

**MASTER**

DYNAMIC SIMULATION OF COAL-BASED COMBINED CYCLE  
PLANTS FOR DEVELOPMENT OF PROCESS CONTROL  
GUIDELINES

G. Narender Reddy

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# DYNAMIC SIMULATION OF COAL BASED COMBINED CYCLE PLANTS FOR DEVELOPMENT OF PROCESS CONTROL GUIDELINES

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## ABSTRACT

Low Btu gasification/combined cycle power generation (LBG/CCPG) plants and the use of dynamic simulation for developing process control guidelines are described. The formulation of mathematical relationships describing the behavior of various processes within an LBG/CCPG plant (model development) and their solution (simulation) are discussed. A simplified fluidized-bed gasifier model is used as an example. Use of the results of such simulation for developing process control system guidelines is also discussed.

## INTRODUCTION

An assessment carried out under the Environmental Control Technology Program at Argonne National Laboratory showed that commercialization of low Btu gasification/combined cycle power generation (LBG/CCPG) plants could begin in the late 1980s contingent upon the solution of several technological problems. An important problem is the development of instrumentation and a process control system that would allow sequential operation of LBG/CCPG plants under varying transient conditions of feed quality, power demand, and upsets. Dynamic process simulation can be used for determining the transient behavior of these plants in terms of the magnitude of variation and rates of change of various critical process parameters.

A proposal submitted to the Department of Energy by Argonne National Laboratory involved the use of dynamic simulation techniques for the development of process control guidelines. Similar work, funded by Electric Power Research Institute (EPRI), has been under way at Fluor in Los Angeles, California, for the past two years. Other organizations such as General Electric Company, Westinghouse, and the University of Delaware are involved in various aspects of simulation of LBG/CCPG plants.

## DESCRIPTION OF LBG/CCPG PLANTS

The assessment of the status of the LBG/CCPG technology has been made by establishing a base case, as summarized in Table I, in terms of the size of the plant, coal characteristics, types of gasifiers, process configuration, and various individual units within the plant such as the raw fuel gas cleaning system and the gas turbine<sup>(1)</sup>. A brief description of the three different gasifiers selected, the fuel gas cleaning system, and the combined gas and steam turbine system is given in the following subsections<sup>(2)</sup>.

Table I. Base Case for Assessment

1. Size of Plant	500 MWe (net)
2. Types of Coal	Midwestern Bituminous Western Sub-bituminous
3. Types of Gasifiers	Moving Bed Fluid Bed Entrained Flow
4. Raw Fuel Gas Cleaning	Low Temperature <250°F
5. Gas Turbine	Inlet Temperature; 2200°F Pressure Ratio; 16:1
6. Environmental Standards	New Source Performance Standards

#### Lurgi Moving-Bed Gasifier

As shown in Figure 1, coal sized to 1-1/2 x 1/4" in the coal preparation plant is conveyed to the feed lock hopper and transferred to the gasifier. The coal flowing down through the gasifier represents a slowly moving bed that has several distinct zones. In the first zone at the top of the gasifier, coal is preheated and dried by contact with the hot crude gas leaving the reactor. As coal moves down and is heated further, devolatilization occurs and gasification commences. The bottom of the bed is a combustion zone where carbon reacts with oxygen to form CO and CO<sub>2</sub>. The oxidation provides the overall heat for the gasification and devolatilization reactions, which are endothermic. Only a negligible amount of unburned carbon remains in the ash.

The gasifier effluent at 1000°F contains appreciable quantities of tars, oils, naphtha, phenols, ammonia, hydrogen sulfide, sulfur compounds, and small amounts of coal and ash dust. The gas flows through a quench scrubber where it is washed with a stream of process condensate, thereby reducing its temperature to 250°F and condensing the high boiling tar fractions. Coal and ash dust are removed with the condensed tar, leaving the fuel gas essentially free of particulate matter.

After further cooling, the gas is scrubbed in an ammonia absorber to remove essentially all of the ammonia and final traces of particulates and water soluble phenols. The fuel gas at 100°F and 305 psig then goes to the desulfurization section.

#### IGT's U-Gas Fluidized-Bed Gasifier

Figure 2 shows the process flow diagram for fuel gas production, using the Institute of Gas Technology's U-Gas fluidized-bed gasifier and raw fuel gas cooling system.

Coal from the preparation plant (crushed and sized to 0 x 1/4") is fed to the pretreater, through a system of feed and lock hoppers, where a small portion is oxidized with air at 800°F. Pretreated coal then overflows directly into the gasifier where fluidization velocities of 1 to 2.5 feet per second are maintained by injecting air and steam at the bottom. Approximately 2.0 pounds of air and 0.5 pounds of steam for each pound of coal are required. Gasification takes place under nonslagging conditions at about 1900°F in the fluidized bed.

Ash agglomerates grow in size and are allowed to fall into a water-filled lock hopper at the bottom of the gasifier. Fines in the product gas, at about 1650°F, are separated by cyclones and cooled to about 600°F. The gas is then scrubbed to remove residual entrained char and finally water washed in the ammonia scrubber. Cleaned gas at 305 psig and 100°F is then sent to the acid gas treatment plant.

#### Foster Wheeler's Entrained-Flow Gasifier

Figure 3 shows the process flow diagram for fuel gas production, using Foster Wheeler's entrained-flow gasifier and the raw fuel gas cooling system.

Pulverized coal, dried to less than 2% moisture, is injected into the upper second stage of the two-stage pressurized (350 psig) slagging gasifier. The upper stage operates at about 1800 to 2100°F and the lower stage at about 2500 to 2800°F.

The first stage is where recycled char reacts with air and steam and generates heat to satisfy the endothermic requirements of the second stage and for keeping the ash in a slag. Coal devolatilization and gasification takes place in the second stage and the raw fuel gas at about 1700°F is passed through a series of cyclones where most of the char is collected. The gas is then cooled to 300°F and the remaining particulate matter removed by water washing. Ammonia is removed in an ammonia absorber and the fuel gas, at 305 psig and about 100°F is sent to the acid gas treatment plant.

#### Acid Gas Treatment Plant

Figure 4 shows the Selexol process flow diagram for removing sulfur compounds from the crude fuel gas. The cooled, ammonia free, crude gas flows through an acid gas absorber where it contacts the Selexol solvent (dimethyl ether of polyethylene glycol) countercurrently over a carbon steel packing. The treated gas from the top of the absorber flows through a knockout drum, which minimizes solvent losses, and is delivered as fuel gas to the gas turbine combustor at about 315 psia and 100°F.

The rich solvent from the absorber flows to a flash drum and then, after being heated by hot, regenerated solvent, flows to the top of the regenerator. In the regenerator, the absorbed H<sub>2</sub>S and CO<sub>2</sub> are stripped, cooled, and sent to the sulfur recovery plant. To maintain the absorption system water balance, demineralized water is added to the regenerator overhead.

## Combined Power Cycle

The operating conditions of a representative combined power cycle system were described earlier. The process flow diagram of a combined cycle system operating at these conditions is shown in Figure 5.

Clean low Btu gas is burned in the combustor. Combustion air is provided by the compressor, driven by the gas turbine, at 235 psia and 843°F in quantities varying from 1400 lb/hr to 1937 lb/hr.

Gas turbine (expander) exhaust at about 949°F and varying pressures then go through the heat recovery steam generator and are exhausted into the atmosphere. The total quantity and quality of steam generated varies with the types of gasifiers and coals used. Depending upon these two factors, the percentages of total power produced in the gas turbine and steam turbine cycles varies from 91.7%/8.3% to 72%/28%.

### By-Product Recovery and Ancillary Facilities

By-product recovery systems and other facilities in a commercial-scale plant include the following: oil/tar recovery system, sulfur and ammonia recovery plants, wastewater treatment facilities, cooling water system, flare facilities, ash disposal ponds, condensate storage, and polishing up facilities.

### MATHEMATICAL MODEL

The development of a mathematical model representing the various interacting systems and devising ways to control an entire coal based combined cycle plant is best accomplished using a *system engineering* type of analysis. This would involve the examination of the following parts of the complex plant as a unit, with all the interactions included, and devising an automatic process control system for it.

1. Coal preparation and pretreatment;
2. Gasifier;
3. Raw gas cleaning and by-product recovery;
4. Acid gas treatment and sulfur recovery;
5. Gas turbine and generator;
7. Steam turbine and generator;
8. Process heat recovery;
9. Recycle gas stream and coal/char transport and feeding;
10. Instrumentation and process control system;
11. Ancillary facilities such as for cooling and boiler feedwater; waste water treatment, waste gas flare, instrument and plant air, etc..

Since this paper discusses only the methodology for the development of process control guidelines using dynamic simulation techniques, systems engineering-type analysis would be beyond its scope. Therefore, a lumped mathematical model for studying the dynamic behavior of an open-loop gasifier will be developed. The dynamic relationships between input and output variables, called *transfer functions* for the gasifier will be derived. Dynamics of the closed-loop system, i.e., the gasifier with a control system that will give some desired dynamic performance, is discussed under

the section on control system guidelines.

The rates of conversion of the various components in coal to the various products in the raw fuel gas are influenced by many variables. For heterogeneous reactions involving solids, important variables include surface area, porosity, gas-solid contact and diffusion characteristics, and temperature. For gaseous phase homogeneous reactions, partial pressures or densities and temperature are of importance. The catalytic effect, mainly of the mineral matter present in coal, is of additional importance in some of the reactions.

