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THE MIXING AND GASIFICATION OF COAL IN ENTRAINED FLOW SYSTEMS

Quarterly Technical Progress Report
for the Period 1 October, 1975 to 31 December 1975

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ABSTRACT

This report presents work accomplished during the fourth quarter to investigate mixing and gasification of coal in entrained flow systems.

Technical visits to European laboratories conducting coal and combustion work are summarized. Review of numerical methods for treating recirculating flows in coal combustors was continued. Fabrication and installation of modifications to the non-reacting facility for measuring particle-gas mixing rates were completed. Fabrication of the low pressure reactor sections was completed while fabrication of inlet sections was initiated. Final design of the high pressure reactor was nearly completed and a fabrication schedule was identified. The primary oxygen preheater was received and the steam generator and secondary steam-oxygen superheater were ordered. Design of the reactor support and service systems were completed and parts ordered and received. Samples of pulverized coal to be used in the test program were analyzed by independent laboratories.

Development of a macroscopic model of coal gasification processes was outlined. Model assumptions, differential equations, and auxiliary equations were formulated. For a specified rate of mixing of primary and secondary streams and rate of recirculation of combustion products, the model includes effects of radiation, ignition, coal pyrolysis, char oxidation, and hydrocarbon reaction. A possible cooperative program for predicting the details of mixing and recirculation in coal gasifiers is also being considered.

OBJECTIVE AND SCOPE OF WORK

Background

Two national goals of great importance to every citizen of the United States are the development of adequate energy supplies and the establishment of a satisfactory living environment. Vast domestic reserves of coal cannot presently be used directly without degrading the environment beyond the limits specified by current environmental quality laws. As a consequence, conversion of this fossil fuel into a more desirable form is an intermediate solution to the problem of meeting energy demands.

As attempts have been made to produce large, clean, economical supplies of gas and oil from coal, a number of different types of coal gasification processes have been proposed, explored and developed. Several of these coal gasification processes involve, either directly or indirectly, the injection of finely powdered coal, suspended in a gas stream, into a reactor where the conversion reactions take place, creating a variety of different products. Associated with such entrained particle processes are technological problems involving the entrainment of the coal. The basic principles of this process are not well understood and require considerable study before rational engineering designs are possible. One problem associated with the entrainment of the coal particles is the influence of the turbulent mixing characteristic of a particle-laden gas stream on the rates of chemical reactions which take place in the reactor, and on the subsequent yield of products. Such mixing problems have been identified (1) as among the most critical and key problems which need to be solved in order to improve the design of entrained gas reactors. While some work has been and is being conducted (2,3) to determine the effects of mixing on the kinetics of direct combustion of pulverized coal, very little work has been reported which deals with the basic processes of coal gasification. The present study deals specifically with the influences of turbulent mixing on coal gasification processes.

Objectives

The general objective of this research program is to develop an understanding of physical and chemical rate processes that occur during gasification of entrained, pulverized coal particles. Specific tasks that have been outlined for accomplishment during the first phase of this study are:

1. Conduct visits to facilities where research and development on entrained coal gasification units are in progress. Identify more specifically the configurations, operating conditions, and input properties of reactants and clarify the nature of potential particle/gas mixing problems.

2. Analyze in detail the configurations, reactant systems, and operating properties in entrained coal gasifiers and char combustors and select a set of variables for a subsequent experimental test program. Variables to be considered will include: (1) operating conditions, such as pressure, residence time and flow rates; (2) configurations, such as injection angle and reactor size; (3) reactant stream conditions, such as temperature, gas phase composition, particle size and particle loading level.

3. Design and construct a laboratory-scale test facility, capable of operation over a range of conditions for study of non-reacting and reacting coal/char/gas systems in different geometries. Include the capability to sample the particle/gas mixtures locally in order to determine the extent of gas mixing, the extent of particle dispersion, the amount of particle reaction, and the local product composition.

4. Conduct a series of non-reacting tests using the laboratory scale facility to determine the gas dispersion rates and recirculation effects for various operating conditions, stream compositions, and geometric configurations.

5. Interpret experimental particle/gas dispersion results and analyze for potential impact on configuration and operating conditions in entrained coal-gasification units.

6. Initiate the development of a computerized mathematical model for describing reacting coal gasification and char combustion processes.

This first phase of this work has been scheduled to be accomplished in a two-year study period. The second phase of the program will emphasize reacting coal gasification tests, and comparison of measurements with model predictions.

Technical Approach

In order to accomplish the tasks outlined above, two entrained flow reactors are being designed and constructed. One reactor will operate at atmospheric pressure while the second reactor will be designed to operate at a peak pressure of 20 atm.

The atmospheric reactor is being constructed principally to study direct coal combustion using funds from a separate project supported by EPRI (3). However, this reactor will also have the capability to gasify coal and combust char at atmospheric pressures. The high pressure reactor, which will require a longer period to design, construct and evaluate, is being developed principally to study entrained coal gasification processes at elevated pressures, and isbeing constructed using funds from this study. The high pressure reactors will have a primary nozzle diameter of 1.27 cm, and will have a coal processing capacity of 13.6-136 kg/hr.

A third test facility to study mixing processes of non-reacting flows is already available at this laboratory and is being used for this project to study mixing of non-reacting, particle-laden flows at atmospheric pressure conditions.

Experimental plans for Phase I require two separate sets of non-reacting tests: (1) A series of non-reacting, atmospheric tests using the existing atmospheric, non-reactive test facility. (2) A series of non-reacting, high-pressure tests using the reactive high pressure test facility being designed as a part of this study. It is also planned that reactive coal gasification checkout tests for atmospheric and higher pressure will be conducted toward the end of this first phase of study. Additional information concerning the basic approach was outlined in the first quarterly progress report (4).

SUMMARY OF PROGRESS TO DATE

Figure 1 shows a summary chart of research activities by task. Progress to date in each of the tasks is summarized below.

Task 1. Facility Visits. Facility visits have been completed. This task included visits with Bureau of Mines, BCRI, Koppers Corporation, Babcock and Wilcox, Foster and Wheeler, and Combustion Engineering in the United States. International Flame Foundation , Cherchar, Bergbau Forschung, BCURA, CERL, National Coal Board Labs and British Gas Corporation facilities were visited in Europe. Contact and interchange is being maintained with U.S. companies.

Task 2. Variable Selection. Development of the test variables and tentative test programs have also been completed and were reported in detail in the first and second quarterly progress reports (3,5). For non-reactive tests, two series of tests with and without recirculation, have been outlined for several different test conditions. Test variables include primary velocity (15, 30 m/sec), secondary velocity (30, 60 m/sec), percent solids in primary stream (40, 60 %), injection angle (0, 30 degrees), secondary/primary density (0.1, 0.47), aft-duct diameter (13-35 cm), and particle size (30, 70μ).

Development of test conditions and test programs have also been completed for the entrained gasification tests. Coal feed rate will be about 140 Kg/hr. Variables will include pressure (1-20 atm), coal type, injection angle (0, 30 degrees), secondary preheat temperature (315, 430 C), secondary velocity (15, 25 m/sec), solids loading level (70-80%), and coal size. The tentative test program includes 54 tests.

Task 3. Facility Design and Construction. Modification of the non-reacting test facility has been completed for the non-recirculating tests. A series of preliminary tests have been conducted using that facility. Design of new components for recirculating, nonreacting tests has been completed and fabrication of these components initiated by the research machine shop.

