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THEORETICAL AND EXPERIMENTAL STUDIES OF FIXED-BED
COAL GASIFICATION REACTORS

Final Report

By
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A. Bhattacharya
L. Salam
M. P. Duduković

September 1983

Work Performed Under Contract No. FG22-80PC30219

Washington University
St. Louis, Missouri

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Summary

A laboratory fixed-bed gasification reactor was designed and built with the objective of collecting operational data for model validation and parameter estimation. The reactor consists of a 4 inch stainless steel tube filled with coal or char. Air and steam is fed at one end of the reactor and the dynamic progress of gasification in the coal or char bed is observed through thermocouples mounted at various radial and axial locations. Product gas compositions are also monitored as a function of time. Results of gasification runs using Wyoming coal are included in this report.

In parallel with the experimental study, a two-dimensional model of moving bed gasifiers was developed, coded into a computer program and tested. This model was used to study the laboratory gasifier by setting the coal feed rate equal to zero. The model is based on prior work on steady state and dynamic modeling done at Washington University and published elsewhere in the literature.

Comparisons are made between model predictions and experimental results. These are also included in this report.

Publications From This Contract

(a) Technical Journals

1. Joseph, B., M. Kim (1982), "Dynamic Modeling of Moving-Bed Gasifiers", Ind. and Eng. Chem., Proc. Des. and Dev., Vol. 22, 212 (1983).
2. "Dynamic Behavior of Moving-Bed Gasifiers" (with M. Kim). Gasification Advanced Research and Technology Development Cross-Cut Meeting. Proceedings, Department of Energy Report No. TR-82/008-003, p. IVA-32, (1982).
3. Joseph, B., "Modeling of Fixed-Bed Coal Gasifiers." Coal Gasification Modeling Workshop Proceedings. Edited by M. Ghate and J. W. Martin. Department of Energy Publication No. DOE/METC/82-24. pp. 352-375. With M. Kim.
4. Joseph, B., "Theoretical and Experimental Studies of Fixed-Bed Coal Gasification Reactors." Second Annual Advanced Gasification Projects Contractors' Meeting Proceedings. Edited by M. R. Ghate and G. R. Friggens. Department of Energy Publication No. DOE/METC/82-51. pp. 137-139. With M. P. Duduković.

(b) Technical Presentations

1. "Dynamic Modeling of the Lurgi Process for Coal Gasification," paper presented at AIChE Meeting, Detroit, August, 1981.
2. "Dynamic Modeling of Moving-Bed Coal Gasifier", Gasification Advanced Research and Technology Crosscut Meeting, Washington, D.C., June, 1981.
3. "Modeling of Fixed-Bed Gasifiers", Invited Paper Presented at the Coal Gasification Modeling Workshop, Morgantown, West Virginia, January 1982.
4. "Theoretical and Experimental Studies of Fixed-Bed Coal Gasification Reactors" (with M. P. Duduković). Second Annual Advanced Gasification Projects Contractors' Meeting, Morgantown, West Virginia, July 1982.
5. "Theoretical and Experimental Studies of Fixed-Bed Coal Gasification Reactors (with M. P. Duduković). Third Annual Advanced Gasification Projects Contractors' Meeting, Morgantown, West Virginia, July, 1983.

(c) Theses

1. "Dynamic Modeling of Moving-Bed Coal Gasifiers", M. Kim, M.S. Thesis, Washington University, August 1981.
2. "An Experimental Investigation of Fixed-bed Coal Gasification", L. Salam, M.S. Thesis, Washington University, August 1983.
3. "Modeling Studies in Fixed-bed Coal Gasification", Ph.D. Thesis in Progress at Washington University.

Introduction

The production of clean fuels from coal is an important step towards meeting the energy requirements of this nation. One of the best known methods for gasifying coal is the moving-bed (also known as fixed-bed) coal gasification process. Although considerable attention has been paid in the recent past to model fixed-bed gasifiers, little or no effort has been made to validate these models using detailed operational data, partly because such data have been difficult to obtain.

This research was undertaken to partially fill this need for accurate models validated with experimental data. To this end, a laboratory fixed-bed reactor was designed and built with the specific objective of collecting dynamic data on its operation. Simultaneously, a two-dimensional model of the reactor was developed, coded into a computer program and tested. The model was used to simulate the laboratory scale gasifier and the results were used to validate the model and estimate parameters.

Improved understanding of the coal gasification process is essential to build more efficient gasifiers and to optimize the performance of existing gasifiers. The optimum operation of gasifiers is known to be in a region where the reactor is very sensitive to input disturbances. The gasifier itself is the front end of the coal gasification plant and hence its performance will have significant impact on the purification and methanation steps that follow. This is particularly significant for combined cycle gasification power plants that may have to follow significant load changes.

2. Experimental Studies: Process Description

The need for accurate models of coal gasification processes has been briefly noted above. Any model simulation has a limited value if it cannot be compared to experimental results. Several experimental vessels have been constructed in an attempt to confirm simulation equations. Work by Westbrook (2) involved construction of a vessel to investigate in-situ gasification of Texas lignite. An attempt was made to confirm the equations of Penberthy and Ramey (9); however, insufficient experimental data prevented this. Work by Lu (10) involved construction of a combustion tube apparatus. The results were compared with a one-dimensional mathematical model. Other models have been developed and compared to limited commercial data. The diversity and complexity of commercial reactors has so far prevented proper verification of coal gasification models.

The objective of this work was to design, construct and operate a bench-scale fixed-bed coal gasifier for data acquisition. The reactor is to be designed in such a manner as to allow collection of data suitable for comparison to the model equations to be described later. The apparatus should be as versatile as possible, and it should allow for the investigation of the effects of coal (char) type and various reactant gas compositions and flowrates.

2.1 INTRODUCTION

The purpose of this chapter is to briefly describe the process of coal gasification as carried out in a bench-scale fixed-bed reactor. The overall process is similar to commercial scale systems requiring similar unit operation processes. No attempt will be made to describe specific equipment in this chapter. This will be covered in Chapter 5. Here only a general process is briefly described. A summary of this is given in Figure 2.1.

2.2 COAL PREPARATION

The solid reactant in this process is coal. As has already been discussed (Section 2.1) coal can have varying compositions. Depending on the manner in which it was mined it also can vary considerably in its size distribution. For these reasons it is necessary to characterize any coal feed used. Standard analyses called ultimate and proximate analysis can be performed on the coal used to give its chemical composition. The proximate analysis determines the weight percentages of volatiles, fixed carbon and ash. The ultimate analysis determines the percentages of carbon, hydrogen, nitrogen, sulfur, oxygen and ash. Examples of these are given in Table 5.1a. These same tests can be performed on any intermediate solids produced in any of the processes. For example the char resulting from devolatilization could be analyzed. Further preparations require separation of the coal to yield a suitable size range. It might also be necessary to wash the coal to remove any dust.

Figure 2.1 Process Description

2.3 GAS FEED PREPARATION

Three reactant gases are required as feed gas to the coal gasifier. The proper preparation of this feed is essential to the process. Water (steam), air and/or nitrogen must be delivered in an accurate consistent fashion. A known flowrate of water must be delivered to a steam generator where it is converted to steam. This steam is then mixed with known flowrates of air and/or nitrogen. This combined stream is mixed and further heated in a preheater. All necessary pressures and temperatures are recorded in the preparation steps. The result of these steps is the delivery of a feed gas of known composition, pressure and temperature. It should also be noted that this feed can be any combination of air, nitrogen and steam.

2.4 DEVOLATILIZATION VESSEL

The main objective of the experiment is to study the gasification of char in the fixed-bed gasifier. Consequently a process must be carried out to devolatilize the coal prior to its gasification. The devolatilization vessel is loaded with a portion of the prepared coal previously described in Section 2.2. If devolatilization is to be carried out in an inert gas environment a nitrogen feed is used. Otherwise, the inlet of the vessel is sealed and the coal gas is simply vented through an exit line. No nitrogen is used. Temperatures are maintained at high enough levels to dry and devolatilize the coal without fusing it. Temperature probes in the vessel record these temperatures continuously. The end product of this process is char. If this char is carefully reloaded in the

devolatilization vessel, experiments can be carried out to determine heat transfer characteristics of char and between char and the vessel wall. These later runs were performed with various nitrogen flowrates.

2.5 GASIFICATION VESSEL

The gasification vessel contains the char bed. The char produced in the devolatilization vessel is used to make this bed. The vessel is constructed in a manner which allows for the introduction of the prepared feed gas. This gas contains air or nitrogen-enriched air and steam at elevated temperature and pressure (above 1 atm). The vessel contains an ignition system capable of igniting and starting the reaction. As the reaction proceeds in the vessel, temperature probes continuously record the temperature at multiple points in the vessel. The product gas exits the vessel and is sent to a downstream process. The unconverted coal and ash remain in the vessel.

2.6 PRODUCT GAS TREATMENT

The gases produced in either the devolatilizer or the gasifier must be properly treated after they exit the vessel. Several processes are performed. The first of these is the cooling of the gas. This also condenses any tars, oil and water. This cooled and condensed stream then flows to a separator where the liquids are removed. The saturated gas exiting the separation process is split into two parts. One part flows to a flare where it is combusted and vented. The second and smaller part is sent to a gas chromatograph where the composition of the product gas is determined. Temperatures, pressures and flowrates are controlled in these downstream processes through valves, gauges and

meters. This ensures proper operating conditions. The liquid product stream is periodically monitored to determine the amount produced. Samples of this liquid are retained.

2.7 PERIPHERALS

Several major pieces of peripheral equipment are required in the gasification/devolatilization processes. The first of these, a gas chromatograph, has already been mentioned. The gas chromatograph is capable of accurately determining the amount of CO, CO₂, H₂, CH₄, N₂ and O₂ that are present in a gas stream. It is used in analyzing the prepared feed gas as well as the product gas. The second peripheral device is a microprocessor (LSI-11). This unit is capable of recording the temperature probe readings at a rate as fast as 17 probes per 3 seconds. These values are displayed on a Cathode Ray Tube (CRT) (or lineprinter at slower rates). After a run is completed the third peripheral unit, a DEC-20 computer is used. The data collected by the microprocessor as well as the data collected from gas chromatograms is transferred via modem to the larger computer. It is the large computer which allows for the proper manipulation of the data. Lastly several smaller safety items are used to protect the operator and may also be considered peripheral equipment.

3. Detailed Description of Experimental Reactor

3.1 INTRODUCTION

The previous chapter gave a general description of how the processes of devolatilization and gasification are carried out. The purpose of this chapter is to describe in detail the equipment that was constructed to affect the general processes described in the previous chapter. Figure 3.1 shows most of the equipment for gasification. The design, construction, and initial operation of the overall apparatus spanned a period of one and a half years. It is hoped that this chapter will help in understanding the reasoning which has led to the current process configuration. While several parts of the process are based on "state of the art" engineering principles, the majority of the items have been selected with cost and availability being the primary consideration.

3.2 COAL PREPARATION

The need for coal preparation has been briefly mentioned in Section 2.2. Runs 1 and 2 described in the results used a subbituminous coal from the Wyodac mine in Campbell, Wyoming. The Department of Energy's Grand Forks Energy Technology Center supplied four 11.4 kg buckets of crushed coal with the specification sheet shown in Section 5.2. The coal was characterized using ultimate, proximate and ash analyses. To retain the original moisture of the coal it was stored in double plastic bags.

