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POLLUTANTS FROM COAL CONVERSION PROCESSES

Final Technical Report for the Period September 1, 1980—August 31, 1983

By
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Work Performed Under Contract No. FG22-80PC30232

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Raleigh, North Carolina

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FINAL TECHNICAL REPORT

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R. M. Felder
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Research Conducted For

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ABSTRACT

A devolatilized Kentucky bituminous coal, a North Carolina peat, and a New Mexico subbituminous coal have been gasified with steam and oxygen in a pilot-scale fluidized-bed reactor. The reactor was operated at pressures of 570-840 kPa (80-120 psia), molar steam-to-carbon feed ratios of 0.6 to 1.9, and average bed temperatures of 795-1010°C (1460-1850°F). The coal feed rate ranged from 14 to 33 kg/hr (30-73 lb/hr).

The reactor effluents were analyzed for major components and potentially hazardous minor components using gas chromatography; tars and wastewaters condensed from the product were analyzed using gas chromatography/mass spectroscopy, capillary column gas chromatography, and high pressure liquid chromatography; and the feed coals, spent chars, and condensed phase streams were analyzed for selected trace metals using atomic absorption spectrophotometry.

The experimental results were used to provide a basis for the formulation and evaluation of a mathematical model of the gasifier. The model assumes instantaneous devolatilization of coal at the top of the fluidized-bed, instantaneous combustion of carbon at the bottom of the bed, and steam/carbon gasification and water gas shift reaction in a single perfectly mixed isothermal stage.

The effects of various operating parameters and phenomena on reactor performance were determined using the model. As would be expected, carbon conversion and make gas production both increase with bed temperature, steam-to-carbon feed ratio, and solid-phase space time. Both also go up with pressure, but above about 1.7 MPa the increases are negligible. At the temperatures studied, the water-gas shift reaction falls short of equilibrium for pressures lower than 2.1 MPa (confirming experimental results), but the reaction is close to equilibrium at pressures above this value.

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INTRODUCTION

A major obstacle to the commercial development of coal gasification processes is the need to remove undesired species -- potentially hazardous pollutants and species that might function as catalyst poisons in downstream processing units -- from the reactor product gas. In the steam/oxygen gasification of coal, the removal is normally accomplished in two stages: raw gas cleanup, in which particulates, tars and other readily condensable species, and water-soluble species are removed; and acid gas removal, in which carbon dioxide and hydrogen sulfide are removed. The final product is an intermediate Btu fuel gas (principally hydrogen, carbon monoxide, and some methane) or a low Btu fuel gas (the above plus nitrogen for an air-blown gasifier), which may either be burned as is or subjected to further processing and upgrading.

A large number of gas cleaning processes have been implemented either commercially or on a pilot scale, and their ability to accomplish the tasks for which they were designed has been demonstrated. However, a number of environmental questions have received relatively little attention in the process development efforts conducted to date. Among these questions are the following:

1. What potentially hazardous minor and trace species are contained in the gaseous, liquid, and solid effluent streams from the gasification reactor?
2. How do the formation rates of these species depend on the coal feedstock used, and on the gasifier operating conditions?
3. How effectively do the various stages and substages of the gas cleaning process remove the identified species from the product gas? Which species are likely to pass through with the final product fuel gas, and in what quantities?
4. How do the pollutant removal efficiencies of different cleaning processes compare?

A coal gasification and gas cleaning pilot plant has been constructed at North Carolina State University, and has been operated by faculty and staff of the Department of Chemical Engineering. The major goals of the project are to provide answers to the four questions cited above.

The pilot plant includes a 15.2-cm (6-in) I.D. continuous fluidized bed reactor; a particulate, condensables, and solubles (PCS) removal system consisting of a cyclone separator, a venturi scrubber, a mist eliminator, and a filter; and an acid gas removal system (AGRS) consisting of absorption and stripping towers and a flash tank for acid-gas removal and solvent regeneration. The gasifier operates at pressures up to 800 kPa (100 psig), and has a feed capacity of 23 kg coal/h (50 lb/h). Process control and data acquisition and logging systems and an extensive analytical laboratory complete the facility(1,2).

The gasifier does not currently simulate any existing commercial fluidized bed unit, in that the coal is fed at the top rather than at some point internal to the bed. This provides a worst-case situation with respect to production of tars and heavy hydrocarbons. In fact, the levels of these species found in the product gas are relatively close to those characteristic of commercial fixed bed gasifiers. In experiments conducted as part of the project, a raw New Mexico subbituminous coal and a North Carolina peat were gasified with steam and oxygen, and the gaseous, liquid, and solid effluents from the reactor were analyzed.

The primary function of the NCSU gasification reactor is to provide a reproducible synthesis gas for studies of the potential environmental impact of coal gasification processes. The development of correlative and predictive models of the gasifier was felt to be an indispensable adjunct to planning and implementing the overall experimental program. As part of the study, a gasifier model was developed and used to correlate the data for gasification of the bituminous char and the New Mexico subbituminous coal.

This report summarizes the results of the reactor experiments, and reports the model correlations of the gasification data for both feedstocks studied.

EXPERIMENTAL

Equipment and Procedures

The compositions of the three gasifier feedstocks used to date and the ranges of operating variables are summarized in Table 1. For all runs, the feed gas temperature was maintained at 540°C (1000°F).

A bituminous coal char was the initial feedstock used for gasification runs. The devolatilized coal, free of tar-forming volatiles, acted as a clean-gasifying material to test the facility. A New Mexico subbituminous coal was the second feedstock studied. Initial runs utilized coal/char mixtures to test the facility's ability to operate with a high-volatile raw coal, and 18 successful runs were completed with the pure coal as feed. Following the coal runs, six runs with a North Carolina peat were made. Most of the results of environmental interest were obtained with the coal and peat feeds, and the results to be presented in this paper therefore concern these two feeds almost exclusively. Results from the char runs are given by Ferrell et al.(3).

The char and coal feeds to the gasifier were ground to a 10x80 mesh size, and had an average particle diameter of 600-900 microns. The peat was obtained milled, and was screened to pass through a 1/4 inch screen. Multiple samples of the feed were taken before each run, sieved, and subjected to proximate and ultimate analyses and analyses for selected trace constituents.

Multiple spent char samples were taken from the char receiver vessel or from the bottom of the reactor after a run, and samples of elutriated dust were taken from the cyclone collection tank. Since the cyclone fines were sometimes slightly damp, it is possible that condensation on the fines occurred during or after shutdown. Analyses performed on these samples were essentially identical to those performed on the feed coal.

A small side stream was drawn off just downstream of the cyclone. During steady state operation, the side stream passed through a packed ice water-cooled trap, and then through a dry test flowmeter. The water condensed in the trap was weighed. The result provided the primary measurement of the water content of the product gas.

The gas emerging from the cold trap was sampled for subsequent analysis by gas chromatography. Samples were taken at operating pressure in one-liter stainless steel bombs, and at lower pressures using one-liter glass bombs. The glass bombs were coated internally with hexamethyldisilizane to reduce the adsorption of trace sulfur, nitrogen, and hydrocarbon species. The analyses were performed using several gas chromatographs, equipped with thermal conductivity, flame ionization, and flame photometric detectors.

The cold trap condensate was separated into tar and wastewater fractions; the tars were additionally fractionated; and the tar fractions and wastewater were analyzed by high pressure liquid chromatography, gas chromatography/mass spectroscopy, capillary column gas chromatography, and various wet chemical methods. A number of sample preparation and analysis methods for tar and wastewater were tested. The paragraphs below provide brief descriptions of the procedures finally used for most of the analyses; additional details of the wastewater and tar analyses are given by Bradley(7) and Hubik(8). Many of the procedures are similar to procedures described by Gangwal et al.(9), whose report serves as a good reference on analysis of coal gasifier effluents.

Wastewater sample preparation consisted of acidification to pH 4, filtering, and separation into base-neutral and acid fractions using a C_{18} sep-pak. The acid fraction of the trap water was analyzed for phenolics using a Waters HPLC. A 30 cm by 5 mm stainless steel C_{18} bondapak column was used with water/methanol as the mobile phase. A linear gradient from 80% water to pure methanol was run over a ten minute interval. The water was enriched with 1% acetic acid and buffered with sodium acetate to a pH of 4. A UV detector was used at 280 nm.

Tar samples were subjected to a solvent partitioning scheme to separate them into acid, basic, and neutral fractions, and the neutrals were further partitioned into nonpolar and polar compounds, and cyclohexane-insoluble compounds. In addition, the tars were analyzed for polynuclear aromatic hydrocarbons using glass capillary gas chromatography with a flame ionization detector, and organic sulfur-containing species were analyzed by gas chromatography with a flame photometric detector.

Feed coal, spent char, and cyclone dust samples were routinely collected and analyzed for arsenic, lead, and mercury, which previous studies had shown to be the most volatile of the potentially hazardous elements present in coal. Solids were prepared for analysis by digesting one-gram samples in a Parr bomb under 30 atm. of oxygen, with enough concentrated nitric acid to have 0.5% HNO_3 in the final dilution. Analyses were performed using a Perkin-Elmer Model 603 atomic absorption spectrophotometer. A graphite furnace was used for the analyses of arsenic and lead, and mercury was measured by a cold vapor method.

Results

Gases

The product gas from the gasifier contained a large amount of unconverted steam. The mole percent of water ranged from 40% to 50% for peat gasification, and from 35% to 53% for the New Mexico coal runs. Table 2 gives average compositions of the gases that emerged from the sample train cold trap, and Table 3 lists quantities of individual hydrocarbons and sulfur-containing species, reported as grams per kilogram of peat or coal fed.

For each coal feedstock, the gas composition showed little variance from run to run. The peat runs yielded a gas with a slightly lower hydrogen content, and a slightly greater content of hydrocarbons heavier than methane. Sulfur gas content was lower for the peat runs, roughly in proportion to the sulfur content of the feed materials. The relative amounts of the principal product gas constituents are comparable to values found in other studies(9).

The performance of the sample train cold trap was paralleled by the performance of the cyclone and venturi scrubber in the pilot plant. The gas leaving the scrubber contained hydrocarbons and sulfur gases, in amounts comparable to those given in Tables 2 and 3, but no measurable polyaromatic hydrocarbons.

Previous studies with a char feed indicated that sulfur conversion could be roughly estimated by equating it to carbon conversion.(3) Sulfur conversion is plotted versus carbon conversion in Figure 1 for the coal and peat gasification runs. Only data from runs having sulfur balances within 20% of closure are included. The proximity of most points to the 45° line indicates that the equation of sulfur and carbon conversions is a reasonable approximation for the gasification of all three feedstocks used in this study.

Production rates of specific sulfur gases in the gasification of the subbituminous coal, reported as milligrams per kilogram of coal fed, are plotted versus average bed temperature in Figures 2 and 3. Despite scatter in the plots, it appears that the H_2S and COS production rates show a slight increase with increasing temperature. The production rates of methyl mercaptan, carbon disulfide, and thiophene show no apparent dependence on temperature, a result confirmed by statistical analysis.

The two gas phase reactions of most importance involving H_2S and COS are:

I. $COS + H_2O = H_2S + CO_2$, $K_1 = [H_2S][CO_2]/[COS][H_2O]$

II. $COS + H_2 = H_2S + CO$, $K_2 = [H_2S][CO]/[COS][H_2]$

Figures 4 and 5 show plots of the experimental values of the constants K_1 and K_2 as defined above. Also shown on the graphs are lines representing the equilibrium data given in Kohl and Riesenfeld (10). The solid points shown on the figures are from char gasification data, and the open circles are for the New Mexico coal. Figures 4 and 5 suggest that Reaction I is quite close to equilibrium, while Reaction II may or may not be. These results suggest that a reasonable method for estimating H_2S and COS levels in coal gasifier effluents is first, to calculate carbon conversion and product gas composition (major species) using existing correlations or models(6), then to assume that sulfur conversion equals carbon conversion, and finally to calculate the H_2S/COS split by taking Reaction I above to be in equilibrium.

In the gasification of New Mexico coal a large number of hydrocarbon gases are produced. Aliphatics up to butene and butane and simple aromatic compounds have been detected in the gasifier make gas stream. Figures 6 and 7 plot some of the hydrocarbon levels versus the average bed temperature. There is considerable scatter in the data; however, the levels appear to increase slightly with increasing temperature.