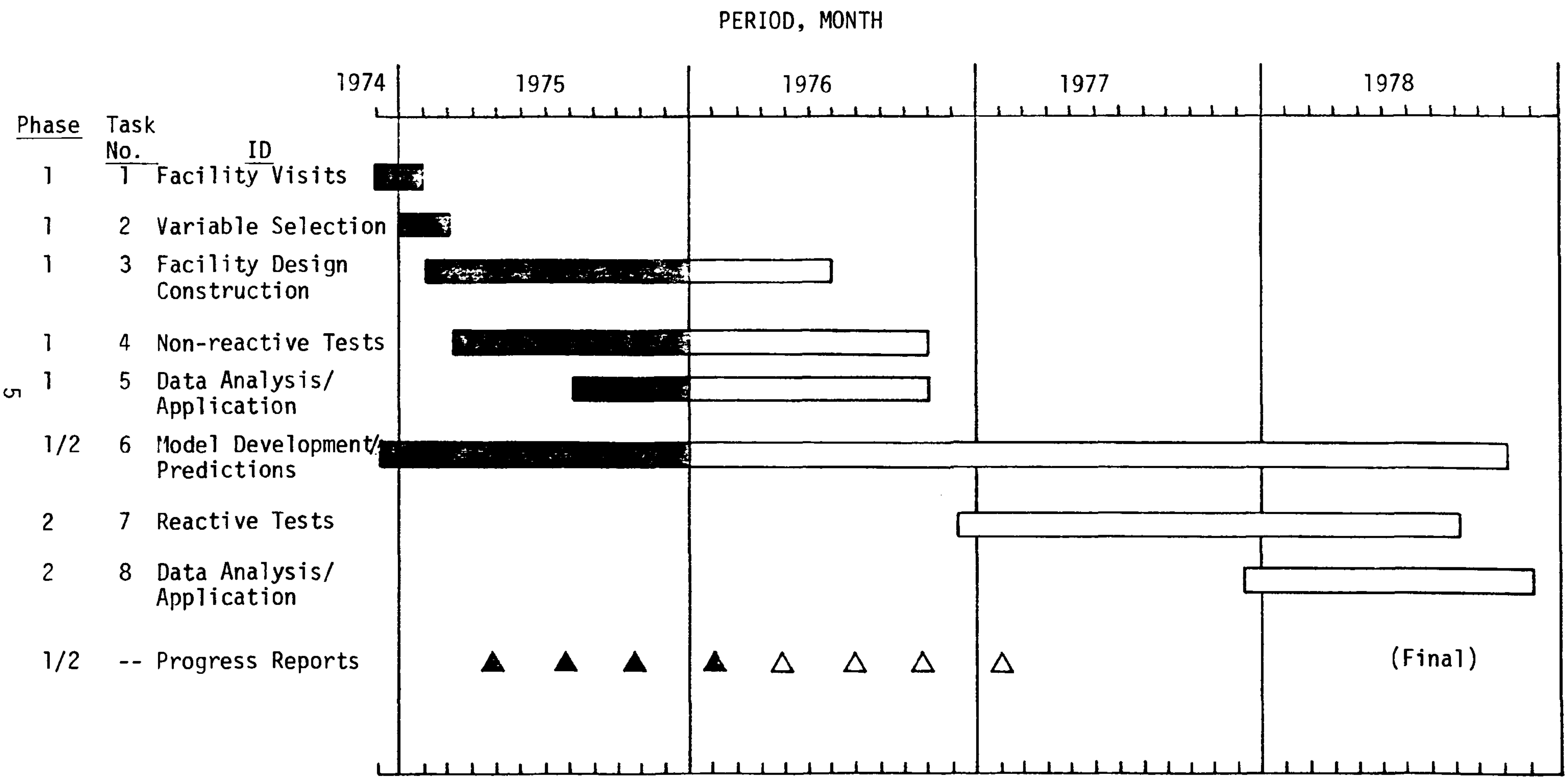


Figure 1. Summary Chart of Research Activities

A major activity has included design of the high pressure coal gasifier. The reactor will be 20 cm inside diameter and approximately 1.5 m long. Inlet sections will be flexible while reactor sections will be interchangeable to permit relocation of the instrument section. The high pressure air system, recording system, control valves, primary heater, ceramic liner, overhead hoist, steam generator and secondary superheater have been designed and fabricated or ordered and received. Design is also complete on the particle removal system, control system, injection system, reactor shell, and structural support system. Detailed construction drawings are being prepared and a fabrication schedule drawn up for the research machine shop which projects completion of high-pressure components by May of 1976. Time required to complete this facility has increased from the original estimates, but is still within contract requirements.

Task 4. Non-Reactive Tests. Twenty-two non-reactive jet mixing tests have been performed to date. These tests have been preliminary facility check-out tests and results indicated problems with the symmetry of the coaxial, particle-laden flows. This difficulty was associated with the secondary flow inlet sections which have been redesigned, constructed, and installed. It is anticipated that final test results will be obtained during the coming study period. This test program will continue to the end of Phase 1.

Task 5. Data Analysis. Analysis of the non-reacting, preliminary test results has been conducted for 22 tests. The bulk of the work for this task will follow the planned experimental program.

Task 6. Model Development. Reviews of the technical literature related to modelling of pulverized coal combustors and gasifiers have been conducted. Areas of emphasis included recirculating flows, coal pyrolysis, coal oxidation, numerical methods, and entrained gasification. Technical assessment of the review will continue. A macroscopic model of pulverized coal gasification has been formulated, including physical assumptions, basic differential equations, and auxiliary equations. Plans for computer solution of this model have been outlined. Also, methods of predicting the detailed structure of recirculating, reacting, particle-laden flows have been considered and a possible cooperative program for development of a practical combustor model is being considered.

Progress Reports. To date, four quarterly reports and an annual summary report have been prepared and submitted to ERDA.

DETAILED DESCRIPTION OF TECHNICAL PROGRESS

Technical Visits and Reviews

During July-October of 1975, L. Douglas Smoot, Professor of Chemical Engineering, Brigham Young University, visited several universities and laboratories in England, France, Germany, and Holland which are interested in coal combustion and gasification and related technologies. The trip was supported in part by Brigham Young University, Electric Power

Research Institute, and Energy Research and Development Administration. Table I provides a short summary of each of the specific laboratory visits relating to coal combustion and gasification. Among the general observations were the following: (1) French activity in coal combustion and technology is declining, with projections for lower uses of coal in the future, due to limited available natural resources. There is some interest in deep mining technology. Previous work on coal pyrolysis is relevant to our present work. (2) German emphasis includes fluidized gasification, including pilot plant development for a combined power plant cycle using coal and nuclear energy. Previous basic work on coal combustion and pyrolysis is of interest. German instrument development and gas phase kinetics work is also relevant. (3) Research emphasis in England includes basic and pilot plant work on fluidized bed combustion and gasification, heavy fuel oil technology, including spray mechanics, gas phase kinetics, and laser-anemometry for study of combusting flows. Previous work on pulverized coal combustion is relevant, but interest and emphasis in coal research is presently not great. European work in MHD cycles seems to have been discontinued.

British pilot plant work with U.S. financial support is continuing for a slagging, high-pressure, Lurgi gasifier. Experimental work at the International Flame Foundation Research Lab has included pulverized coal, but presently emphasizes fuel oils.

A technical discussion was held in December with Dr. David Pratt, Washington State University. Modelling of recirculating flows was emphasized in this discussion. Plans for more detailed discussions were set for January, 1976. Plans were also made for a technical visit with Dr. Jost Wendt, University of Arizona, during January, to discuss coal combustion and pollutant formation.

Technical review during the last report period has emphasized modelling of recirculating flows. Among the references reviewed are Refs. 6-12. Several of these references relate to new techniques developed by Spalding and co-workers at Imperial College.

Non-reacting Tests.

The objectives of the atmospheric, non-reacting tests are: (1) To measure the rates of turbulent mixing of a particle-laden primary jet with a secondary air jet for a range of test conditions similar to that used in pulverized coal combustors; (2) To measure the influence of recirculation on the rates of mixing of the particle-laden jets. These non-reacting tests also relate directly to the pulverized coal combustion study (3). Results of these tests will provide useful information for interpretation of the reacting tests to follow. While some non-reacting tests will be conducted in the high-pressure coal gasifier presently being designed for this study, the initial non-reacting tests will be conducted with an existing test facility used in previous jet mixing studies at this laboratory (14). The proposed non-reacting tests will be conducted in two parts: (1) without recirculation effects (where the primary and secondary jet exhausts entirely fill the mixing chamber) using parallel and non-parallel flow configuration; (2) with recirculation effects, using a mixing chamber that is larger in diameter than the secondary jet.