### Kinetic Model

Figure 6 shows a schematic diagram of the U-Gas fluidized-bed gasifier including the pretreater. Overall gasification, possible in this type of an arrangement, has been assumed by Johnson<sup>(4)</sup> to occur in three consecutive stages: 1) devolatilization, 2) rapid-rate methane formation, and 3) low-rate gasification. Since devolatilization would start in the pretreater and since the hydrogen partial pressure in an air-blown gasifier is quite low for rapid rate methanation (accounting for a significant part of the methane in the effluent gas), low-rate gasification in the fluidized-bed will be considered for developing a model. The following three basic reactions are assumed to take place in the low-rate gasification of char or devolatilized coal<sup>(4)</sup>.



Reaction 1 is the conventional steam-carbon reaction which is the only one that occurs in pure steam at elevated pressures or with gases containing steam at low pressures. Reaction 2, the only reaction that could occur in pure hydrogen or in hydrogen-methane mixtures, depends greatly on the hydrogen partial pressure. The stoichiometry of reaction 3 limits its occurrence to systems in which both steam and hydrogen are present. Even though this reaction is a sum of reactions 1 and 2, it has been considered by Johnson<sup>(4)</sup> and others to be an independent reaction to facilitate correlation of experimental data. Correlations developed by Johnson to describe the kinetics of the above three reactions will be used. The reaction rate expression for the conversion of total base carbon is:

$$\frac{dX}{dt} = f_L k_T (1 - X)^{2/3} \exp(-\alpha X^2) \quad (4)$$

where:

X = total base carbon conversion fraction; ratio of mass of carbon gasified to mass of fixed carbon in feed;

t = time;

$f_L$  = relative reactivity factor for low-rate gasification which depends on the particular carbonaceous solid and temperature;

$k_T$  = overall rate constant,  $\text{min}^{-1}$

$\alpha$  = kinetic parameter which depends on gas composition and pressure.

The overall rate constant is given by:

$$k_T = k_1 + k_2 + k_3 \quad (5)$$

where in  $k_1$ ,  $k_2$ , and  $k_3$  are individual rate constants for reactions (1), (2), and (3).  $f_L$ ,  $k_1$ ,  $k_2$ ,  $k_3$ , and  $\alpha$  can further be defined as functions of temperature and pressure in the gasification zone as follows:

$$f_L = f_0 \exp\left(\frac{8467}{T_0}\right) \quad (6)$$

$$k_1 = \frac{\exp\left(9.0201 - \frac{31,705}{T}\right) \left(1 - \frac{P_{CO} P_{H_2}}{P_{H_2O} K_1^E}\right)}{\left[1 + \exp\left(-22.2160 + \frac{44,787}{T}\right) \left(\frac{1}{P_{H_2O}} + 16.35 \frac{P_{H_2}}{P_{H_2O}} + 43.4 \frac{P_{CO}}{P_{H_2O}}\right)\right]^2} \quad (7)$$

$$k_2 = \frac{P_{H_2}^2 \exp\left(2.6741 - \frac{44,787}{T}\right) \left(1 - \frac{P_{CH_4}}{P_{H_2}^2 K_2^E}\right)}{\left[1 + P_{H_2} \left(\exp -10.4520 + \frac{19,976}{T}\right)\right]} \quad (8)$$

$$k_3 = \frac{P_{H_2}^{0.5} \exp\left(12.4463 - \frac{44,544}{T}\right) \left(1 - \frac{P_{CH_4} P_{CO}}{P_{H_2} P_{H_2O} K_3^E}\right)}{\left[1 + \exp\left(-6.6696 + \frac{15,198}{T}\right) \left(P_{H_2}^{0.5} + 0.85 P_{CO} + 18.62 \frac{P_{CH_4}}{P_{H_2}}\right)\right]^2} \quad (9)$$

$$\alpha = \frac{52.7 P_{H_2}}{1 + 54.3 P_{H_2}} + \frac{0.521 P_{H_2}^{0.5} P_{H_2O}}{1 + 0.707 P_{H_2O} + 0.5 P_{H_2}^{0.5} P_{H_2O}}$$

where:

- $f_0$  = relative reactivity factor for low-rate gasification which depends on the particular carbonaceous solid
- $T_0$  = maximum temperature to which coal in the pre-treater was exposed prior to gasification, °R
- $T$  = reaction temperature, °R
- $P_{H_2}, P_{H_2O}, P_{CO}, P_{CH_4}$  = partial pressures of  $H_2$ ,  $H_2O$ ,  $CO$ , and  $CH_4$ , atm
- $K_1^E, K_2^E, K_3^E$  = equilibrium constants for reactions 1, 2, and 3 considering carbon as graphite.

### Dynamic Model

The basic method of determining the dynamic response of the gasifier is to write first the equations for conservation of mass and energy\* in the gasifier at any given instant of time. The use of transport-rate equations then introduces the time variable and, by use of conversion equations, the response equation can be converted into the particular variables that are desired to be related. As these have to be manipulated and solved to determine the temporal response of the output variable, it is desirable that the final equation should be linear and with constant coefficients.

Figure 7 shows a fluidized-bed gasifier as a backmix reactor with the various input and output streams and a combustion zone that can be considered to be of negligible volume<sup>(5)</sup>. The equations describing the reactor are:

Reactor total continuity:

$$\frac{dV}{dt} = F_{s_1} + F_{s_3} + F_{g_2} - F_{s_2} - F_{g_1} \quad (11)$$

Reactor component (carbon) continuity equation:

$$\begin{aligned} \frac{d(V C_{s_2})}{dt} = & F_{s_1} C_{s_1} + F_{s_3} C_{s_3} - F_{s_2} C_{s_2} - F_{g_1} C_{s_4} \\ & - V C_{s_2} f_L k_T (1 - X)^{2/3} \exp(-\alpha X^2) \end{aligned} \quad (12)$$

\* Conservation equations for momentum are excluded to simplify the model. It should be noted, however, that gas turbines in combined cycle plants are mass flow machines and therefore a realistic model should take into consideration conservation of momentum equations.

Since the reactor was assumed to be a backmix reactor, carbon concentration of outflow streams should be the same. Therefore

$$C_{s_2} = C_{s_4} \quad (13)$$

Assuming total recycle of char gives

$$F_{s_3} C_{s_3} = F_{g_1} C_{s_4} \quad (14)$$

In a fluidized-bed reactor a minimum bed height (volume) has to be maintained for specific carbon residence time and conversion rates. If the height falls below this minimum, then the outflow would have to be shut off completely and would increase proportionally as the bed height increases above the minimum. Therefore

$$F_{s_2} + F_{g_1} = K(V - V_{\min}) \quad (15)$$

Reactor total energy equation:

$$\begin{aligned} \rho \frac{d}{dt} (Vh) = & \rho_1 F_{s_1} h_1 + \rho_2 F_{g_2} h_2 + \rho_3 F_{s_3} h_3 - \rho(F_{s_2} + F_{g_1})h \\ & - UA(T - T_0) + \lambda VC s_2 f_L k_T (1 - X)^{2/3} \exp(-\alpha X^2) \end{aligned} \quad (16)$$

Again for a backmix reactor

$$T_{g_1} = T \quad (17)$$

$$T_{s_2} = T \quad (18)$$

The quantity of unreacted carbon going to the combustion zone, i.e.,  $F_{s_2} \times C_{s_2}$  depends on the heat required to be generated in that zone. Since the carbon concentration in the reactor and the outflows are the same, the ratio of the two outflows would be fixed for a specific set of operating conditions. Therefore

$$\frac{F_{g_1}}{F_{s_2}} = Y \left( \frac{F_{s_1}}{F_{g_2}} \right) \quad (19)$$

In the above equations 11-19:

V = volume of the reactor or fluidized bed, ft<sup>3</sup>

T = temperature in the reactor, °R

- $F_{s_i}$  = reactor inflow and outflow streams containing solid char,  $\text{ft}^3/\text{min}$   
 $F_{g_i}$  = predominantly gaseous phase inflow and outflow streams,  $\text{ft}^3/\text{min}$   
 $C_{s_i}$  = solid char concentration, moles/ $\text{ft}^3$   
 $K$  = constant; function of the bed level control system used  
 $V_{\text{min}}$  = minimum fluidized bed volume,  $\text{ft}^3$   
 $T_{s_i}$  = temperature of streams containing solid char,  $^{\circ}\text{R}$   
 $T_{g_i}$  = temperature of streams containing predominantly gases,  $^{\circ}\text{R}$   
 $h$  = enthalpy of material in the reactor, Btu/lb  
 $h_i$  = enthalpies of various feed streams, Btu/lb  
 $\rho$  = density of the material in the reactor,  $\text{lb}/\text{ft}^3$   
 $\rho_i$  = densities of various feed streams,  $\text{lb}/\text{ft}^3$   
 $UA(T-T_0)$  = heat transfer between the reactor and surrounding, Btu/min  
 $\lambda$  = heat of reaction for the endothermic gasification reactions, Btu/mole of carbon reacted  
 $Y$  = proportionally constant.

All of the equations of state are defined simply rather than as polynomials of pressure, temperature, and composition.

$$h = C_p T \quad (20)$$

$$h_i = C_{p_i} T_i \quad (21)$$

$$\rho = \frac{MP}{RT} \quad (22)$$

$$\rho_i = \frac{M_i P_i}{RT_i} \quad (23)$$

where:

$$C_p = \text{heat capacity of the material in the reactor at temperature } T, \text{ Btu}/\text{lb-}^{\circ}\text{R}$$

- $C_{p_i}$  = heat capacity of the stream  $i$  at temperature  $T_i$ ,  
 Btu/lb-°R
- $M$  = average molecular weight of the material in the reactor
- $P$  = absolute pressure of the reactor, psi
- $M_i$  = average molecular weight of stream  $i$
- $P_i$  = absolute pressure of stream  $i$ , psi
- $R$  = gas constant, lb<sub>f</sub> - ft/mole °R.