A complete run requires 20 kg of coal to be screened. Generally 6.5 kg is found to fall between 8 and 20 mesh (2.362 and 0.833 mm). 2.5 kg is greater than 8 mesh with the remaining portion being a fine

Figure 3.1 Process Flow Design

Legend for Figure 3.1

R1, R4	- Meco Type or Dubbi-Stage Nitrogen Regulators (with pressure gauges P1, P4)	X5	- 2-1/2" x 30" (6.35 x 76.2 cm) copper pipe separation vessel
R2, R3	- Meco Type A-6 Dubbi-Stage Air Regulators (with pressure gauges P2, P3)	X7	- 250 cc glass gas washing bottle (with water)
R5	- Meco Type or Dubbi-Stage Helium Regulator (with pressure gauge P5)	X8	- Bunsen burners
T1, T4	- AGC size 200 compressed nitrogen cylinders	CC	- Gow Mac series 500 gas chromatograph with gas sampling valve
T2, T3	- AGC size 200 compressed breathing air cylinders	a	- 1/4" (6.35 mm) copper tubing - N ₂ for pressurizing water reservoir
T5	- AGC size 300 compressed helium cylinders	b	- 1/4" copper tubing - gas manifold for charging reservoirs
V1	- Valve to control water flow from reservoir	c	- 1/4" copper tubing - water deliver to evaporator
V2	- Valve to control charging rate of reservoir	d	- 1/4" Tygon tubing - calibration drain
V3	- Valve to calibrate flowmeter F1	e	- 1/4" copper tubing - evaporator drain
V4	- Valve to interrupt water delivery to evaporator	f	- 1/4" stainless steel (s.s.) tubing, insulated - carried steam from evaporator to preheater
V5	- Valve to drain evaporator	g	- hot air/N ₂ line inside preheater
V6, V7, V8	- Valves to control gas delivery from tanks T2, T3, T4	h	- 3/8" (9.53 mm) copper tubing - N ₂ /air feed line
V9	- Valve to draw gas sample of feed	i	- 3/8" s.s. tubing, insulated - hot mixed feed gas
V10	- Valve to pressure check system	j	- 1/8" (3.18 mm) s.s. tubing, insulated - hot gas sampling line
V11	- Valve to interrupt feed gas flow from T2, T3, T4	k	- 3/8" s.s. tubing, uninsulated - cold line for pressure gauge and safety valve
V12	- Valve to control product gas sampling flow	l	- 3/8" s.s. tubing, insulated - reactor inlet line
V13	- Valve to drain condenser	m	- 3/8" copper tubing - hot product gas line
V14	- Kunkle model 264 steel relief valve with 100 psig set point	n	- 3/8" copper tubing - condensed product gas line
V15	- Valve to control natural gas delivery to Bunsen burner	o	- 1/4" copper tubing - condenser cooling water - in
V16	- Valve to control system back pressure	p	- 1/4" copper tubing - condenser cooling water - out
P6	- Water pressure delivery gauge (0-60 psig)	q	- 3/8" copper tubing - condensate drain
P7	- Reactor inlet gas pressure (0-60 psig)	r	- 3/8" copper tubing - dry product gas line
P8	- Product gas pressure gauge (0-16 psig)	s	- 1/4" Tygon tubing - product gas sampling line to wash bottle
P9	- Feed gas delivery pressure (0-30 psig)	t	- 1/4" Tygon tubing - washing product gas line to GC
F1	- Brooks Sho-dade (2-1355-V w/B-1-13 AA and s.s. float) flowmeter for water flowrates 0-4.96 cm ³ /sec	u	- 1/8" copper tubing - purged sample gas line
F2	- Brooks (1110-08H2GLA w/R-8N-25-2 and s.s. RV float) flowmeter for product gas flowrates 0-1.47 m ³ /hr (3.22 scfm)	v	- 1/8" copper tubing - Helium carrier gas line
F3	- Brooks (1110-08H2GLA w/R-8N-25-2 and s.s. spool float) flowmeter for feed gas flowrates 0-3.77 m ³ /hr (2.22 scfm)	w	- 3/8" copper tubing - product gas line to Bunsen burner
TC1	- Gardman (JP, chromal/alumel) automatic time proportioning temperature (0-600°C) controller for evaporator	x	- 3/8" Tygon tubing - natural gas line to Bunsen burner
TC2	- Gardman (JP, chromal/alumel) automatic time proportioning temperature (0-800°C) controller for preheater (or devolatilizer)	81	- Terminal board - thermocouple extension wire to ribbon cable
S	- On/off switch for TC2 and outlet controlled by TC2	82	- LSI-11 microprocessor
CP1	- Control panel #1	83	- Tape drives - #0) Programs #1) Data storage
CP2	- Control panel #2	84	- 12 volt tape drive power supply
T1 - T12	- Chromal/alumel thermocouples located in gasifier	85	- Infotronics (CRS-309) integrator
T13	- Feed gas chromal/alumel thermocouple, 1/16" diameter (1.59 mm)	86	- Omni-Scribe (8-3000) strip chart recorder
T14	- Cooled product gas chromal/alumel thermocouple, 1/16" diameter	87	- Switching box to set LSI-11 baud rate and configure computer lines
Tc1	- Evaporator thermocouple for TC1, 1/16" diameter	88	- CRT (9600 baud) or line printer (300 baud)
Tc2	- Preheater thermocouple for TC2, 1/16" diameter	89	- Royal-Vadic (VA 3430) modem for 1200 baud data file transfer to DEC-20
X1	- 2-1/2" x 60" (6.35 x 152.4 cm) copper pipe water reservoir	910	- Telephone jack
X2	- Evaporator	b1	- Thermocouple output voltages (ribbon cable)
X3	- Preheater	b2	- Data to tape storage
X4	- Gasifier	b3	- Power line to tape drive
X5	- Condenser	b4	- Gas chromatograph output
		b5	- Integrator monitored, chart input
		b6	- LSI-11 to switching box
		b7	- Switching box to output device
		b8	- Switching box to modem
		b9	- Modem to DEC-20 via telephone line

powder. It should be noted that the weights given above are only approximations. While the fines are too small for fixed-bed use, the oversize coal may be crushed to the 8 to 20 mesh range. The coal is screened using a set of 20.32 cm (8 in) diameter Tyler sieves. The sieves are set inside a 20 liter (5 gallon) plastic bucket. A small pipe is set between the bottom sieve pan and the bucket bottom. The bucket is mounted on a Eberbach 6010 shaker. Approximately 300 gms (500 cm^3) of coal at a time is loaded on the top tray. The bucket is covered with a lid to prevent the spread of coal dust. The screening process is carried out to separate the fines first. After the coal is devolatilized it is rescreened to remove the oversized particles. The oversized particles are more friable as char and are crushed at this point rather than in the harder state as coal. The crushed oversized char is then rescreened. The process of crushing and rescreening is repeated until no oversized char remains. The final yield after devolatilization and screening is approximately 3.3 kg of char. Samples of the char are sent to Galbraith Laboratories (Knoxville, Tennessee) for ultimate and proximate analyses. All coal and char are stored in metal cans with air-tight plastic lids (coffee cans).

3.3 FEED GAS PREPARATION

The basic requirements for the feed gas preparation were briefly noted earlier. The preparation steps are divided into the four areas of: water delivery, evaporation, dry gas delivery, and steam/dry gas preheating. The approximate range of flowrates was calculated based on an assumed reactor size.

The first step requires delivery of a well metered amount of water in a smooth continuous manner. Initially a 50 ml continuous syringe pump was used. However, the pump was unable to withstand the 0.2393 to 0.3082 MPa (20 - 30 psig) back-pressure. A peristaltic pump withstood the back-pressure but was not capable of delivering intermediate flowrates. The system that is currently used involves a nitrogen pressured copper pipe water reservoir. If the vessel is maintained at 0.6164 MPa (60 psig) the back-pressure has minimal effect on the water delivery rate. The vessel is charged with tap water prior to a run. The vessel pressure is maintained with a line supplied from a nitrogen cylinder. The delivered water flows from the reservoir through a flowmeter and needle valve. The valving downstream of the flowmeter permits calibration of the water delivery system.

The water is delivered to the next preparation step where it is flash-evaporated. Figure 3.2 shows the evaporator that is used. The evaporator is essentially an electrically heated packed-bed heat exchanger. Water is introduced into the bottom of the vessel and contacts the hot pipe wall and hot packing. The water flashes into steam and exits the top of the vessel. The internal tubes simply increase the hot surface area in the vessel. A centrally mounted thermocouple is fixed in the vessel. The thermocouple is connected to a temperature controller to maintain the vessel at 500°C. Stainless steel was used for the vessel's construction because of its high melting temperature and resistance to corrosion. While copper or brass are excellent heat transfer materials they corrode rapidly at such high temperatures in the presence of water. The evaporator is capable of flashing up to

- A - Hoskins (FD-303A) combustion tube furnace, 1-3/4" x 12" (4.45 x 30.48 cm) chamber with maximum 1000°C and 0.55 kw rating
- B - 1" x 12-3/8" (2.54 x 31.43 cm) 304 stainless steel pipe
- C - Bushings welded inside pipe ends (stainless steel)
- D - 304 stainless steel reducing bushings (3/4" MPT to 1/4" FPT) used as endplugs
- E - Vessel support washer
- F - Exit fitting and thermocouple mounting (stainless steel)
- G - 1/16" (1.59 mm) thermocouple (chromel/alumel)
- H - 13 - 1/4" x 11" (0.635 x 27.94 cm) stainless steel tubes
- I - Inlet fitting (stainless steel)

Figure 3.2 The Evaporator

5 cm³/min of water. Above this flow the evaporator will have a portion of the tube filled with water and boiling occurs rather than flashing.

Other arrangements were considered for evaporation but none proved feasible. Rotating evaporators were limited to too low a pressure and were not capable of continuous feed. Commercial boilers well exceeded the desired flowrates. It should also be noted that consideration was given to metering the steam flowrate rather than the water but condensation associated with this measurement would result in uneven delivery. Thus the present arrangement was considered best.

The air/nitrogen feed is delivered from a set of three compressed gas cylinders. Two cylinders contain air. The third cylinder contains nitrogen. No oxygen cylinder is used, thus preventing accidental delivery of pure oxygen. The gasifier is not capable of withstanding the temperatures associated with a pure oxygen feed. Nitrogen is used to dilute the air feed or in the case of an emergency to cool down the reactor. The tanks are teed together and the combined gas flows to a flowmeter and pressure gauge. If a dilute air mixture is to be delivered the flowmeter is used to deliver the approximate relative flow from each cylinder. However, the slightly different pressure drop between each cylinder and the flowmeter limit the accuracy of this method. Chromatographic sampling of the feed is needed to accurately determine the feed composition. The flow through the flowmeter is considered to be at ambient conditions and no temperature correction is needed. Typical feed pressures are 0.2393 to 0.3772 MPa (20 to 40 psig).

The steam feed and air/nitrogen feed flow to the last part of the feed preparation process. The air/nitrogen feed must be heated before it is mixed with the steam to prevent condensation from occurring. Figure 3.3 shows the piece of equipment which is used. The preheater is similar to the evaporator. The cold air/nitrogen feed is heated in a long coil. The hot gas and steam are teed together and flow together through a pipe. The pipe is fixed inside the coil to allow the entire assembly to be mounted inside a large combustion tube furnace. The inside pipe helps in mixing the two streams as well as heating them further. A thermocouple fixed inside the furnace is connected to a temperature controller and thus maintains an operating temperature of 550°C. The hot combined stream exits the furnace and is sent to the reactor. This line has a sampling line teed into it to allow for a sample to be drawn by syringe for chromatographic analysis. Also teed into the final feed line, just upstream of the reactor, is a pressure gauge and safety relief valve. Since these are rated at temperatures below that of the feed they are teed via a long piece of tubing. To keep this pressure tap line cool it is not insulated. The remainder of the hot feed line and steam line are insulated. The tubes are wrapped first with a layer of Kaowool 2600 refractory wool, and then enclosed in preformed calcium silicate insulation tubes.