TABLE 1

Summary of Technical Visits

No.	Laboratory/ Location/Contact	Date Of Visit	Nature of Work/ Size	Observations, Comments Interests, and Activities
1.	International Flame Research Foundation, Ijmuiden, Holland; Mr. S. Michelfelder	July 11, 1975	Experimental pc-oil test facility with probing; sponsored by 150 member companies.	Solvent refined coal,p.c.NO_x tests (EPA); large scale (2-4 megawatt).
2.	Centre D'E'tudes et Recherches Des Charbonnages De France (CERCHAR), Creil, France M.P. Pumoutet, M.R. Chauvin	Aug. 7, 1975	Coking, power plants, mining, utilization, chemistry; 640 personnel.	Low coal emphasis since 1968 Koppers plant in 1950's: deep mining interest; previous basic pyrolysis and ignition work.
3.	University of Stuttgart, DFVLR Labs., Germany Dr. Thomas Just Mr. Heinrich Reidelbach	Sept. 16, 1975	Basic research work, instrument development general energy sources; 80 people.	Methane kinetics, direct measurement of NO_x, laser-fluorescence for turbulence, coal pyrolysis
4.	Bergbau Forschung GMBH, Essen-Kray, Germany Dr. Karl Van Heck Dr. Paul Feistel	Sept. 26, 1975	Coal utilization coal production mine safety 1250 people	Previous basic pyrolysis work coking, fluid bed combustion, combined coal gasification, nuclear power cycle.
5.	British Coal Utilization Research Association Latherhead, England Mr. Raymond Hoy	Sept. 30, 1975	Fluidized bed gasification; U.S. Company investment; 70 people	High pressure gasification (COED) two stage with char combustion; pilot plant operation; discontinued MHD work.
6.	Central Electricity Research Labs Leatherhead, England Mr. Ken H. Joliffe Dr. Michael Neddleton	Oct. 1, 1975	Total English power generation responsibility; central lab. 350 scientists	Heavy fuel oil combustion, H_2SO_4 mist control; safety; explosions; atmospheric dispersion; previous p.c. in shock tubes; power transmission; low coal emphasis.
7.	National Coal Board, Stoke Orchard, Eng. Dr. Gibson Mr. Jack Owen	Oct. 2, 1975	Coke production coal combustion coal gasification coal liquifaction 500 people	Fluidized bed gasification small scale and pilot scale small appliance coal applications combined cycle interest supercritical extraction
8.	British Gas Corporation Solihull, England Dr. J.A. Lacy Dr. Henry Stroud	Oct. 3, 1975	SNG and gas applications; LNG storage and safety; gas production/combustion; 350 people.	Lurgi plant (Westfield) liquid HC derivations catalytic processes oil based SNG
9.	University of Birmingham, England Dr. John Botterill	Oct. 4, 1975	Chemical Engineering fluidized bed mechanics 30 academic staff	fluid bed heat transfer; referenced Sept. 1975, Fluid Bed Combustion Conference, London

TABLE 1 cont.

No.	Laboratory/ Location Contact	Date of Visit	Nature of Work/ Size	Observations, Comments Interests, and Activities
10.	Aston University Birmingham, England Prof. Doug Elliott	Oct. 6, 1975	Mechanical Engineering combustion and heat transfer in fluid beds	shallow bed development extended surface heat transfer centrifugal fluid combustor.
11.	Leeds University Leeds, England Prof. Alan Williams Dr. Dixon-Lewis	Oct, 7-8, 1975	Fuel and Combustion Science Department 11 academic staff	HC gas kinetics, shock tubes, computations, fluid beds, turbulence noise, radiation, fuel sprays, combustion.
12.	British Gas Corp Westfield Develop. Center, Scotland Mr. John McNaughton Dr. Terry Brooks	Oct. 10, 1975	Lurgi pilot plant 14 U.S. companies 50-100 people	Previous operation - 4 Lurgis-350 psia; new slagging gasifer development-3-6 times through-put: operation by spring, 1976 methanation plant.
13.	Safety in Mines Research Establishment Buxton, England and Sheffield, England Dr. D. Rae Dr. G. Artingstall	Oct. 13-14, 1975	Mine safety, explosion suppression; mine venilation.	1000 ft. test gallery - mine explosions, water spray barrier development work on all dust explosions stirred reactor coal combustor previous work on explosions.
14.	University of Sheffield, England Prof. J.N. Beer Dr. N.A. Chigier	Oct. 15-16, 1975	Chemical Engineering and Fuel Technology, engineering research 12 academic staff	flames, kinetics and ions spray dynamics/size distribution, previous work on p.c. combustion; radiation, particulate emissivity, laser ana-mometry, fluidized beds, NO_x.
15.	Imperial College London, England Prof. Brian Spalding Dr. Douglas Napier	Oct. 20-21, 1975	Mechanical/ Chemical Engineering 12/20 academic staff	methane/air quenching unsteady jet development complex combustor computations laser anamom try, combustion chemistry, spray mechanics, fluidized bed combustion
15.	Southampton University, England Prof. Kenneth Bray Dr. Norman Pratt	Oct. 22-23, 1975	Aeronautical Engineering 12 academic staff	Reaction with turbulence, shock tube kinetics/high pressures, laser anamometry turbulent jet computations
17.	CERL Marchwood Engineering Labs Southampton, England Dr. D. Swift Hook Mr. Peter Street	Oct. 24, 1975	Engineering laboratories for Central Electricity Generating Board	p.c. furnace radiation model; p.c./oil fired large scale experimental furnace; super-critical extraction; coal/oil pyrolysis atmospheric dispersion

During the last quarter of study, efforts were continued to complete required facility modifications as described in the previous quarterly progress report (5). The purpose of these modifications was to adapt the facility to the proper range of test conditions and to eliminate an asymmetric flow problem which developed as a result of implementing test conditions required for this study. The fabrication and installation of the parts necessary in this modification have been completed. System control and vacuum difficulties were also resolved and the test facility was made ready for testing. At the end of the study period, a check-out test was conducted using an argon/air mixture without particles. The facility functioned well and test results indicated that the asymmetric flow problem had been corrected. During the coming study period, final testing will be initiated.

Reacting, Gasification Tests

Design and Construction. During this past quarter, detailed design has continued on the various components of the high pressure gasification system. Table 2 summarizes the status of the components that comprise the high-pressure gasifier unit. Design work has been completed on the reactor and most of the associated components.

The general dimensions chosen for the reactor were 0.3m O.D. by 1.4m long. The reactor will be built in interchangeable sections which will give the flexibility of probing for gas and particulate samples every 0.15m along the axis of the reactor. Figure 2 is an elevation drawing of the reactor with the primary-secondary injection system and the reactor shell and outlet. Figures 3-5 show design details of the top section, a typical reactor section and the bottom section, respectively.

Preparation of final working drawings for reactor components was initiated during the study period. Fabrication of these component parts, according to OSHA standards for high pressure vessels will be initiated during the coming quarter.

Design details have also been completed for the feeder. In order to have the capability of running for 20-25 minutes at the desired 136 kg/hr feed rate, the design diameter of the feeder has been increased from 0.4m to 0.5m. Capabilities of installing a stirrer in the top and filling from the top have been provided. A cross-section drawing of the feeder is shown as Figure 6. Final construction drawings were initiated with fabrication to start in the next quarter.

Also during this past quarter, the primary oxygen preheater was received while designs on the steam generator and secondary oxygen steam preheater were completed and these components were ordered. Further, the hoist rail was installed and the structural support and service systems for the reactor were designed, order and received. In addition, the overhead hoist system was installed and several control and instrumentation components were received.

TABLE 2

Design Status of High Pressure Gasifier Components

Design Item	Status	Comments
Coal/Char Feeder	Design complete	Detailed drawings being prepared
High Pressure Air Line and System	Construction and installation complete	
Particulate Removal System	Design complete	Awaiting fabrication in machine shop - parts not yet received
Instrumentation - Recording System	Design complete	Ordered per specifications - certain components received
Primary and Secondary Control Valves	Design complete	Ordered per specifications and received
Automatic Controllers and Control System	Design complete	
Primary Heater	Design complete	Ordered and received
Primary-Secondary Injection System	Design complete	Detailed drawings being prepared
Reactor Shell	Design nearing completion	To be fabricated in machine shop - parts and materials not yet received
Ceramic Reactor Lining	Design and testing near completion	Cylindrical cast ceramic shells
Sampling Probes	Design nearing completion	Water-cooled, direct water quench probes
Overhead Hoist System	System installed	
Structural Supports and system piping	Design essentially complete	Construction initiated
Steam Generator System	On order	Design complete
Steam Superheater	On order	Design complete