An examination of equations 11-19 shows that there are nine unknowns --  $V$ ,  $F_{s_2}$ ,  $F_{g_1}$ ,  $C_{s_2}$ ,  $C_{s_3}$ ,  $C_{s_4}$ ,  $T_{s_L}$ ,  $T_{g_1}$ , and  $T$  in the nine equations. Therefore, the system is *specified* and a solution can be obtained. The forcing functions or the variables that must be specified are  $F_{s_1}$ ,  $C_{s_1}$ ,  $T_{s_1}$ ,  $F_{g_2}$ ,  $T_{g_2}$ ,  $F_{s_3}$ , and  $T_{s_3}$ . The rest of the parameters in the equations must be known for simulating the reactor.

## SIMULATION

The mathematical model of the reactor shown in Figure 7 consists of nine equations that have to be solved for simulating its dynamic behavior.

In general two basic methods have been used to solve mathematical models of chemical processes<sup>(6)</sup>: a *simultaneous* one in which all equations for all process units in a comprehensive model are solved simultaneously, and a *modular* one, in which the overall process model is constructed piece by piece from equations associated with the individual units. If systems engineering approach was used for the analysis of a combined cycle plant, then either method could be used depending on the type of various computer programs available for solving the equations.

Most of the computer programs for steady state simulation, mainly for calculating material and energy balances, use the modular approach that allows the user to write individual routines to model new units added to those already available as a part of either the executive program or in the subroutine library. About 29 different steady state simulation programs have been listed by Peterson, et al.<sup>(7)</sup> as a result of their survey of programs for simulation, design, equipment sizing, cost estimation, economic evaluation, as well as service routines for physical-property calculations, data regression, and equation solving. They also listed 7 dynamic simulation programs and 3 programs specifically written for simulating various aspects of coal conversion and process technologies.

Programs available for dynamic simulation, using either the *simultaneous* or *modular* approach include DYN SYS (version 2), DYSCO, PRODYC, UCANS, GEMSCOPE, etc. A brief description of these programs and the person to contact for further information is given in Reference 7. GEMSCOPE, developed by Prof. Seborg at the University of Alberta, seems to be the only program

that can assist directly with the design of control systems. PRODYC has sub-routines for handling valves (with controller) and signal transmission delays.

Apart from these, the building block type preprogrammed packages are also available, based on which a person could develop his own executive program. For example, one of the principal difficulties in digital simulation is in integration. This has to be done numerically and involves approximating continuous differential equations with discrete finite difference equations. However, a number of general simulation languages, such as MIMIC, MIDAL, and LEANS, are available that do not require detailed knowledge of numerical integration. A number of such subroutines, along with those for solving a set of implicit simultaneous algebraic equations, are discussed by Franks in his book on modeling and simulation(8).

Simulation of the backmix reactor representing a fluidized-bed coal gasifier, for which a mathematical model was developed in the previous section, was not undertaken because of time and monetary constraints. However, the methodology will be discussed as follows.

The first step toward solving equations 11-19 would be to examine them for possibly further simplification. An information-flow block diagram is then drawn showing the natural arrangement of the equations and how each one is to be used, i.e., the variable it solves for and the interrelationship between the equations. Numerical values for all the parameters are then selected from the physical properties file or through a function generator subroutine or from the input data to the general program. Initial conditions along with steady state values for the variables are assigned. The method for solving implicit simultaneous equations is selected for use along with the numerical integration method, to solve the complete set of equations. For the differential equations at each instant in time, either the Euler or the fourth order Runge-Kutta numerical integration scheme is used to calculate new values for the variables. Other integration techniques can also be used depending on the accuracy desired in relation to the optimum usage of computer time. Finally, new values of these variables plotted against time would indicate the dynamic behavior of the fluidized-bed gasifier. A check of the model's accuracy can also be made by comparing these values with those obtained from experiments or pilot plants.

A systems engineering type of analysis for the combined cycle plant would allow the development of interrelated mathematical models for the individual units, which, when solved, would simulate the dynamic behavior of the complete plant. As mentioned earlier, this approach would be the best for determining the load following capability and the transient behavior during startup, shutdown and upsets, of coal based combined cycle plants.

## CONTROL SYSTEM GUIDELINES

An integrated coal based combined cycle plant is much more complicated to operate than a conventional plant even if it is built for base-load application. The relatively short residence time of coal, char, and gases in the gasifier, the differences in the reaction rates of various reactions taking place, the variations in process dynamics of systems for gas cleaning, the gas turbine combustor, the heat recovery steam generator, etc. and the economically unfeasible storage of low Btu gas makes it mandatory that a sophisticated control system be developed for the plant to operate sequentially under various loads and feed quality.

It has been stated by Luyben<sup>(9)</sup> that at present 80 to 90% of the control loops in a plant are usually designed, installed, tuned, and operated quite successfully by simple, rule-of-thumb, experience generated techniques. The other 10 to 20% of the loops are those that require plant testing, computer simulation, and detailed controller design to achieve a specific performance. Considering the complexity of an integrated combined cycle plant and the electricity generator response required for a plant operated on a large interconnection, it is very likely that the rule-of-thumb design of 80 to 90% of the control loops in the plant may not allow for achievement of the desired performance. Therefore, development of a sophisticated control system by using dynamic modeling and process simulation techniques is justifiable.

In this section of the paper, using as an example the gasifier model, after further simplification, developed in the section on mathematical modeling, the development of control system guidelines is discussed. These guidelines are in the form of transfer functions discussed by Luyben<sup>(9)</sup> in detail.

In Johnson's<sup>(4)</sup> kinetic model, the overall rate constant,  $k_T$ , is given as a function of temperature and partial pressures of various product gases and the reaction rate expression in terms of the base carbon conversion fraction. This expression is highly nonlinear and would take extensive mathematical manipulation to linearize it so that transfer functions for the perturbation variables could be derived. Therefore, a simple rate expression for a first order reaction will be used with the specific reaction rate constant,  $k$ , assumed to follow the Arrhenius dependent function.

Considering equations 12 and 16, substituting;

$$f_{\alpha} k_T (1 - X)^{2/3} \exp(-\alpha X^2) = \beta \exp\left(-\frac{E}{RT}\right) \quad (24)$$

and further simplifying we have;

$$\frac{d(VC_{s_2})}{dt} = F_{s_1} C_{s_1} - F_{s_2} C_{s_2} - VC_{s_2} \beta \exp\left(-\frac{E}{RT}\right) \quad (25)$$

$$\frac{\rho d(V C_p T)}{dt} = \rho_1 F_{s_1} C_{p_1} T_{s_1} + \rho_2 F_{g_2} C_{p_2} T_{g_2} + \rho_3 F_{s_3} C_{p_3} T_{s_3} - \rho(F_{s_2} + F_{g_1}) C_p T - UA(T - T_0) + \lambda V S_{s_2} \beta \exp\left(-\frac{E}{RT}\right) \quad (26)$$

where:

$\beta$  = constant preexponential factor, same units as  $k$

$E$  = activation energy, Btu/mole.

Linearizing equation 25 and writing it in terms of perturbations in  $C_{s_1}$ ,  $F_{s_1}$ ,  $C_{s_2}$ ,  $F_{s_2}$ , and  $T$ , we get

$$V \frac{dC_{s_2}}{dt} = \bar{F}_{s_1} C_{s_1} + \bar{C}_{s_1} F_{s_2} - (\bar{F}_{s_2} + V \bar{k}) C_{s_2} - \bar{C}_{s_2} F_{s_2} - \left( \frac{V \bar{k} \bar{C}_{s_2} E}{RT^2} T \right) \quad (27)$$

The variables with overscore refer to steady state values used in the Taylor series expansion. It should be noted that truncation errors resulting from discarding higher order partial derivatives may have to be considered in some cases when modeling real systems.

Similarly, equation 26 is linearized to give

$$\begin{aligned} \rho C_p V \frac{dT}{dt} &= \rho_1 C_{p_1} \bar{F}_{s_1} T_{s_1} + \rho_1 C_{p_1} \bar{T}_{s_1} F_{s_1} + \rho_2 C_{p_2} \bar{F}_{g_2} T_{g_2} \\ &+ \rho_2 C_{p_2} \bar{T}_{g_2} F_{g_2} + \rho_3 C_{p_3} \bar{F}_{s_3} T_{s_3} + \rho_3 C_{p_3} \bar{T}_{s_3} F_{s_3} \\ &- \rho C_p \bar{F}_{sg} T - \rho C_p \bar{T} F_{sg} - UA(T - T_0) \\ &+ \lambda V \bar{k} C_{s_2} + \frac{\lambda V \bar{k} \bar{C}_{s_2} E}{RT^2} T \end{aligned} \quad (28)$$

where:

$$\bar{F}_{sg} = \bar{F}_{s_2} + \bar{F}_{g_1}$$

$$F_{sg} = F_{s_2} + F_{g_1}$$

Equation 27 can be further reduced to

$$\frac{dC_{s_2}}{dt} = a_1 C_{s_1} + a_2 F_{s_2} + a_3 C_{s_2} + a_4 T \quad (29)$$

where:

$$a_1 = \frac{\bar{F}_{s_1}}{V}, \quad a_2 = \frac{\bar{C}_{s_1} - \bar{C}_{s_2}}{V}, \quad a_3 = -\frac{\bar{F}_{s_2}}{V} + \bar{k} \quad \text{and}$$