3.4 DEVOLATILIZATION VESSEL

Figure 3.4 shows a detailed sketch of the devolatilizer. The vessel is used to devolatilize approximately 2.8 kg of coal at a time. The process is an endothermic one and therefore requires a large heat input. A nitrogen feed from the preheater has a maximum temperature

- A - 1/4" (6.35 mm) stainless steel tube - hot air/nitrogen/steam exit
- B - 1/4" stainless steel tube - steam enters
- C - Cold air/nitrogen enter coil
- D - Lindberg (MJ024) combustion tube furnace with a 3" x 24" (7.62 x 60.96 cm) chamber. Maximum 1000°C and 2.0 kw rating
- E - 1/4" x 50' (6.35 mm x 15.24 m) stainless steel tube in a 3" (7.6 cm) coil
- F - Stainless steel exit fitting
- G - Copper gasket
- H - Stainless steel bushing welded inside pipe end
- I - Stainless steel reducing bushing for endplug (1-1/4" NPT to 1/4" FPT)
- J - 2" O.D. x 15" (5.08 x 31.8 cm) 304 stainless steel pipe (1/16" wall)
- K - Stainless steel inlet fitting tee
- L - 1/4" stainless steel tube - hot air/nitrogen enters pipe

Figure 3.3 The Preheater

Figure 3.4 The Devolatilizer

of 400°C and falls well below typically needed values of 800°C. The electrically heated wall overcomes this problem. All heat is supplied through the wall and no nitrogen feed is needed for heating purposes. The vessel is maintained at constant temperature by a thermocouple and temperature controller. The same preheater controller is used by plugging the devolatilizer into the controller outlet. It should be noted that the controller insures that the thermocouple is maintained at a constant temperature. Since the reactor wall is very close (~ 0.6 cm) to the heated surface the wall temperature is not uniform. Three thermowells are mounted inside the vessel and a fourth is positioned on the outside wall. Normally devolatilization is done with no nitrogen purge, the product gas is simply vented to the fume hood. The wall temperature is maintained at 800°C and the process is considered complete when the thermocouples in the bed level off near this value. A second indication of completion is an absence of gas bubbles when the venting line is immersed in a water bath.

After char production is completed and the char is screened (see Section 3.2), a portion of the char is reloaded into the devolatilizer. The bed is loaded to a specific depth. The wall temperature is set at an appropriate value and various nitrogen flowrates are introduced at known temperatures from the preheater. Each flow condition is allowed to come to steady state and the temperature profiles for various depths are recorded. The four 1.59 mm chromel/alumel thermocouples may be moved up and down inside the wells to accomplish this. In addition to a profile for the bed, a profile is also obtained for the outside of the vessel wall. The maximum level the thermocouples may

be inserted is 18 cm above the bottom of the vessel. The data on the bed temperature profile can be used to obtain estimates for k_{eff} and U_{wall} . Lastly it is noted that the support rod and rings are fixed to a large ringstand which itself is fixed to an adjustable stool. This arrangement greatly facilitates the positioning of the apparatus.

3.5 GASIFICATION VESSEL

The purpose of the gasifier is to constrain a fixed-bed of coal (or char) so that it may be gasified. Since the reactions are carried out at temperatures as high as 1300°C it is necessary to carefully consider the design and materials that will be used. Figure 5.5 shows the gasifier that is used. The refractory insulated vessel has a 8.91 cm diameter, 100 cm long bed. The vessel has been operated at temperatures as high as 1200°C.

When choosing the dimensions for the bed several factors were considered important. First it was desired to construct a reactor with a bed sufficiently large to house two thermowells each capable of positioning six thermocouples. The smallest thermocouples available are 0.01 inch (0.25 mm) and are too fragile for this application. The 0.02 inch (0.51 mm) thermocouples are more appropriate. Six of these require a thermowell 3/16 inch (0.476 cm) in diameter. As shown in Appendix 10.1, scaling calculations are performed for several reactor dimensions. In these calculations several assumptions are made. They are, i) a superficial gas velocity of 1 ft/sec (30.5 cm/sec) is desired, ii) a molar oxygen/water feed ratio of 1.0, iii) a 10 hour run requiring no more than two air cylinders, and iv) operating

Figure 3.5 The Gasifier

Legend for Figure 3.5

A	- 1 cm thick x 19 cm diameter 304 stainless steel top cover
B	- 6 - bolt holes
C	- 1/4" FPT for stainless steel inlet fitting (centered)
D	- 1/4" FPT for stainless steel ignition lead fitting (2 cm from center)
E	- 1/8" (0.3175 cm) compressed asbestos (casp) gasket seals basket flange bolt holes H and cover
F	- 19 O.D. x 7.75 cm I.D. steel top flange 1 cm thick
G	- 6 - 1/4"-20 threaded bolt holes
H	- 6 - recessed bolt holes
I	- 3 - 1/8" casp gasket seals and shims top flange
J	- 14.9 O.D. x 11.6 cm I.D. steel retaining flanges (1 cm thick) welded inside each end of steel shell
K	- 10.8 O.D. x 7.6 cm I.D. stainless steel basket flange (0.0051 cm thick) welded to basket
L	- 6 - 1/4"-20 threaded bolt holes
M	- 12.7 x 10 cm stainless steel sheet (0.0051 cm thick) rolled and welded to form a 7.6 cm diameter tube for basket wall
N	- Asbestos braided copper ignition leads
O	- 1/2" (1.27 cm) Diamonite (95% alumina grinding media) ceramic beads
P	- 1/4" x 12" (0.535 x 30.4 cm) Incoloy sheathed tubular heater bent to form 5.7 cm loop with 7 cm perpendicular legs
Q	- 6" O.D. x 47.7" (15.24 x 121.2 cm) steel pipe for outside wall (0.1651 cm wall)
R	- 1" x 24" x 48" (2.54 x 60.96 x 121.92 cm) Kaowool 2600 refractory blanket wraps liner twice
S	- Preformed refractory sleeves (Kaowool 2600), split and slid over liner. Refractory cement fills resulting gap
T	- 3-3/4" O.D. x 48" (9.525 x 121.92 cm) 304 stainless steel liner (0.3048 cm wall)
U	- 1/8" casp gasket seals bottom flange
V	- 1/8" casp gasket seals liner bottom
W	- Bottom flange same as F with 9.75 cm shoulder 7 mm deep
X	- Same as A for bottom cover
Y	- 1/8" FPT for stainless steel thermowell fitting
Z	- 1/4" FPT for stainless steel exit and thermowell tee fitting
AA	- 3/16" O.D. (0.4762 cm) Inconel thermowells 117 and 122 cm
BB	- Aluminum thermocouple plug mounting block with set screw
CC	- Perforated stainless steel basket bottom (4 x 7/32" holes/inch)

Thermocouple Locations From Top of Well (Bed)

1. 113.0 cm	7. 105.1 cm
2. 91.8 cm	8. 85.7 cm
3. 71.1 cm	9. 65.7 cm
4. 51.1 cm	10. 44.4 cm
5. 29.8 cm	11. 24.3 cm
6. 11.0 cm	12. 4.8 cm

Note all thermocouples are 0.02" (0.0508 cm) diameter Inconel sheathed chromel/alumel rated at 1150°C.

conditions and results of Wilson and Bissett (11) are applicable. It is furthermore assumed that the char behaves the same as coal but merely has the higher carbon content assumed to be 80%. This assumption is the least valid but for scaling purposes is appropriate. The results of the calculations show that a 3" (7.62 cm) diameter bed yields a superficial velocity close to 1 ft/sec. It also yields a bed length of 26" (67 cm). While a 4" (10.16 cm) diameter bed also yields a superficial velocity near 1 ft/sec, the relatively short bed length requires more closely positioned thermocouples and thus they must be positioned more accurately. For this reason the 3" (7.62 cm) bed was chosen. It should also be noted that this diameter yields a tube to particle diameter ratio of about 50. This ratio is sufficient to minimize wall effects (12). The final reactor, as already noted, has a slightly larger diameter and length. The longer length is simply a design precaution. The larger diameter is based on the availability of the larger diameter pipe.

The reactor is designed to operate as near to adiabatic conditions as possible, thus, heat losses from the bed must be minimized. Heat losses through the wall are minimized by using a refractory in the vessel wall. Heat losses through the ends of the vessel are prevented by a layer of ceramic beads. While the beads can rest at the bottom of the bed they must be suspended at the top. A basket is used to accomplish this. These beads are also needed to protect the flanges and covers from overheating by radiation from inside the bed. The beads in the basket also help flatten the velocity profile of the feed gas. The last function the basket serves is to fix the ignition coil at the top of the bed.

A major problem with composite walls involves finding a design that can accommodate the different thermal expansion coefficients associated with the different layers. The steel liner is at higher temperatures than the outside steel shell. The liner will elongate to a greater extent and if it is not free to travel in the outer shell, it will be damaged. For this reason no seal is made on the top of the liner. The large pressure drop associated with gas flow through the refractory prevents the gas from bypassing the bed. The seal at the bottom of the liner is simply an added precaution. Since the liner is not sealed the outside shell must be air-tight. The compressed asbestos gaskets accomplish this. They serve to prevent gas flow between flanges and through bolt holes as well. The vessel is mounted on a steel stand which permits the vessel to be rotated end-over-end. This allows the bottom flange, bottom cover and thermowells to be easily mounted.

Lastly, it is noted that the reactor was initially constructed with a 7.62 cm $\text{Al}_2\text{O}_3/\text{SiO}_2$ liner (Ispen Ceramics, I-MULL 900) instead of the present 304 stainless steel liner. While the ceramic liner is better suited for the high temperatures it proved unable to withstand the thermal shock associated with the rapid temperature rise in a section of the bed. The ceramic liner cracked repeatedly.

3.6 PRODUCT GAS TREATMENT

The product gases that are produced in the gasifier (or devolatilizer) contain water vapor, tars and ash. To determine the product gas flowrate and composition, the stream must be cooled and cleaned. The equipment downstream of the reactor is designed to accomplish this.

The first piece of equipment is a packed-bed condenser and is sketched in Figure 3.6. The hot product gas enters the top of the vessel and flows downward contacting the inside vessel wall and ceramic packing. The outside vessel wall is cooled by a water-filled copper coil. The inside gas temperature is lowered causing the water and tars to condense. The cooled saturated stream exits the bottom of the vessel. The cooling coil is split into three parallel flow segments to maintain the lowest possible wall temperature.

The cooled stream is sent to a liquid separator. The vessel is a simple version of a knock-out drum. A 2" x 30" (6.35 x 76.2 cm) copper pipe is capped at both ends. A 1/4" NPT inlet fitting is mounted in the side of the pipe. The dry gas and condensate exit the top and bottom of the pipe respectively through 1/4" NPT exit fittings. The dry product gas is sent to the product gas flowmeter. The temperature and pressure are also measured so the flowmeter reading can be corrected for non-standard conditions. The condenser must be operated in a manner that maintains the temperature of the measured gas below 204°C which is the maximum allowable temperature for the flowmeter.

The product gas is split after exiting the flowmeter. A small portion is sent to a water wash bottle and then introduced into the gas chromatograph. The bulk of the product stream is sent to a Bunsen burner. The product gas is generally unable to sustain a flame on its own. To ensure complete combustion a natural gas burner is impinged on the product gas jet. The combusted gases are vented to a fume hood.

A	- 1/4" (6.35 mm) copper tube - inlet cooling water teed to three cooling coils
B	- 6 - bolt holes
C	- 7 cm, 304 stainless steel plate (top cover) 2 mm thick
D	- 3.82 I.D x 7 cm O.D., 304 s.s. flange, 2 mm thick
E	- 6 - threaded bolt holes
F	- 1/8" (0.3175 cm) cusp gaskets (top and bottom)
G, H, I	- three 16-2/3' (5.08 meter) long 1/4" copper cooling coils touching outside vessel wall
J	- 1/4" copper tube - exit cooling water teed to three cooling coils
K	- Bottom cover same as C
L	- 1/4" FPT for exit gas fitting
M	- Stainless steel wire mesh to retain packing
N	- Welded steel block for inlet fitting
O	- 3 mm ceramic beads
P	- 1/4" FPT for feed gas fitting
Q	- 1-1/2" x 36" (3.81 x 91.44 cm), 304 stainless steel pipe (0.1587 cm wall)

Figure 3.6 The Condenser

3.7 PERIPHERALS

The product gas sampling line is analyzed to determine the volume fractions of N_2 , O_2 , H_2 , CH_4 , C_2H_6 , C_2H_4 , CO and CO_2 . A Gow Mac series 500 thermal conductivity gas chromatograph is configured with a gas sampling and a column series/bypass valve. The chromatograph uses a 243.8 cm (8 ft) 5A molecular sieve in series with a 182.8 cm (6 ft) Porapak Q column with helium as a carrier gas. Both are 6.35 mm (1/4") stainless steel columns. The chromatograph is calibrated using single component mixtures of the individual gases in nitrogen with the one exception of CO_2 in air. Levels of 10% were used for CH_4 , CO , H_2 and CO_2 (in air) with 1% for C_2H_4 and C_2H_6 . The CO_2 sample is also used to calibrate O_2 in nitrogen. Appendix 10.2 lists the operating conditions of the chromatograph and the area correction factors determined from calibration. Several sample chromatograms of actual product gases are also given. The chromatograms are recorded by both a chart recorder and an integrator. Area percentages are calculated based on the integrator output. The chart output is used only for qualitative purposes.

