-6 Simplified Schematic of Rankine Steam Cycle

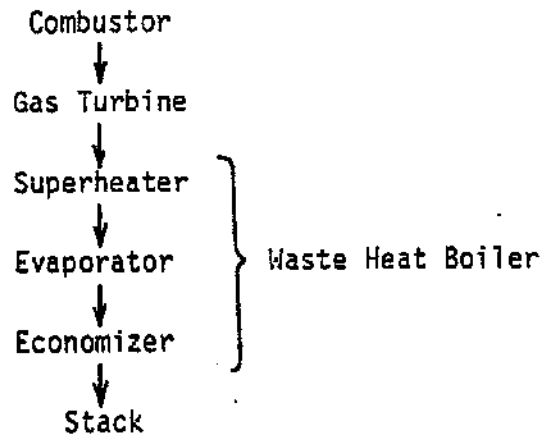


Figure 2.1-7 Path of Gas in Waste Heat System

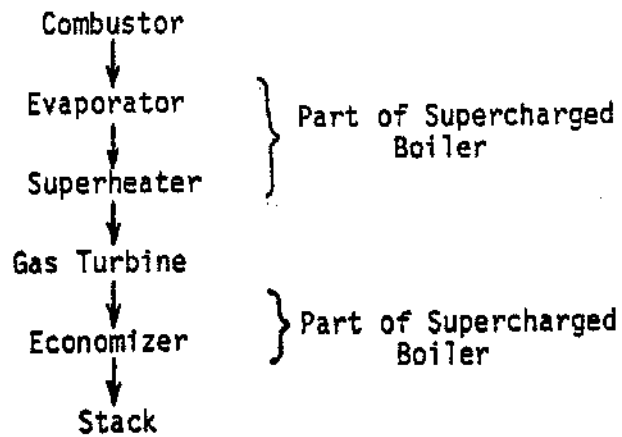


Figure 2.1-8 Path of Gas in Supercharged Boiler System

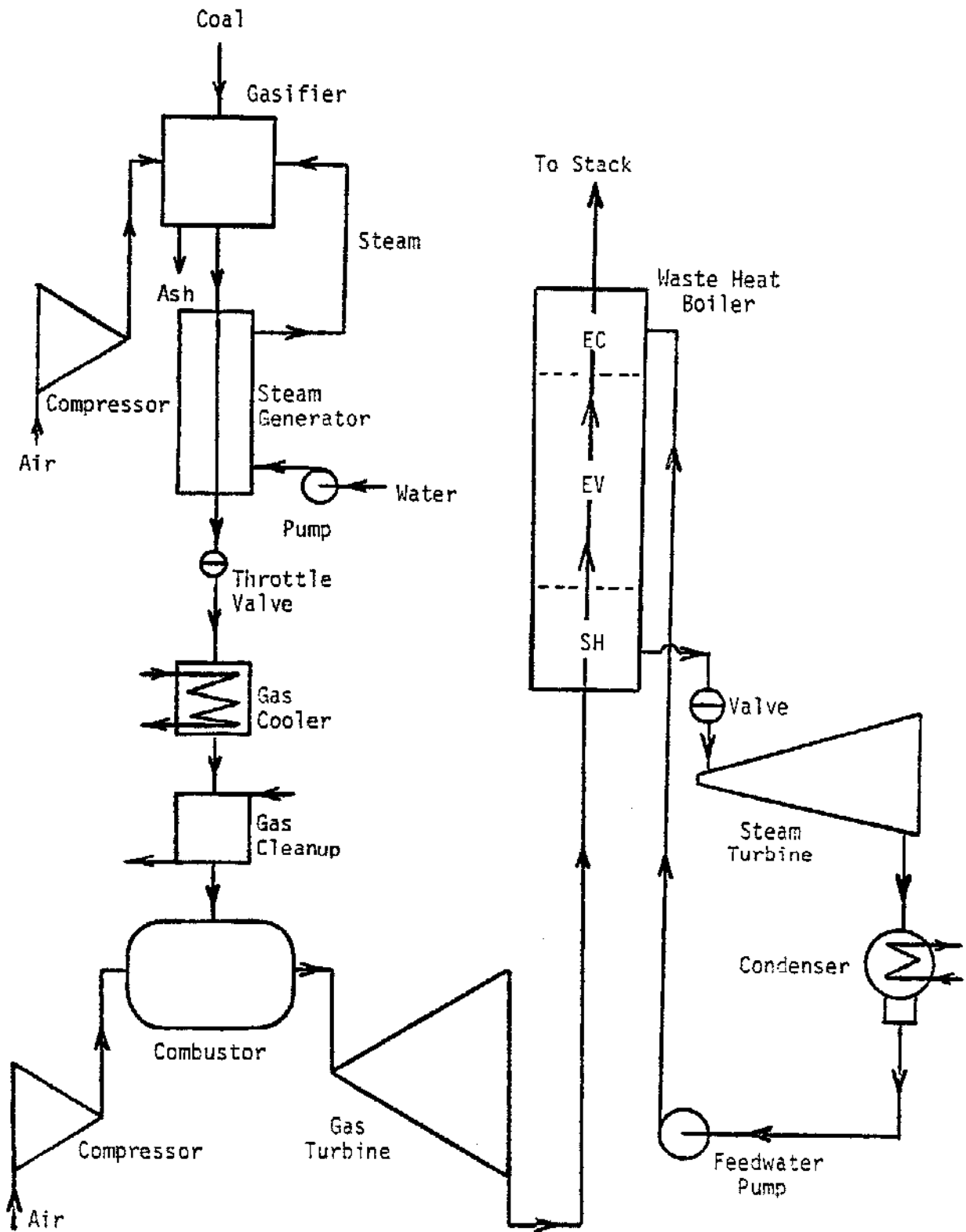