Wastewater

Table 4 shows results of the routine wastewater analyses performed for the coal and peat runs, and indicates the production levels of the principal wastewater components. The results for both coal and peat are nearly the same, except for those pertaining to dissolved carbon (carbon, COD, TOC, and TVC). Plots of production levels of various species versus temperature show no clear trends.

The base/neutral extract of the condensate contains most of the polyaromatic hydrocarbon compounds in the wastewater, and the acid extract contains most of the phenolic compounds. Table 5 lists the phenolic compounds identified in the wastewater from the gasification of New Mexico coal. The major species were quantified using HPLC, with results given in Table 6. The proportions of phenol, cresols, and xylenols shown in this table are quite similar to those reported by Gangwal et al.(9) for wastewaters from the semibatch gasification of a Wyoming subbituminous coal.

Figures 8 and 9 show the results of GC/MS analyses of the base-neutral and acid fractions of a wastewater sample from peat gasification. Many other peaks appeared in the scan that could not be positively identified.

In studies of effluents from an entrained flow gasifier, Hansen et al.(11) found that as in our system, higher molecular weight organics were removed effectively by the raw gas cleaning system; however, in their system the organics were removed primarily through adsorption on the particulate matter in the make gas, and the filtered wastewater was relatively clear. The substantially higher concentrations of organics observed in the present studies are attributable both to the greater production rate of organics at the lower temperatures characteristic of fluidized bed gasification, and to the lower concentration of particulates in the fluidized bed product gas.

Tar

In the gasification of the subbituminous coal, tar production varied from 0.10 to 0.14 g tar/g coal fed (dry ash-free basis), and for peat gasification the tar production varied from 0.052 to 0.089 g tar/g peat(DAF). For peat, the tar production rate increased with increasing temperature, while the rate for coal showed no correlation with run conditions. Tar partitioning results are shown in Table 7. Generally, the tar from the peat gasification contained more acidic compounds and fewer high molecular weight PNA compounds, although the differences were not great.

Tar compositions determined by capillary column chromatography are given in Table 8 for three coal runs and a peat run. (The run number prefix GO signifies a coal run, and GOP a peat run.) Results are shown for analysis of tar samples collected both from the sample train following the cyclone (designated "Trap" in the table) and from the receiving tank following the venturi scrubber (designated "PCS"). Table 9 presents the quantitative identification of organic sulfur compounds in the tar from one of the coal runs. Concentrations of sulfur compounds in the peat tar were too low for analysis.

The tar analyses indicate that significant amounts of polyaromatics are in the gas stream as it leaves the reactor, and emerge primarily in the venturi scrubber condensate. It appears that compounds with boiling points higher than that of naphthalene are not present in the gas stream past the PCS system.

Forney et. al.(12), who studied the Synthane coal gasification process for the gasification of a subbituminous coal, found the same types of compounds appearing in the tar as were found in the present studies. In both cases, naphthalene constituted the most prevalent polyaromatic hydrocarbon in the tar. Research by Stompel et. al.(13) on tars from fluidized-bed pyrolysis of a subbituminous coal resulted in the identification of approximately 150 compounds ranging form 2- to 5-rings and from C_{10} to C_{30} in an aromatic hydrocarbon subfraction, which agrees well with the compound structures and molecular weight ranges indicated in our studies with subbituminous coal.

Workers at the Research Triangle Institute, who performed the tar partitioning and capillary GC analyses on our samples, also performed gasification studies employing a bench-scale fixed-bed gasifier, gasifying both Montana and Wyoming subbituminous coals.(9) The distribution of fractions from partitioning the fixed-bed gasification tars was different from those obtained in the present fluidized-bed gasification study, while the distribution of organic acids and bases was similar for both processes. There were more neutrals in the fixed-bed tars, and the fluidized-bed tars contained more components soluble in methylene chloride but not in cyclohexane.

Solomon(14,15) notes a correlation between proximate analysis values for fixed carbon and aromatic carbon concentration in coals. He also suggests that there is a resemblance between tar and parent coal; that tar consists of aromatic "momomers" released from the coal "polymer". Greater tar yields would be expected from coals with greater degrees of aromaticity. Results of tar analyses in the present study are consistent with these observations. There was less fixed carbon in the peat (26%) than in the subbituminous coal (36%), implying a less aromatic structure for the former material. As noted above, tar yields from peat were in fact lower than those from subbituminous coal; moreover, the peat tars contained fewer high molecular weight aromatic constituents and fewer fused rings. Studies currently under way which involve gasification of a Texas lignite follow the same product distribution pattern.

Compounds Condensed from AGRS Feed Stream

During an integrated run, the gases leaving the PCS system pass through a dehydrator and are then compressed to about 35 atm. Following the compressor, the gases are cooled to approximately 10°C and pass through a small knockout drum. A sample of the liquid collected in the knockout drum after a coal run was analyzed by GC-MS. Compound identification results are given in Table 10. Similar species were seen in the compressor knockout liquids from peat runs.

While a variety of hydrocarbon compounds were found in the compressor knockout drum fluid, no aromatic compounds heavier than substituted benzenes were observed. The absence of PNA's and heavy hydrocarbons in the compressor knockout indicates that the scrubbing, cooling, and filtering operations of the PCS system are effective in removing these species.

Trace Metal Volatilization

Analyses for arsenic, lead, and mercury were carried out for coal and peat runs, with the results shown in Table 11. Most of the trace metal mass balance closures are below 100%, indicating the strong possibility that substantial quantities of these volatile metals are present in the gas stream. Methods are currently under development to trap and analyze these metals in the gas stream, but gas stream analyses were not attempted for the peat runs.

While no definite conclusions can be drawn from the results of two runs, it can be seen that for all three metals, the peat char was depleted to a greater extent than the coal char, though the gasification conditions and the final carbon conversion in both runs were almost the same. One possible explanation is that the metals are not as strongly bound to the organic matrix in peat as they are in coal, and hence are more easily devolatilized. Additional data, however, are needed before any firm conclusions can be reached.

The cyclone dust from peat gasification was similarly enriched in all three metals to a larger degree than in coal gasification. A possible explanation for the relatively large amounts of these metal elements in the cyclone dust is that they are volatilized in the gasifier and then tend to condense on the particulates collected in the cyclone separator.

MODELING

Formulation of the Model

The goal of the modeling studies was to formulate the simplest possible model which incorporates the principal gasification reactions and the gross physical characteristics of the reactor, and to determine the degree to which the gasifier performance could be correlated by this model. A well-mixed fluidized-bed model was used for this purpose. The model assumes instantaneous devolatilization and oxidation, followed by gasification in a perfectly mixed bed. The model takes as input the average reactor bed temperature and pressure; the bed dimensions; feed rates of coal, steam, oxygen, and nitrogen; solids holdup in the bed; and ultimate analysis of the feed coal, and calculates carbon conversion and make gas flow rate and composition.

Devolatilization is presumed to occur instantaneously at the point where the coal enters the bed. The extent of devolatilization and composition of the volatile products are taken from rapid pyrolysis data obtained in a separate study at N.C. State University(16), and additional data of Friedman et al.(17) for a western subbituminous coal close in composition to the one used in this study.

After devolatilization has occurred, the following reactions are presumed to take place:

$$C + H_2O = CO + H_2 \quad (1)$$

$$C + 2H_2 = CH_4 \quad (2)$$

$$2C + H_2 + H_2O = CO + CH_4 \quad (3)$$

$$CO + H_2O = CO_2 + H_2 \quad (4)$$

$$C + 1/2O_2 = CO \quad (5)$$

$$C + O_2 = CO_2 \quad (6)$$

$$S + H_2 = H_2S \quad (7)$$

$$H_2S + CO_2 = COS + H_2O \quad (8)$$

Reactions 5 and 6 are the oxidation steps required to supply heat for the remaining reactions. These two reactions are assumed to occur instantaneously in a zone of negligible volume separate from the gasification zone. All oxygen in the feed gas is taken to be consumed to form CO and CO_2, with the combustion product distribution being governed by the relation:

$$C + aO_2 = (2-2a)CO + (2a-1)CO_2$$

where a, the combustion product distribution coefficient, is an adjustable model parameter. A value of a = 0.5 indicates that all CO is formed, while a = 1.0 indicates that only CO_2 is formed.

Reactions 1, 2, and 3 are the reactions with which Johnson(18) at the Institute of Gas Technology correlated gasification kinetics data. The Johnson kinetic expressions are summarized in the body of the report. They include as an adjustable parameter a char reactivity coefficient, f_o, which has values ranging from 0.3 for low-volatile bituminous coal char to about 10 for North Dakota lignite(18).

Reaction 4 is the water-gas shift reaction. A model option allows the assumption of shift reaction equilibrium or the use of kinetic rate equations. The rate expression used is that given by Wen and Tseng(19) and contains an adjustable parameter, f_{wg}, which accounts for the varying catalytic activities of different chars.

The rate of reaction 7 is estimated by assuming that the sulfur conversion equals the carbon conversion, and that all converted sulfur forms hydrogen sulfide by reaction 7 The flow rate of COS is then determined by assuming equilibrium of reaction 8.

In summary, the model has three adjustable parameters: the intrinsic char reactivity factor, f_o; the CO/CO_2 combustion product distribution parameter, a; and the water gas shift reactivity factor, f_{wg}. The other coefficients of the various rate and equilibrium equations are prescribed by the model. Details of these equations and of the model computational procedure are given in the report.

Results

The coal reactivity coefficient, f_o, the combustion product distribution coefficient, a, and the water gas shift reactivity parameter, f_{wg}, were evaluated by using a Pattern Search routine(20) to minimize a function of the sum of squared deviations between predicted and measured values of gasifier performance variables, including carbon conversion, dry make gas flow rate, and mole fractions of hydrogen, carbon monoxide, and carbon dioxide in the make gas. The runs with the best mass balance closures were chosen to provide the data base for the parameter estimation. For the Kentucky bituminous char, the following parameter values were obtained.

$$f_o = 0.276$$

$$a = 0.828$$

$$f_{wg} = 1.29\times10^{-5}$$

The value of a given above indicates that 66% of the carbon oxidized forms CO_2 and 34% forms CO. An equation by Arthur(21) predicts a = 0.57 at 760°C and a = 0.52 at 1100°C, while several gasification studies have assumed a = 1.0(22-25).

The value of $f_{wg} = 1.29\times10^{-5}$ indicates that the shift reaction rate is approximately five orders of magnitude less than the rate typically obtained in catalytic shift reactors. Wen and Tseng(19) used a shift reactivity value of 1.7×10^{-4} in modeling the gasification of a bituminous coal by the Synthane process. The larger value used by Wen and Tseng may be attributed to the differences in the coals used in both studies.

Using the optimal parameter values, the model was run for all char runs. Plots of predicted vs measured values of carbon conversion, dry make gas flow rate, and sweet gas heating value are shown in Figures 10-12. (The sweet gas is defined as the dry make gas with the CO_2 and H_2S removed.) The close proximity of the points to the 45 degree line is gratifying in view of the simplicity of the model.

The same optimization procedure used to determine the optimal parameters for char was employed to find the optimal parameter values for the New Mexico subbituminous coal, using the fast pyrolysis product data of Friedman, et al.(17) to calculate the devolatilization gas product distributions. The resulting parameter values were:

$f_o = 4.20$

$a = 1.00$

$f_{wg} = 1.2 \times 10^{-4}$

The char reactivity parameter for coal is much larger than that obtained for the Kentucky char. The combustion coefficient does not differ greatly for the coal and the char; however, the shift reactivity parameter is an order of magnitude greater for the coal than for the char. A possible reason for the greater shift reactivity of the New Mexico coal compared to the char is the different ash contents of the two materials: the coal had an feed ash content of 22.6%, while the ash content of the char was only 10.7%. The minerals in the ash fraction of coal serve as catalysts for the shift reaction. In addition, during gasification the coal was converted to a greater extent than the char, giving an even larger difference in ash contents. The shift reactivity parameter obtained in this study for a subbituminous coal agrees well with the value used by Wen and Tseng(19) for a bituminous coal (f_{wg} = 1.7×10^{-4}).