$$\text{and } a_4 = -\frac{\bar{k} E \bar{C}_{s_2}}{RT^2}$$

Similarly, equation 28 is reduced to

$$\begin{aligned} \frac{dT}{dt} = & b_1 T_{s_1} + b_2 F_{s_1} + b_3 T_{g_2} + b_4 F_{g_2} + b_5 T_{s_3} \\ & + b_6 F_{s_3} + b_7 F_{s_2} + b_8 F_{g_1} + b_9 T + b_{10} C_{s_2} \end{aligned} \quad (30)$$

where:

$$b_1 = \frac{\rho_1 C_{p1} \bar{F}_{s_1}}{\rho C_p V}, \quad b_2 = \frac{\rho_1 C_{p1} \bar{T}_{s_1}}{\rho C_p V}, \quad b_3 = \frac{\rho_2 C_{p2} \bar{F}_{g_2}}{\rho C_p V},$$

$$b_4 = \frac{\rho_2 C_{p2} \bar{T}_{g_2}}{\rho C_p V}, \quad b_5 = \frac{\rho_3 C_{p3} \bar{F}_{s_3}}{\rho C_p V}, \quad b_6 = \frac{\rho_3 C_{p3} \bar{T}_{s_3}}{\rho C_p V},$$

$$b_7 = b_8 = -\frac{\bar{T}}{V}, \quad b_9 = \left( \frac{\lambda \bar{k} \bar{C}_{s_2} E}{\rho C_p R \bar{T}^2} - \frac{\bar{F}_{s_2}}{V} - \frac{\bar{F}_{g_1}}{V} - \frac{UA}{\rho C_p V} \right),$$

$$b_{10} = \frac{\lambda V \bar{k}}{\rho C_p V}.$$

In equations 29 and 30, the variables  $C_s$ ,  $T_{s_1}$ ,  $F_{s_1}$ ,  $T_{g_2}$ ,  $F_{g_2}$ ,  $T_{s_3}$ , and  $F_{s_3}$  are considered input variables or, as defined earlier, the forcing functions. Also, as specified by equation 19, the ratio of outflows,  $F_{g_1}/F_{g_2}$ , was considered to be a function of the input flow rates  $F_{s_1}/F_{g_2}$ . Therefore  $F_{g_1}$  and  $F_{s_2}$  can also be considered as input variables. The output variables are

$C_{s_2}$  and  $T$ . It is obvious now that eighteen different transfer functions are required to relate the nine input variables to the two output variables. Putting it in another way, the solid carbon content and temperature of the outflows from the backmix reactor are a function of the nine input variables.

The transfer functions in the Laplace domain can be defined as  $G_{a_i}(s)$  and  $G_{b_i}(s)$ . Then

$$\begin{aligned}
 C_{s_2}(s) = & G_{a_1}(s)C_{s_1}(s) + G_{a_2}(s)T_{s_1}(s) + G_{a_3}(s)F_{s_1}(s) \\
 & + G_{a_4}(s)T_{g_2}(s) + G_{a_5}(s)F_{g_2}(s) + G_{a_6}(s)T_{s_3}(s) \\
 & + G_{a_7}(s)F_{s_3}(s) + G_{a_8}(s)F_{s_2}(s) + G_{a_9}(s)F_{g_1}(s)
 \end{aligned} \tag{31}$$

and

$$\begin{aligned}
 T(s) = & G_{b_1}(s)C_{s_1}(s) + G_{b_2}(s)T_{s_1}(s) + G_{b_3}(s)F_{s_1}(s) \\
 & + G_{b_4}(s)T_{g_2}(s) + G_{b_5}(s)F_{g_2}(s) + G_{b_6}(s)T_{s_3}(s) \\
 & + G_{b_7}(s)F_{s_3}(s) + G_{b_8}(s)F_{s_2}(s) + G_{b_9}(s)F_{g_1}(s)
 \end{aligned} \tag{32}$$

To find these transfer function equations 29 and 30 are Laplace transformed and solved simultaneously.

$$sC_{s_2} = a_1C_{s_1} + a_2F_{s_2} + a_3C_{s_2} + a_4T \tag{33}$$

$$\begin{aligned}
 sT = & b_1T_{s_1} + b_2F_{s_1} + b_3T_{g_2} + b_4F_{g_2} + b_5T_{s_3} + b_6F_{s_3} \\
 & + b_7F_{s_2} + b_8F_{g_1} + b_9T + b_{10}C_{s_2}
 \end{aligned} \tag{34}$$

$$\begin{aligned}
 C_{s_2}(s) = & \left[ \frac{a_1(s - b_9)}{s^2 - s(a_3 + b_9) + a_3b_9 - a_4b_{10}} \right] C_{s_1}(s) \\
 & + \left[ \frac{a_4b_1}{s^2 - s(a_3 + b_9) + a_3b_9 - a_4b_{10}} \right] T_{s_1}(s)
 \end{aligned}$$

$$\begin{aligned}
& + \left[ \frac{a_4 b_2}{s^2 - s(a_3 + b_9) + a_3 b_9 - a_4 b_{10}} \right] F_{s_1}(s) \\
& + \left[ \frac{a_4 b_4}{s^2 - s(a_3 + b_9) + a_3 b_9 - a_4 b_{10}} \right] T_{g_2}(s) \\
& + \left[ \frac{a_4 b_4}{s^2 - s(a_3 + b_9) + a_3 b_9 - a_4 b_{10}} \right] F_{g_2}(s) \\
& + \left[ \frac{a_4 b_5}{s^2 - s(a_3 + b_9) + a_3 b_9 - a_4 b_{10}} \right] T_{s_3}(s) \\
& + \left[ \frac{a_4 b_6}{s^2 - s(a_3 + b_9) + a_3 b_9 - a_4 b_{10}} \right] F_{s_3}(s) \\
& + \left[ \frac{a_4 b_7 + a_2(s - b_9)}{s^2 - s(a_3 + b_9) + a_3 b_9 - a_4 b_{10}} \right] F_{s_2}(s) \\
& + \left[ \frac{a_4 b_8}{s^2 - s(a_3 + b_9) + a_3 b_9 - a_4 b_{10}} \right] F_{g_1}(s)
\end{aligned} \tag{35}$$

Similarly,

$$\begin{aligned}
T(s) & = \left[ \frac{b_{10} a_1}{s^2 - s(a_3 + b_9) + a_3 b_9 - a_4 b_{10}} \right] C_{s_1}(s) \\
& + \left[ \frac{b_1(s - a_3)}{s^2 - s(a_3 + b_9) + a_3 b_9 - a_4 b_{10}} \right] T_{s_1}(s) \\
& + \left[ \frac{b_2(s - a_3)}{s^2 - s(a_3 + b_9) + a_3 b_9 - a_4 b_{10}} \right] F_{s_1}(s) \\
& + \left[ \frac{b_3(s - a_3)}{s^2 - s(a_3 + b_9) + a_3 b_9 - a_4 b_{10}} \right] T_{g_2}(s)
\end{aligned}$$

$$\begin{aligned}
& + \left[ \frac{b_4(s - a_3)}{s^2 - s(a_3 + b_9) + a_3b_9 - a_4b_{10}} \right] F_{g_2}(s) \\
& + \left[ \frac{b_5(s - a_3)}{s^2 - s(a_3 + b_9) + a_3b_9 - a_4b_{10}} \right] T_{s_3}(s) \\
& + \left[ \frac{b_6(s - a_3)}{s^2 - s(a_3 + b_9) + a_3b_9 - a_4b_{10}} \right] F_{s_3}(s) \\
& + \left[ \frac{b_7(s - a_3) + b_{10}a_2}{s^2 - s(a_3 + b_9) + a_3b_9 - a_4b_{10}} \right] F_{s_2}(s) \\
& + \left[ \frac{b_8(s - a_3)}{s^2 - s(a_3 + b_9) + a_3b_9 - a_4b_{10}} \right] F_{g_1}(s) \quad . \quad (36)
\end{aligned}$$

Figure 8 shows the block diagram for the transfer functions of a fluidized-bed gasifier derived after making some assumptions to simplify the mathematical model.

Transfer functions for the closed-loop reactor can also be derived by specifying different controlled variables and an equal number of manipulative variables. For example, if the temperature of the reactor  $T$  and the carbon content of the outflow streams,  $C_{s_2}$ , are to be controlled by manipulating the feed flow rate,  $F_{s_1}$ , and the temperature of the gas stream from the combustion zone,  $T_{g_2}$ , then the following transfer functions for feedwater type controllers can be obtained. Disturbances are assumed to be feed quality, i.e., carbon concentration, and temperature of feed stream,  $C_{s_1}$  and  $T_{s_1}$ , respectively.