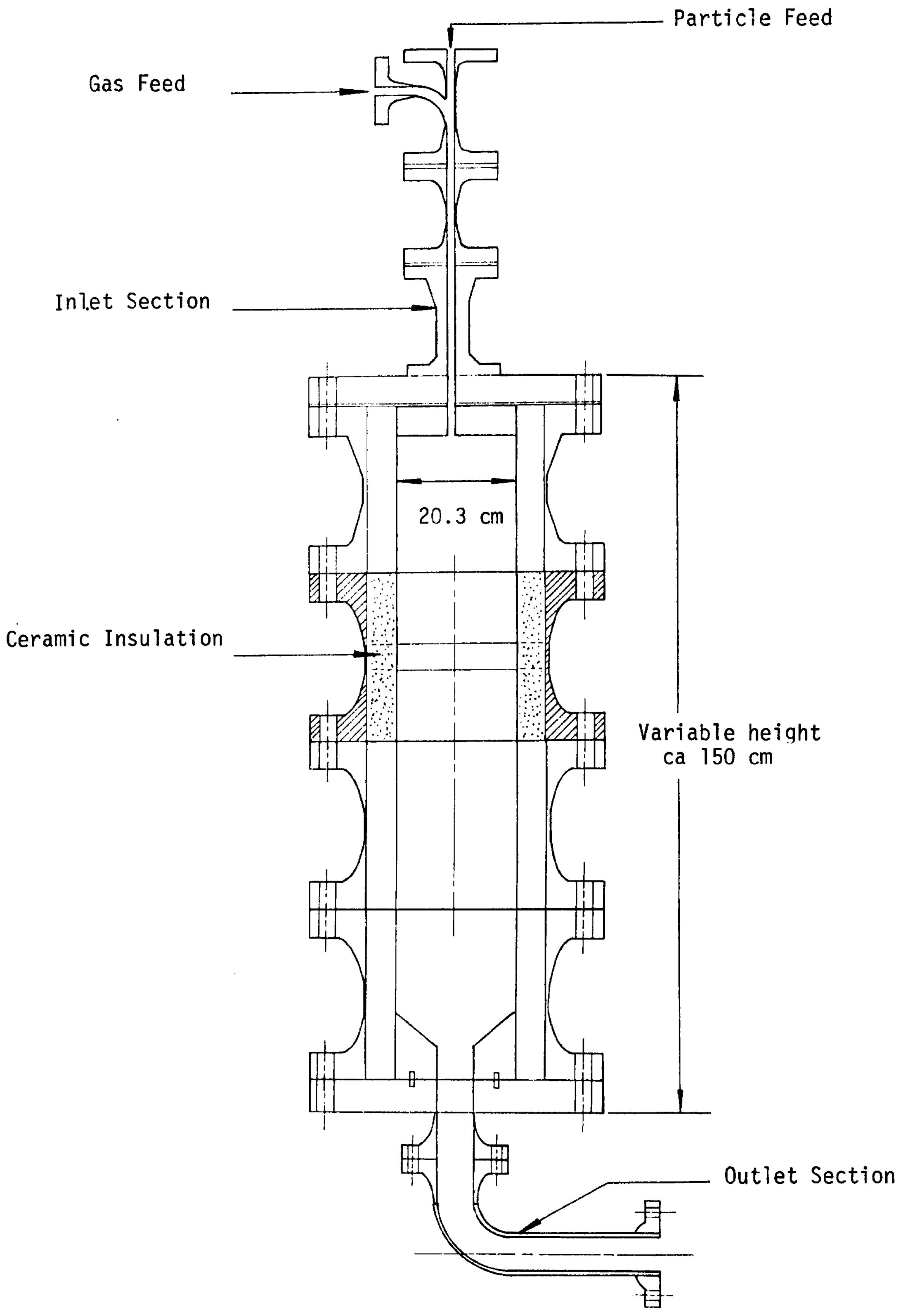


Figure 2. ERDA High Pressure Reactor -- Overall System Design.

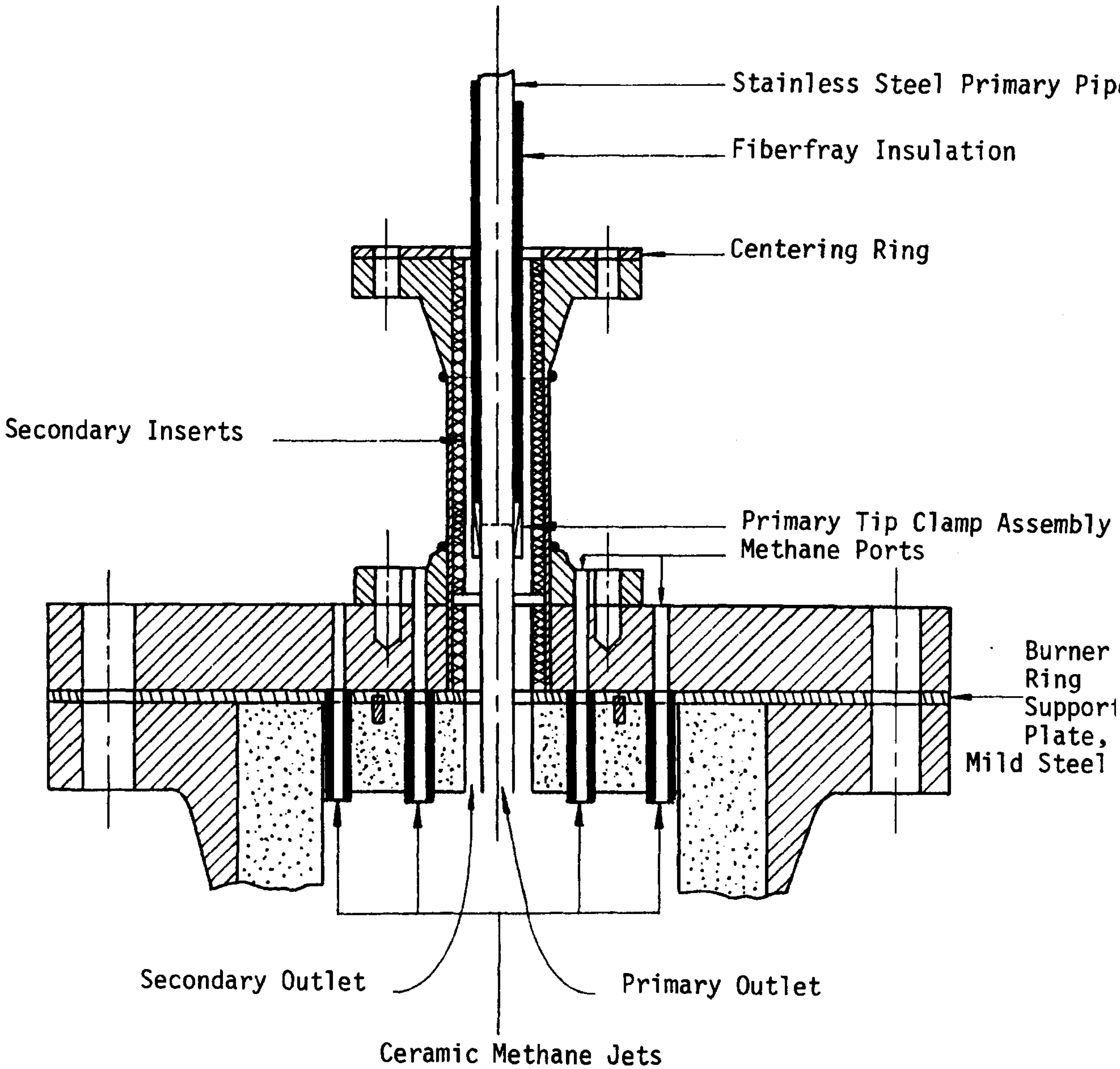


Figure 3. Gasifier Reactor Top Plate and Primary/Secondary Assembly.