Figure 2.3-1 Simplified Schematic of Adiabatic Gasifier Integrated with Waste Heat Boiler Combined Cycle (Configuration 1)

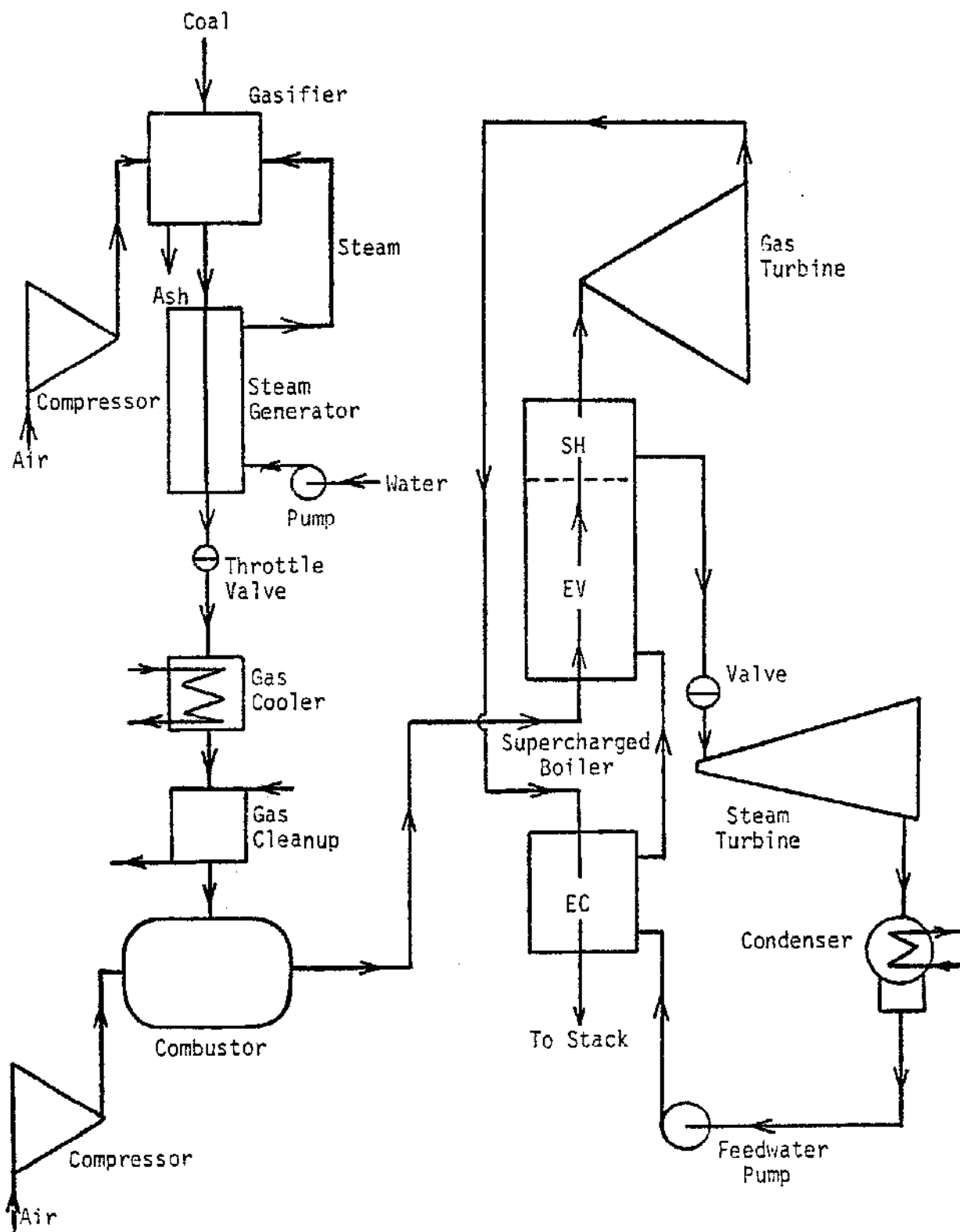


Figure 2.3-2 Simplified Schematic of Adiabatic Gasifier Integrated with Supercharged Boiler Combined Cycle (Configuration 2)