The model was used to correlate the New Mexico coal run data using the optimal parameter values. In general, the agreements between model predictions and experimental measurements were excellent. Comparisons of predicted and measured reactor variables are shown in Figures 13 and 14.

For each run, the water-gas shift equilibrium ratio was calculated from both experimental measurements and model predictions of the gas composition. A plot of the predicted vs experimental values of this ratio is given in Figure 15. The substantial degree of scatter may be attributed to the simplicity of the model, and equally to the fact that the mole fractions which are the constituents of K_{wg} are interdependent, so that an experimental error in one of them affects the values of the others.

The significance of this plot emerges when it is compared with Figure 16, which shows the values of K_{wg} predicted assuming shift equilibrium. This assumption leads to overprediction of K_{wg} and lends support to the conclusion that the shift reaction should not be assumed to proceed to equilibrium.

SUMMARY AND CONCLUSIONS

The pilot plant facility has been used for 18 runs with a New Mexico subbituminous coal and 6 runs with a North Carolina peat. Sampling and chemical analysis methods were developed for all feed and effluent streams. Methods used for the sampling and analysis of gaseous streams proved satisfactory for the major gases and for all minor gaseous components present in concentrations greater than a few parts per million. Detailed chemical compound analyses for solid and liquid streams are generally satisfactory, but are still under development.

The sulfur conversion can be roughly estimated by equating it with the carbon conversion for New Mexico coal and North Carolina peat. The distribution between H_2S and COS in the make gas may be predicted by assuming that the reaction,

$$COS + H_2O = H_2S + CO_2$$

is at equilibrium at the temperature at the top of the fluidized bed.

In the gasification of New Mexico coal a variety of hydrocarbon gases are produced, including aliphatics up to butene and butane and simple aromatic compounds. Production rates of these hydrocarbons generally increase with increasing reactor bed temperature.

The concentrations of various species in the water condensate from the sample train have been normalized to determine rates of evolution in milligrams per kilogram of coal fed to the gasifier. No clear trends with reactor temperature are evident, indicating that for the temperature range covered, the reactor temperature has little effect on the formation rates of wastewater species. Comparison of coal and peat wastewater component concentrations showed no major differences except for dissolved carbon (carbon,COD,TOC,TVC), which was present to a greater extent in the wastewater from peat gasification.

Wastewater samples were analyzed by high pressure liquid chromatography (HPLC) for phenolics, and base/neutral and acid wastewater extracts were analyzed by GC/MS. As anticipated, the base/neutral extract was found to contain the majority of the PAH's, while the acid extract contained most of the phenolics. Coal wastewater showed greater amounts of PAH's than peat wastewater.

Production rates of tar were calculated from cold trap data. The tar rate, calculated as g tar/kg feed, was greater for coal than for peat. The tar production rate for peat increased with increasing temperature, while that for coal showed no correlation with run conditions. Peat tars contained fewer high molecular weight PNA's, but greater amounts of acidic compounds compared to coal. The sulfur content of peat tars was too low to be detected. No detectable polynuclear aromatic compounds are in the gases leaving the PCS system, as evidenced by the absence of these compounds in the compressor knockout drum condensate. Both the tar and wastewater analyses are consistent with a correlation of tar and aromatic hydrocarbon production levels with the aromatic structure of the coal feed, with the proximate fixed carbon content serving as an index of the degree of aromaticity.

Trace element analyses indicate that substantial fractions of the arsenic, lead, and mercury in the feed coal are volatilized in the gasifier. Mass balance closures on these elements are not yet satisfactory, however, and refinements in sampling procedures will be necessary before quantitative conclusions can be drawn regarding the extent of volatilization.

In the gasification of a New Mexico subbituminous coal, roughly 66% of the char oxidized prior to gasification forms CO_2 and the balance forms CO. The water-gas shift reaction rate is approximately five orders of magnitude less than the rate typically obtained in catalytic shift reactors.

A simple model which treats devolatilization and oxidation as instantaneous and considers the gasification zone to be a perfect mixer provides a good correlation of the gasifier output with process conditions.

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TABLE 1
GASIFIER FEEDSTOCKS AND RUN CONDITIONS

	Coal Char	N.M. Coal	N.C. Peat
Rank	Bituminous	Subbituminous	Peat
Origin	Western Ky.	Fruitland, NM	Creswell, NC
Supplier	Peabody Coal Co.	Utah Int. Co.	First Colony Farms
Pretreatment	Devolatilized at 2000°F	none	partially dewatered
Proximate Analysis			
Fixed Carbon	86.0	36.2	26.3
Volatile Matter	2.4	31.1	46.3
Moisture	0.9	9.7	22.8
Ash	10.7	23.0	4.6
Ultimate Analysis			
Carbon	83.8	50.2	45.9
Hydrogen	0.6	4.2	4.3
Oxygen	2.2	20.7	44.1
Nitrogen	0.1	1.1	0.9
Sulfur	2.6	0.8	0.2
Ash	10.7	23.0	4.6
Run Conditions			
Bed Temp, °C	920 - 1030	875 - 990	860 - 940
Pressure, kPa	630 - 840	795 - 840	795 - 825
Coal feed, kg/hr	11 - 30	18 - 30	17 - 33
Molar S/C feed ratio	0.63 - 1.55	0.97 - 1.90	0.57 - 1.70
Bed height, m	1.0 - 1.3	0.8 - 1.0	0.4 - 0.5
Feed gas velocity, m/s	0.17 - 0.46	0.24 - 0.37	0.15 - 0.24

analyses in weight percent

TABLE 2
COMPOSITIONS OF MAKE GASES FROM GASIFICATION OF NEW MEXICO COAL AND NORTH CAROLINA PEAT
Mole %, dry basis

	New Mexico Coal	North Carolina Peat
CO	17.0	16.1
H_2	31.8	27.9
CH_4	6.6	6.4
CO_2	22.5	22.6
N_2	20.5	25.2
H_2S	0.2650	0.0500
COS	0.0080	0.0025
CS_2	0.0002	0.0002
CH_3SH	0.0020	0.0030
C_2H_5SH	0.0002	----
Thiophene	0.0025	0.0015
Ethylene	0.4180	0.5400
Ethane	0.5040	0.6700
Propylene	0.1400	0.2900
Propane	0.0420	0.0840
Butylene	0.0490	----
Butane	0.0220	0.0380
Benzene	0.0810	0.0880
Toluene	0.0480	0.0590
Ethylbenzene	0.0010	----
Xylenes	0.0045	----

TABLE 3
GASEOUS PRODUCTS OF THE GASIFICATION OF NEW MEXICO COAL AND NORTH CAROLINA PEAT
Grams per kg of feed

Species	N.M. Coal	N.C. Peat
H_2S	2.7 - 9.8	0.8 - 1.1
COS	0.14 - 0.56	0.06 - 0.09
CS_2	0.003 - 0.018	0.00 - 0.009
CH_3SH	0.02 - 0.16	0.05 0.12
C_2H_5SH	0.005 - 0.012	---
Thiophene	0.07 - 0.61	0.05 - 0.11
Methane	42 - 105	47 - 57
Ethylene	3 - 11	6 - 9
Ethane	5 - 17	1 - 10
Propylene	1.7 - 5.0	3 - 11
Propane	0.6 - 1.5	0.8 - 3.0
Butylene	1.5 - 2.0	---
Butane	0.4 - 1.9	0.5 - 2.1
Benzene	0.9 - 8.1	2.5 - 4.5
Toluene	0.9 - 6.2	1.7 - 5.7
Xylenes	0.2 - 0.5	---
Ethylbenzene	0.05 - 0.10	---

TABLE 4
TRAP WATER ANALYSES FOR COAL AND PEAT

	Concentration mg/l except pH		Production Level g/kg feed	
	Peat	Coal	Peat	Coal
pH	8.2 - 8.9	8.0 - 8.7	---	---
Nitrogen	4700 - 9800	5400 - 8200	3.5 - 6.5	5 - 9
Ammonia	3900 - 8000	3900 - 7400	2.8 - 5.2	4.0 - 8.3
Cyanide	37 - 75	10 - 270	0.02 - 0.04	0.01 - 0.3
Cyanate	600 - 1770	360 - 7200	0.3 - 1.5	0.4 - 6.8
Thiocyanate	230 - 430	100 - 700	0.13 - 0.45	0.1 - 0.7
Sulfate	2 - 20	10 - 300	0.001 - 0.023	0.02 - 0.28
Sulfite	6 - 60	10 - 70	0.004 - 0.07	0.007 - 0.08
Chloride	50 - 180	10 - 130	0.03 - 0.14	0.01 - 0.2
Fluoride	12 - 120	6 - 30	0.01 - 0.06	0.004 - 0.02
Carbon	10400 - 18000	2500 - 7500	7.4 - 12.2	2.1 - 8.5
COD	30500 - 39600	950 - 10300	21 - 36	1 - 11
TOC	9300 - 13600	1200 - 6800	6 - 11	1 - 7
TVC	2500 - 11000	900 - 2400	2 - 7	0.8 - 2.7

TABLE 5
PHENOLIC COMPOUNDS IDENTIFIED IN COAL GASIFICATION WASTEWATER

phenol
2-methylphenol
4-methylphenol
2,5-dimethylphenol
2-ethylphenol
4-ethylphenol
2,5 dimethylphenol
3,5-dimethylphenol
2,4-dimethylphenol
catechol
resorcinol
hydroquinone
1H-indole
5-methylresorcinol
4-methylcatechol
3-methylcatechol
4-ethylresorcinol
3,4,5-trimethylphenol
1,4-dimethoxybenzene
2,2'-bifuran
7-methyl benzofuran
ethenyl benzaldehyde
1-naphthalenol
2-naphthalenol
ethanone, 1-(4-hydroxyphenol)
ethanone, 1-(2-hydroxyphenyl)
4,5-dimethylresorcinol
furan, 3-phenyl
benzonitrile, 4-hydroxy
ethanone, 1-(2,4-dihydroxyphenyl)
benzene
benzonitrile, 4-hydroxy
benzene, 1-methyl-2(methylthio)
benzenemethanamine, N-methyl-N-nitroso
2-propyn-1-ol, 3-p-tolyl
2,4(1H,3H)-pyrimidinedione, 6-methyl

TABLE 6
TRAP WATER PHENOLICS ANALYSES

Compound	Average Concentration, mg/l	Average Emission Rate, g/kg coal
Phenol	950	0.97
Cresol	450	0.44
Xylenol	300	0.23
Catechol	250	0.22
3-Methylcatechol	200	0.11
Ethylphenol	170	0.17
Resorcinol	150	0.12
4-Methylcatechol	120	0.11
5-Methylresorcinol	90	0.06
Indole	70	0.09
Hydroquinone	70	0.06
4-Ethylresorcinol	50	0.11
Naphthol	30	0.03

TABLE 7
TAR PARTITIONING RESULTS
Wt%

GOP-4B	GO-69B	GO-70	GO-76	GO-76	GO-78	
Acids	10.9	34.7	16.5	11.2	17.3	22.5
Bases	20.9	27.5	4.7	6.7	6.1	4.4
Total neutrals	68.3	37.7	78.8	80.1	76.7	*
Non polar	25.1	5.5	24.7	30.0	11.5	16.6
PNAs	36.0	26.7	10.7	11.5	26.9	15.8
Polar	7.2	5.5	15.3	15.2	16.5	20.8
Cyclohexane Insolubles	--	--	28.1	23.4	21.8	*

* - Analytical difficulties with the cyclohexane-insoluble species precluded a material balance for the neutral fraction of the peat-derived tar.