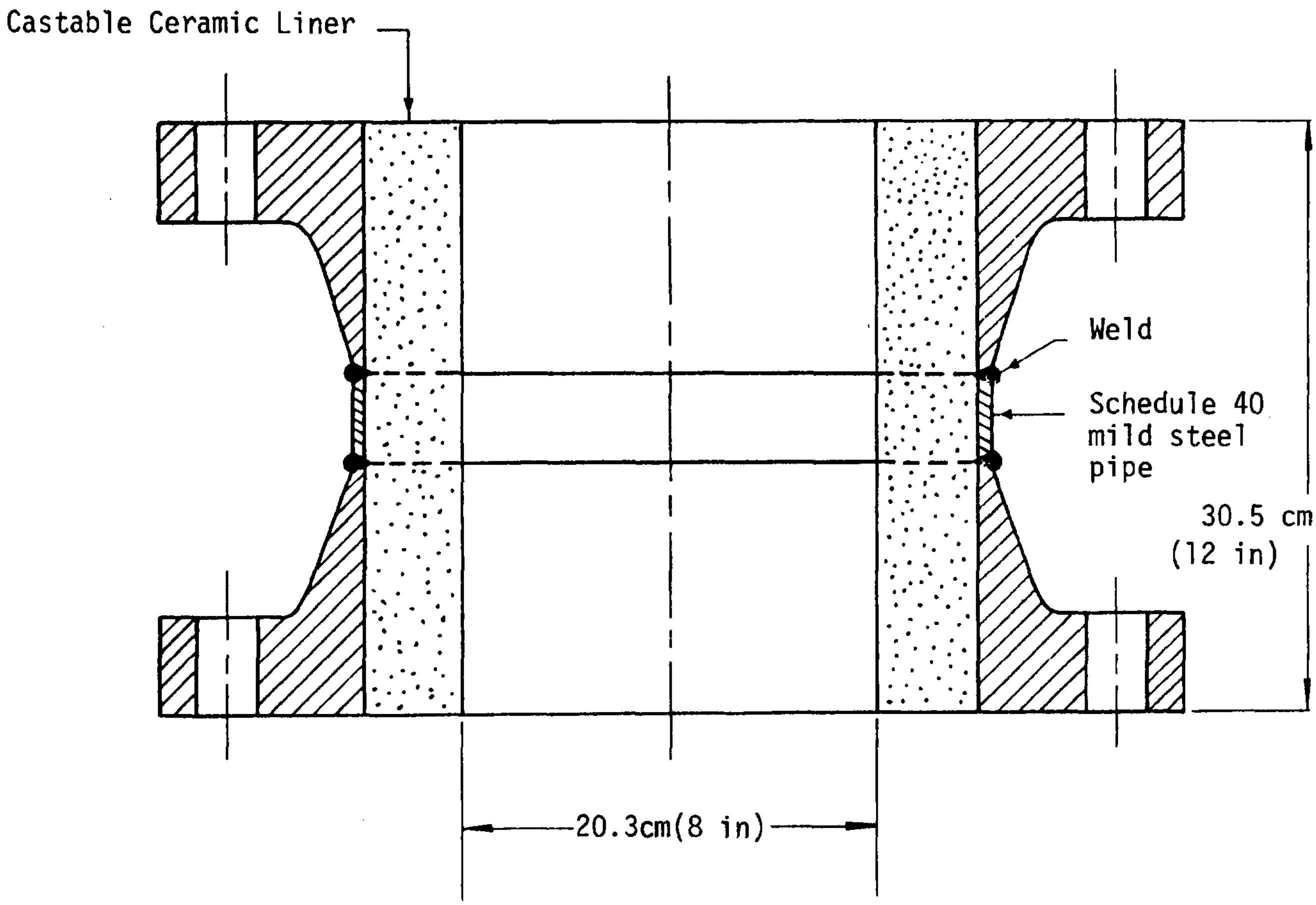


Figure 4. Gasifier Reactor Section - (One Component)