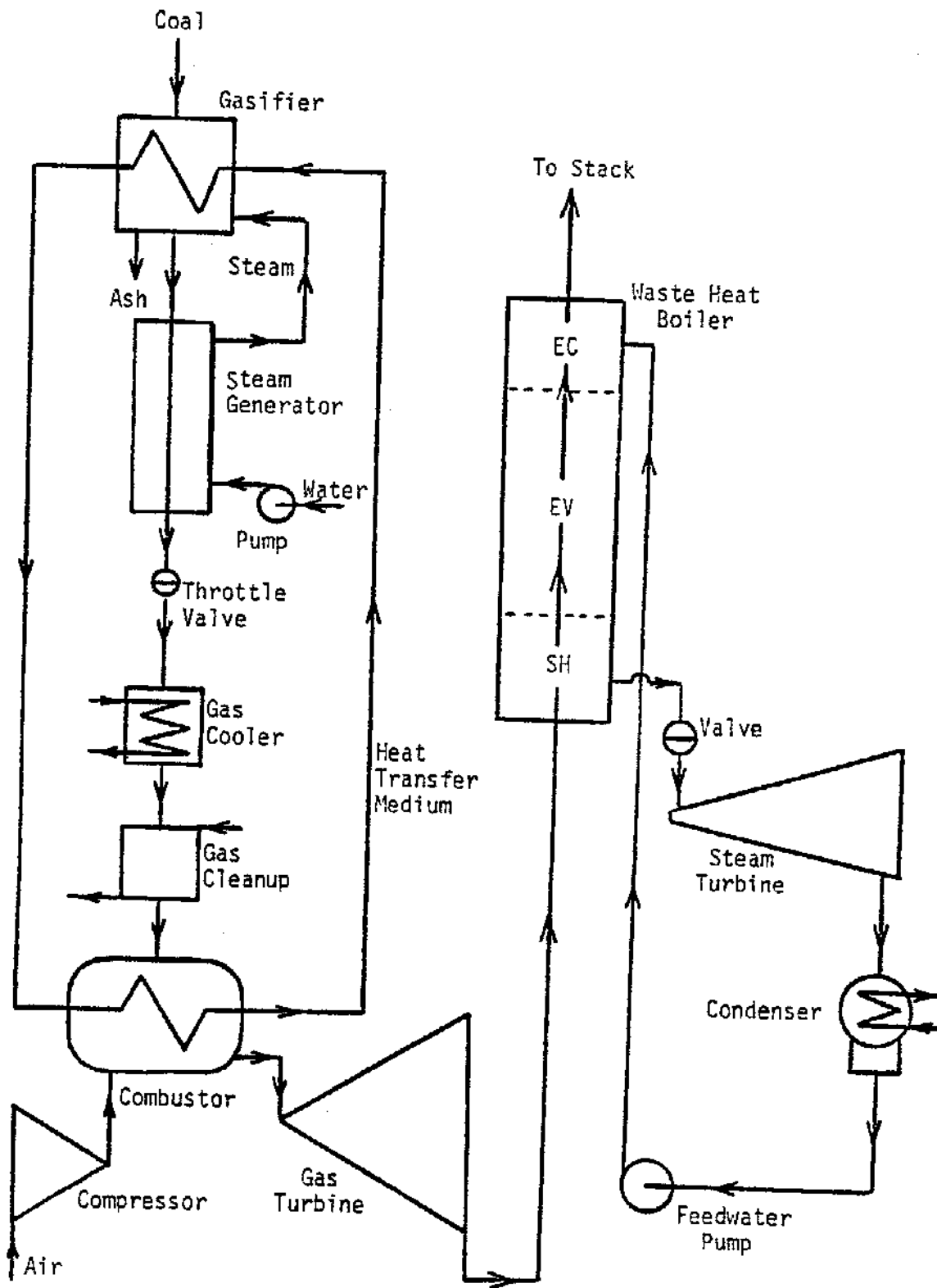


Figure 2.3-3 Simplified Schematic of Endothermic Gasifier Integrated with Waste Heat Boiler Combined Cycle (Configuration 3)