Eighteen type K (chromel/alumel) thermocouples are positioned in the various pieces of equipment. A Digital LSI-11 microprocessor has been programmed to record on tape, and print to an output device any sixteen of these. The set of sixteen (or less) can be sampled once every 3 to 59 seconds. For the faster rates the CRT must be used because of its higher baud rate. When the main program called system, say is executed, the user is prompted for various heading information.

A switching box is used to select the baud rate for the LSI-11 output. The box also configures the LSI-11 so that it may output the data file to the DEC-20 via a modem.

While the LSI-11 collects and stores the temperature data, it is not large enough to permit the desired manipulations for graphic output. It is necessary to transfer the data file to the larger DEC-20 system. Several copies of the data file are transferred. Occasional noise on the telephone lines can garble the data. The transferred files are compared and checked for inconsistencies and a new file, free of errors, is created. The gas chromatograph results are manually entered into a data file and a third program converts the results to volume percentages using the proper correction factors. Finally a graphics package is used to graph the gas composition and temperature profiles as a function of time.

Several other items are used when operating the reactors. All coal is handled using latex gloves while wearing a dust mask. In addition a small vacuum is used to collect any dust which rises when coal samples are loaded into the storage containers or vessels. Lastly a Bendix/Gastec piston-type gas detector is used to periodically check the room for carbon monoxide concentrations.

4. EXPERIMENTAL PROCEDURE

4.1 INTRODUCTION

The previous chapter described in detail the various pieces of equipment that are used to achieve the end result of coal gasification. There are three procedures that are carried out. They are i) char production, ii) char profiles and iii) gasification. Char production requires screening of the coal, devolatilization, and rescreening. A portion of the char is reloaded into the devolatilizer and temperature profiles are recorded for several nitrogen flowrates through the bed. These procedures are adequately described in the previous chapter and will not be discussed here. The remainder of this chapter describes the gasification procedure and flowmeter calibration procedure. The procedures described are for the most recent run and differ somewhat from the early runs. The major difference is the improved instrumentation of the latest run.

4.2 CALIBRATION

Three flowmeters are used in the overall process. While all three are rated at 2% accuracy, calibration is necessary. The water flowmeter is calibrated using a graduated cylinder and stopwatch. Figure 10.3 in Appendix 10.5 shows the resulting calibration curve. It should be noted that this curve is not linear. Calibration of the two gas flowmeters is somewhat more difficult. The first step requires connecting a 3/8" (9.52 mm) tube between the feed gas preparation section and the product gas treatment section. This tube replaces the reactor. A 3" (7.62 cm) glass bubble column is attached to the product gas Bunsen burner line. Both gas flowmeters are calibrated

simultaneously for a number of different flowrates.

4.3 GASIFICATION

The operation of the gasifier is critical if the data collected is to be reliable. The first step requires loading and sealing the reactor vessel. The volume of the char is measured and the length of the bed is calculated. The bottom flange and cover are bolted into place. The thermowells are then inserted. In the upright position two 3/8" (9.52 mm) stainless steel tubes are inserted over the thermowells. Each of these tubes exit the top of the reactor and are used to help position the thermowells. The bottom of the reactor is filled with 1/2" (12.7 mm) ceramic beads to the level required to allow the char bed top to be positioned directly below the ignition coil. A stainless steel mesh is inserted on the top of the beads. The mesh prevents any char from exiting the bed. The preweighed char is loaded several inches at a time. Each portion is slightly agitated by tapping on the side of the reactor with a piece of wood. This agitation insures uniform loading of the bed. When the bed is loaded the thermowell guide tubes are removed. The bed is then topped off with a portion of char fines. The top flange is bolted into place. The basket is inserted and filled with beads. The ignition leads are sealed and the top cover is then bolted onto the top of the reactor. It is important to record the position and weight of the char bed.

The next step requires preheating of several pieces of equipment. The gas chromatograph requires approximately two hours to reach proper operating temperatures. The preheater also requires a similar warm-up

period. The last piece of equipment that requires a warm-up period is the evaporator. A period of one hour is required for it.

When all the equipment is up to temperature the reactor is connected to the upstream and downstream sections of the apparatus. The system is pressure tested at 30 psig with a pure nitrogen feed. Pure air (no steam) is then fed to the reactor for a 15 minute period. The water is then introduced into the evaporator at the desired flowrate. The air and water flowrates are readjusted over a 7 minute period until the flows have equilibrated. The ignition coil is then connected for 5 minutes and the reactions are started.

The LSI-11 is implemented just prior to the start of the pure air feed. The sampling time is generally set at 50 second intervals. Chromatograms are begun just prior to ignition and continue throughout the entire run with 3 to 4 samples tested every hour. Feed and product gas flowrates and pressures are recorded 3 to 6 times an hour. The reactor pressure is also recorded several times every hour. The water feed flowrate and condensate weight are recorded every ten minutes. More frequent sampling is used if transients are noticed in the operating conditions.

The reactions are terminated by suspending the air and water feed and introducing pure nitrogen for 10 minutes. The system is then left pressurized with the nitrogen and allowed to cool. All equipment is also turned off.

After the reactor has cooled, the top of the vessel is opened. The basket is removed and the level of the unconverted bed is measured. The unconverted char, ash and ceramic beads are then carefully removed

from the bed. The ceramic beads are removed by screening and the ash and char are weighed. The ash and char are loaded into a combustion tube furnace and completely combusted. The remaining ash is weighed and recorded. The reduction in weight represents the unconverted quantity of carbon remaining in the bed.

5. SUMMARY OF MAJOR EXPERIMENTAL RESULTS AND DISCUSSION

5.1 INTRODUCTION

Two complete runs were made using char in the gasifier. Several instrumentation problems were present during the first run. The problems prevented accurate measurements of the gas flowrates in and out of the gasifier. The second run performed on July 24, 1983 was more successful and is discussed here in detail. The results of the first run are provided in Appendix 1.

5.2 CHAR PRODUCTION

Three batches of char were produced for the most recent run using the devolatilization procedure previously described. The coal used to load the devolatilizer is a Wyodac coal and is characterized in Table 5.1. The data sheet was supplied with the coal. The operating conditions for the three batches are summarized in Table 5.2. The weight reduction during the runs is also given. The coal gas evolved during these runs was analyzed and a typical composition is given in Table 5.3. A char sample (equal portions from each batch) is characterized by ultimate and proximate analyses. These results are given in Table 5.4.

It is apparent from Table 5.2 that the weight reduction remains constant within 0.4%. While the weight loss is a function of temperature and run duration, the devolatilization is essentially complete after three hours. It therefore serves no purpose exceeding this period and future runs should be performed in a manner similar to the last batch. The coal gas compositions are similar to those given earlier in Table 2.1c. The gases produced result primarily from the cracking of the volatile

Table 5.1

Coal Analysis

Mine. Wyodak
 Town. Campbell
 County. Campbell
 State Wyoming
 Abbreviated ID. Wyo 1
 Sample Date 7-15-78
 Bin # 3500

Proximate Analysis:

As Received

Moisture 31.87
 Volatile Matter. 32.46
 Fixed Carbon 30.16
 Ash. 5.51
 Heating Value (Btu/lb) 7978

Ultimate Analysis:

Moisture-free

Ash. 8.09

Moisture- and Ash-free

Hydrogen 5.75
 Carbon 74.05
 Nitrogen 1.39
 Sulfur 0.53
 Oxygen (by diff) 18.28
 Heating Value MAF (Btu/lb) . . 12,742
 H/C Ratio. 0.93

Ash Analysis - Wt % of Ash:

SiO₂ 33.85
 Al₂O₃. 16.66
 Fe₂O₃. 5.07
 TiO₂ 1.03
 P₂O₅ 1.44
 CaO. 22.46
 MgO. 6.52
 Na₂O 1.75
 K₂O. 0.31
 SO₃. 10.86

Table 5.2

Operating Conditions and Results for Char Production Runs

(Devolatilization) 5/24, 5/25, 6/3/83

Coal Type: Wyodac (Campbell, Wyoming)

Run	Grams Loaded	Grams Removed	Weight % Remaining	Run Duration (hrs.)	Final Temperature (°C)
5/24/83	2849.0	1188.0	0.4170	7.0	817
5/25/83	2823.5	1172.0	0.4148	8.5	841
6/3/83	3049.5	1271.0	0.4168	3.0	860

Table 5.3

Typical Coal Gas Composition (Water Free)

<u>Species</u>	<u>Percentage</u>
H ₂	62.94
CO ₂	14.06
CO	10.51
CH ₄	10.15
N ₂	1.11
C ₂ H ₆	0.76
O ₂	0.25
C ₂ H ₄	0.24

Table 5.4
Analyses of Produced Char

Ultimate Analysis

% Moisture	1.15
% Carbon	81.76
% Hydrogen	1.46
% Nitrogen	0.97
% Chlorine	less than 0.01
% Sulfur	0.53
% Ash	11.55
% Oxygen (by diff.)	2.58

Proximate Analysis

% Moisture	1.15
% Ash	11.55
% Volatile Matter	8.71
% Fixed Carbon	78.59

matter which is liberated at the high temperatures. The char characterization confirms the reduction of the volatile matter and moisture content.

5.3 TEMPERATURE PROFILES IN DEVOLATILIZER

Temperature profiles in the devolatilizer are measured to estimate the heat transfer coefficients in the system. A portion of the char is reloaded into the devolatilizer to obtain these profiles. Table 5.5 summarizes the results of one such run. It is important to note the increase in wall temperature at lower depths in the bed. This effect can be accounted for by considering an energy balance on a unit cross sectional segment of the vessel and bed. Energy enters the segment by radiation from the heating elements. Energy also enters and exists the segment by convection from the nitrogen gas. Other modes of energy transfer do occur, however, they are secondary to those noted above and are neglected. The temperature controller ensures that for the segment where the thermocouple is fixed, the vessel wall temperature is held constant. This is accomplished by controlling the amount of radiation to the segment. Since the same amount of energy is radiated to all segments the same amount of energy should be conducted into the char for each segment. If the wall heat transfer coefficient is constant then the temperature gradient between the wall and the char bed should be constant. Since a net energy flux occurs through the wall the temperature of the bed (and gas) increase at lower depths. Thus to maintain the same temperature gradient near the wall the temperature of the wall must increase. The rate of increase, however, decreases at lower levels. The decrease in the rate of increase parallels the

Table 5.5

Char Profile Results

Char Type: Wyodac 8-20 mesh (2.362-0.833 mm)

Char Loaded: 1443.5 gms

Char Removed: 1311.0 gms (9.18% weight reduction)

Vessel Inside Radius (R): 5.715 cm

Nitrogen Flowrates: A-1.605 m³/hr, B-2.166 m³/hr (standard conditions)

Vessel Pressure: A-0.2393 MPa, B-0.2807 MPa

Inlet Gas Temperature: 25°C

Depth from Top of Bed	RUN A				RUN B			
	Wall	r/R			Wall	r/R		
		0.888	0.640	0.298		0.888	0.640	0.298
4 cm	604°C	519°C	339°C	357°C	607°C	497°C	305°C	313°C
5	620	534	360	370	612	508	315	319
6	633	549	388	389	630	523	337	333
7	643	563	411	408	639	540	360	345
8	653	576	436	425	649	555	383	361
9	669	594	461	446	658	569	404	375
10	677	603	481	464	663	578	423	389

flattening of the radial bed profile. At steady state the net gain of energy in the nitrogen gas passing through a segment must be constant and equal to the same amount for every segment. Thus as temperatures begin to increase near the center of the bed the outside temperature cannot increase at as great a rate.