The transfer functions, in the Laplace domain, for the four feedforward controllers, i.e.,  $F_{a_1}(s)$ ,  $F_{a_2}(s)$ ,  $F_{b_1}(s)$ , and  $F_{b_2}(s)$ , as shown in Figure 9 would be

$$F_{s_1}(s) = F_{a_1}(s)C_{s_1}(s) + F_{a_2}(s)T_{s_1}(s) \quad (37)$$

and

$$T_{g_2}(s) = F_{b_1}(s)C_{s_1}(s) + F_{b_2}(s)T_{s_1}(s) \quad (38)$$

These transfer functions can be obtained by setting  $C_{s_2}$  and  $T$  equal to zero in equations 31 and 32 along with the terms that contain variables other than

those listed above. After considerable algebraic manipulation, the transfer functions in terms of  $G_{a_i}$  and  $G_{b_i}$  are obtained.

$$F_{s_1}(s) = \frac{G_{a_1}G_{b_4} - G_{a_4}G_{b_1}}{G_{a_4}G_{b_3} - G_{a_3}G_{b_4}} C_{s_1}(s) + \frac{G_{a_2}G_{b_4} - G_{a_4}G_{b_2}}{G_{a_4}G_{b_3} - G_{a_3}G_{b_4}} T_{s_1}(s) \quad (39)$$

and

$$T_{g_2}(s) = \frac{G_{a_3}G_{b_1} - G_{a_1}G_{b_3}}{G_{a_4}G_{b_3} - G_{a_3}G_{b_4}} C_{s_1}(s) + \frac{G_{a_3}G_{b_2} - G_{a_2}G_{b_3}}{G_{a_4}G_{b_3} - G_{a_3}G_{b_4}} T_{s_1}(s) \quad (40)$$

From equation 37 and 39 and 38 and 40, we obtain the transfer functions for the four feedforward controllers.

$$F_{a_1}(s) = \frac{G_{a_1}G_{b_4} - G_{a_4}G_{b_1}}{G_{a_4}G_{b_3} - G_{a_3}G_{b_4}} \quad (41)$$

$$F_{a_2}(s) = \frac{G_{a_2}G_{b_4} - G_{a_4}G_{b_2}}{G_{a_4}G_{b_3} - G_{a_3}G_{b_4}} \quad (42)$$

$$F_{b_1}(s) = \frac{G_{a_3}G_{b_1} - G_{a_1}G_{b_3}}{G_{a_4}G_{b_3} - G_{a_3}G_{b_4}} \quad (43)$$

$$F_{b_2}(s) = \frac{G_{a_3}G_{b_2} - G_{a_2}G_{b_3}}{G_{a_4}G_{b_3} - G_{a_3}G_{b_4}} \quad (44)$$

Substitution of  $G_{a_i}$ 's and  $G_{b_i}$ 's and the  $a_i$ 's and  $b_i$ 's would give these transfer functions in terms of the various process variables.

An evaluation of the stability of the closed loop system can be made by examining whether the roots of the polynomial in  $s$  of the denominator of the transfer function, i.e., its poles, lie in the left or right half of the  $s$  plane. The system is considered stable if these roots lie in the left half of the  $s$  plane. The Routh stability criterion or direct substitution methods can be used to determine the stability or instability of the system in either the closed or open loop configuration.

## CONCLUSIONS

An evaluation of the status of technology of coal based combined cycle plants has shown that its commercial application could be in the late 1980s. However, a few technological problems remain to be solved. One of such problems was found to be the development of an automatic process control system that would allow sequential operation of an integrated combined cycle plant under varying conditions of load and feed quality.

The use of mathematical modeling and dynamic simulation for the development of process control guidelines were described. Since actual simulation was not undertaken, transient response curves for the various critical process parameters could not be developed. Such curves would have allowed a better understanding of the dynamics of the plant.

Using as an example a simplified fluidized-bed gasifier (modeled as a backmix reactor), process transfer functions for a number of process variables were derived for an open loop system. The system was closed by four feedforward controllers, and the transfer functions for the controllers in terms of process parameters were also derived. These transfer functions can be used as guides for the design of a control system for the fluidized-bed gasifier. A systems engineering approach would permit the development of such process control guidelines for an integrated coal based combined cycle plant.

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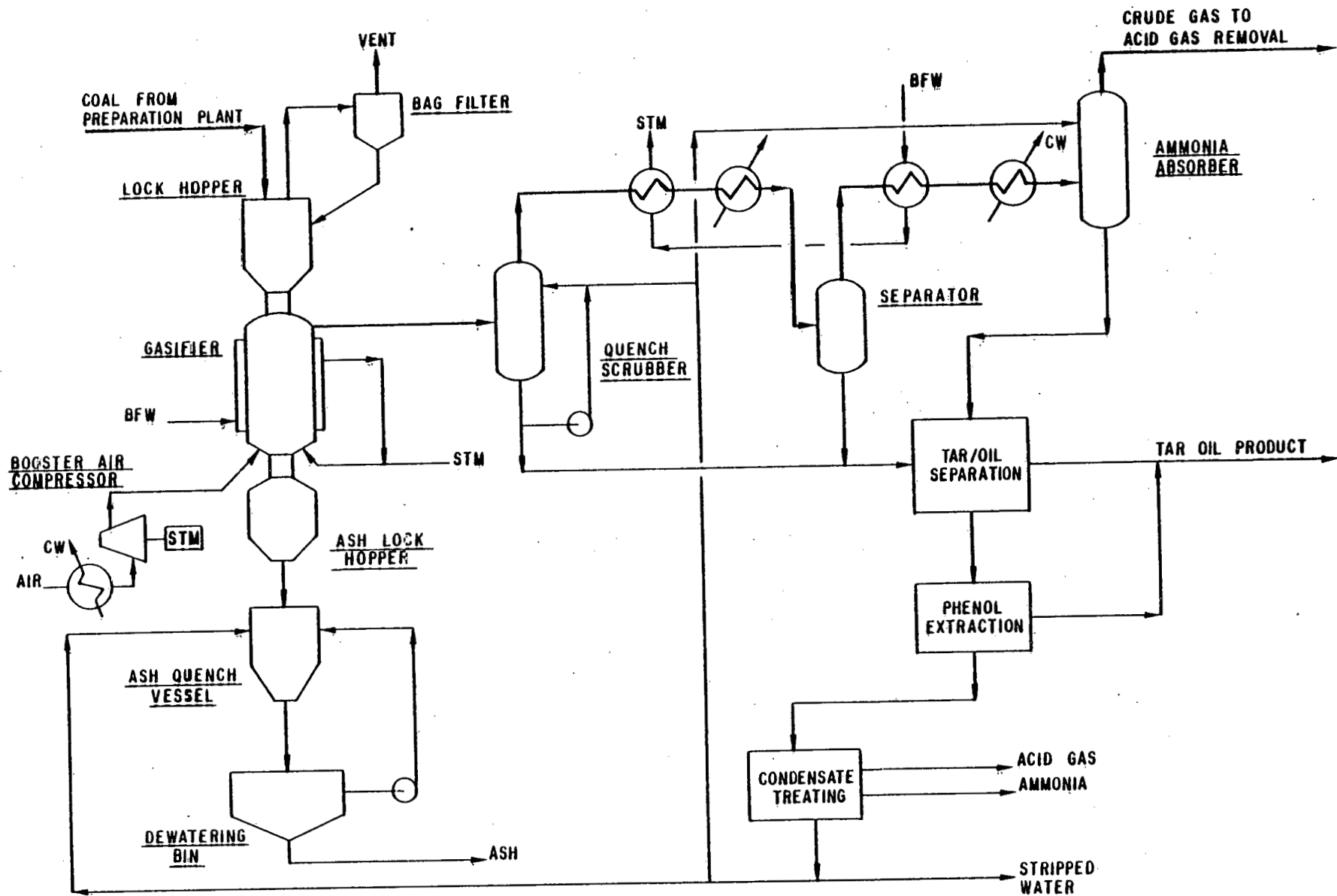