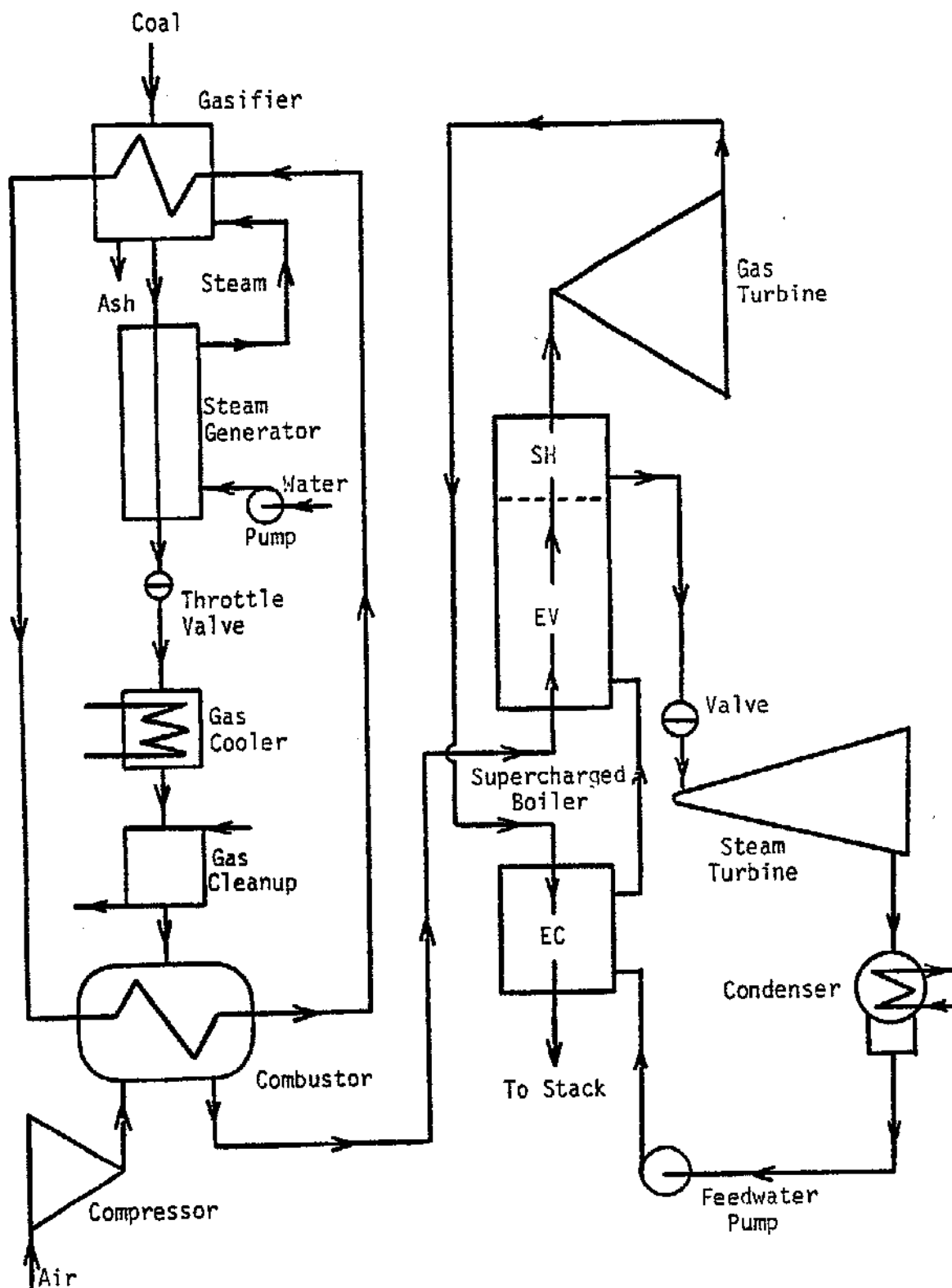


Figure 2.3-4 Simplified Schematic of Endothermic Gasifier Integrated with Supercharged Boiler Combined Cycle (Configuration 4)

CHAPTER 3
MATHEMATICAL MODELING OF COMPONENTS

3.1 Introduction

An obvious first step in the analysis of the systems described in Chapter 2 is the representation of each component in a particular cycle by a mathematical model. Because many components appear several times within a particular cycle and because a particular component is used in more than one cycle, it is advantageous to keep the models separate. We shall find it better to model each component, where possible, as a single entity. For example, the modeling of a two-stage intercooled compressor is accomplished by separately modeling a single stage compressor (which is then used twice) and an intercooler. This point will be more obvious in Chapter 4, where the models are cast into the form of subroutines.

It is important to remember that we are interested only in the steady-state thermodynamics of the four cycles. Consequently, the models will provide only a limited amount of information about a particular component. For example, the model for the adiabatic gasifier provides information like the air and steam flow rates and the outlet gas composition, but does not provide information like the size of the gasifier.

As expected, some of the models are more complex than others. The gasifier, combustor, waste heat boiler, and supercharged boiler models are among the most complicated. These particular ones will be described in considerable detail. Because the mathematical solution of the equations which represent the gasifier model is nearly identical to that of the combustor model, both of these are treated in Section 3.2, with the common method of solution also given. In Sections 3.3 and 3.4, the waste heat boiler and the supercharged boiler

models are developed, respectively. The more simple components are described and modeled in Sections 3.6 to 3.16.

3.2 Gasifier and Combustor

3.2.1 General Comments

These models are very similar in the sense that the same types of equations are provided by (1) mass balances on each of the elements, (2) the assumption of equilibrium of the various gaseous species, and (3) an energy balance. This approach results in 16 non-linear algebraic equations to describe the gasifier, and 21 similar equations for the combustor. Of course, there are 16 and 21 unknowns for the gasifier and combustor, respectively.

As discussed in Section 2.2, provisions must be made to operate the gasifier in two specific modes: adiabatic gasification of coal with steam and air and endothermic gasification of coal with steam. And, as discussed in Section 2.1, provisions must also be made to operate the combustor in two different modes: one in which the combustor outlet temperature is specified (the excess air is then calculated), and the other in which the excess air is specified (the outlet temperature is then calculated). These last two modes correspond to uses in the waste heat system and supercharged boiler system, respectively. As discussed in the next few sections, these provisions on the gasifier and combustor models are easily implemented.