It can be seen that an irregularity exists in the topmost bed depths. The two innermost temperatures are inverted. This would appear to result from the fact that the top of the bed was not completely flat, varying in depth as much as a centimeter. It is also possible that radiation to the bed played a significant role. The top of the bed is located below the top of the heating elements. Thus the hot vessel wall might have radiated to the top of the bed. The radiation would be greatest at the center of the bed where the angle of incidence is greatest. These difficulties can be avoided in future runs by using greater care in leveling the top of the bed and then protecting it from radiation and further movement by covering it with a thin layer of refractory wool. Lastly, one experimental difficulty encountered prevented further data collection for this run. The thermocouples began to freeze in the thermowells. For future runs smaller, 0.04 inch (1.02 mm), thermocouples are recommended.

5.4 GASIFICATION

On July 24, 1983 the gasification of the char previously described in Tables 5.2, 5.4, and 5.5 was performed. Table 5.6 summarizes the operating conditions of the gasification run. The initial set of operating conditions for the run resulted in dangerously high temperatures and were altered to lower the peak temperatures. The composition of the

Table 5.6

Summary of Operating Conditions

For Gasification Run 072483

Char Loaded: 3645.7 gms devolatilized Wyodac char
 Char Composition: 83.56% Carbon
 11.97% Ash
 2.33% Oxygen > Moisture included
 1.02% Hydrogen
 0.62% Nitrogen
 0.50% Sulfur

Time 0-45 min.

	Air Flowrate:	1.478 m ³ /hr*
INLET	Water Flowrate:	3.48 gm/min
	O ₂ /H ₂ O:	2.12 gm/gm (1.192 mol/mol)
OUTLET	Product Gas Flowrate:	2.055 m ³ /hr*
	Total Condensate:	0 gm

Time 45-580

	Air Flowrate:	1.206 m ³ /hr*
INLET	Water Flowrate:	3.48 gm/min
	O ₂ /H ₂ O:	1.73 gm/gm (0.975 mol/mol)
OUTLET	Product Gas Flowrate:	2.022 m ³ /hr*
	Total Condensate:	382.2 gms

Unreacted Carbon: 697.8 gms
 Reactor Pressure: 0.1910 MPa
 Original Bed Length: 85.7 cm
 Final Bed Length: approximately 12.0 cm

* at 25°C, 0.1013 MPa

char bed is shown in Table 5.4. The temperature profiles are plotted as a function of time in Figures 5.1 and 5.2. The gap in this data at 6 hours was a result of stopping the normal LSI-11 operation to save the data file. While this is not a normal procedure, it was feared that an electrical storm passing the University might cause a power outage and loss of the data. Figure 5.3 shows the product gas as a function of time. Not shown in the figure, however, is the trace amount (average of 0.07%) of methane produced.

Figures 5.2 and 5.3 indicate that the front propagates at approximately 10 and 7 cm/hr for the two flow conditions respectively. The slower rate is due to the decreased air flowrate. It is also apparent that at the second set of operating conditions the temperature peaks gradually lower and broaden at lower bed depths. This is more pronounced for the outside temperatures. The broadening and lowering of the peaks can be accounted for as dispersion in the solid phase energy balance. The steel liner's thermal mass greatly contributes to this effect near the wall and thus accounts for the more pronounced effect near the wall.

Several other points should also be noted. The first of these relates to the feed gas temperature. While the Figures 5.1 and 5.2 indicate a temperature of 350°C this is in fact the temperature of the feed as it exits the preheater. The inlet feed gas temperature would be less than 350°C. Thermocouple #12 (Figure 5.2) would indicate that the feed is at most about 180°C since it does not fall below this value. It is also important to note that after a peak has been reached the bed above this point collapses due to reduction in volume when char is

Figure 5.1 Gasification Temperature Profiles For Run 072483 (TC #1 - TC #6)

Figure 5.2 Gasification Temperature Profiles For Run 072483 (TC #7 - TC #12)

Figure 5.3 Product Gas Compositions for Run 072483

converted to ash. The decreasing halves of the profiles indicated the cooling of the thermowells and liner wall not the cooling of the ash. Lastly, there are some minor fluctuations observed in the temperature profiles. In the earlier run (see Appendix 1) these fluctuations were more pronounced. It was postulated that these fluctuations were due to fluctuations in the steam flowrate. Prior to the most recent run two changes were made to remedy this problem. The pressured water reservoir was operated at 80 psig (0.653 MPa) rather than the previous setting of 60 psig (0.515 MPa). An additional change was to slightly loosen the top fitting on the water reservoir permitting the nitrogen to purge the reservoir. Both of these changes caused the water delivery to be less sensitive to back-pressure fluctuations. While some fluctuations are still present they are considerably smaller. Part of the decrease might also be due to the higher air flowrates present in the most recent run. The earlier run shown in Appendix 10.6 was at a lower gas flowrate and the relative amount of water was greater, thus fluctuations are more important.

The product gas compositions shown in Figure 5.3 remain relatively constant during the majority of the run. The effect of the higher air flowrate at earlier times is not possible to determine due to too few data points during this period. Two compositions which differ from typical values shown (see Table 5.3) are those of hydrogen and oxygen. Typical hydrogen percentages for the operating conditions (11) are around 15%. The values obtained here are almost double this. The error results from the gas chromatograph's poor sensitivity to the hydrogen peaks. A very large adjustment is needed in quantifying the hydrogen peak. This

correction factor could introduce significant error in the hydrogen results. One possible solution is to use a heavier carrier gas rather than helium. Argon is suitable, however, the sensitivity for the heavier components is decreased with a heavier gas. While a higher detector temperature and bridge current could be used the improvement is minimal. A better solution would be to have a second set of columns using argon as the carrier gas. The second set could be used to better determine the hydrogen percentage. During a run samples could be alternated between the two sets of columns.

The appearance of oxygen in the product stream would appear to indicate some bypassing of the bed. Whether or not the bypassing occurred in the bed or through the insulated wall is difficult to determine. Since it is unlikely that any oxygen could pass through the char bed without reacting the latter explanation is the most reasonable. As the bed length is reduced the pressure drop associated with the bed decreases. The decreased pressure drop would decrease the amount of bypassing. The steady decrease in oxygen as time increases would support this idea. The bypassing might be corrected in several ways. The easiest solution would be to use a larger char particle size or shorter length beds. Both of these would help decrease the pressure drop through the bed. A second solution would involve increasing the resistance to flow through the refractory. If the liner is temporarily plugged and a portion of ceramic cement is poured in the top of the gap between the liner and the retaining flange, the cement can be forced into the refractory by passing gas through the sealed reactor. The third solution would be to redesign the reactor. This alternative will be discussed in the next chapter.

The results of two gasification runs using Wyodac coal indicate that the experimental facility is capable of producing data for model development and verification. The runs also identified several inadequacies in instrumentation which must be corrected to obtain better material balance closure and more reliable product gas composition measurements. The results are considered sufficient for indicating front velocities, temperature profiles in the bed, and the ratio of carbon monoxide and carbon dioxide in the product gas.

The first run lacked proper instrumentation to determine the gas flowrates accurately. Hence it is recommended that the results of the first run only be used in a qualitative fashion. With several modifications the second run yielded better results. The observed temperature profiles correspond to typical literature values. The inability, however, to close the material balance is indicative that several instrumentation problems still exist. The primary problem appears to be the gas chromatograph's poor sensitivity to hydrogen. A more sophisticated gas chromatograph with dual columns should correct this problem. The entire amount of error cannot however be accounted for by this problem alone. The feed and product gas flowrates also appear to be slightly in error. Recalibration of the flowmeters might improve the measurements. A more expensive solution would be to use mass flowmeters or controllers. This would eliminate the effect of back-pressure fluctuations. The hydrogen error does not invalidate the entire set of results. The relative amounts of the components excluding hydrogen are valid. While the hydrogen values are not quantitatively correct they can still be used in a qualitative manner.

Measurement of temperature profiles in the char bed inside the devolatilizer can be used for estimates of the heat transfer coefficient at the wall and the effective radial conductivity of the bed. A problem with nonuniform heating of the vessel can introduce errors as large as 10°C. This error will be reflected in property estimates. Calculations by Bhattacharya (8) on parameter estimates from these profiles indicate that the values obtained are very close to some of the recently published literature on heat transfer properties of char beds.

The use of the results from the second run for model development should be approached carefully. The appearance of oxygen in the product stream is indicative of some degree of bypassing of the feed gas. Suitable model adjustments should be made for this. Alternately, calculations can be made to adjust the measured feed gas flowrate to the actual flowrate through the bed. These calculations would be valid if the sensible heat removed from the hot zone by the bypassing air is negligible.

In addition to the previously noted modifications needed to produce more reliable results, a new reactor must be designed if future runs will require higher temperatures. The current reactor is limited to 1200°C by the maximum use temperatures of the 304 stainless steel liner and chromel/alumel thermocouples. Ceramic liners are the best material for extending the maximum allowable temperatures. Problems with thermal shock prevent use of extruded or cast ceramic materials. This problem does not occur with refractory (ceramic) wool tubes. The replaceable refractory tubes could be housed in a stainless steel pipe. If diameter tolerances are kept sufficiently close, bypassing between the pipe and refractory tubes can be prevented. Ceramic thermowells could be mounted through the

stainless steel pipe wall permitting more accurate positioning than the current flange mounted wells. Platinum/rhodium type thermocouples could be inserted in the wells. The bed would be sealed by flanging the stainless steel pipe. The entire assembly could then be fixed inside a heavily insulated housing if additional insulation is needed. This would depend on the thickness of the refractory liner. A reactor of this kind should be able to operate at temperatures as high as 1600°C.

In conclusion, the current facility has been demonstrated to be fully operational and is sufficient for early model development. It is noted, however, that several major modifications are necessary in the apparatus before final dynamic models could be applied.

6. Mathematical Modeling of the Fixed-Bed Gasifier

The major events that occur in a fixed-bed gasifier are: drying, devolatilization, combustion and gasification. Among these, drying and devolatilization are hard to model, primarily because of the extremely complex and uncertain nature of the processes themselves. Accordingly, it was felt that gasification of devolatilized (and dried) coal should be carried out, to remove as much uncertainty from the model as possible.

The combustion reaction (exothermic) and gasification reactions (net endothermic) are shown in Table 6.1. Some reactions involving sulfur, nitrogen, etc., are ignored as they do not have a significant bearing on the product gas composition. The molar ratio of carbon monoxide/carbon dioxide in the combustion reaction follows an Arrhenius temperature relation (Arthur (13), Rossberg (14)). The parameter γ accounts for this dependency.

The development of Yoon (6), Cho (3), Kim (5) is followed for the evaluation of reaction rates. The char-oxygen and char-steam reactions are assumed to follow the shrinking core model; the others are assumed to be kinetically controlled.

6.1 Material and Energy Balance Equations

Axial mixing effects in both material and energy flow may be present because of turbulence and the presence of the solid phase, and may be accounted for by superposing an "effective" transport mechanism on the overall transport by plug flow. However as discussed by Yu, axial dispersion is negligible according to the criteria developed by Young and Finlayson (15) unless the gas flow rate is very low. Radial dispersion of mass in the gas phase may be assumed to be negligible in comparison with the convective contributions. Radial dispersion for the energy

Table 6.1. Major Reactions in the Gasifier

balance may not be neglected because there is a substantial temperature profile radially, especially since non-adiabatic reactors are being considered. Additionally, since temperatures in gasifiers regularly reach very high values (about 1300 K) it would be expected that radial dispersion of heat would play a substantial role.

Under the assumption that the gas and solid phases are at the same temperature, the energy balance can be written as:

$$\frac{1}{r} \frac{\partial}{\partial r} \left[k_R r \frac{\partial T}{\partial r} \right] - \left(\sum_{i=2}^m F_i C_{pi} \right) \frac{\partial T}{\partial z} - \sum_{j=1}^n R_j \sum_{i=1}^m \alpha_{ij} H_i = C_l C_{pl} \frac{\partial T}{\partial t}$$

Here α_{ij} is the stoichiometric coefficient of species i in reaction j . Gas-phase accumulation terms have also been neglected - this should not result in major inaccuracies since the residence time of gases in the reactor is of the order of a few seconds whereas the reactor operation time runs into hours.