Fig. 1 PROCESS FLOW DIAGRAM - LURGI GASIFIER AND GAS COOLING  
 BFW-BOILER FEED WATER, CW-COOLING WATER, STM-STEAM

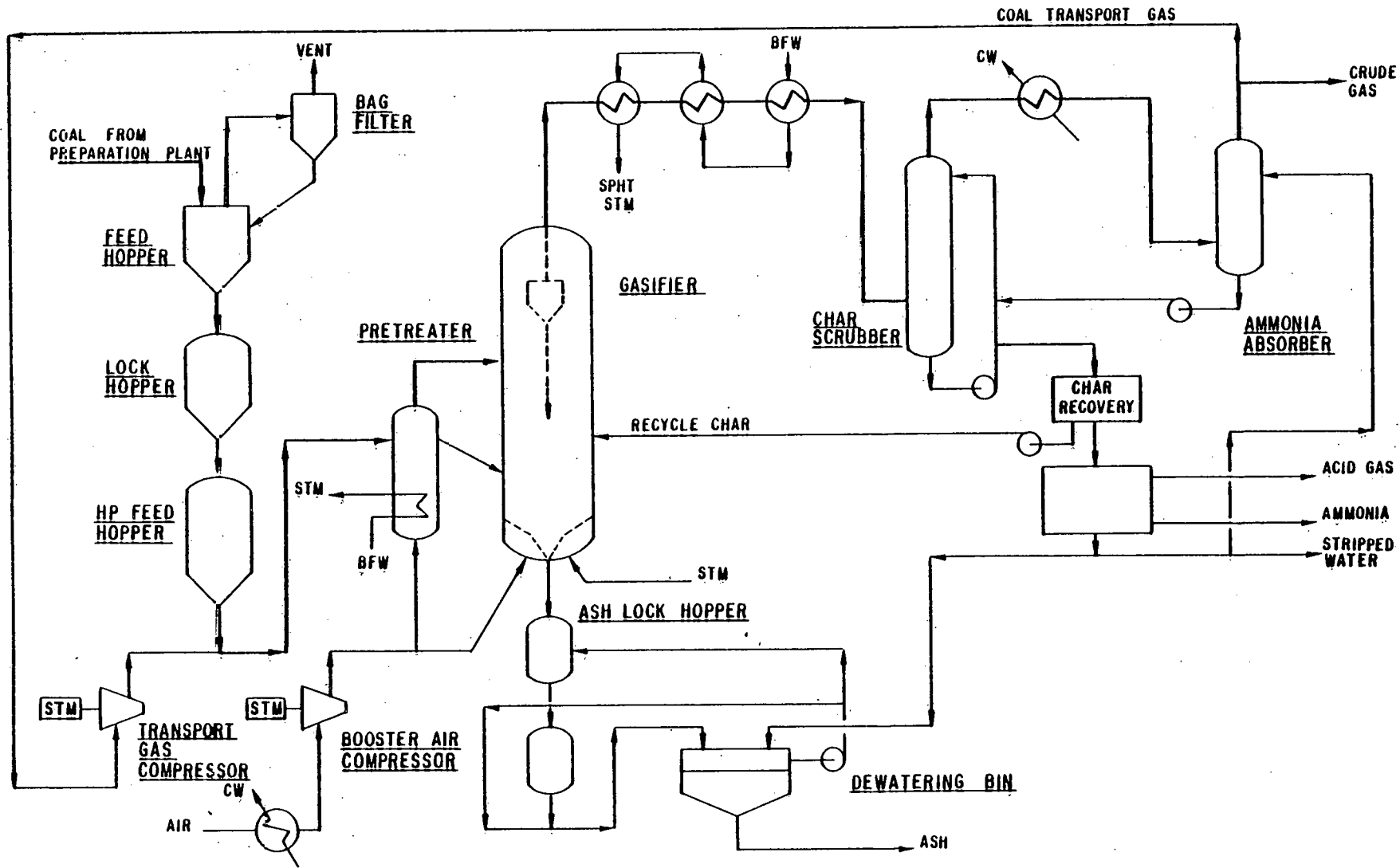


Fig. 2 PROCESS FLOW DIAGRAM - U-GAS GASIFIER AND GAS COOLING

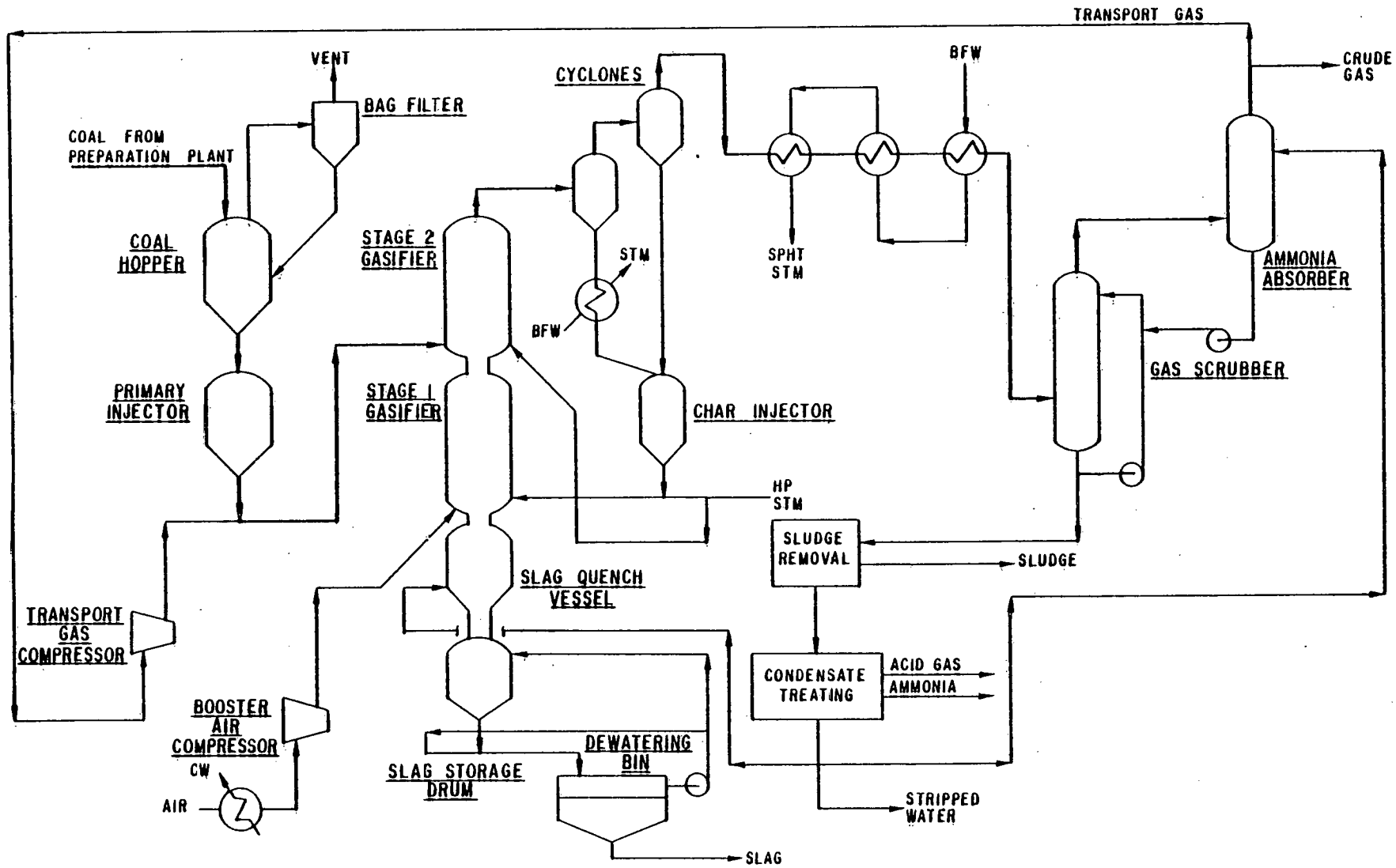


Fig. 3 PROCESS FLOW DIAGRAM - FOSTER WHEELER GASIFIER AND GAS COOLING