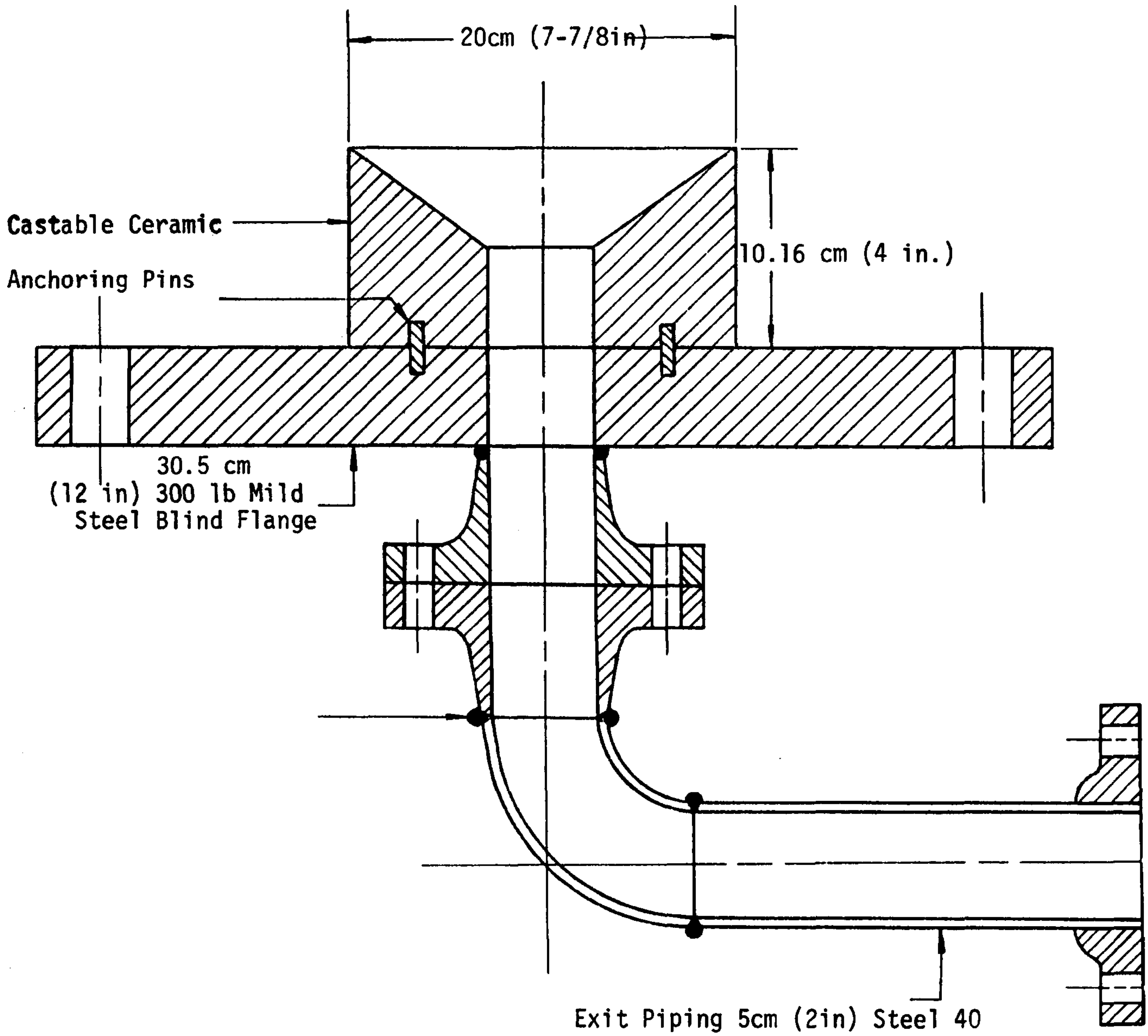


Figure 5. Gasification Reactor - Bottom Details

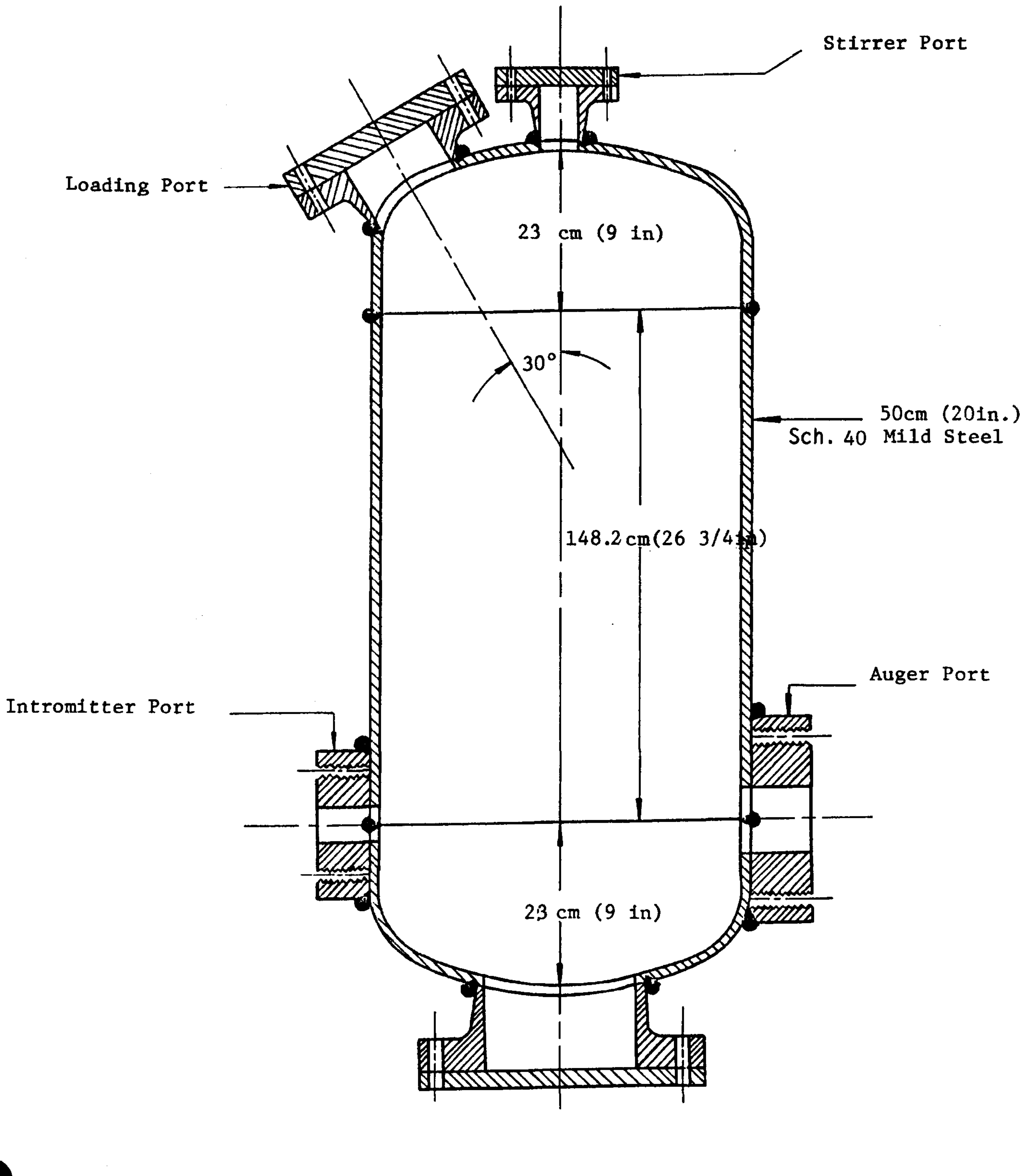


Figure 6. High Pressure Coal Feeder

Coal Analysis. Approximately 7000 kg of pulverized (70% - 200 mesh) high volatility Bituminous coal was received from Utah Power and Light Company. It is planned to conduct the bulk of the experimental tests for this test program and the related EPRI combustion program (3) using this coal. During the past quarter, analysis of the quality and variability of this coal was initiated. Seven barrels were randomly chosen and sampled at different levels in each barrel. The coal from different levels was well mixed and portions were sent to different laboratories for ultimate analysis. The results from two of these barrels are shown in Table 3. The consistency between barrels, the reproducibility among laboratories, and the sample analysis reproducibility are all considered to be very good. During the next study period, the size distribution of the coal will be investigated together with obtaining more data on the proximate and ultimate analyses of coal samples.

Coal Gasifier Model Development

Model Basis. During this past study period, the basis for a computerized model for predicting characteristics of entrained coal gasifiers was developed. The model uses the integrated or macroscopic form of the general conservation equations (13) for a volume element inside the gasifier as illustrated in Figure 7. The following aspects of pulverized coal gasification have been included in the model: (1) mixing of primary and secondary streams; (2) recirculation of reacted products; (3) pyrolysis and swelling of coal; (4) oxidation of the char by oxygen, steam and carbon dioxide; (5) heat transfer between the coal/char particles and gases; (6) variation in composition of inlet gases and solids; (7) variation in coal/char particle size; (8) oxidation of the hydrocarbons produced from coal pyrolysis. A summary of key model assumptions and conditions is given in Table 4.

Model Equations. Differential mass, energy and momentum balances have been developed for particle and gas phases and are summarized in Table 5. This set of first-order, non-linear equations requires also a large number of auxiliary, algebraic equations as component model parts. These equations describe the following aspects of the coal gasifier process: (1) enthalpy-temperature relationships; (2) physical properties including heat capacity, thermal conductivity, diffusivity, and viscosity; (3) radiative interchange inside the gasifier; (4) equations of state and mass flow continuity; (5) convective and conductive heat interchange among the gases, particles and walls; (6) rates of pyrolysis and oxidation of coal and char; (7) rates of oxidation of gaseous hydrocarbon products. A summary of these equations is given in Table 6. A detailed nomenclature of symbols is also provided at the end of the report. Since these equations are newly formulated, it is anticipated that some changes will result as the model is analyzed and organized for computer coding. During the next study period, refinements to the model will be made and computer solutions will be initiated.

Prediction of Mixing and Recirculation. The gasifier model outlined above requires input information concerning the rate of mixing of the primary coal/carrier stream with the oxidizers (e.g. CO_2, H_2O, O_2) and the rate of recirculation of combusted products inside the gasifier. Techniques have only recently been developed to predict these properties directly as a part of the model output (6-12). While no such comprehensive model exists for entrained coal gasification processes, most of the component parts for this model seem to be available.

TABLE 3

Ultimate Analysis of Pulverized
Bituminous Coal from Independent Laboratories

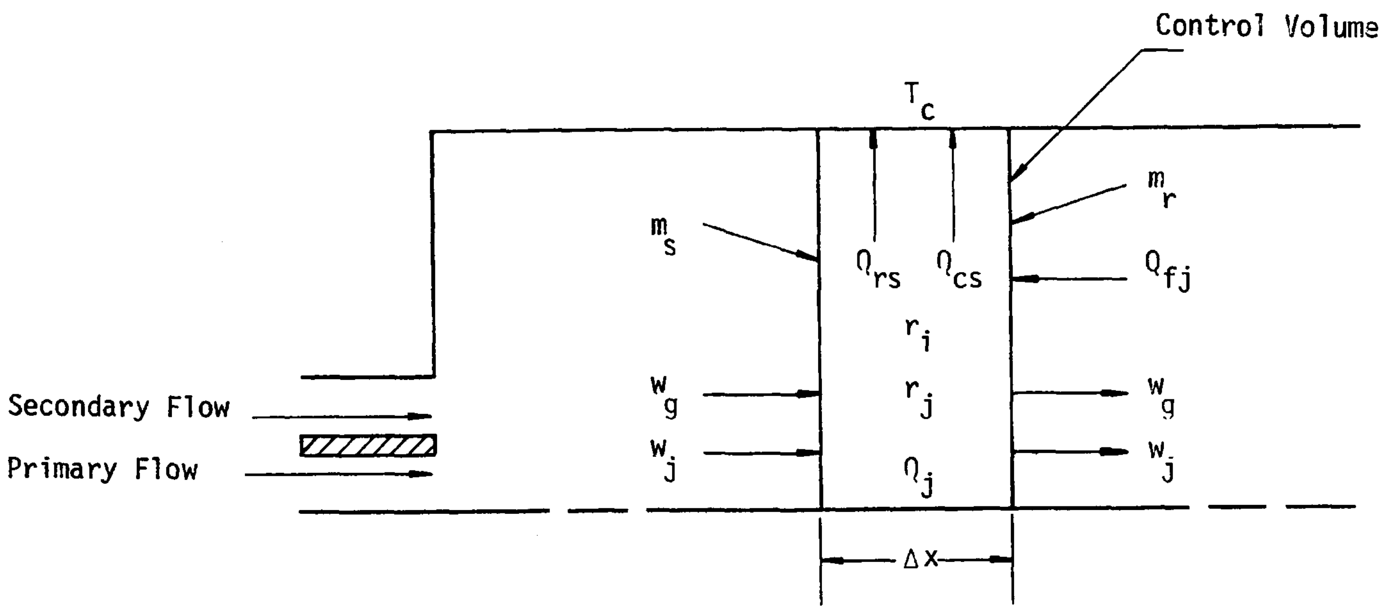
Barrel No. 2 — Weight Percent

Element	Lab 1	Lab 2		Lab 3
		1	2	
C	71.5	70.8	70.8	70.7
H	5.5	5.6	5.6	5.6
O	12.8	12.3	12.2	11.7*
N	1.4	1.4	1.5	1.4
S	0.4	0.6	0.7	0.6
Ash	----	9.3	9.2	10.6

Barrel No. 31 — Weight Percent

Element	Lab 1	Lab 2
C	71.7	71.0
H	5.6	5.6
O	12.4	12.4
N	1.4	1.5
S	0.4	0.6
Ash	----	8.0

*Oxygen determined by difference



m_s = rate of flow of secondary stream into control volume
w_g = rate of gas flow into control volume
w_j = rate of particle flow into control volume
m_r = rate of recirculated product flow into control volume
Q_j = heat transferred by conduction between gas & particles
r_j = rate of pyrolysis and oxidation of coal/char
r_i = rate of reaction of gas species
Q_{cs} = rate of heat loss by convection
Q_{rs} = rate of heat loss by radiation
Q_{fj} = rate of radiative heat transfer in reactor
T_c = wall temperature

Fig. 7 Schematic Diagram of Macroscopic Coal Gasification Model

TABLE 4

Summary of Key Assumptions
for Macroscopic Coal Reaction Model

1. Steady-state, compressible gas, with uniform pressure or pressure variation.

2. Particles and gases in dynamic equilibrium.

3. Secondary gases and recirculated products input along reactor with instantaneous mixing at each interval of specified reactor area (or pressure distribution).

4. Multiple particle sizes or types.

5. Particle phases and gas as separate continua.

6. Neglegible gas conduction, diffusion, and thermal diffusion, gravity effects, particle interactions, wall friction, viscous dissipation, work on surroundings, gas phase radiation, particle-phase convective losses, kinetic energy.