Besides the above, one other energy balance may be written for the wall of the reactor. Eigenberger (16) has shown that the effect of heat accumulation in the wall (of a tubular reactor with a highly exothermic reaction) has a considerable influence upon the transient behavior of the reactor. Eigenberger's analysis was for disturbances imposed on reactors operating at steady state, but it is felt that for gas-solid reactors (which are not steady since there is a moving front) having walls with high thermal capacity the effect would be not minimal. Consequently, we write the energy balance for the wall as:

$$\frac{\partial T_w}{\partial t} = \frac{2R_1 U_{eff}}{\rho_w C_w (R_2^2 - R_1^2)} (T|_{r=R_1} - T_w) + \frac{2R_2 U_c}{\rho_w C_w (R_2^2 - R_1^2)} (T_c - T_w) + \frac{\lambda_w}{\rho_w C_w} \frac{\partial^2 T_w}{\partial z^2}$$

The solid phase material balance equation can be written as:

$$\sum_{j=1}^n \alpha_{1j} R_j = \frac{\partial C_s}{\partial t}$$

For the gas phase we have:

$$-\frac{\partial F_i}{\partial z} + \sum_{j=1}^n \alpha_{ij} R_j = 0 \quad i = 2, \dots, m$$

There are no dispersion terms in the above, and no accumulation terms except for the solid-phase terms.

The boundary and initial conditions are as follows:

Boundary Conditions:

$$\text{at } z = 0 \quad F_i = F_{i0} \quad i = 2, \dots, m$$

$$T = T_0$$

$$\frac{\partial T_w}{\partial z} = 0$$

$$\text{at } z = 1 \quad \frac{\partial T_w}{\partial z} = 0$$

$$\text{at } r = 0 \quad \frac{\partial T}{\partial r} = 0$$

$$\frac{\partial F_i}{\partial r} = 0 \quad i = 2, \dots, m$$

$$\frac{\partial C_1}{\partial r} = 0$$

$$\text{at } r = R_1 \quad \frac{\partial T(z)}{\partial r} = \frac{U_{\text{eff}}}{k_{\text{eff}}} (T - T_w)$$

$$\frac{\partial F_i}{\partial r} = 0 \quad i = 2, \dots, m$$

Initial Conditions:

$$\text{at } t = 0 \quad T = T_0$$

$$F_i = 0$$

$$C_1 = C_{10}$$

$$T_w = T_0$$

6.2 Solution Procedure

There are three independent variables in our system of equations: t , r and z . The z -dimension is easy to handle, because the set of equations (with the exception of the wall energy balance) are of first order in z , with specified conditions at $z = 0$. Therefore any integration scheme (Runge-Kutta, etc.) may be used. Collocation is inappropriate, as the profiles are very steep at the combustion region. It was decided to use Gear's algorithm (which utilizes a predictor-corrector scheme) for a number of reasons: the possibility of having (1) variable step size without a large number of function evaluations, and (2) error estimations which are fairly accurate.

Before specifying any integration technique for the z direction however, the equations have to be converted from PDEs to ODEs. One of the best ways of doing so is orthogonal collocation, and this was the

method used for the r -dimension. It may be noted here that this was the technique used by Yu, albeit in a slightly more elaborate form.

For the time frame, an explicit Euler scheme was used. Kim used a semi-implicit method for his moving-bed simulations, but for the case with no solid flow (i.e. for a fixed-bed) an explicit method is adequate - provided the time steps are small.

The wall equation was dealt with on an individual basis, because of the difficulty of dealing with a second-order differential equation. For this equation, finite differencing was applied for both the z and t dimensions.

The procedure therefore, is as follows:

1. Assume char-conversion and wall temperature profiles along the length of the reactor (z -dimension). For example, char-conversions could be zero everywhere, and wall temperature could be T_a (the ambient temperature) everywhere.
2. Integrate the energy balance and gas-phase material balance equations for each radial collocation point from $z = 0$ to $z = L$.
3. Take a time step: that is, update the char conversion and wall temperature profiles.
4. Repeat the (2) - (3) cycle until conversion is complete (or in the case of moving beds, until steady state is reached).

7. Results of Simulation Study

7.1 Moving-bed simulation (with coal feed $\neq 0$)

There are two cases that will be reported.

(i) Going from one steady state to another. This new steady state may be caused by a disturbance in one of its inputs (eq. feed gas flow rate or composition, coal flow rate, etc.). In this work, only a change in the coal flow rate is considered.

Figures 7.1 and 7.2 show some of the dynamic profiles for an increase in coal flow rate from 725 Kgmoles/hr of Wyoming Coal to 750 Kgmoles/hr. Reactor dimensions are the same as used in Yoon, Cho. The total time taken is 15 hours of real time.

We can see (Figure 7.1(a)) that coal conversion near the wall of the reactor is less than that near the center of the reactor (the plots are for two radial collocation points, the inner being at $r/R = 0.3938$ and the outer at $r/R = 0.8031$) = that is, there is a radial profile. The magnitude of this profile is a function of the two heat transfer parameters k_{eff} and h_{eff} . For this work, the numbers proposed by Yu (34.2 kJ/mhrK and 1116.0 kJ/m²hrK respectively) were used.

(ii) Going from startup to a steady state. The difference between (i) and this is that coal conversion profiles are originally set to zero. A little care is required for this simulation because the updating process of coal conversion profiles may become unstable, depending on the time step taken, and the coal flow rate.

Figure 7.3 shows the dynamic conversion profiles for startup, for a coal flow rate of 725 Kgmoles/hr of Wyoming coal. The bed dimensions are the same as in (i). The total time taken in this case was 28 hours.

In this case, we can see the separation that occurs in the profiles as time goes on, even though all profiles were identical at time zero. Of course, the separation is a factor of the values needed for h_{eff} and k_{eff} .

7.2 Fixed-bed Simulation (no coal feed)

Since there can be no steady state in this case, there is essentially only one possibility: simulation from startup to exhaustion of coal in the bed. One difference between this and the moving-bed simulations is that in this case the wall of the gasifier was considered, since for our experimental runs it was estimated that the wall was a major heat sink. Also, the numbers used for h_{eff} to k_{eff} were calculated from experiments conducted on a similar bed of coal as the experimental gasifier here at Washington University. These numbers are significantly different from the ones used by Yu.

Figures 7.4, 7.5 and 7.6 show some of the dynamic profiles for this case. The coal conversion profile for the outer collocation point (Figure 7.4b) shows that complete conversion does not occur. The average conversion here is about 0.95 - the jagged peaks that show up are due to the discretization in the time frame. It is expected that if time steps are made smaller, the profiles will become smoother. For this case, the time step was 0.1 hrs.

Figures 7.5 and 7.6a show the temperature profiles. The maximum temperatures at the two radial collocation points differ by as much as 150 K, unlike the moving-bed case (where the maximum temperatures were the same). The wall temperature initially starts off at a high temperature at $z = 0$, because of the heat given to it during startup. However, the profiles settle down as time proceeds, and a peak of roughly 800 K is

got. It should be noted here that the solid phase accumulation term in the energy balance becomes important for the fixed-bed case, because this is the only term in the energy balance that "retains" the temperatures in the previous time-step.

Figure 7.6b is an example of the gas-flux profiles: in this case, steam flux as a function of reactor axial distance is shown. Note that conversion of steam is less towards the outside of the reactor than the inside.

7.3 Comparisons with Experimental Data

Two figures (Figure 7.7 and 7.8) are included here for comparison purposes. Figure 7.7 has the central thermocouple temperatures (at four z locations specified in Lyle Salam's Thesis (Appendix 2) plotted as a function of time. The major difference between the experimental and predicted temperatures occur after the reaction front has passed the particular location, with the predictions being substantially lower than the actual temperatures. A major reason for this is that the walls of the gasifier as well as the thermowell walls probably retain a lot of heat; the drop in the measured temperatures, therefore, is much less than what the model equations would predict.

Figure 7.8 shows the center line temperature profile after two hours of operation. Here, the measured temperatures can only be plotted as four points (since we only have four z -locations where thermocouples are present), and have been shown as circles. One of the circles has been left open because that measurement is not felt to be a true representation of the bed temperature, for reasons mentioned in the previous paragraph.

Comparison between the results of Run 050283 and the simulation model are reported in this section. The comparisons are restricted to

temperature profiles since product gas compositions were not measured accurately in this run. As seen from Figure 7.7, there is general agreement between the model predictions and the experimental results.

Corresponding figures for the exterior collocation point have not been plotted because there is a great deal of uncertainty in the radial location of the thermocouple readings.

During the course of various simulations it was found that the predictions for the resistances (involved in the shrinking-core model) yielded reaction rates which were much too high for the combustion reaction and much too low for the $C + H_2O$ reaction. Of particular concern was the prediction for k_g , the mass transfer resistance of the gas film around the particle. This was so because the particle Reynold's number (at conditions existing in the gasifier at Washington University) was much too low (~ 5.0) for the expression used by Sen Gupta and Thodos (17) to be valid. Therefore, a factor (FACTOR 1) was defined such that the resistance was always equal to or greater than $0.3758 \cdot \text{FACTOR 1}$ (in our simulations, $\text{FACTOR 1} \approx 0.2$ worked well). (See Appendix 3). FACTOR 2 was used to account for the fact that more water was being used in the gasifier than the predictions showed. Since the limiting resistance was the intrinsic reaction rate term, this term was sought to be decreased by increasing the rate by a factor, FACTOR 2 (we have used $\text{FACTOR 2} \approx 10.0 - 15.0$). It should be noted here however, that for conditions existing in the larger gasifiers (e.g the moving-bed Lurgi gasifier simulated in this report) the factors were 0.0 and 1.0 respectively.

Other sources of problems are the reaction rates expressions themselves. For conditions in the gasifier at Washington University, the

reverse reactions generally were much larger than the forward reactions right after the combustion zone, resulting in predictions of fairly large amounts of carbon deposition. Since this was not felt to be the case, the reverse reactions were removed. They, however, were present in the Lurgi gasifier simulation.

7.4 Evaluation of Heat Transfer Parameters

Two parameters - the effective thermal conductivity and the effective wall heat transfer coefficient - are required to solve the energy balance equation. There has been a fair amount of work done in the area of estimation of these parameters (Coberly and Marshall (18), Kwong and Smith (19), Plantz and Johnson (20), Burnell et. al. (21), Yagii and Kunii (22), etc.). All of these works correlate the two parameters in some way or the other to the mass flow rate of gas, the most usual variable being $\frac{d_p G}{\mu_{avg}}$. However, experimental data is limited to regions where $\frac{d_p G}{\mu_{avg}}$ is greater than 30, whereas in the gasifier at Washington University, a representative value is 3.

Yu, quoting Yoon, used the value 9.5 W/m K for k_{eff} whereas calculations using the correlations developed by Plantz and Johnson and Merrick (23) for example, yield the value 1.04 W/m K and 1.102 W/m K respectively (for the correlation of Plantz and Johnstone, a value of 150 was used for $\frac{d_p G}{\mu}$). The correlations for effective wall heat transfer coefficient are even more sensitive to mass flow rates, and some of the proposed correlations have very poor fits (eg. Coberly and Marshall). Furthermore, the problem of low $\frac{d_p G}{\mu}$ values is present here too.

Taking all these inconsistencies into account, it was decided that the two parameters should be determined experimentally, at conditions at

or near those existing in the gasifier. The method of parameter estimation is described next.

The experimental setup is as shown in the Figure. Cold gas (temperature T_{in}) enters a cylindrical

vessel packed with coal. The walls of the vessel are heated, and kept at a constant temperature, T_w . Temperature measurements are taken at various z and r locations, when steady state has been reached.

The equation governing this system is:

$$k_{r,eff} \left(\frac{\partial^2 T}{\partial r^2} + \frac{1}{r} \frac{\partial T}{\partial r} \right) = G C_p \frac{\partial T}{\partial z}$$

Boundary Conditions are:

$$r = 0 \quad : \quad \frac{\partial T}{\partial r} = 0$$

$$r = R \quad ; \quad -k_{r,eff} \frac{\partial T}{\partial r} = h_{w,eff} (T - T_w)$$

$$z = 0 \quad : \quad T = T_{in}$$

The assumptions involved in the above formulation include:

- (i) the system is homogeneous
- (ii) there is no axial dispersion of heat
- (iii) parameters (like $k_{r,eff}$, $h_{w,eff}$, C_p) are independent of temperature.