3.2.1.1 Gasifier Model

The endothermic mode for the gasifier will be shown later to be a special case of the adiabatic mode. Therefore, the most general gasifier

model can be obtained by assuming that coal is to be reacted with air and steam, subject to the adiabatic constraint.

The question arises, however, of how one should obtain the enthalpy of the coal, which is needed for the energy balance. This problem is resolved by using the Dulong approximation for enthalpy determination purposes which is accurate to about 3 percent¹⁸. The Dulong approximation may be summarized as follows. The carbon given by the ultimate analysis is assumed to be fixed carbon. All the oxygen is assumed to combine with the necessary amount of hydrogen to form water vapor with the remaining hydrogen forming only diatomic hydrogen gas. The nitrogen and sulfur are assumed to be in the form of their respective elemental gaseous compounds and the moisture is taken as liquid water. (The sensible heat associated with the ash will be accounted for by using a suitable specific heat.)

The basic reaction for the adiabatic mode is



Let us normalize the calculation by assuming a unit mass of coal, whose ultimate analysis is given. That is, the weight fraction is given for the following: carbon (C), hydrogen (H), oxygen (O), nitrogen (N), sulfur (S), liquid water (H₂O), and ash. Also let us assume that the composition of the air by weight fraction is also specified, with provisions for nitrogen (N₂), oxygen (O₂), argon (Ar), and water vapor (H₂O). The steam which is required by the gasifier is assumed to be pure superheated water vapor (H₂O). The power gas which is produced is assumed to have the following chemical species present: hydrogen (H₂), carbon monoxide (CO), methane (CH₄), water vapor (H₂O), carbon dioxide (CO₂),

nitrogen (N_2), argon (Ar), hydrogen sulfide (H_2S), carbonyl sulfide (COS), and ammonia (NH_3). Finally, the ash in the coal is assumed to exit from the gasifier at some specified temperature presumably no higher than the gas exit temperature.

We are now in a position to write the mass balance equations. Since we have present C, H, O, N, S, and Ar, we expect to have six such equations. Let w_{ci} be the weight fraction of component i in the coal, where i takes on values from 1 to 7 as summarized in Table 3.2-1. Let v_{ci} be the molecular

Table 3.2-1
Meaning of Subscripts Applied to Coal

| Subscript (c_i) | Component in Coal |
|---------------------|-------------------|
| c1 | C |
| c2 | H |
| c3 | O |
| c4 | N |
| c5 | S |
| c6 | $H_2O(l)$ |
| c7 | Ash |

weight of component i in the coal, where again i is defined according to Table 3.2-1. Similarly, we define w_{ai} and v_{ai} to be the weight fraction and the molecular weight of species i , respectively, for the air. As shown in Table 3.2-2, i now takes on values of 1 to 4. Furthermore, let

Table 3.2-2
Meaning of Subscripts Applied to Air

| Subscript (a_i) | Species in Air |
|---------------------|----------------|
| a1 | N_2 |
| a2 | O_2 |
| a3 | Ar |
| a4 | $H_2O(g)$ |

w_a be the mass of air required, and let w_s be the mass of steam required each per unit mass of coal. The molecular weight of steam (or water) will be denoted as v_s . Having defined the necessary parameters associated with the reactants, we now turn to the products.

Let n_{gi} be the number of moles of species i formed per unit mass of coal, where i now takes on values of 1 to 10, as defined in Table 3.2-3.

Table 3.2-3
Meaning of Subscripts Applied to Power Gas

| Subscript (g_i) | Species in Gas |
|---------------------|-------------------------|
| g_1 | H ₂ |
| g_2 | CO |
| g_3 | CH ₄ |
| g_4 | H ₂ O(g) |
| g_5 | CO ₂ |
| g_6 | N ₂ |
| g_7 | Ar |
| g_8 | H ₂ S |
| g_9 | COS |
| g_{10} | NH ₃ |

Let N_g be the sum of the n_{gi} from $i = 1$ to 10; that is,

$$N_g = \sum_{i=1}^{10} n_{gi}$$

Note then that N_g is the total number of moles of power gas produced per unit mass of coal. The composition of the power gas by mole fraction (y_{gi}) is then given by

$$y_{gi} = n_{gi}/N_g.$$

Now based on a unit mass of coal, the number of moles of C in the reactants is simply w_{C_1}/v_{C_1} and the number of moles of C in the products

is given by $n_{g2} + n_{g3} + n_{g5} + n_{g9}$. These two expressions must be equal in order to satisfy the mass balance requirement on carbon and the mass balance equation for C becomes

$$\frac{w_{C1}}{v_{C1}} = n_{g2} + n_{g3} + n_{g5} + n_{g9} \quad (3.2-1)$$

The mass balance on H is slightly more complicated because hydrogen appears in all three reactants. The number of moles of H in the coal is $w_{C2}/v_{C2} + 2w_{C6}/v_{C6}$, while the air, $2w_a w_{a4}/v_{a4}$, and due to the reactant steam, $2w_s/v_s$. The number of moles of H in the products is given by $2n_{g1} + 4n_{g3} + 2n_{g4} + 2n_{g8} + 3n_{g10}$. Again the sum of moles of H in the reactants must equal the sum of the moles of H in the products so the mass balance equation for H is

$$\frac{w_{C2}}{v_{C2}} + \frac{2w_{C6}}{v_{C6}} + 2w_a \frac{w_{a4}}{v_{a4}} + 2w_s \frac{1}{v_s} = 2n_{g1} + 4n_{g3} + 2n_{g4} + 2n_{g8} + 3n_{g10} \quad (3.2-2)$$