TABLE 8
TAR ANALYSES
Wt%

	RUN GO-76 (PCS)	RUN GO-76 (TRAP)	RUN GO-78 (TRAP)	RUN GOP-4 (TRAP)
naphthalene	1.30	2.11	2.10	6.06
benzothiophene	0.06	0.09	0.08	0.02
quinoline	0.09	0.16	0.13	0.20
2-methylnaphthalene	0.60	0.79	0.97	3.17
1-methylnaphthalene	0.37	0.52	0.81	1.22
biphenyl	0.14	0.16	0.28	0.74
acenaphthylene	0.53	0.71	0.60	0.80
acenaphthene	0.30	0.34	0.26	1.83
dibenzofuran	0.46	0.53	0.53	2.58
fluorene	0.51	0.53	0.43	1.74
phenanthrene	0.67	0.62	0.47	1.70
anthracene	0.32	0.38	0.49	0.56
fluoranthene	0.32	0.36	0.23	0.53
pyrene	0.25	0.26	0.17	0.14
benzo(a)anthracene	0.07	0.16	0.05	0.07
chrysene	0.09	0.13	0.04	0.04
triphenylene	0.03	0.06	0.02	0.02
benzo(b)fluoranthene	0.05	0.11	0.01	
benzo(k)fluoranthene	0.01	0.06	0.01	
benzo(e)pyrene	0.01	0.05	0.01	0.50
benzo(a)pyrene	0.03	0.11	0.02	
perylene	0.01	0.05	0.01	
dibenzothiophene	0.08	0.07	0.09	ND

NA - not analyzed for
ND - not detected

TABLE 9
SULFUR SPECIES IN TAR FROM SUBBITUMINOUS COAL GASIFICATION
Wt%

thiophene	0.01
methylthiophenes	0.02
C_2-thiophenes	0.03
C_3-thiophenes	0.03
benzothiophene	0.13
C_1-benzothiophenes	0.05
C_2-benzothiophenes	0.06
C_3-benzothiophenes	0.05
dibenzothiophenes	0.09
napthothiophenes	0.08
phenanthrothiophenes	0.06
naphthobenzothiophenes	0.09
Total	0.70

TABLE 10
COMPOUNDS IDENTIFIED IN COMPRESSOR KNOCKOUT DRUM LIQUID

1-pentene
hydrocarbon
benzene
hydrocarbon
toluene
cyclo C4-C5
hydrocarbon
ethyl benzene
dimethyl benzene
substituted benzene
C_8 hydrocarbon
C_9 hydrocarbon
propyl or ethyl methyl substituted benzene
propyl or ethyl methyl substituted benzene
1-decene
2-propyl benzene
1-ethyl-4-methyl benzene

TABLE 11
MASS BALANCE RESULTS FOR ARSENIC, LEAD, AND MERCURY

	Peat		Coal	
	ppm	mg/hr	ppm	mg/hr
Arsenic				
Input - Feed	1.9	50	3.5	66
Output:				
Char	2.1	10	3.6	22
Cyclone dust	12.0	37	5.8	10
Cold Trap:				
Tar	2.2	4	2.4	4
Solids	*	*	7.1	1
Water	*	*	0.19	4
Total		51		42
Mass Balance Closure: % of Input		102		62
Lead				
Input - Feed	6.4	167	7.1	132
Output:				
Char	3.3	16	4.8	29
Cyclone dust	20.0	62	5.7	10
Cold Trap:				
Tar	6.1	10	2.0	3
Solids	41.0	12	15.6	2
Water	*	*	0.01	<1
Total		100		44
Mass Balance Closure: % of Input		60		33
Mercury				
Input - Feed	0.52	13.8	0.058	1.1
Output:				
Char	0.29	1.4	0.048	0.29
Cyclone dust	0.064	1.98	0.054	0.09
Cold Trap:				
Tar	0.79	1.37	1.47	2.36
Solids	8.1	2.42	5.33	0.67
Water	*	*	0.003	0.08
Total		7.17		3.49
Mass Balance Closure: % of Input		52		317