The governing equation is fairly easy to solve and may be treated in a number of ways. For this work, radial collocation is applied to transfer the equation into a set of ordinary differential equations in z , which can be solved. We can therefore numerically predict the temperature at any z -location, at specified radial collocation locations.

Measurements were taken at collocation locations and samples are shown in Table 5.5. An error vector $\underline{e}$, each element of which is the difference in the predicted and calculated values, is calculated next. Minimization of the sum of squares ($\underline{e}^T \underline{e}$) is now done by a gradient search, the parameters for the search being $k_{r,eff}$ and $h_{w,eff}$.

The experimental setup for this analysis was not very elaborate, and as a result, the wall temperature could not be kept at a constant value. To account for this, the boundary condition at $r = R$ was rewritten as:

$$-k_{r,eff} \frac{\partial T}{\partial r} = h_{w,eff} (T - T_w(z))$$

where $T_w(z)$ is now fitted as a polynomial in z ,

$$T_w(z) = f_1 + f_2 z + f_3 z^2 + \dots$$

Minor modifications are now required to be made in the algorithm, but the procedure remains essentially the same.

The data shown in Table 5.5 was used to evaluate the best values for $k_{r,eff}$ and $h_{w,eff}$. The results are as follows:

Case A: Gas flow rate 0.0593 Kgmol/hr

$$k_{r,eff} = 2.263$$

$$h_{w,eff} = 235.6$$

$$error = 4.25 * 10^{-2}$$

Case B: Gas flow rate 0.0823 Kgmol/hr

$$k_{r,eff} = 2.495$$

$$h_{w,eff} = 274.9$$

$$error = 8.46 * 10^{-2}$$

"error" here refers to the sum of the squares of the individual errors, in a non-dimensional form. It is not possible to get the error to zero because of many reasons: major among them being the fact that $k_{r,eff}$ and $h_{w,eff}$ are really not constants, and also many assumptions are involved in this analysis, as mentioned before.

Figure 7.1(a) Solid conversion profiles for two-point radial collocation, for an increase in coal flow rate. (b) Temperature profiles (in K) at the same points. Total time $T = 15$ hrs.

MOVING-BED GASIFIER. WYOMING COAL

Figure 7.2. Examples of gas flux (Kgmol/hr m²) profiles for an increase in coal flow rate. (a) Steam flux (b) oxygen flux. Total time T = 15 hrs.

MOVING-BED GASIFIER, WYOMING COAL

Figure 7.3(a) Coal conversion profiles as a function of time for startup. Two-point collocation was used. (b) Final steady state for the two points.

FIXED-BED GASIFIER, WYOMING COAL

Figure 7.4 Coal conversion profiles, two point radial collocation. (a) Interior collocation point (b) Exterior collocation point.

FIXED-BED GASIFIER, WYOMING COAL

Figure 7.5 Temperature (kelvin) profiles, two point radial collocation.
 (a) Interior collocation point (b) Exterior collocation point.

FIXED-BED GASIFIER, WYOMING COAL

Figure 7.6(a) Temperature profile of the wall (K) as a function of time.

(b) Example of gas flux (Kgmol/m²hr) profile on a function of time.

GASIFICATION RUN 050293

Figure 7.7. Comparison between experimental and predicted temperature profiles; as a function of time.

TEMPERATURE PROFILE AFTER 2 HOURS

Figure 7.8. Comparison between experimental and predicted temperatures at a particular time.

8. NOMENCLATURE

C_l	concentration of solid
C_p	specific heat of species i
C_{l0}	initial solid concentration
C_w	specific heat of wall
F_i	flow rate of speis i
$h_{w,eff}$	effective wall heat transfer coefficient
k_{eff}	effective radial thermal conductivity
m	no. of gaseous species
n	no. of reactions
r	radial coordinates
R_j	reaction rate of reaction j
R_1, R_2	inner and outer radii of wall
t	time
T	temperature
T_c	temperature of ambient air
T_w	temperature of wall
T_0	inlet temperature of gas
U_c	wall-air heat transfer coefficient
U_{eff}	effective heat transfer coefficient
z	axial coordinate

Greek Alphabet

α_{ij}	stoichiometric coefficient of species i in reaction j
λ_w	thermal conductivity of wall
ρ_w	density of wall

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Appendix 1. Program Documentation

- 1.1 Program Description
- 1.2 Program Structure
- 1.3 Description of Subroutines
- 1.4 Sample Input File and Description
- 1.5 Sample Output File and Description
- 1.6 Program Listing

1.1 Program Description

This program simulates the dynamic behavior of a fixed-bed (moving-bed) char gasifier. Basically the program does the following: Given

- (i) char characteristics and feed rate
- (ii) steam and air feed rate
- (iii) characteristics of gasification reactor
- (iv) initial operating condition of the gasifier

the program computes

- (i) the temperature profile (both axially and radially); product gas compositions and char conversion profiles.

The model is based on mass balances on each of the gaseous and solid species, and a heat balance equation. Radial dispersion of heat is incorporated. Collocation is used in the radial direction and the resulting PDEs are solved by Gear's method of integration in the axial direction and Euler's method of integration in the time domain.

The program consists of about 1500 lines of Fortran code and executes typically in about 1.5 hrs of CPU time (on a DEC-20 computer) for a dynamic simulation of moving beds. The program was coded by A. Bhattacharya, graduate student in chemical engineering department.

1.2 Program Structure

The program structure is shown in Figure 1.2.1. MAIN is the main program, and calls a sequence of subroutines which perform various tasks:

- (i) Reading of data, done by INPUT
- (ii) Calculation of collocation matrices and quadrature weights, done by MATRIX
- (iii) Gasification, done by GASIFY

(iv) Calculation of output values, done by OUTPUT

(v) Taking a step in time, done by TSTEP

(iii), (iv) and (v) are repeated in sequence until conversion is complete. The individual subroutines are described in Appendix 1.3.

The logical unit numbers and the corresponding file names are given in Table A1.2.1. Unit numbers 20-22 correspond to sequential files, whereas 25-27 correspond to direct access files. INDAT.DAT is the only input data file, and a sample is described elsewhere. OUTDAT.DAT contains overall dynamic information at certain z locations for the run, and is also described later. PROF.DAT contains the solid conversion -, the bed temperature - (at all collocation points) and the wall temperature profiles at each of one hundred equidistant z locations. This file therefore, can be used to re-start the program.

PLOT1.DAT, PLOT2.DAT and PLOT3.DAT are direct access files which are only there so that a plotting package existing here in the Chemical Engineering Department at Washington University (Author: Yoshio Yamashita) may be used. As such, PLOT1 contains the profiles of each independent variable at each collocation point at specified times. PLOT2 contains the outlet flow rates of each gaseous species at each time step. PLOT3 contains the extrapolated temperature profiles at $r = 0$ and $r = R$ at specified times.

Restarting the program can be done with the help of PROF.DAT. Simply changing lines 33 to 242 of INDAT.DAT with lines 1-210 of PROF.DAT will usually be enough, unless the heat terms (the 4th and 5th number on the CALCulation control line) are non-zero. If these terms were non-zero (i.e. start-up was being simulated), they should be set to zero.

Table A1.2.1

<u>LOGICAL UNIT #</u>	<u>I/O</u>	<u>FILE NAME</u>
20	I	INDAT.DAT
21	O	OUTDAT.DAT
22	O	PROF.DAT
25	O	PLOT1.DAT
26	O	PLOT2.DAT
27	O	PLOT3.DAT

1.3 Description of Subroutine

INPUT	Reads input data
MATRIX	Sets up the calculation of weight matrices for collocation and calculates the weight matrixes, quadrature weight for collocation
JACOBI	
DFOPR	
INTRP	Calculates the quadrature weights
DGELG	Simultaneous linear equation solver; required for quadrature weight calculation
CASIFY	Performs the gasification
INIT	Sets all variables to conditions at $z = 0$
DIFSUB	Integrates a set of first-order ODEs
MATINV	Dummy routines required for DIBSUB
PEDERV	
DIFFUN	Evaluates the values of the derivatives
OXYGEN	Evaluate v , the stoichiometric coefficient for oxygen in the combustion run
SPHT	Evaluates the specific heats of gaseous species
COEF	Supplies the stoichiometric coefficients of all species
DELTAH	Supplies the heats of reaction
ENTHPY	Calculates the enthalpy of each species
KPRIME	Supplies the effective thermal conductivity and wall heat transfer coefficients
RRATE	Calculates the reaction rate
CORREL	Calculates the values of all parameters (like diffusivities, mass transfer coefficients, etc.)
PARP	Evaluates the partial pressures of each gaseous species
MOLFR	Evaluates the mole fractions of each gaseous species
FUNC	Does a calculation in the evaluation of effectiveness factor
SSTORE	Stores all profiles at specified grid points

INTERP	Interpolates the profiles to find values at all grid points
OUTPUT	Creates most output files
TSTEP	Performs the time-step
THOMAS	Solves a set of simultaneous linear equations which are tridiagonal in nature, using the Thomas algorithm

1.4 Sample Input File and Description

The input data file need not be written in any particular order (except the ESSE segment, which has to come first) since segments are identified by key words. Their description is as follows:

ESSENTIAL PARAMETERS

Number of components, number of reactions

TITLE:

Title of the run

REACTOR PARAMETERS

Length, inner diameter of wall, outer diameter of wall, temperature of surroundings, effective heat transfer coefficient, entering gas temperature, solid temperature, pressure in reactor, thermal conductivity of wall.

CALCULATION CONTROL

Time of run, time step size, number of iterations after which output is to be recorded, heat required for startup, heat added to wall at startup, z-location where heat is added, number of time steps for which heat is added minus one.

KINETIC CONSTANTS

First line: k_0 for reactions 1 through 6

Second line: E for reactions 1 through 6

PROXIMATE ANALYSIS OF COAL

Water, volatile material, ash

ULTIMATE ANALYSIS OF COAL

C, H, O, S, N

FLOW RATES

Steam, oxygen, nitrogen, coal flow rates

ENTHALPY COEFFICIENTS

Heat of formation and specific heat coefficients in the formula

$C_p = a + bT + CT^2$ (T in kelvin) for each of the eight species: Coal.

H₂O, CH₄, O₂, H₂, CO, CO₂, N₂.

COAL PARAMETERS

Particle size, heating value, density, specific heat, weight of coal in the gasifier

EQUILIBRIUM DATA

First line: k_o for equilibrium constants of reaction

Second line: E for equilibrium constants of reaction

PROFILES

First 100 lines: char conversion profiles for each collocation point

Second 100 lines: temperature profiles for each collocation point

next 10 lines: wall temperature profile (10 successive z-locations on each line).

Note: (a) All units are SI

(b) Some of the segments are unnecessary now, but have been put in in case some means of devolatilization can be incorporated.

Interactive parameters required:

N Number of radial collocation points (max: 10)

FACTOR1 Factor to be put on mass transfer resistance for
C + O₂ reaction

FACTOR2	Factor to be put on intrinsic resistance for $C + H_2O$ reaction
TRIAL	Temperature after which heat (for startup) is to be shut off
EFFCON	Effective conductivity
EFCOEFF	Effective wall heat transfer coefficient
EPS	Tolerance criterion for DIFSUB, the integrating routine
ALPHA BETA	α and β in $CH_\alpha O_\beta$

1.5 Sample Output File and Description

There are seven columns in the profile section that need to be explained. They are in order of appearance: temperature, steam flux, methane flux, oxygen flux, hydrogen flux, carbon monoxide flux, and carbon dioxide flux.

Lines are to be read in sets of $N + 1$ (where N is the number of interior collocation points). The first line is for the innermost collocation point; the others come in order.

The line describing the outlet flow rates have the following order:
 H_2O , CH_4 , O_2 , H_2 , CO , CO_2 , N_2 .

The 11 lines following the flow rates are the coal conversion profiles for the N collocation points.