Similarly for O, N, S, and Ar we get, respectively,

$$\frac{w_{C3}}{v_{C3}} + \frac{w_{C6}}{v_{C6}} + w_a \left(2\frac{w_{a2}}{v_{a2}} + \frac{w_{a4}}{v_{a4}} \right) + \frac{w_s}{v_s} = n_{g2} + n_{g4} + 2n_{g5} + n_{g9} \quad (3.2-3)$$

$$\frac{w_{C4}}{v_{C4}} + 2w_a \frac{w_{a1}}{v_{a1}} = 2n_{g6} + n_{g10} \quad (3.2-4)$$

$$\frac{w_{C5}}{v_{C5}} = n_{g8} + n_{g9} \quad (3.2-5)$$

and

$$w_a \frac{\omega_{a3}}{v_{a3}} = n_{g7}. \quad (3.2-6)$$

Because mole fractions will appear in the equilibrium equations, it is advantageous to work with mole fractions rather than mole numbers. Therefore, we divide Equations (3.2-1) to (3.2-6) by N_g . However, we then solve equation 3.2-1 for N_g , which can be used in the remaining five equations. Accordingly,

$$N_g = \frac{\omega_{c1}/v_{c1}}{y_{g2} + y_{g3} + y_{g5} + y_{g9}}. \quad (3.2-7)$$

The five remaining equations, Equations (3.2-2) to (3.2-6), are changed only in that the left-hand side of each is multiplied by the reciprocal of N_g , with N_g given by Equation (3.2-7), and each n_{gi} is replaced by y_{gi} . The final form of the mass balance equations is as follows:

$$\left\{ \frac{\omega_{c2}}{v_{c2}} + 2 \frac{\omega_{c6}}{v_{c6}} + 2w_a \frac{\omega_{a4}}{v_{a4}} + \frac{2w_s}{v_s} \right\} \left\{ \frac{\omega_{c1}}{v_{c1}} (y_{g2} + y_{g3} + y_{g5} + y_{g9}) \right\} \\ = 2y_{g1} + 4y_{g3} + 2y_{g4} + 2y_{g8} + 3y_{g10} \quad (3.2-8)$$

$$\left\{ \frac{\omega_{c3}}{v_{c3}} + \frac{\omega_{c6}}{v_{c6}} + w_a \left(2 \frac{\omega_{a2}}{v_{a2}} + \frac{\omega_{a4}}{v_{a4}} \right) + \frac{w_s}{v_s} \right\} \left\{ \frac{\omega_{c1}}{v_{c1}} (y_{g2} + y_{g3} + y_{g5} + y_{g9}) \right\} \\ = y_{g2} + y_{g4} + 2y_{g5} + y_{g9} \quad (3.2-9)$$

$$\left\{ \frac{\omega_{C4}}{\nu_{C4}} + 2w_a \frac{\omega_{a1}}{\nu_{a1}} \right\} \left\{ \frac{\omega_{C1}}{\nu_{C1}} (y_{g2} + y_{g3} + y_{g5} + y_{g9}) \right\} = 2y_{g6} + y_{g10} \quad (3.2-10)$$

$$\left\{ \frac{\omega_{C5}}{\nu_{C5}} \right\} \left\{ \frac{\omega_{C1}}{\nu_{C1}} (y_{g2} + y_{g3} + y_{g5} + y_{g9}) \right\} = y_{g8} + y_{g9} \quad (3.2-11)$$

$$\left\{ w_a \frac{\omega_{a3}}{\nu_{a3}} \right\} \left\{ \frac{\omega_{C1}}{\nu_{C1}} (y_{g2} + y_{g3} + y_{g5} + y_{g9}) \right\} = y_{g7} \quad (3.2-12)$$

The sixth equation, of course, is provided by the fact that the sum of mole fractions must equal unity, or

$$\sum_{i=1}^{10} y_{gi} = 1 \quad (3.2-13)$$

This completes the six equations provided by the mass balances.

At this point, we see that there are twelve unknowns: the ten mole fractions, the steam flow, and the air flow. Additional equations are provided by invoking the assumption of thermodynamic equilibrium. The validity of this assumption is established in Section 5.8.

