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MEASURING AND MODELING SOLIDS MOVEMENT
IN A LARGE, COLD FLUIDIZED BED TEST FACILITY

Fifth Quarterly Report, October 1—December 31, 1980

By
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Robert V. Mrazek
Stephen D. Crane

December 1980

MASTER

Work Performed Under Contract No. AC01-79ET13152

Oregon State University
Dept. of Chemical Engineering
Corvallis, Oregon

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MAGNETIC SOLIDS FLOW METER

Previous reports have presented tests which show that the magnetic mass flow meter developed at OSU to study the movement of solids in a fluidized bed is capable of reproducibly measuring the mass flow of magnetic solids. A test apparatus was used to measure the velocity of circulating loops of magnetic solids, and the results showed that the response was directly proportional to both the linear velocity, and the cross-sectional area of the loop; thus the overall response is proportional to the mass flux.

Before the device can be used to give unambiguous results in an operating fluidized bed, three tasks remain. They are:

1. Shortening the response time between the application of the magnetizing pulse and the measuring of the induced voltage caused by the motion of the magnetized solids.
2. Eliminating flow obstructions which could affect the velocity of solids in the vicinity of the pickup coil.
3. Eliminating to the greatest extent possible the errors produced by the passage of bubbles.

Two modifications which shorten the response time have already been made, and the response time will be shortened even more by the use of a new probe which has the added benefit of eliminating the presence of flow-obstructing coils external to the in-bed tubes. The new probe should also reduce errors caused by the passage of bubbles. A computer program is now being developed which will predict the voltage that should be detected by the pickup coil for any specified geometry of magnetizer coils, pickup coils, and moving solids. For any given geometry, the program will calculate the field of the magnetized particles using

the measured magnetic inductance properties of the particles themselves. Thus we will be able to estimate the error caused by a bubble passing the probe.

The changes already made shorten the response time in the electronic circuitry. They were completed before the data presented in a subsequent section was collected. Before any further data on solids movement is collected, we hope to have completed the remaining tasks.

Reducing Current Decay Time in the WRITE Coils

When the magnetizing pulse is cut off, it is necessary to wait until the current in the WRITE coil decays to a sufficiently small value so that it is not picked up by transformer action in the READ coil. In previous experiments, the current pulse was produced by a linear voltage amplifier. At the end of the pulse the voltage dropped to zero and the current decayed exponentially down to zero with a time constant equal to the inductance of the coil divided by its resistance. The modification shown in Figure 1 improves the response of the amplifier by the use of current feedback instead of voltage feedback. An operational amplifier is used to drive the power amplifier. The feedback signal is the current through the WRITE coils. This current produces a small voltage across a 0.1 ohm resistor, which is fed back to the negative input of the driver amplifier. At the end of the magnetizing pulse the signal input to the amplifier falls to zero but because of the inductance of the coil, the current does not immediately go to zero. Thus, a positive voltage appears at the negative input of amplifier A-1, thereby causing the output of amplifier A-3 to become negative. Because of the very

FIGURE 1

BLOCK DIAGRAM OF DRIVER AMPLIFIER TO DECREASE DECAY TIME AND CURRENT LEVEL CONTROL.

large gain of the driver amplifier, the output from the power amplifier remains negative until the current falls to a very low value. The current then continues to decay all the way to zero but with a time constant which is equal to the inductance of the coil divided by its resistance and divided also by the gain of the driver amplifier.

Figures 2a and 2b, respectively, show the record pulses using the linear voltage amplifier and the current feedback arrangement.

Reducing the Recording Pulse Width

The rise time of the recording pulse depends upon the inductance of the WRITE coils. When the coils are completely surrounded by iron the inductance is high and the rise time is maximal. If there is less iron in the vicinity of the coils, then the inductance is smaller and the current in the WRITE coils reaches a saturating value in a shorter time. Once this saturating current has been established, there is no need to prolong the pulse. In order to take advantage of this effect, the electronics were modified so that the magnetizing pulse is switched off when the magnetizing current reaches a predetermined level, sufficient for saturating the iron in the vicinity of the WRITE coil. In order to protect the coil from possible overheating, the length of the recording pulse is limited to two milliseconds and the current will shut off after this time even if it has not reached the required saturating value. The shortened record pulse is shown in Figure 2c.

Modified Coil Designs to Improve Response Time and Eliminate Flow Obstruction

A new coil arrangement has been designed and is currently being

Figure 2. Recording pulse (a) using a linear voltage amplifier (b) using a current feedback amplifier (c) with "level-switching" circuit.

built and will be tested during the next quarter. It is shown in Figure 3. In this design all the coils--the WRITE coil and the detector coils--are located inside one of the in-bed tubes.