7. Rate limiting steps include upstream radiation, rate of gross oxidizer/fuel mixing, rate of product recirculation, rate of coal particle pyrolysis, rate of char oxidation (w/O_2, CO_2, H_2O), and rate of gaseous hydrocarbon oxidation.

8. Gas phase in quasi-equilibrium (except hydrocarbons).

9. Specified gas and particle ignition temperatures.

10. Coal pyrolysis by parallel activated processes with high and low activation energies.

11. Coal particle swelling proportional to extent of pyrolysis.

12. Spherical-like particles of uniform local particle temperature with constant char diameter burnout and with internal and external surface reaction.

13. Irreversible particle and gas-phase hydrocarbon reactions.

TABLE 5

SUMMARY OF MODEL DIFFERENTIAL EQUATIONS

No.	Type	Equation	No. of Eqns.
1	Gas Element Continuity (k^{th})	$d(w_g \omega_k)/dx = A \sum_j r_{jk} + m_{sgk} + m_{\rho gk}$	k
2	j^{th} Particle Phase	$dw_j/dx = -Ar_j + m_{sj} + m_{\rho j}$	j
3	Gas Energy	$d(w_g h_g)/dx = h_{sg} m_{sg} + h_{\rho g} m_{\rho g} + A(\sum_j Q_j - Q_{cb} + \sum_j r_j h_{jg})$	1
4	Particle Energy	$d(w_j h_j)/dx = m_{sj} h_{sj} + m_{\rho j} h_{\rho j} + A(Q_{fj} - Q_{rb} - Q_j - r_j h_{jg})$	j
5	Gas Momentum	$d(w_g v)/dx + d(pA)/dx = m_s v_s + m_\rho v_\rho + vA \sum_j r_j$	1
6	Particle Number	$d(vn_j)/dx = (m_{\rho j}/\alpha_j A)$	j
7	Gas Specie Continuity (i^{th})	$d(w_g \omega_i)/dx = A[(\sum_m r_{im}) + \sum_j r_{ji}] + m_{si} + m_{\rho i}$	i
8	Total Gas Continuity[1]	$d(w_g)/dx = A \sum_j r_j + m_{sg} + m_{\rho g}$	1
9	Particle Mass[2]	$d(\alpha_j)/dx = -(r_j/n_j v)$	1
10	Coal Mass	$d(\alpha_{cj})/dx = -(r_{cj}/n_j v)$	1
11	Char Mass	$d(\alpha_{hj})/dx = -(r_{hj}/n_j v)$	1
12	Moisture Mass	$d(\alpha_{wj})/dx = -(r_{wj}/n_j v)$	1

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1 Sum of Eqs 1 over k elements

2 Sum of Eqns 10-12 for total particle change

TABLE 6
Auxiliary Equations for
Coal Reaction Model

No.	Type	Equation
13	State	$p/\rho_g = RT_g/M_g$
14	Gas mass flow	$w_g = \rho_g vA$
15	Particle mass flow	$w_j = \rho_j vA$
16	Gas element and specie fractions	$\sum_k \omega_k = 1;\ \sum_i \omega_i = 1$
17	Gas temperature	$T_g(h_g, C_{pi}, \omega_i)$
18	Particle temperature	$T_j(h_j, C_{pj})$
19	Particle-gas heat transfer	$Q_j = 12[B_j/(\exp B_j - 1) k_g (T_j - T_g)\rho_j/\rho_{\sigma j} d_j^2$
20	Convective heat loss to surroundings	$Q_{cb} = 4\bar{h}(T_g - T_b)/D_s$
21	Radiative heat loss to surroundings	$Q_{rb} = (4\sigma\varepsilon_b \bar{T}_j^4/D_s)\{1-\exp[E_\lambda(\pi/4)(D_s/2)\sum_j d_j^2 n_j]$
22	Transpiration parameter	$B_j = r_j C_{pg}/2\pi d_j k_g n_j$
23	Radiative heat transfer in reactor	$Q_{fj} = (\pi/4) I_{qt} n_j d_j^2 \varepsilon_j$
24	Local radiative intensity	$I_{qt} = \sum_p I_{pq} - I_{qo}$
25	Radiative emission	$I_{po} = (\sum_j a_j T_j^4)_p\ \sigma\Delta x_p$
26	Radiative intensity component	$I_{pq} = I_{po} \exp[-\sum_p^q (\sum_j a_j)_p \Delta x_p]$
27	Radiative absorption coefficient	$a_j = (\pi/4)\ \varepsilon_j n_j d_j^2$

TABLE 6, Continued

No.	Type	Equation
28	Particle density	$\rho_j = \rho_{cj} + \rho_{hj} + \rho_{aj} + \rho_{wj}$
29	Coal density	$\rho_{cj} = \alpha_{cj} n_j$;
30	Moisture density	$\rho_{wj} = \alpha_{wj} n_j$
31	Char density	$\rho_{hj} = \alpha_{hj} n_j$
32	Ash density	$\rho_{aj} = \alpha_{aj} n_j$
33	Particle mass	$\alpha_j = \alpha_{hj} + \alpha_{cj} + \alpha_{aj} + \alpha_{wj}$
34	Particle reaction rate	$r_j = r_{hj} + r_{cj} + r_{wj}$
35	Net char reaction rate	$r_{hj} = \sum_m \phi_m r_{cjm} - \sum_\ell (r_{hj\ell})$
36	Oxidizer-char reaction rate	$r_{hj\ell} = (\phi_\ell M_h A_j C_{o\ell} n_j)/[(1/k_c)+(1/k_\ell)]$
37	Kinetic char rate	$k_\ell = A_\ell \exp(-E_\ell/RT_j)$
38	Char mass transfer coefficient	$k_c = [2D_{om} B_j/d_j(\exp B_j - 1)]$
39	Total coal reaction rate	$r_{cj} = \sum_m r_{cjm} = -[\sum_m (r_{hjm} + r_{vjm})]$
40	Volatiles reaction rate	$(1/r_{vjm}) = (1/r_{vjmd}) + (1/r_{vjmk})$
41	Volatiles diffusion rate	$r_{vjmd} = K_{vjm} A_j \rho_{\sigma j} n_j / d_j$
42	Volatiles kinetic rate	$r_{vjmk} = k_{mj} Y_{mj} \rho_{cj}$
43	Char production rate	$r_{hjm} = r_{vjm} (1-Y_{mj})/Y_{mj}$
44	Gas element production	$r_{jk} = \sum_m \phi_{khcm} r_{hcm} + \sum_\ell \phi_{k\ell} r_{jh\ell} + \sum_m \phi_{jkvm} r_{jmv}$

45	Coal kinetic rate	$k_{mj} = A_{mi} \exp(-E_{mj}/RT_j)$
46	Gas specie production	$r_{ji} = \sum_m \phi_{im} r_{cjm}$
47	Gas specie conductivity	$k_i = (5/4)\ [C_{pi} + (R/2M_i)]\ \mu_i$
48	Gas mixture conductivity	$k_g = \sum_j [X_i\ k_i / \sum_k X_k \phi_{ik}]$
49	Gas specie viscosity	$\mu_i = 2.67 \times 10^{-5} (M_i T_g)^{1/2} / \sigma_i^2\ \Omega_\mu$
50	Interaction parameter	$\phi_{ik} = (1/8)^{1/2}\ [1+(M_i/M_k)]^{-1/2}\ [1+(\mu_i/\mu_k)^{1/2}(M_k/M_i)^{1/4}]^2$
51	Gas mixture viscosity	$\mu_g = \sum_i [X_i \mu_i / \sum_k \phi_{ik}]$
52	Gas heat capacity	$C_{pi} = f(T)$
53	Mixture heat capacity	$C_{pg} = \sum_i \omega_i\ C_{pi}$
54	Gas molecular weight	$M_g = [\sum_i \omega_i / M_i]^{-1}$
55	Heat transfer coefficient	$(\bar{h} D_s / k_g) = 0.023\ (Re_g)^{0.8}\ (Pr_g)^{2/3}$
56	Reynolds No.	$Re_g = (D_s v \rho_g / \mu_g)$
57	Prandtl No.	$Pr_g = (C_{pg} \mu_g / k_g)$
58	Particle diameter	$d_j = d_{jo}\ [1 + \gamma(\alpha_{cjo} - \alpha_{cj})/\alpha_{cjo}$
59	Specie diffusivity	$D_{ik} = 1.86 \times 10^{-3} T_g^{3/2}\ [(1/M_k) + (1/M_i)]^{1/2} p \sigma_{ik} \Omega_d$
60	Mixture diffusivity	$D_{im} = (1 - X_i) / \sum_i (X_k / D_{ik})$
61	Particle enthalpy	$h_j = (\alpha_{cj} h_{cj} + \alpha_{hj} h_{hj} + \alpha_{aj} h_{aj} + \alpha_{wj} h_w) / (\alpha_{cj} + \alpha_{hj} + \alpha_{aj} + \alpha_{wj})$