The species assumed to be present in the power gas imply that five independent reactions are taking place. Using (s) to denote the solid phase and no phase designation to imply the gas phase, we may assume the following arbitrary (but independent) reactions:



Then the equilibrium condition for each reaction can be written. For example, for the reaction in Equation (3.2-13a), we could write

$$K_p = \frac{(y_{\text{CH}_4} P)}{(y_{\text{H}_2} P)^2} \quad (3.2-14)$$

where again y_i denotes the mole fraction of species i and P is the total pressure in atmospheres since the equilibrium constant, K_p , is assumed to be based on atmospheres. For a given reaction, the equilibrium constant, which is a function of temperature only, can be obtained from an appropriate handbook. In Equation (3.2-14), it is assumed that the mixture behaves like an ideal gas; otherwise, the mole fraction and pressure products would be replaced by the fugacities. Because the carbon is in the solid phase, there is no " $RT \ln$ " correction on the Gibbs free energy for solid carbon and, therefore, Equation (3.2-14) is valid as written. Similar equations could be written for the remaining reactions.

Although the equilibrium equations in the form of Equation (3.2-14) could be used directly in the solution to our problem, it is better to modify them to effect a more general solution strategy. One such modification would be to use the logarithmic form of the equilibrium equations. For example Equation (3.2-14) would become

$$\ln K_p = \ln(y_{\text{CH}_4 P}) - 2\ln(y_{\text{H}_2 P}). \quad (3.2-14a)$$

However, we would then need to have K_p for each reaction. While this is a trivial point for Equation (3.2-14a) since we conveniently have a formation reaction, this is an important consideration for reactions like that in Equation (3.2-13e). If the equilibrium constant for this kind of reaction is not found in any handbook, then we would have to reconstruct it from the formation reactions. In addition, taking equilibrium constants from many sources is undesirable, since there is no guarantee that the data would be consistent among the various sources. We shall use an alternate approach which does not have either of the above mentioned deficiencies and *which does not depend on the reactions chosen*. For this alternate method we shall see that we need to specify only the participating chemical species and not the reactions.

Smith and Van Ness¹⁹ describe a method for obtaining the equilibrium composition of a mixture of gases where several reactions are actually proceeding. This method is really based on the fact that at equilibrium the Gibbs free energy for the system is a minimum. This condition, however, is subject to the constraints provided by the mass balances.

Since we have a minimization problem subject to constraints, the method of Lagrange multipliers is directly applicable.

Let us briefly outline the derivation of this equilibrium condition. Let $G(n_1, n_2, \dots, n_n)$ represent the total Gibbs free energy for the system with the mole numbers of the various species i represented by the n_i . Let the m mass balance equations be

$$f_1(n_1, n_2, \dots, n_n) = 0$$

$$f_2(n_1, n_2, \dots, n_n) = 0$$

⋮

⋮

⋮

$$f_m(n_1, n_2, \dots, n_n) = 0$$

and since we have m constraints, then we introduce m Lagrange multipliers, $\lambda_1, \lambda_2, \dots, \lambda_m$. If we want to minimize G , then we may minimize $G + \sum_{k=1}^m \lambda_k f_k$ since the f_k are zero and we have not changed the function to be minimized. Differentiating this new function with respect to each of the n_i in turn gives n equations which must hold at the minimum (or maximum). These equations are

$$\frac{\partial G}{\partial n_i} + \sum_{k=1}^m \lambda_k \frac{\partial f_k}{\partial n_i} = 0 \quad (i = 1, 2, \dots, n)$$

Then n "equilibrium" equations and the m constraint equations ($f_\ell = 0$ for $\ell = 1, 2, \dots, m$) are used to solve for the n_i which minimize $G(n_1, n_2, \dots, n_n)$. When this method is applied to our equilibrium

problem, the equilibrium condition becomes for gas phase reactions

$$\Delta G_{f_{g_i}}^{\circ}(T_e) + RT_e \ln(y_{g_i} \phi_{g_i} P) + \sum_k \lambda_k a_{ik} = 0 \quad \text{for } i = 1, 2, \dots, N \quad (3.2-15)$$

where the meaning of the nomenclature is as follows. We first note that the fugacity coefficients for a solution, ϕ_{g_i} , have been introduced. Since we assume our gaseous mixture to behave like an ideal gas, all the ϕ_{g_i} are unity. The meaning of the subscript is unchanged from its previous definition in Table 3.2-3, except that we do not write an equilibrium equation for Ar ($i=7$), since argon is inert. The standard Gibbs free energy of formation at temperature T_e for species i is denoted by $\Delta G_{f_{g_i}}^{\circ}(T_e)$. Like the equilibrium constant, K_p , this parameter is a function of temperature only. The Gibbs free energy of formation is assumed to be zero for the elemental compounds; for example, $\Delta G_f^{\circ} = 0$ for H_2 , N_2 , and so forth. R is the universal gas constant, and T_e is the absolute temperature at which the reactions are proceeding. Of course, the product RT_e must be in consistent units with the values for the Gibbs free energy. The argument of the natural logarithm is essentially the fugacity, f_{g_i} , of the species i , which, because of the ideal gas assumption, reduces to the product of the mole fraction and system pressure in atmospheres, or the partial pressure in atmospheres. The λ_k 's are the Lagrange multipliers. One Lagrange multiplier should be introduced for each constraint provided by the mass balances. So one might expect to have six Lagrange multipliers for the adiabatic gasifier; that is λ_C , λ_H , λ_O , λ_N , λ_S , and λ_{Ar} .