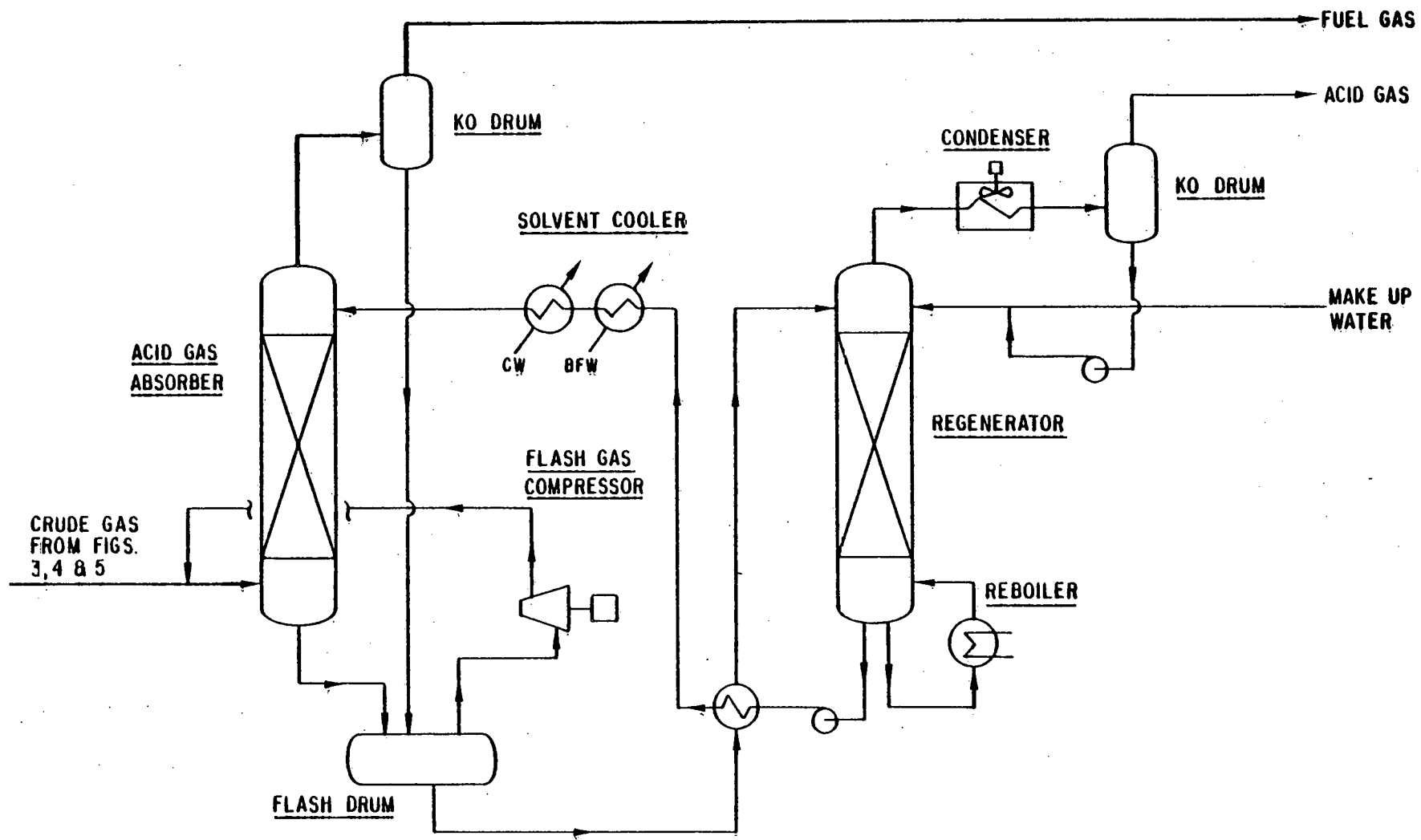


Fig. 4 SELEXOL PROCESS FLOW DIAGRAM

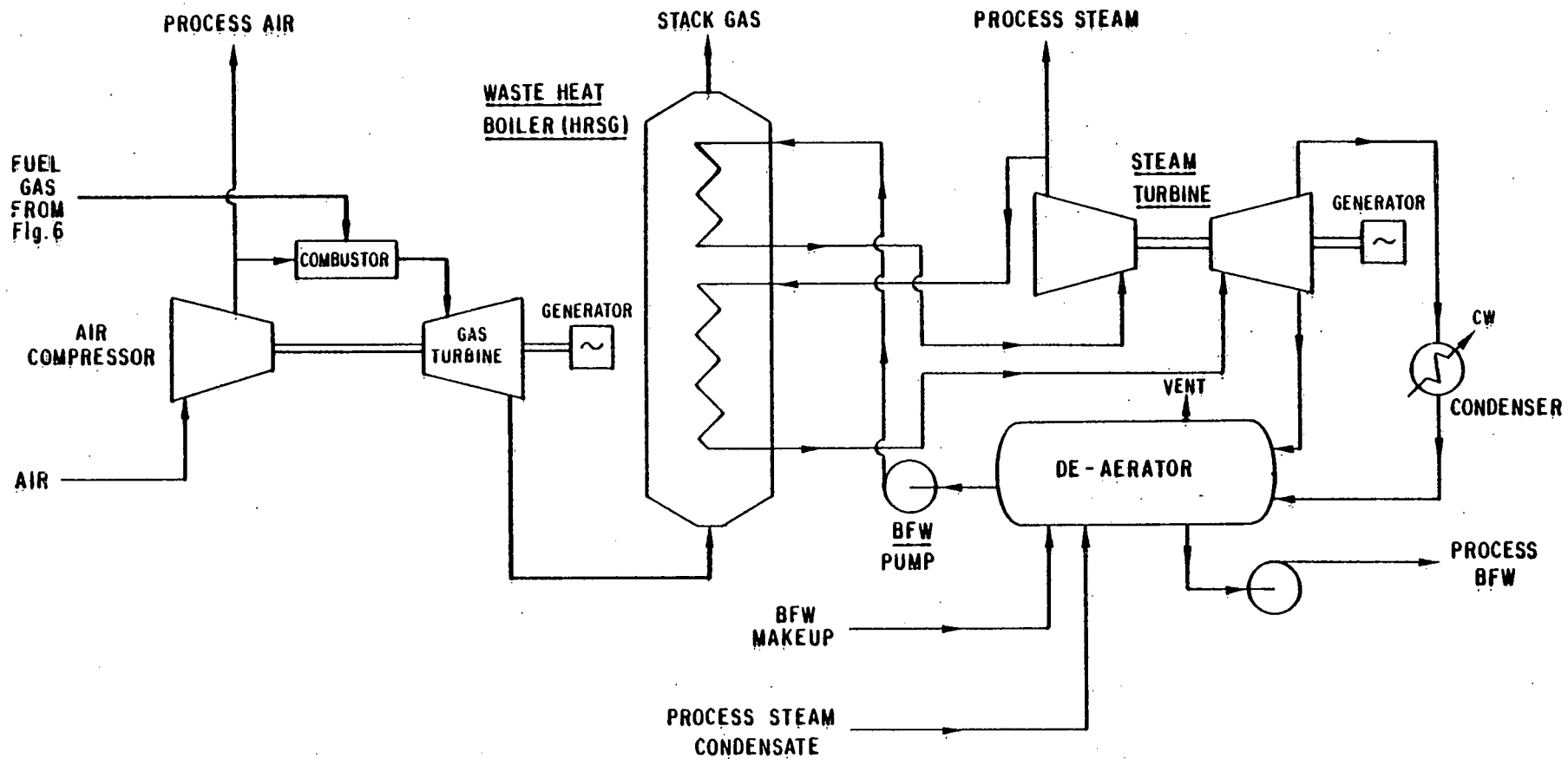


Fig. 5 PROCESS FLOW DIAGRAM FOR THE COMBINED CYCLE SYSTEM

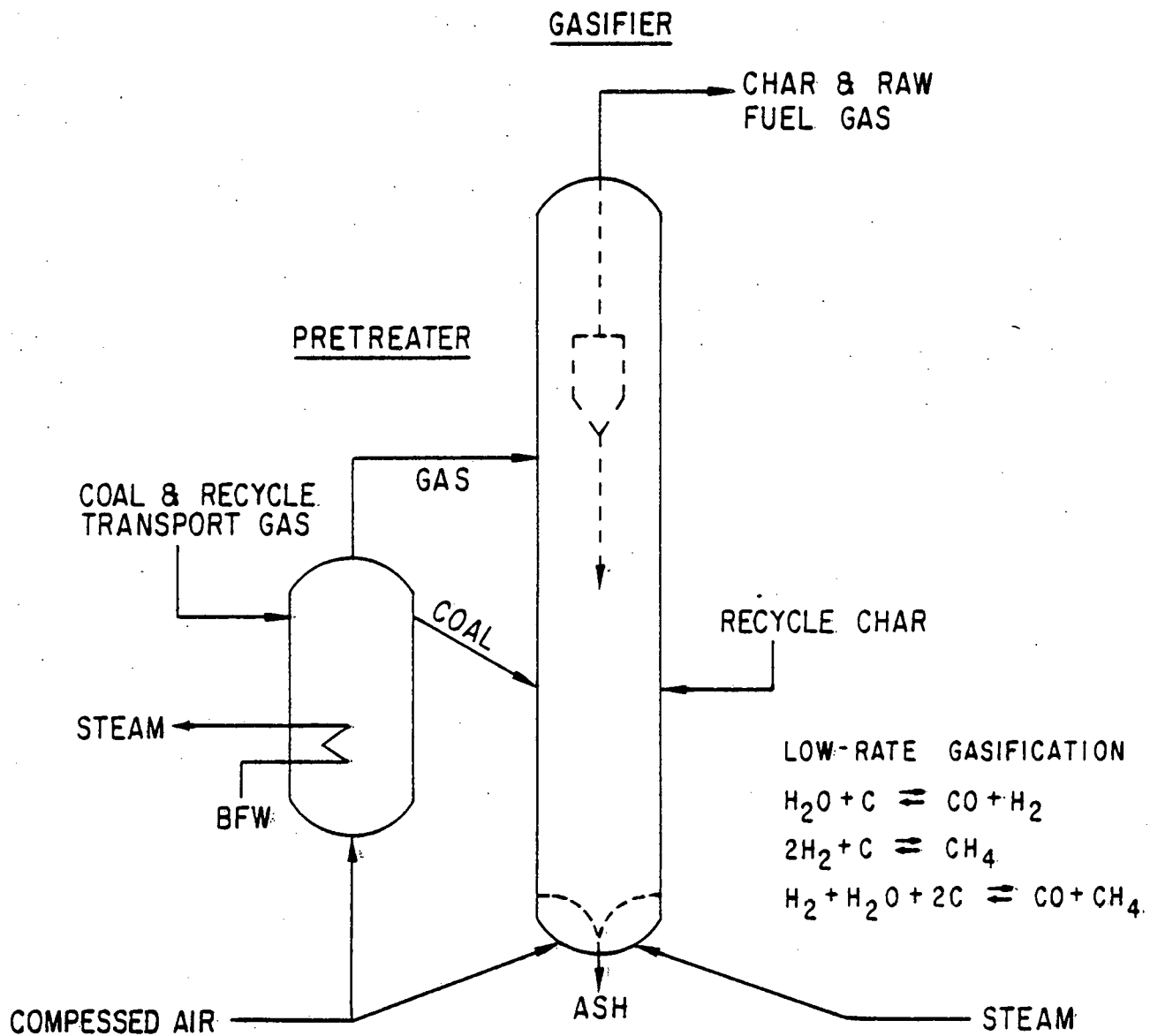


FIG. 6 IGT's FLUIDIZED BED U-GAS GASIFIER

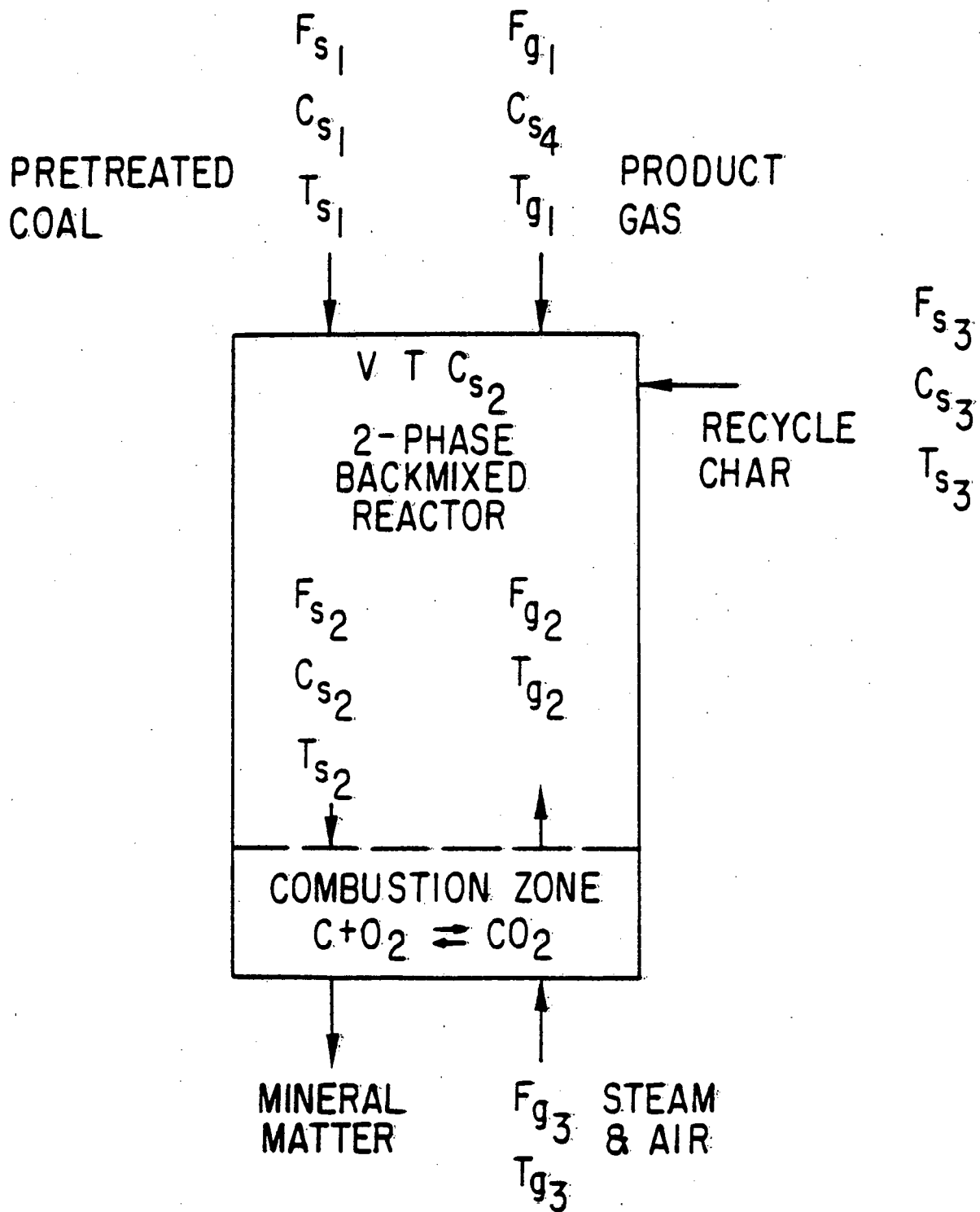


FIG. 7. FLUIDIZED-BED GASIFIER SHOWN AS A BACKMIXED REACTOR