FIGURE 1

SULFUR CONVERSION VERSUS CARBON CONVERSION

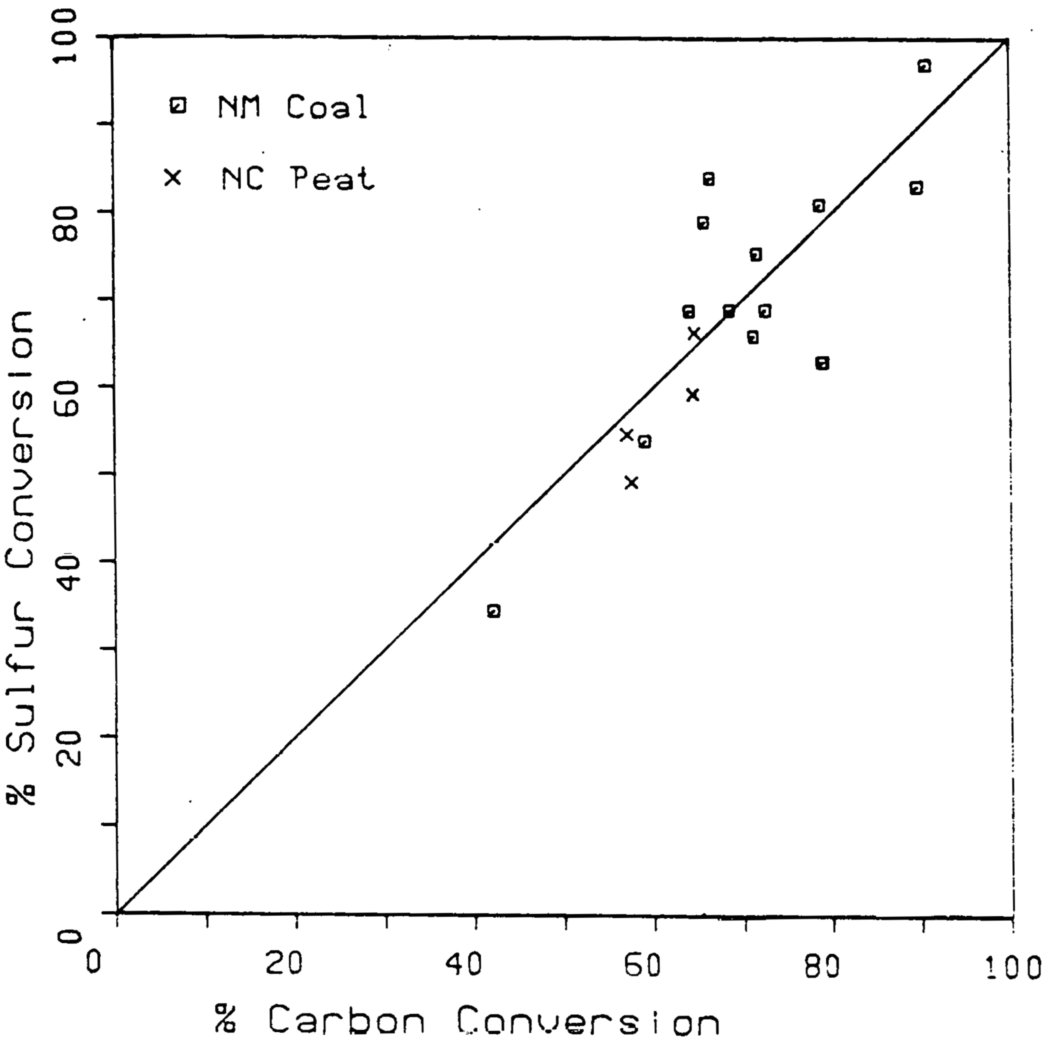

FIGURE 2

PRODUCTION RATES OF HYDROGEN SULFIDE AND CARBONYL SULFIDE IN SUBBITUMINOUS COAL GASIFICATION

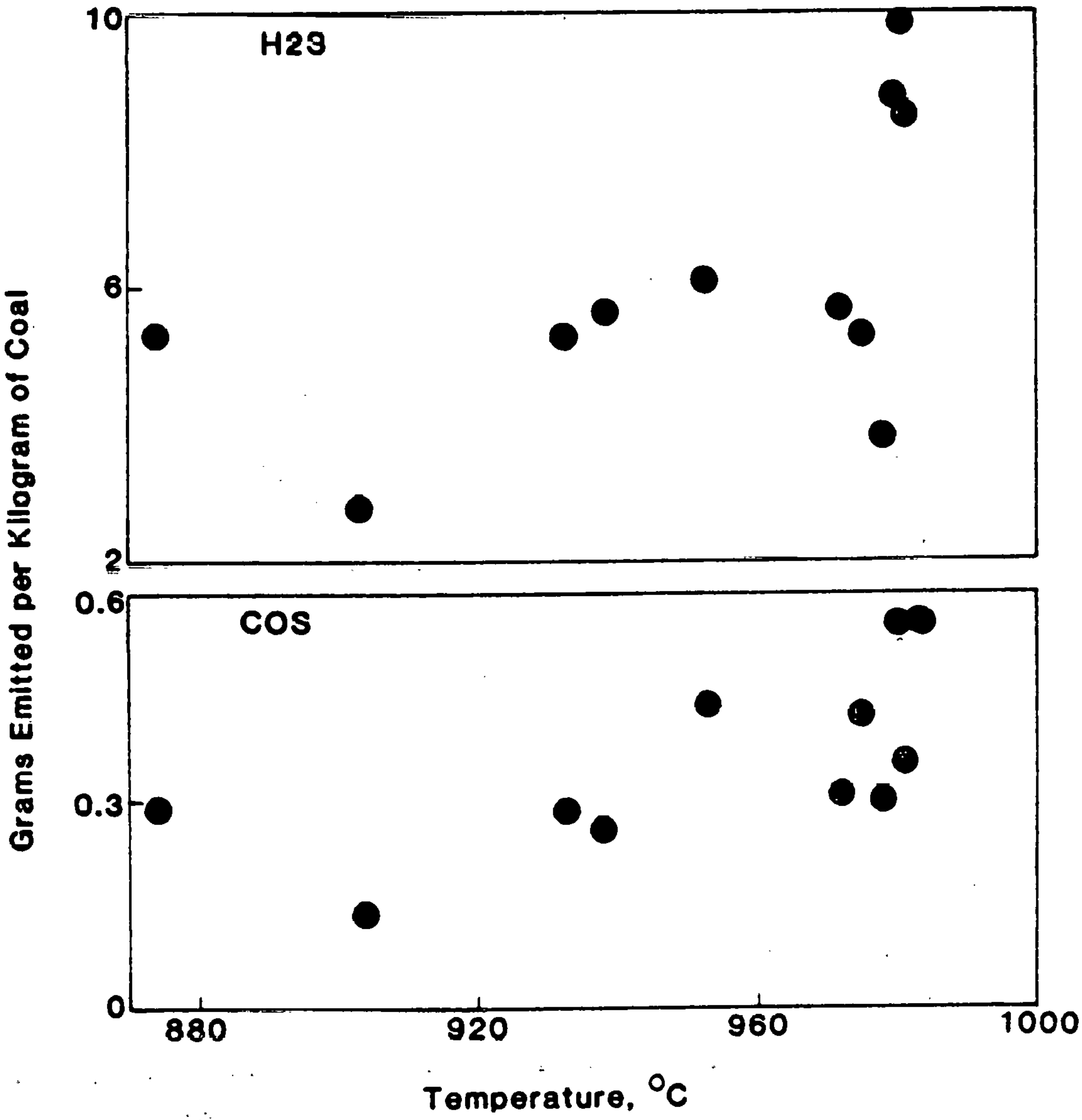

FIGURE 3

PRODUCTION RATES OF METHYL MERCAPTAN, CARBON DISULFIDE, AND THIOPHENE IN SUBBITUMINOUS COAL GASIFICATION

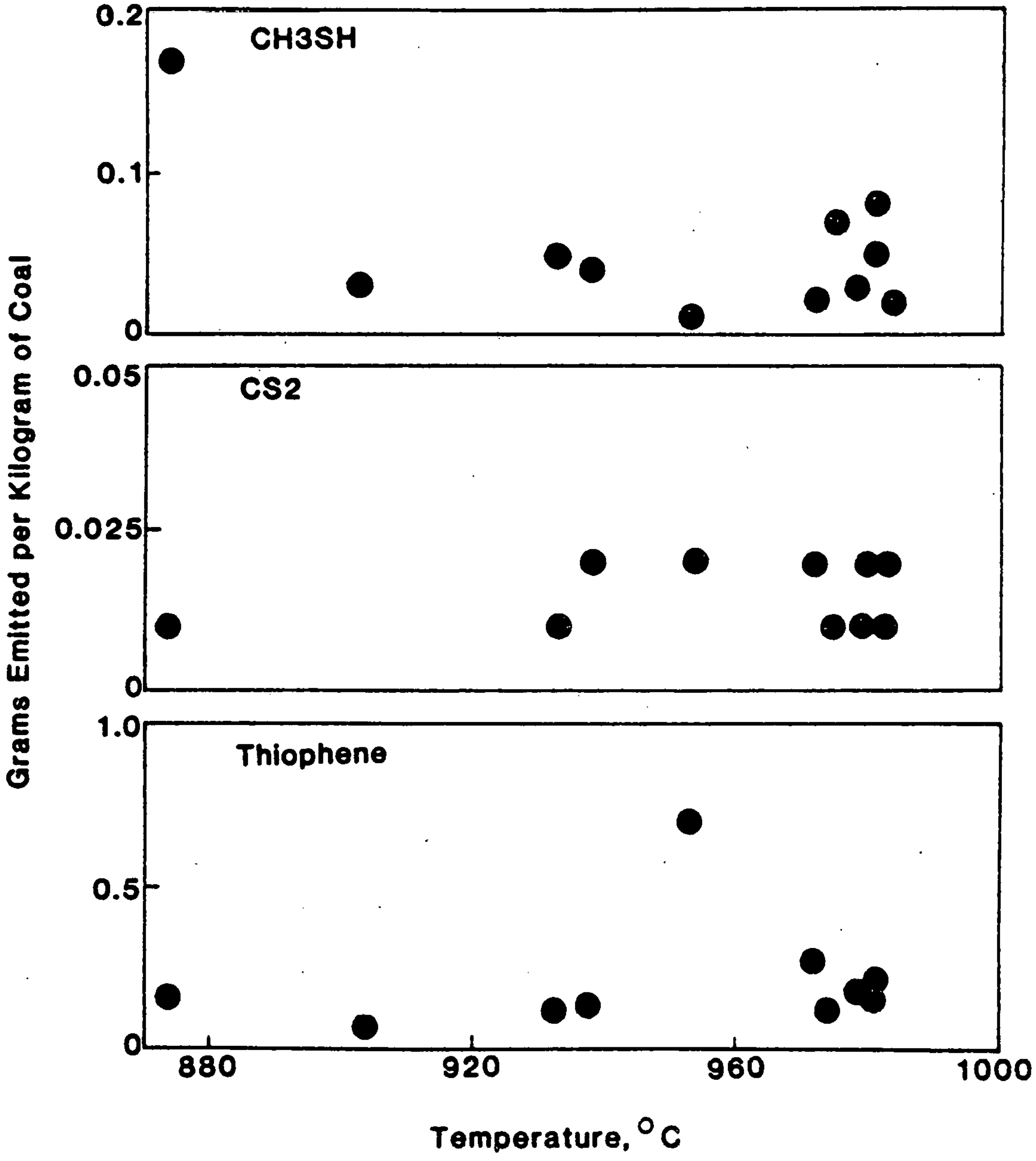

FIGURE 4

CONCENTRATION RATIO FOR H_2S-CO_2 SHIFT REACTION

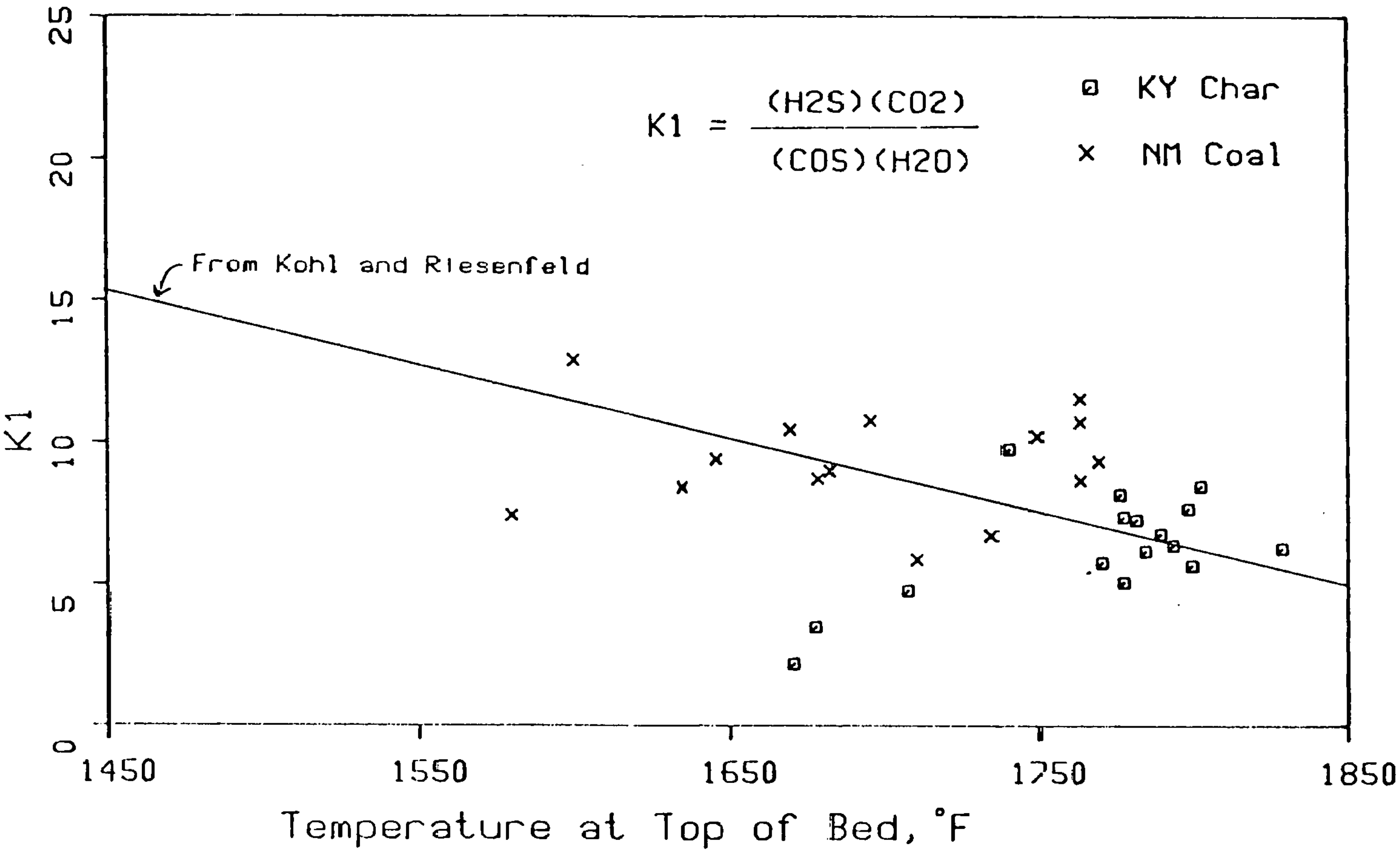

FIGURE 5

CONCENTRATION RATIO FOR H_2S-CO SHIFT REACTION

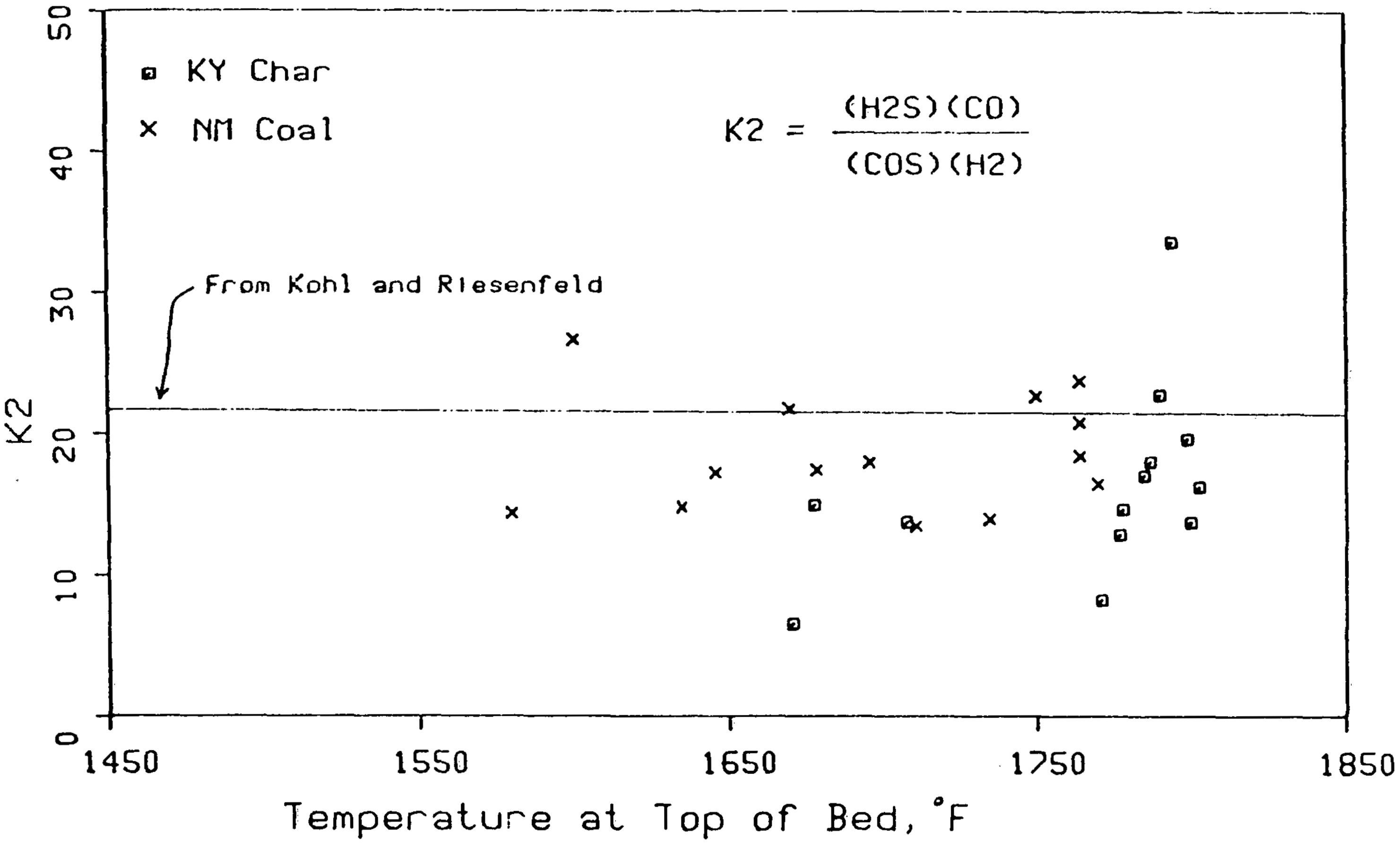

FIGURE 6

PRODUCTION RATES OF METHANE, ETHANE, AND ETHYLENE
IN SUBBITUMINOUS COAL GASIFICATION

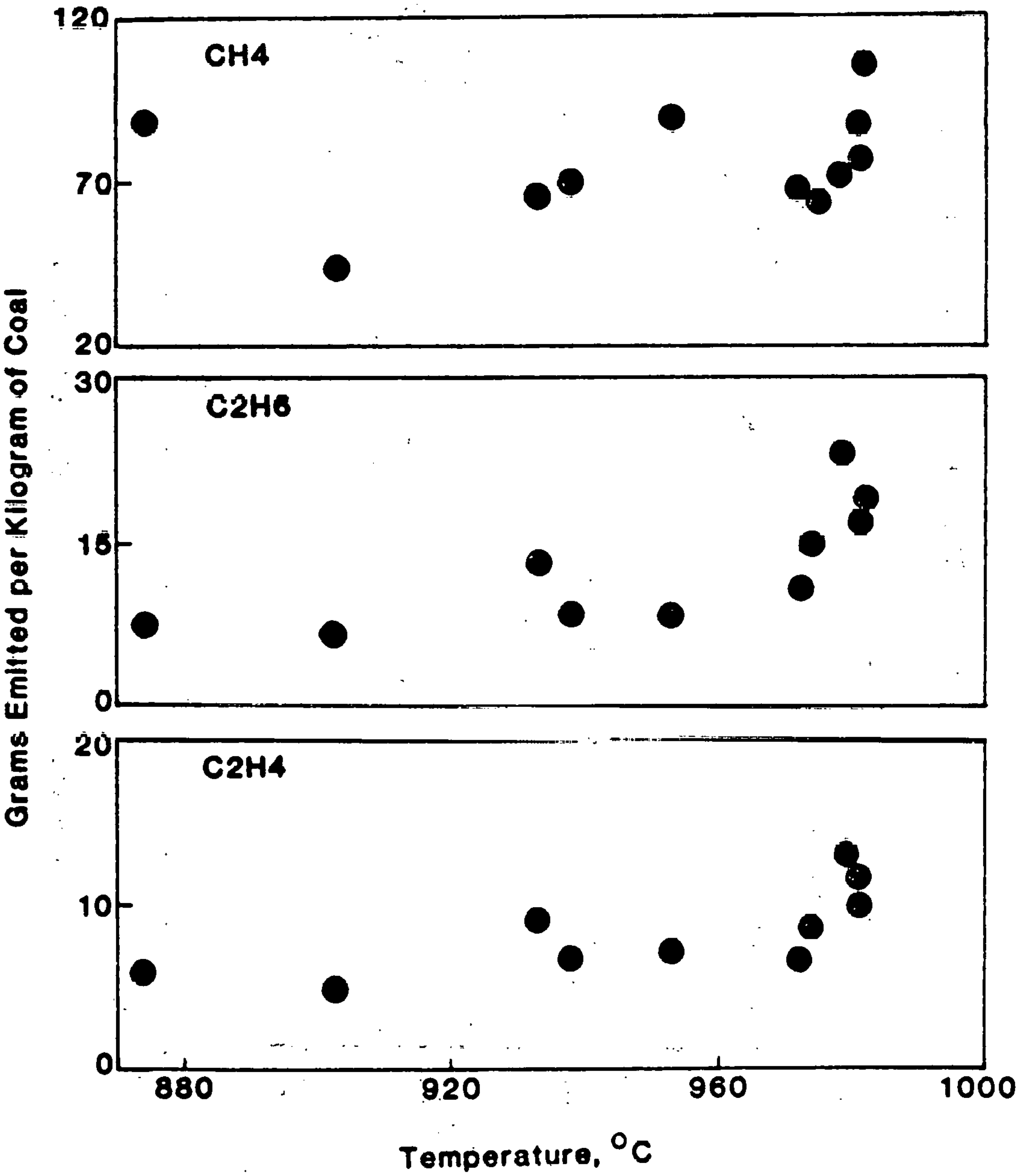

FIGURE 7

PRODUCTION RATES OF BENZENE AND TOLUENE
IN SUBBITUMINOUS COAL GASIFICATION

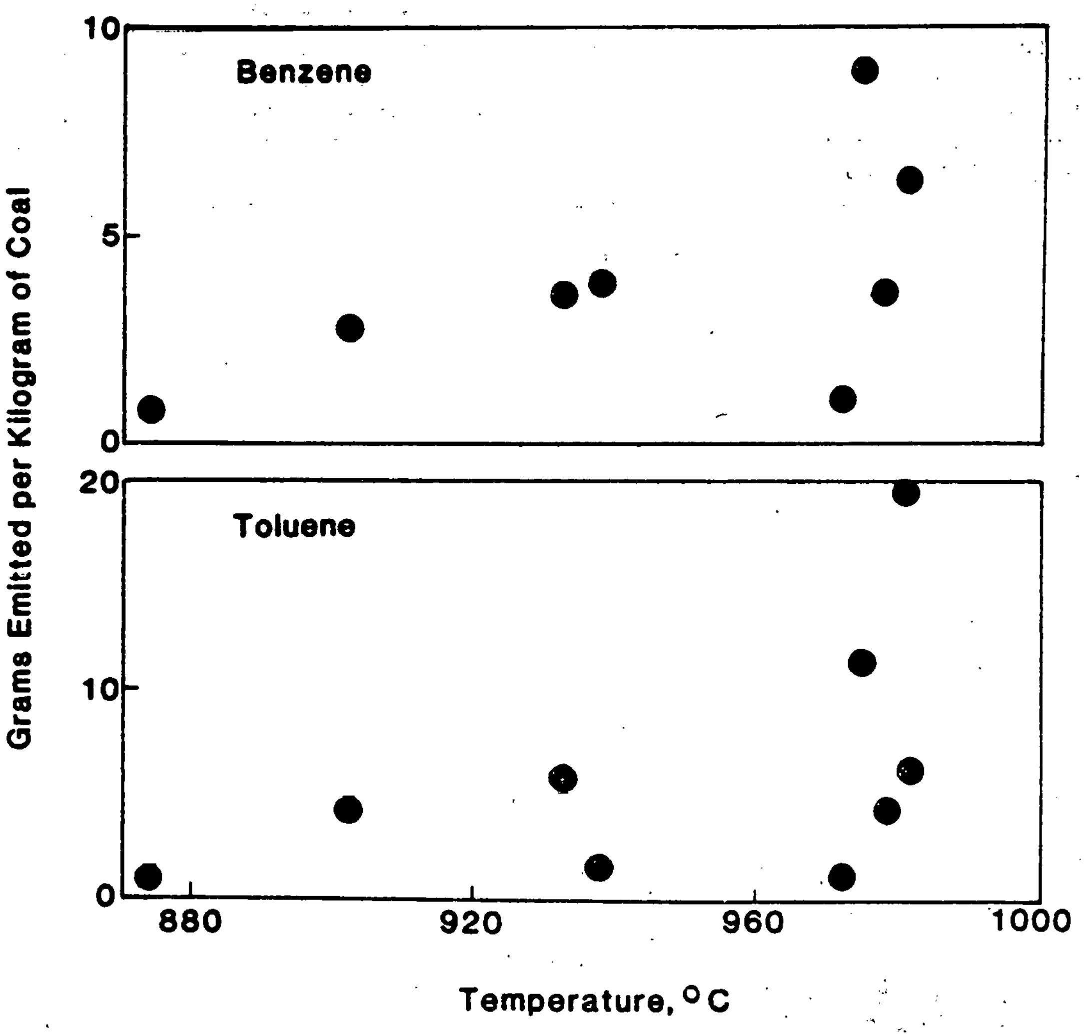

FIGURE 8

ANALYSIS OF BASE-NEUTRAL FRACTION OF WASTEWATER FROM PEAT GASIFICATION

Peak No	Compound	Peak No	Compound
1	pyridine	17	phenol
2	toluene	18	?
3	cyclopentanone	19	napthalene