However, as already mentioned, argon is inert and so λ_{Ar} is meaningless. We shall show later that taking λ_C to be zero is consistent with Equation (3.2-14). From the definition of the λ_k we see that the subscript k is associated with a particular elemental atom present in the system. The a_{ik} represent the number of atoms of element k per molecule of species i . Table 3.2-4 gives this matrix for the gasifier model.

Table 3.2-4
Assignment of Values to the a_{ik}
for the Gasifier Model

| Species | i | Element (k) | | | | |
|------------------|----|-------------|------|------|------|------|
| | | C(1) | H(2) | O(3) | N(4) | S(5) |
| H ₂ | 1 | 0 | 2 | 0 | 0 | 0 |
| CO | 2 | 1 | 0 | 1 | 0 | 0 |
| CH ₄ | 3 | 1 | 4 | 0 | 0 | 0 |
| H ₂ O | 4 | 0 | 2 | 1 | 0 | 0 |
| CO ₂ | 5 | 1 | 0 | 2 | 0 | 0 |
| N ₂ | 6 | 0 | 0 | 0 | 2 | 0 |
| Ar | 7 | 0 | 0 | 0 | 0 | 0 |
| H ₂ S | 8 | 0 | 2 | 0 | 0 | 1 |
| COS | 9 | 1 | 0 | 1 | 0 | 1 |
| NH ₃ | 10 | 0 | 3 | 0 | 1 | 0 |

Now Equation 3.2-15 can be readily applied to each of the reacting species assumed to be present in the gasifier. For generality, the fugacity coefficients, $\hat{\phi}_{g1}$, will be kept in the equations with the understanding that each will be taken to have a value of unity. Also, it is advantageous to divide the equilibrium equations by RT_e . The reason for doing this will be explained in Subsection 3.2.2. The equilibrium equations become

$$\frac{\Delta G_{f, H_2}^s(T_e)}{RT_e} + \ln(y_{g1} \hat{\phi}_{g1} P_g) + 2\lambda_H/RT_e = 0 \quad (3.2-16)$$

$$\Delta G_{f,CO}^{\circ}(T_e)/RT_e + \ln(y_{g_2} \hat{\phi}_{g_2} P_g) + \lambda_0/RT_e = 0 \quad (3.2-17)$$

$$\Delta G_{f,CH_4}^{\circ}(T_e)/RT_e + \ln(y_{g_3} \hat{\phi}_{g_3} P_g) + 4\lambda_H/RT_e = 0 \quad (3.2-18)$$

$$\Delta G_{f,H_2O}^{\circ}(T_e)/RT_e + \ln(y_{g_4} \hat{\phi}_{g_4} P_g) + 2\lambda_H/RT_e + \lambda_0/RT_e = 0 \quad (3.2-19)$$

$$\Delta G_{f,CO_2}^{\circ}(T_e)/RT_e + \ln(y_{g_5} \hat{\phi}_{g_5} P_g) + 2\lambda_0/RT_e = 0 \quad (3.2-20)$$

$$\Delta G_{f,N_2}^{\circ}(T_e)/RT_e + \ln(y_{g_6} \hat{\phi}_{g_6} P_g) + 2\lambda_N/RT_e = 0 \quad (3.2-21)$$

$$\Delta G_{f,H_2S}^{\circ}(T_e)/RT_e + \ln(y_{g_8} \hat{\phi}_{g_8} P_g) + 2\lambda_H/RT_e + \lambda_S/RT_e = 0 \quad (3.2-22)$$

$$\Delta G_{f,COS}^{\circ}(T_e)/RT_e + \ln(y_{g_9} \hat{\phi}_{g_9} P_g) + \lambda_0/RT_e + \lambda_S/RT_e = 0 \quad (3.2-23)$$

$$\Delta G_{f,NH_3}^{\circ}(T_e)/RT_e + \ln(y_{g_{10}} \hat{\phi}_{g_{10}} P_g) + 3\lambda_H/RT_e + \lambda_N/RT_e = 0 \quad (3.2-24)$$

The total number of equations for the adiabatic gasifier model is now fifteen, but we have introduced four more unknowns, namely λ_H , λ_0 , λ_N , and λ_S , making the total number of unknowns sixteen. The energy equation provides us with the sixteenth equation.

Before we consider the energy equation, let us first show that our taking λ_C to be zero is consistent with the equilibrium condition expressed by Equation (3.2-14). Multiplying Equation (3.2-16) by 2 and subtracting the resulting equation from Equation (3.2-18) gives (taking $\hat{\phi}_{g_i}=1$):

$$\Delta G_{f,CH_4}^{\circ}/RT_e + \ln(y_{CH_4} P) - 2\Delta G_{f,H_2}^{\circ}/RT_e - 2\ln(y_{H_2} P) = 0$$