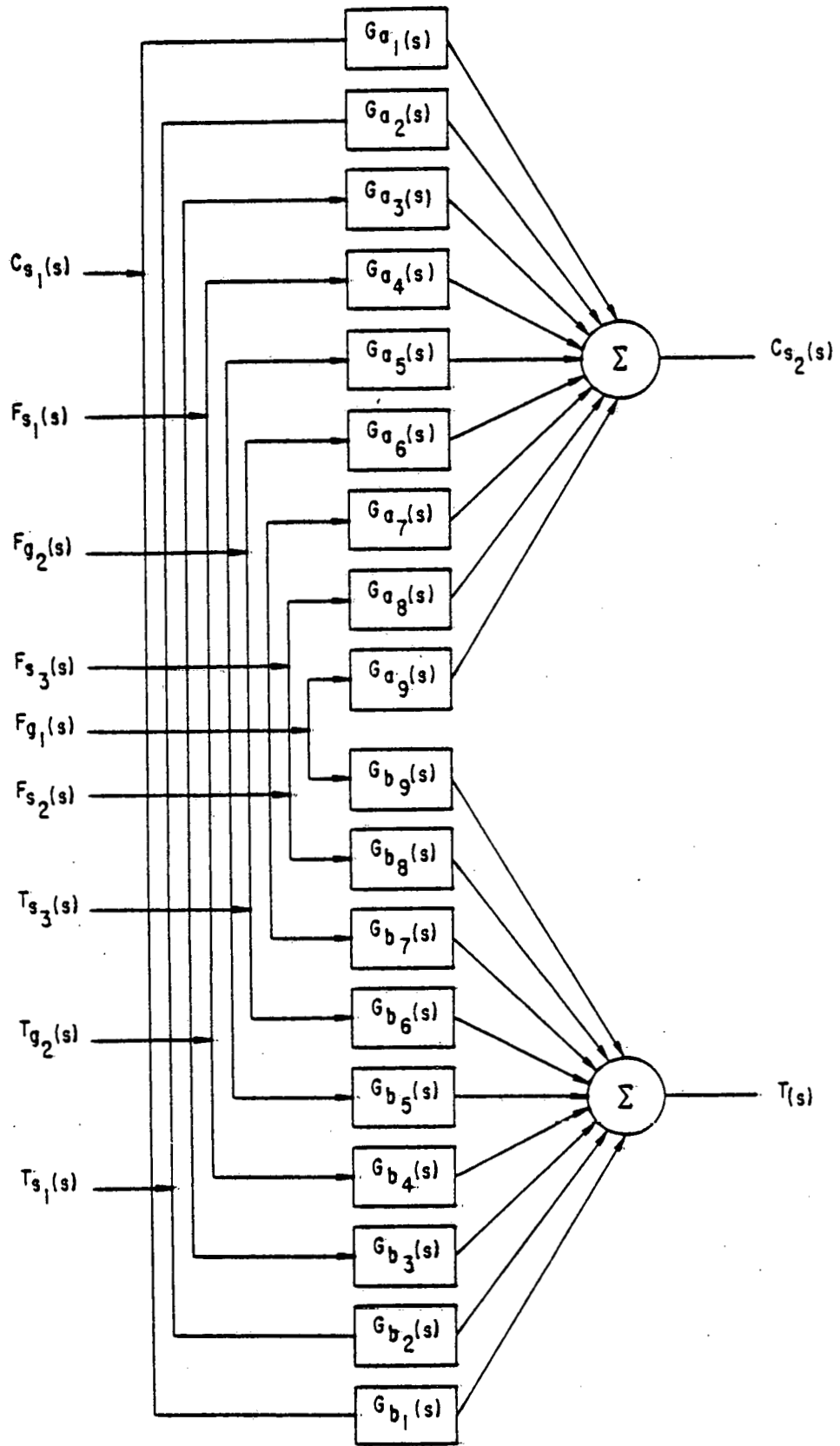


FIG. 8. BLOCK DIAGRAM SHOWING TRANSFER FUNCTIONS FOR INPUT AND OUTPUT VARIABLES

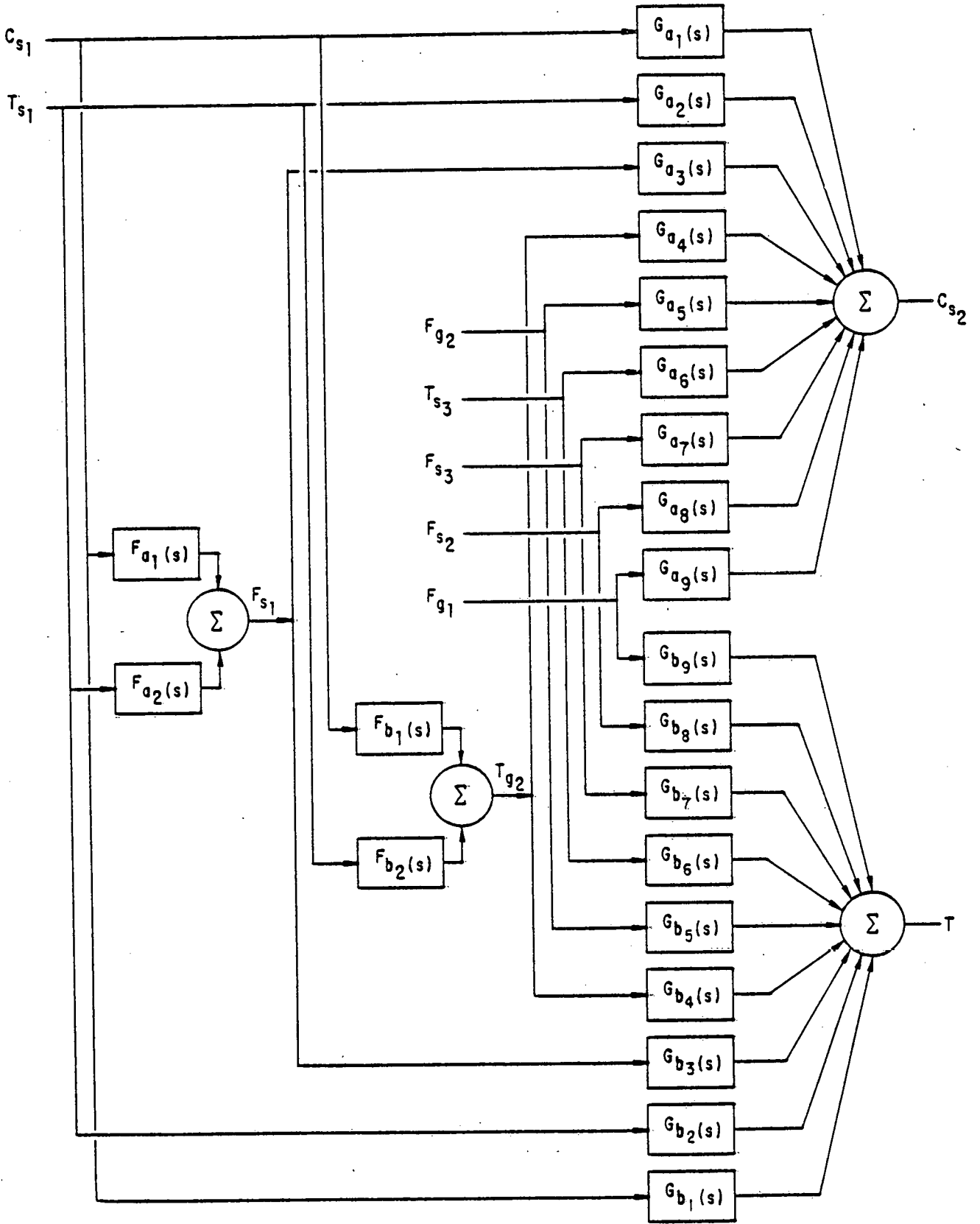


FIG. 9. BLOCK DIAGRAM SHOWING TRANSFER FUNCTIONS FOR FEEDFORWARD CONTROLLERS FOR CONTROLLING T AND  $C_{s2}$  BY MANIPULATING  $F_{s1}$  AND  $T_{g2}$