4	methylpyridine	20	?
5	3-ethylcyclopentene	21	quinoline or isoquinoline
6	2 (1H)-pyridinone	22	ethyl substituted phenol
7	hydrocarbon	23	dihydro substituted inden-1-one
8	1-(1H-pyrazol-4-yl)-ethanone	24	methylnapthalene
9	3,5-dimethylpyridine	25	methylnapthalene
10	3-methyl-2-cyclopenten-1-one	26	benzeneacteonitrile
11	5-methyl-2-furancarboxaldehyde	27	biphenylene or acenaphthylene
12	hydrocarbon	28	1,2-dihydroacenapthylene
13	benzofuran	29	dibenzofuran
14	hydrocarbon	30	9H-fluorene
15	1-propynylbenzene	31	phenanthene or anthracene
16	1-phenylethonone		

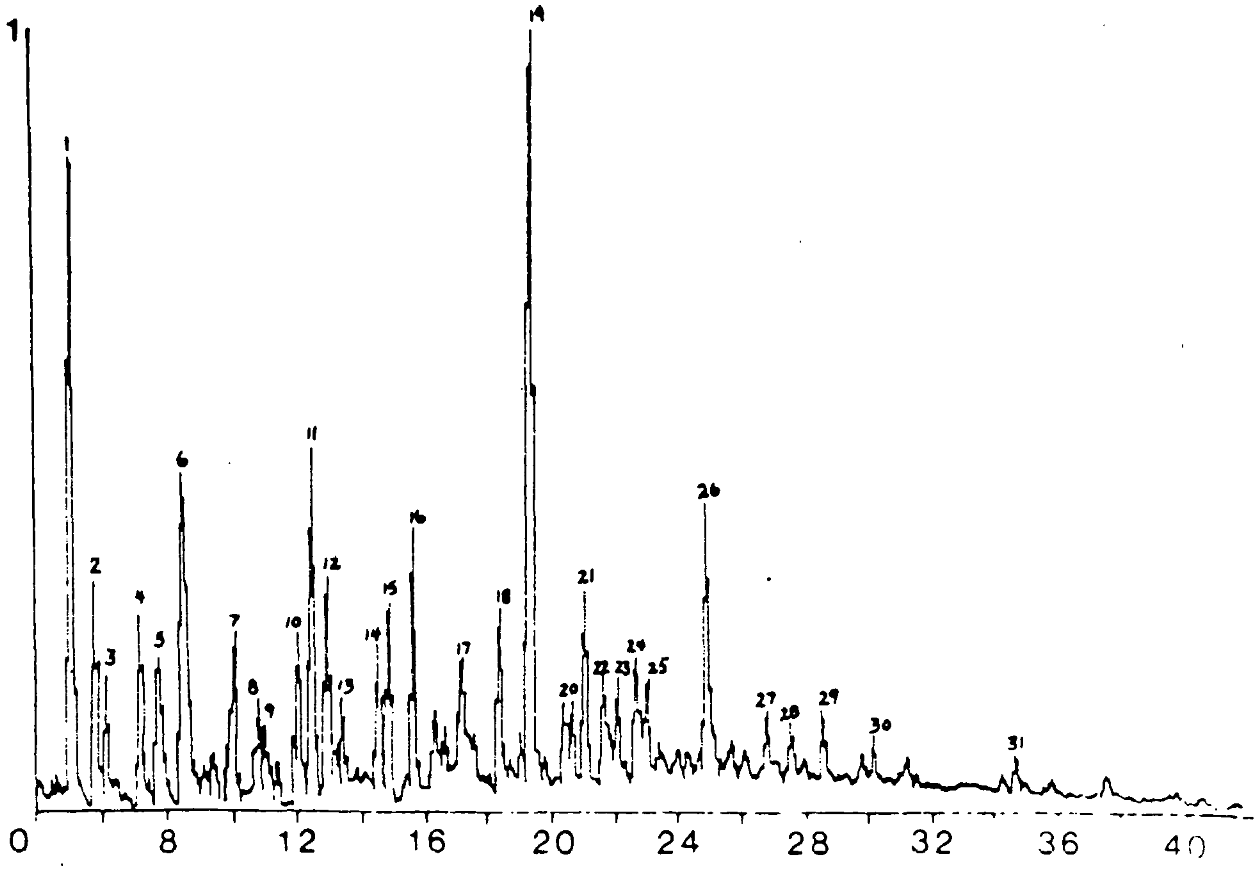

FIGURE 9

ANALYSIS OF ACID FRACTION OF WASTEWATER FROM PEAT GASIFICATION

Peak No	Compound
1	phenol
2	2-methoxyphenol
3	2,6-dimethyl or ethyl substituted phenol
4	methyl substituted phenol
5	dimethyl substituted phenol
6	ethyl or dimethyl substituted phenol
7	1-(2,4-dihydroxyphenyl)ethanone
8	methylethyl or propyl substituted phenol
9	3,4-dimethoxyphenol
10	sulfur containing hydrocarbon
11	hydroxy-methoxyphenyl substituted ethanone
12	hexanedioic acid ester