TABLE 6 Continued

62	Gaseous h... reaction rate (reaction 1)	$r_{hcm} = (5.52 \times 10^8/p$ $C_{hcm}^{1/2} C_{O_2} T_g \exp(-12,200/T_g)/M_{hcm}$
63	Hydrocarbon concentration	$\rho_{hcm} = \omega_m \rho_g$; $C_{hcm} = \rho_{hcm}/M_{hcm}$
64	Particle temperature	$T_j = h_j/C_{pj}$
65	Particle heat capacity	$C_{pj} = \omega_{hj} C_{phj} + \omega_{cj} C_{pcj} +$ $\omega_{wj} C_{pwj} + \omega_{aj} C_{paj}$
66	Coal product enthalpy in gas phase (volatiles)	$h_{jcq} = h_{jc} + \Delta h_c$
67	Char product enthalpy in gas phase	$h_{jhg} = h_{jh} + \Delta h_h$
68	Moisture enthalpy in gas phase	$h_{jwg} = h_{jw} + \Delta h_w$
69	Particle enthalpy	$h_{jg} = r_{jc} h_{jcg} + {}_{jh} h_{jhg} + r_{j\omega} h_{j\omega g}/$ $(r_{jc} + r_{jh} + r_{jw})$
70	Particle area	$A_j = \pi \zeta_j d_j^2$
71	Moisture vaporization rate	$r_{jw} = [12B_j/\exp G_j - 1)]\ C_g N_w (X_{wj} - X_{wg}).$ $D_{wg} \rho_j / d_j^2\ (1 - X_{wj}) \rho_{\sigma j}$
72	Coal enthalpy	$h_{cj} = \int C_{pcj} dT_j + h_{cj}^{\circ}$
73	Char enthalpy	$h_{hj} = \int C_{phj} dT_j + h_{hj}^{\circ}$
74	Moisture enthalpy	$h_{wj} = \int C_{pwj} dT_j + h_{wj}^{\circ}$
75	Ash enthalpy	$h_{aj} = \int C_{paj} dT_j + h_{aj}^{\circ}$
76	Molar gas concentration	$C_g = p/RT_g$
77	Moisture equilibrium	$X_j = p_{ej}/p$

During the past report period, technical discussions were held with Spalding and co-workers of Imperial College, England, and with Pratt and co-workers of Washington State University (WSU). A technical meeting has been scheduled with Pratt and Crowe (WSU) during January, 1976, to explore the possibility of a cooperative effort in developing such a model. If this effort appears to be feasible, it will probably be recommended as a part of the second phase of this proposed study.

PLANS FOR THE NEXT STUDY PERIOD

During the fifth quarter of this investigation, the following plans have been identified:

1. Continue technical review and analysis of coal literature with emphasis on treatment of reacting, recirculating flows.

2. Complete check-out of modified non-reacting flow facility and initiate collection and analysis of experimental data.

3. Complete shop construction of non-reactive facility components for study of recirculating flows.

4. Complete working drawings of high pressure gasifier components and initiate fabrication and installation of components.

5. Complete installation of reactor structural systems, together with installation of the atmospheric reactor and associated components.

6. Review coal gasification model equations, and initiate computer solution development and debugging.

7. Visit Washington State University and discuss possible cooperative programs for development of generalized model for describing mixing and recirculation in entrained coal gasifiers.

NOMENCLATURE

SYMBOL	UNITS	DEFINITION	SOURCE
A	cm^2	effective duct area	input
A_j	cm^2	j^{th} particle area	Aux. Eq.[1]
a_j	cm^{-1}	particle absorption coefficient	Aux.Eq.
A_{mj}	sec^{-1}	pyrolysis pre-exponential factor	input
A_ℓ	cm/sec	surface reaction pre-exponential factor	input
B_j	--	transpiration parameter for j^{th} particle type	Aux.Eq.
C_{pi}	cal/g°	heat capacity of i^{th} gas specie	thermochem input
C_{pg}	cal/g°K	heat capacity	thermochem output
C_{o_2}	$gmol/cm^3$	oxygen molar concentration	thermochem output
C	$gmol/cm^3$	total molar concentration	thermochem output
d_j	cm	j^{th} particle diameter	Aux. Eq.
D_s	cm	reactor diameter (physical)	input
D_{om}	cm^2/sec	oxidizer diffusivity in mixture	Aux. Eq.
D_{ik}	cm^2/sec	binary diffusivity	Aux. Eq.
D_{im}	cm^2/sec	diffusivity of i^{th} specie in mixture	Aux. Eq.
E_λ	--	absorption efficiency factor	input
$E_\ell (E_{mj})$	cal/gmol	activation energy for ℓ^{th} (m_jth) reaction	input

1 - Aux. Eq. ≡ auxiliary equation of Table 6

NOMENCLATURE, CONTINUED

SYMBOL	UNITS	DEFINITION	SOURCE
h	cal/g	static enthalpy	dependent variable (Eq. 3&4)
Δh	cal/g	heat of reaction	input
h_m	cal/sec°K cm^2	mean heat transfer coefficient	Aux. Eq.
I	cal/cm^{2}sec	radiation intensity	Aux. Eq.
k_g	cal/sec°Kcm	gas thermal conductivity	Aux. Eq.
k_i	"	gas specie i thermal conductivity	Aux. Eq.
k_c	cm/sec	mass transfer coefficient	Aux. Eq.
k_ℓ	cm/sec	surface kinetic rate coefficient	Aux. Eq.
k_{mj}	sec^{-1}	pyrolysis reaction coefficient	Aux. Eq.
K_v	cm^2/sec	volatiles diffusion parameter	input
m	g/cm sec	rate of mass addition	input
M	g/gmol	molecular weight	input
n_j	cm^{-3}	number density of jth particle	dependent variable (Eq 6)
p	atm	static pressure	Eq. 5
Pr_g	--	Prandtl No.	Aux. Eq.
Q	cal/cm^{3}sec	volumetric heat transfer rate	Aux. Eq.
R	cal/gmol°K, etc	universal gas constant	input
r	g/cm^{3}sec	volumetric reaction rate	Aux. Eq.
Re_g	--	Reynolds number	Aux. Eq.

NOMENCLATURE, CONTINUED

SYMBOL	UNITS	DEFINITION	SOURCE
T_b	°K	wall temperature	input
T_g	°K	gas temperature	thermochem output
T_j	°K	j^{th} particle temperature	Aux. Eq.
v	cm/sec	velocity in x-direction	dependent variable (Eq 5)
w	g/sec	mass flow rate	Aux. Eq.
x	cm	distance along burner	independent variable
X_i	--	mole fraction-gas phase	thermochem output
Y	--	mass fraction-particle phase	input
α_j	g	mass of j^{th} particle	dependent var. (Eqs. 9-12)
γ	--	swelling coefficient	input
Δ	--	incremental change	--
ε	--	emissivity	input
μ	g/cm sec	viscosity	Aux. Eq.
ρ	g/cm^3	density	Aux. Eq.
σ_{ik}	A°	collision diameter	input
σ	$cal/cm^2\ sec°K^4$	Stephan-Boltzman Constant	input
ϕ	--	stoichiometric coefficient	input
ϕ_{ik}	--	interaction parameter	Aux. Eq.
ζ_j	--	particle surface area factor	input
ω	--	mass fraction	dependent var. (Eq. 1,7)
Ω	--	collision integral	input

Subscripts	Definition
a	ash
b	boundary, wall, surroundings
c	convection
c	coal
d	diffusion
e	equilibrium or vapor
f	flame (hot region)
g	gas
h	char, carbon
hc	hydrocarbon
i	i^{th} specie
j	j^{th} particle type or phase
k	kinetic
k	k^{th} chemical element
ℓ	ℓ^{th} reaction
m	m^{th} reaction
m	hydrocarbon coefficient
m	mixture
n	hydrocarbon coefficient
o	initial
o	oxidizer
p	p^{th} increment in x direction
q	q^{th} increment in x direction
r	radiation
s	secondary
σ	solid
t	total
v	volatiles
w	moisture
x	ignition
μ	viscosity
ρ	recirculation

NOMENCLATURE, CONTINUED

Subscripts

Symbol	Definition
v	volatiles
w	water
μ	viscosity

1 metric units are shown; in the english-engineering system gm-lbs, cm-ft, sec-sec, °K-°R, gmol-lb, mol, cal-BTU

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