SAMPLE INPUT FILE

```

00100 ESSENTIAL PARAMETERS FIRST:NO. OF COMPONENTS, NO. OF RXNS
00200      8,6
00300 TITLE:
00400 TRIAL RUN: FIXED BED GASIFIER
00500 REACTOR PARAMETERS:L,DI,DT,TA,UT,TS,P,COND
00600      3.043,3.658,3.8,496.0,340.0,644.0,644.0,2533.0,19.0
00700 CALCULATION CONTROL:T,DT,IPDPTN,Q,htad1,PDSN,NO. OF T-STEPS
00800      15.0,0.10,5,0.0d+10,0.0D+03,1.0
00900 KINETIC CONSTANTS:K0 & AE FOR RXNS 1 THROUGH NRCTN
01000      .1464D+05, .3704D+04, .2931D-03, .2931D-03, .6360D+08, .01543
01100      .1465D+05, .1465D+03, .6715D+08, .6715D+08, .1130D+09, .4070D+08
01200 PROX. ANALYSIS OF COAL(AFTER DEV. AT 900 F): WATER, VOL. MAT., ASH
01300      0.1272,0.1981,0.1331
01400 ULTIMATE ANALYSIS OF THE COAL: C,H,O,S,N
01500      0.7147,0.0493,0.0902,0.0313,0.0135
01600 FLOW RATES: STEAM, OXYGEN, NITROGEN, COAL (MCLAR FLOWS)
01700      1274.93,197.5,0.0,750.0
01800 ENTHALPY COEFFICIENTS: HQF, CPA, CPR, CPC FOR COMPONENTS
01900      0.3000D+03, 0.1000D+02, 0.1000D-01, 0.1000D-06
02000      -0.2419D+06, 0.2936D+02, 0.1105D-01, 0.1921D-06
02100      -0.7485D+05, 0.1341D+02, 0.7703D-01, -0.1875D-04
02200      0.0D+00, 0.2560D+02, 0.1325D-01, -0.4205D-05
02300      0.0D+00, 0.2907D+02, -0.9201D-03, 0.1931D-05
02400      -0.1105D+06, 0.2657D+02, 0.7578D-02, -0.1119D-05
02500      -0.3936D+06, 0.2653D+02, 0.4243D-01, -0.1429D-04
02600      0.0D+00, 0.2702D+02, 0.5312D-02, -0.2887D-06
02700 COAL PARAMETERS: DP,HV,DENSITY,SPHT,WT
02800      0.01,-277E0.,1.0,1.0,27000.0
02900 EQUILIBRIUM DATA: (INCLUDING CO/CO2 RATIO)
03000      0.3139D+10, 0.1233D+12, 0.1453D-07, 0.2650D-01, 0.2512D+04
03100      0.1353D+09, 0.1605D+09, -0.9144D+09, -0.3299D+08, 0.4190D+08
03200 PROFILES:CHAR CONVERSION,TEMPERATURE & WALL TEMPERATURE
03300      0.1000D+01 0.9995D+00
03400      0.1000D+01 0.9993D+00
03500      0.1000D+01 0.9992D+00
03600      0.1000D+01 0.9997D+00
03700      0.1000D+01 0.9996D+00
03800      0.1000D+01 0.9995D+00
03900      0.1000D+01 0.9993D+00
04000      0.1000D+01 0.9991D+00
04100      0.1000D+01 0.9989D+00
04200      0.1000D+01 0.9984D+00
04300      0.1000D+01 0.9978D+00
04400      0.1000D+01 0.9970D+00
04500      0.1000D+01 0.9959D+00
04600      0.1000D+01 0.9945D+00
04700      0.1000D+01 0.9929D+00
04800      0.1000D+01 0.9898D+00
04900      0.1000D+01 0.9862D+00
05000      0.1000D+01 0.9813D+00
05100      0.1000D+01 0.9745D+00
05200      0.1000D+01 0.9659D+00
05300      0.1000D+01 0.9536D+00
05400      0.1000D+01 0.9403D+00
05500      0.1000D+01 0.9256D+00
05600      0.1000D+01 0.9093D+00
05700      0.1000D+01 0.8909D+00
05800      0.1000D+01 0.8707D+00
05900      0.1000D+01 0.8494D+00
06000      0.9995D+00 0.9993D+00

```

VALUES OF INTERACTIVE PARAMETERS

N	=	2
FCTRI	=	0.0
FCTR2	=	1.0
TRIAL	=	900.0
EFFCON	=	34.2
EFFCOEF	=	116.0
EPSS	=	1.0
ALPHA	=	0.0
BETA	=	0.0
BED TYPE:		2

Total time of minutes $\approx$ 1 hour, 20 minutes on the DEC-20

Sample Output File, 2-point Collocation

1 TIME= 4.50

MAX. TEMP. FOR 2TH CELL. PT. OCCURRED AT Z= 0.2900 . PROFILES HERE ARE:

0.64920+03 0.12130+03 0.10910-14 0.17820+02 0.26750-02 0.10880-01 0.15710-01
0.11240+04 0.97430+02 0.49250-01 0.60400+01 0.23780+02 0.86980+01 0.19390+02

MAX. TEMP. FOR 1TH CELL. PT. OCCURRED AT Z= 0.5100 . PROFILES HERE ARE:

0.11280+04 0.94350+02 0.73440-01 0.55650+01 0.26820+02 0.10330+02 0.20590+02
0.10170+04 0.60700+02 0.24170+01 0.16210-05 0.53730+02 0.24830+02 0.35740+02

0.64440+03 0.12130+03 0.73530-13 0.17840+02 0.20250-03 0.10990-02 0.14960-02
0.66660+03 0.12130+03 0.10690-10 0.17470+02 0.33530-01 0.24190+00 0.27060+00
0.49610+03 0.12130+03 0.12990-10 0.17390+02 0.40680-01 0.29350+00 0.32840+00
0.64550+03 0.12130+03 0.33350-16 0.17840+02 0.25410-03 0.25580-02 0.42300-02
0.89340+03 0.11920+03 0.53510-05 0.13630+02 0.21440+01 0.30750+01 0.37440+01
0.49620+03 0.11870+03 0.54590-05 0.12730+02 0.26040+01 0.37330+01 0.45460+01
0.64990+03 0.12130+03 0.33240-14 0.17820+02 0.31490-02 0.13650-01 0.19210-01
0.11220+04 0.93350+02 0.82530-01 0.51010+01 0.27800+02 0.10690+02 0.21370+02
0.49620+03 0.87360+02 0.10020+00 0.21750+01 0.32760+02 0.12990+02 0.25950+02
0.67030+03 0.12130+03 0.57090-11 0.17560+02 0.32210-01 0.18240+00 0.21000+00
0.10480+04 0.87550+02 0.10520+01 0.18030+00 0.51650+02 0.24170+02 0.32460+02
0.49620+03 0.56030+02 0.12730+01 0.00000+00 0.62730+02 0.29310+02 0.39380+02
0.82830+03 0.12020+03 0.60610-06 0.14900+02 0.10990+01 0.23070+01 0.23350+01
0.10200+04 0.62270+02 0.22170+01 0.93530-03 0.54510+02 0.24700+02 0.35010+02
0.49620+03 0.49940+02 0.26930+01 0.00000+00 0.66030+02 0.29500+02 0.42020+02
0.11260+04 0.39570+02 0.40350-01 0.65590+01 0.22660+02 0.82830+01 0.19510+02
0.10170+04 0.60310+02 0.33110+01 0.26340-05 0.53880+02 0.24810+02 0.35690+02
0.49620+03 0.52710+02 0.40120+01 0.00000+00 0.60580+02 0.28350+02 0.29370+02
0.10590+04 0.67570+02 0.59590+00 0.25130+00 0.51760+02 0.24930+02 0.31960+02
0.10170+04 0.59790+02 0.43440+01 0.18090-07 0.52840+02 0.24960+02 0.35120+02
0.49620+03 0.58120+02 0.50630+01 0.00000+00 0.53070+02 0.24970+02 0.37020+02
0.10300+04 0.61160+02 0.22310+01 0.65910-02 0.55570+02 0.26060+02 0.24880+02
0.10160+04 0.58330+02 0.53140+01 0.00000+00 0.51810+02 0.25030+02 0.26520+02
0.49620+03 0.58390+02 0.59620+01 0.00000+00 0.51000+02 0.24870+02 0.26870+02
0.10240+04 0.59450+02 0.35310+01 0.00000+00 0.54800+02 0.26930+02 0.35310+02
0.10160+04 0.58040+02 0.62220+01 0.00000+00 0.50830+02 0.25170+02 0.36890+02
0.49620+03 0.57730+02 0.67350+01 0.00000+00 0.49980+02 0.24790+02 0.37240+02
0.10280+04 0.57330+02 0.46340+01 0.00000+00 0.54100+02 0.26870+02 0.35150+02
0.10160+04 0.57260+02 0.70710+01 0.00000+00 0.49910+02 0.25240+02 0.37250+02
0.49620+03 0.57140+02 0.75610+01 0.00000+00 0.49010+02 0.24890+02 0.37480+02

OUTLET FLOW RATES(KGMO/L/HR) ARE:

0.60390+03 0.65500+02 0.00000+00 0.54000+03 0.27130+03 0.38740+03 0.00000+00
1 0.1000+01 0.5290+00
10 0.1000+01 0.9920+00
20 0.1000+01 0.9020+00
30 0.1000+01 0.5370+00
40 0.9950+00 0.1700+00
50 0.9220+00 0.1100+00
60 0.5780+00 0.8200-01
70 0.1470+00 0.5930-01
80 0.6560-01 0.3970-01
90 0.3380-01 0.1920-01
100 0.1760-02 0.1240-02

Figure 1.2.1 Program Structure

APPENDIX 2

Early Results

This Appendix summarizes the results from the first gasification run on May 2, 1983. Table 10.4 summarizes the operating conditions for the run. The feed and product gas flowrates are marked with question marks to denote the uncertainty in these values. The uncertainty resulted from the improper location of the pressure gauges for the two flowmeters. Therefore, the flowrates could not be properly calibrated. Figures 10.5 and 10.6 show the bed temperatures for the run. Figure 10.7 shows the product gas compositions.

Table 10.5

Summary of Operating Conditions

for Gasification Run 050283

Char Loaded: 2868 gms devolatilized Wyodac char.
 Char Composition: The char used was devolatilized to an average of 705°C. Average weight reduction was 53.4% during devolatilization.

Time 0-295 min

INLET	Air Flowrate:	1.410 m ³ /hr* (?)
	Water Flowrate:	3 gm/min
	O ₂ /H ₂ O:	2.15 gm/gm (1.21 mol/mol)
OUTLET	Product Gas Flowrate:	1.970 m ³ /hr* (?)

Time 295-440 min

INLET	Air Flowrate:	2.548 m ³ /hr* (?)
	Water Flowrate:	3 gm/min
	O ₂ /H ₂ O:	3.89 gm/gm (2.19 mol/mol)
OUTLET	Product Gas Flowrate:	2.973 m ³ /hr* (?)

Solids Remaining: 453.5 gms char and ash
 Total Condensate: 206 gms
 Original Bed Length: 70 cm
 Final Bed Length: ~ 2 cm
 Reactor Pressure: 0.1668 MPa, 0.2942 MPa

* at 25°C 0.1013 MPa

Figure 10.5 Gasification Temperature Profiles for Run 050283 (TC #1 - TC #6)

Figure 10.6 Gasification Temperature Profiles for Run 050283 (TC #7 - TC #12)

Figure 10.7 Product Gas Compositions for Run 050283

APPENDIX 3

DESCRIPTION OF FACTOR1 and FACTOR2

These factors are used in the reaction rate calculation. FACTOR1 puts a lower limit on the resistance due to gas film mass transfer. This was necessary so that the total resistance (in the SCM model used for the char + O₂ and char + H₂O reactions) did not become too low - which would result in unreasonably high reaction rates. It is felt that the correlation used to predict k_g , the gas-film mass transfer coefficient is inaccurate or invalid at the low values of particle Reynolds numbers that are present in the experimental gasifier.

FACTOR2 is a multiplicative factor on the char stream intrinsic reaction rate. This was introduced because more steam was being used in the reactor than was being predicted by the model. Since we used char - and not coal - it is a possibility that the kinetic expression used is in error.

It should be noted that these factors were in fact not used for the Lurgi simulation. For this, we used FACTOR1 = 0.0 (: the lower limit = 0) and FACTOR 2 = 1.0 (so not multiplicative factor). It should also be noted that the model does not include devolatilization: so the outlet compositions may be somewhat different from the usual values (for example, low CH₄).