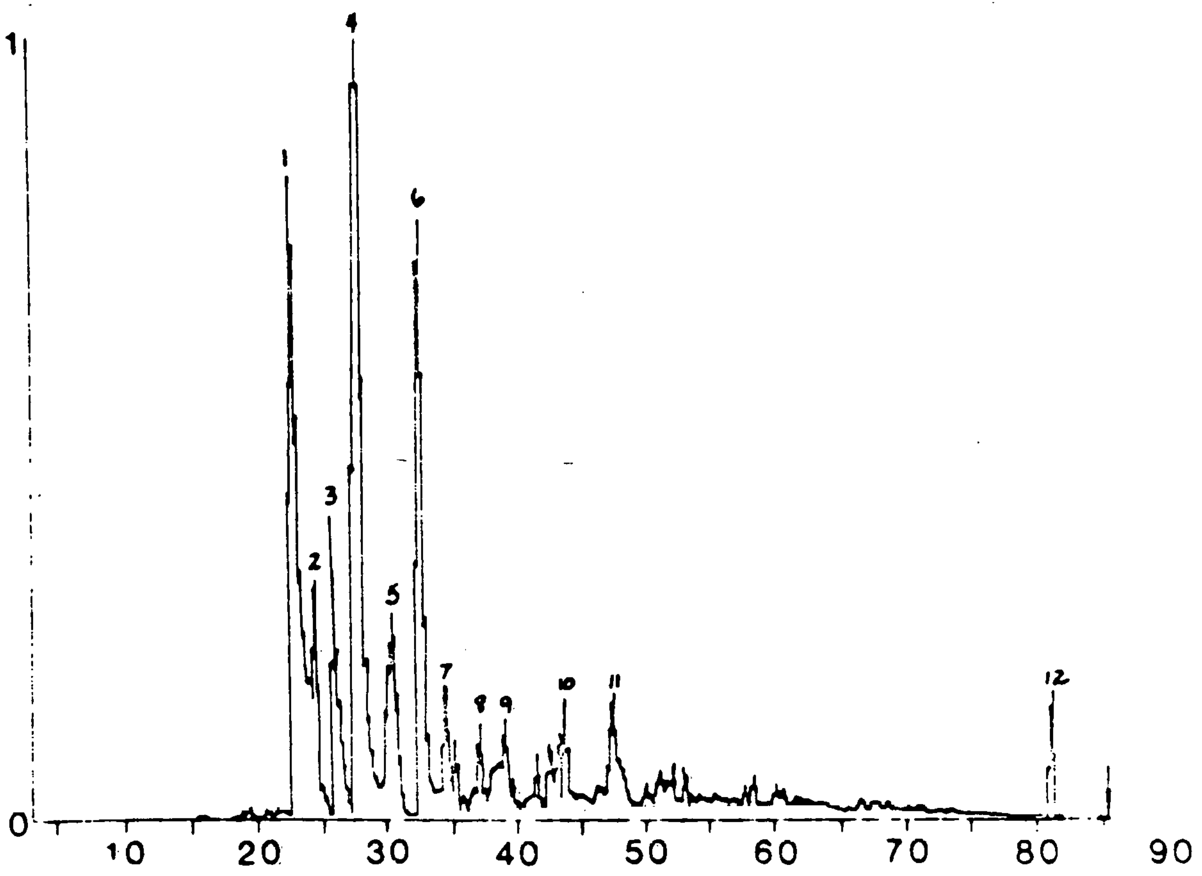

FIGURE 10

PREDICTED VS. EXPERIMENTAL CARBON CONVERSION FOR KY. CHAR

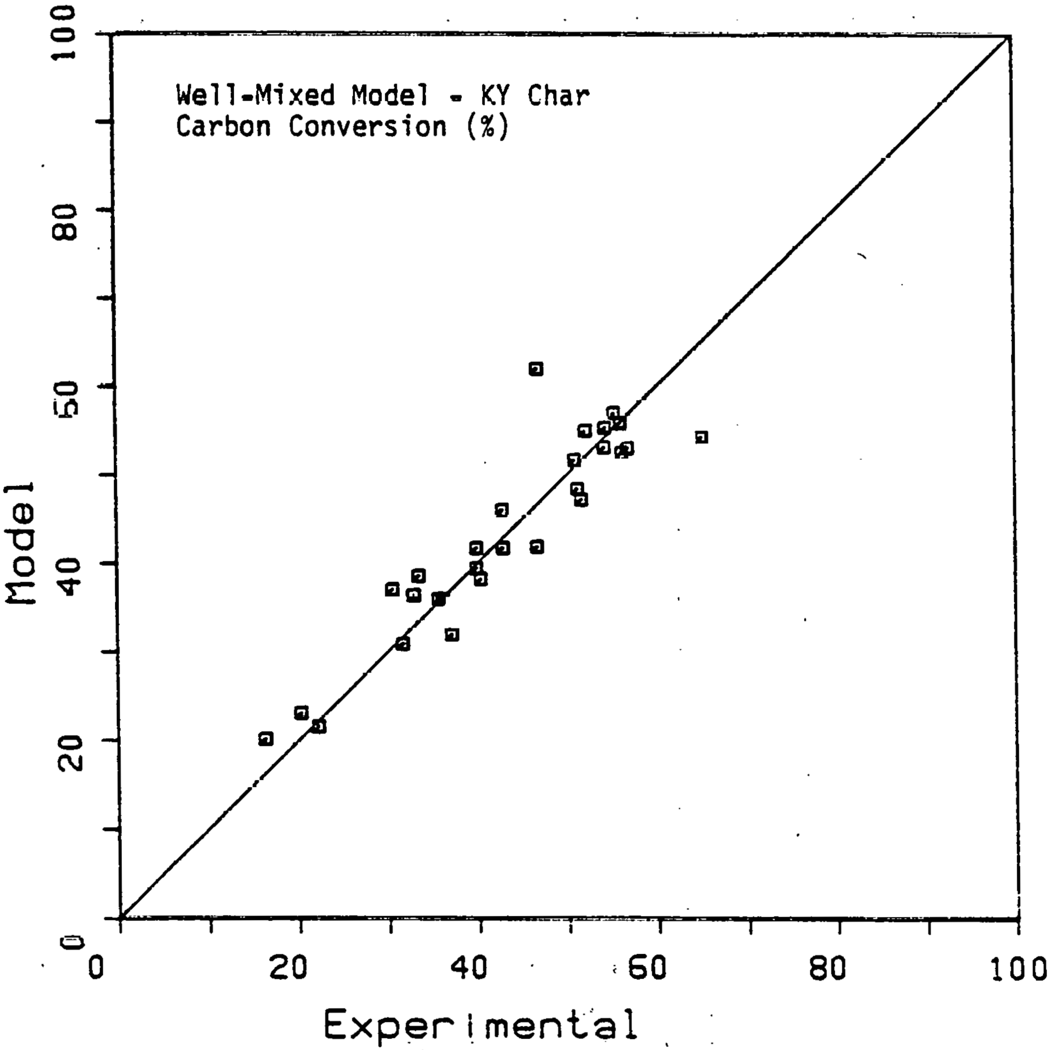

FIGURE 11

PREDICTED VS. EXPERIMENTAL GAS PRODUCTION RATE FOR KY. CHAR

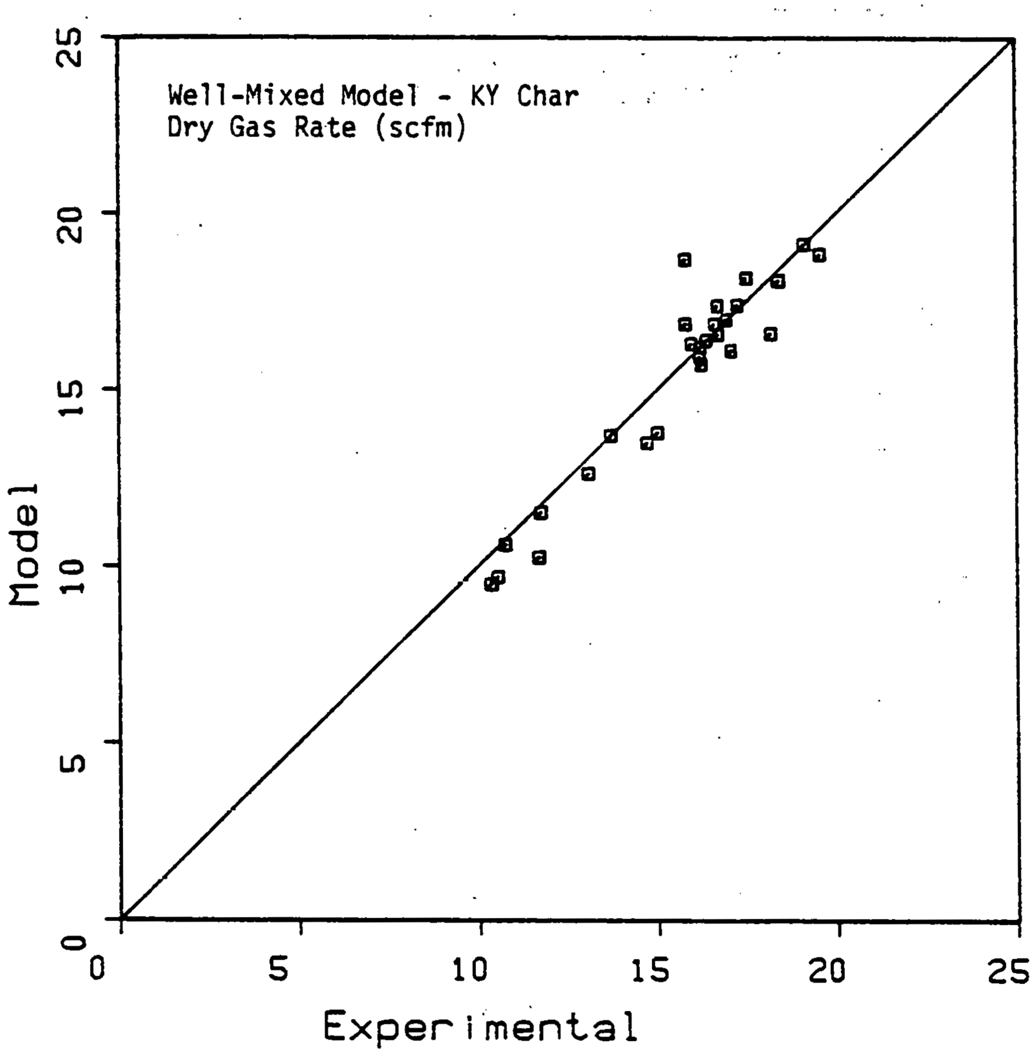

FIGURE 12

PREDICTED VS. EXPERIMENTAL MAKE GAS HEATING VALUE FOR KY. CHAR

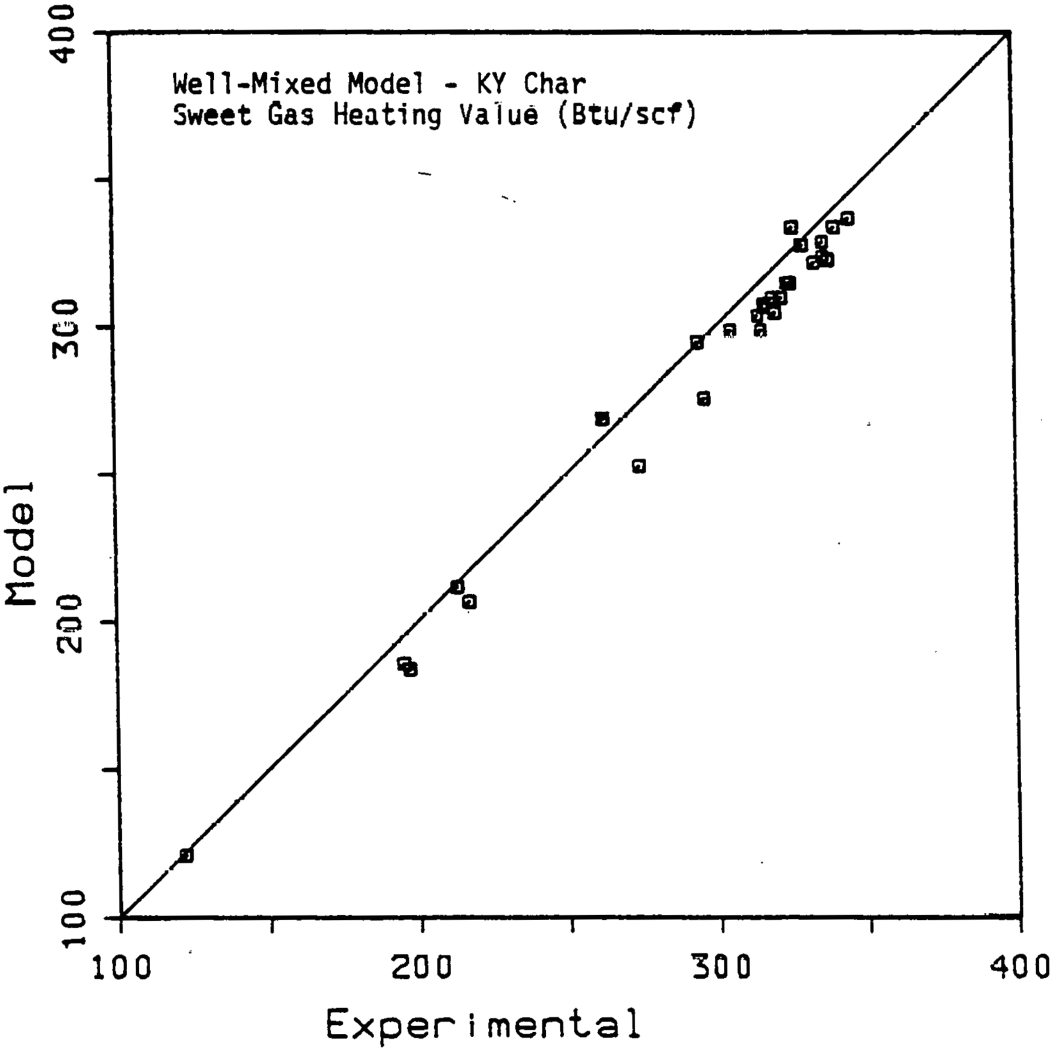

FIGURE 13

PREDICTED VS. EXPERIMENTAL CARBON CONVERSION FOR NM COAL

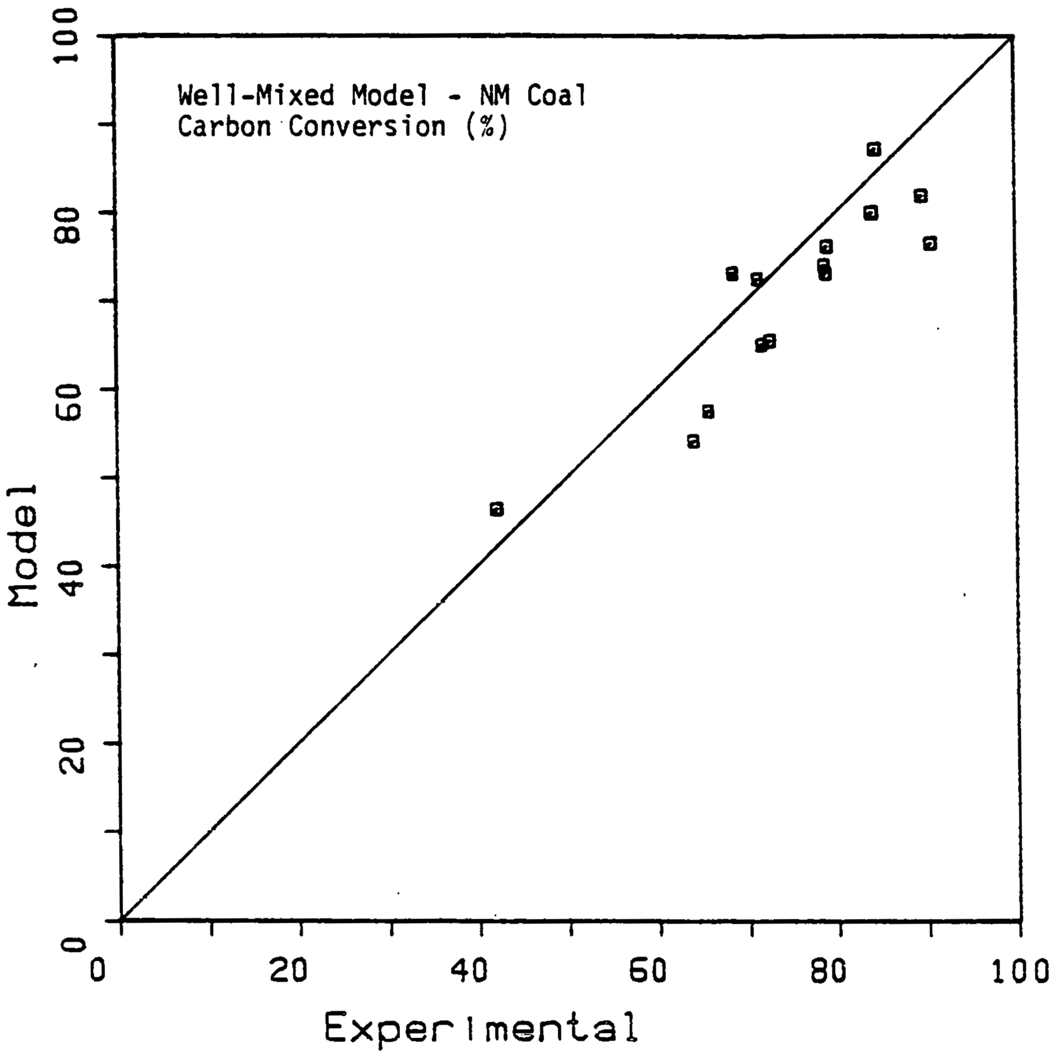

FIGURE 14

PREDICTED VS. EXPERIMENTAL GAS PRODUCTION RATE FOR NM COAL

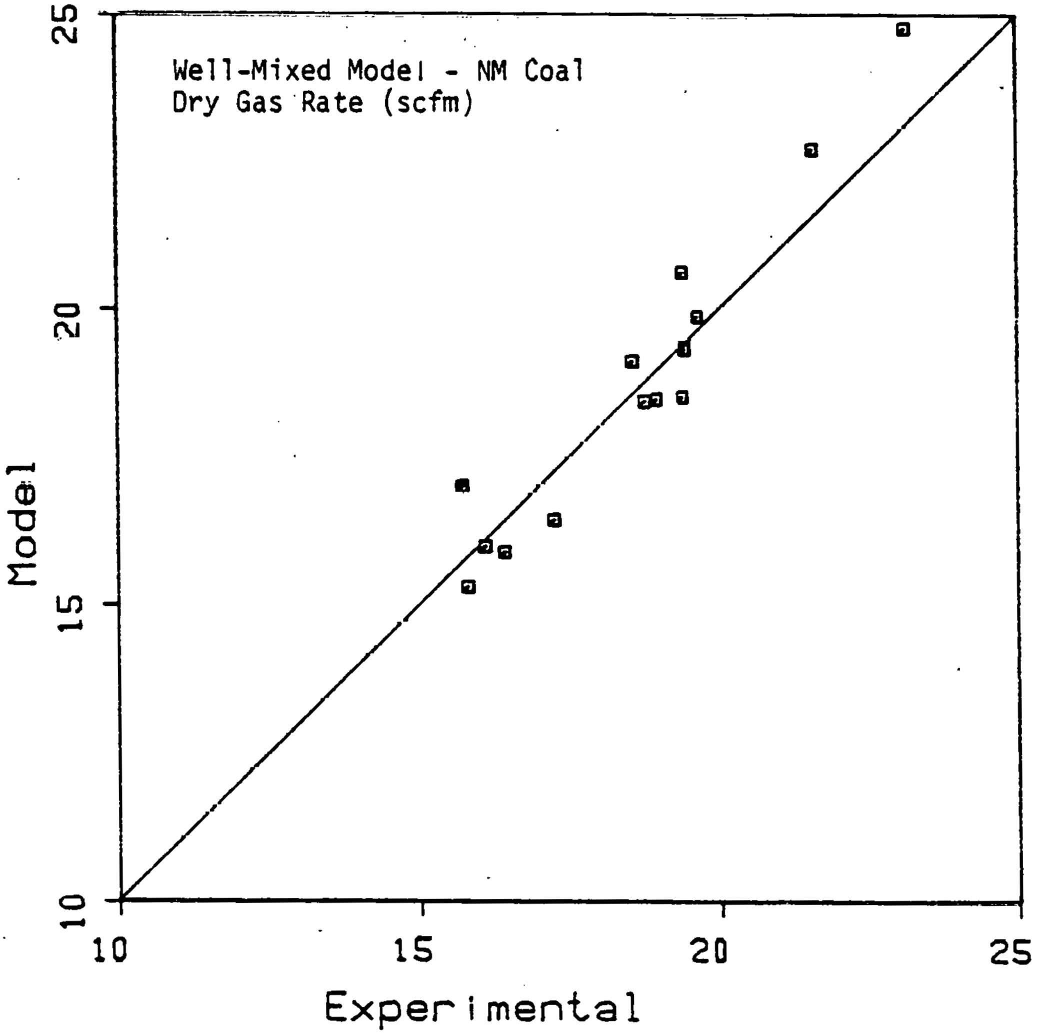

FIGURE 15

PREDICTED VS. EXPERIMENTAL K_{wg} VALUE FOR NM COAL

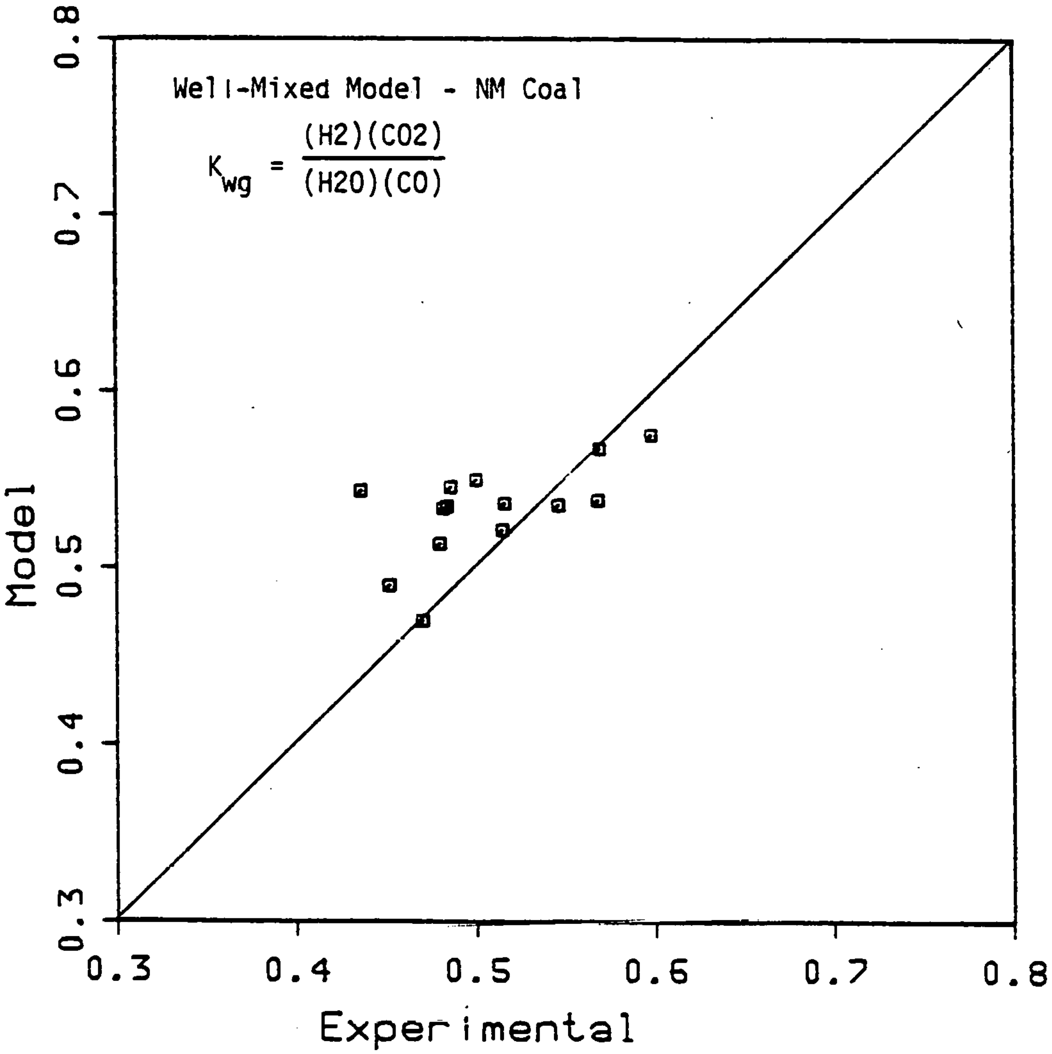

FIGURE 16

EQUILIBRIUM VS. EXPERIMENTAL K_{wg} VALUE FOR NM COAL