In the new arrangement, the coils are located in both the horizontal and vertical plane in the shape of an H. The upright legs of the H are the READ coils which are connected in parallel. The horizontal portion of the H is the WRITE coil. When energized, it creates a magnetic field whose lines are shown dashed in Figure 3b. When the magnetizing coil is no longer energized, the ferromagnetic material along the lines of force will maintain a certain amount of permanent magnetism. The lines of force of this permanent magnetic field should parallel the lines of force created by the WRITE coil. The READ coils are arranged to detect the upward (or downward) movement of solids next to the tube wall. Upward movement of the solids will result in the lines of force from the magnetized solids cutting the detector coil. Because the direction of the lines of force is reversed for the top and bottom leg of each detector coil, the induced voltages are added. The orientation of the detector or READ coils at right angles to the WRITE coil has the further advantage of minimizing the transformer pickup between them.

The field is quite intense and the field lines are nearly horizontal at the points where they cross the detector coils. Thus, the sensitivity (which depends on the number of lines of force per second which cut the detector coil) should be quite good. Because of the compact design, it should be possible to achieve magnetic saturation of the moving iron in the vicinity of the coil. The magnetic flux, in fact,

Figure 3. "H" coil design for magnetic solids velocity measurement.

ought to be so high that any material in the vicinity of the pickup coil will be magnetized by a field which is not distorted by the presence of any bubble. It should be noted that for larger coils the field strength is necessarily weaker, and the ferromagnetic material will have a greater effect in determining the shape of the field itself. Thus if the field is weak and a bubble is present, a magnetizing field line will have a different shape than they would have if the bubble were not present. In the new design the field intensity should be well above that required for saturation of the iron in the vicinity of the tube and hence distortion of the field by a void in the ferromagnetic material will be minimized. A second advantage of the small coil is its inherently lower inductance. Because of this, the magnetizing current should rise to its maximum value in a shorter time and it should also decay in a shorter time, thus enabling the magnetizing pulse to be shortened, and the delay between magnetization and reading also to be shortened.

A final advantage of the new design over the previous designs is the fact that the magnetic lines of force produced by the magnetized solids close on themselves through the nonmagnetic tube. In effect, this introduces a large air gap which ought to minimize the nonlinear effects in field strength caused by the presence of bubbles, and thereby reduces the error caused by the passage of bubbles near the probe.

Computer Simulation of Magnetic Flux Lines

According to electromagnetic theory, magnetic flux satisfies the equation

$$\nabla \cdot \vec{B} = 0$$

where B is the flux density. Thus every line of magnetic flux must close on itself (unlike electrical field lines which can terminate on charged particles). In the absence of ferromagnetic material, the lines of force conform to a potential field. Inside ferromagnetic material, however, the magnetic flux has two components given by the equation

$$B = \mu_0 \vec{H} + \vec{J}$$

The sum of $\mu_0 \vec{H}$ and $\vec{J}$ just inside the surface of a magnetic body precisely equals the flux $\vec{B}$ on the air side of the boundary. The quantities $\vec{H}$ and $\vec{J}$ are related because the magnetic force $\vec{H}$ causes partial alignment of magnetic fields within the ferromagnetic substance to produce an additional magnetic flux, $\vec{J}$. (In the absence of any aligning force, the domains tend to take on random alignments so that no appreciable field is produced.) The relationship between $\vec{H}$ and $\vec{J}$ can be found experimentally by constructing a closed magnetic path of the ferromagnetic material (usually a torrus) and subjecting the material to a uniform external magnetizing force provided by an electric current (usually flowing through a torroidal coil). The magnetic flux within the coil ($\vec{J}$ or $\vec{B}$) is then measured while the magnetizing force ($\vec{H}$) is varied by changing the current through the coil. A typical result is shown in Figure 4. The curve shows hysteresis; i.e., the magnetic flux B depends not only on the magnetic force F but also on its history. As the magnetizing force increases, the lower curve is followed; as the magnetizing force decreases, the upper

Figure 4. Typical B-H curve for ferromagnetic material.

curve is followed. In addition to hysteresis, the ferromagnetic material also exhibits saturation when all the internal magnetic domains are aligned. When the current is increased beyond this saturating level, then the further increase in flux is no more than would occur in air, i.e.,

$$\Delta \vec{B} = \mu_0 \Delta \vec{H}$$

A finite difference picture (in two dimensions) for modeling the behavior of the ferromagnetic material is shown in Figure 5. Because there is no such thing as a magnetic insulator, the gridwork necessarily continues to infinity in all directions. (The magnetic effects, however, are limited and it is sufficient to restrict our attention to a region near the ferromagnetic material of interest.) Connecting adjacent horizontal or vertical points is a "resistor" whose value $1/\mu_0$ is the proportionality factor between magnetizing force H and magnetic flux B in a vacuum. At every grid point the net magnetic flux must equal zero. Inside the ferromagnetic domain there is an additional magnetic flux J (shown schematically as a current generator between adjacent points). The value of J is related to the local H value by the BH curve for the magnetic material. At a boundary between air and the ferromagnetic material, the fluxes from both paths within the magnetic material must sum and must be equal to the flux conducted by the external resistance $1/\mu_0$.

A computer program corresponding to this finite difference model is now being developed and will be used along with measured $B-H$ data to

Figure 5. Finite difference model for calculating field of magnetized iron.

predict the shape and the density of magnetic flux lines near the magnetic probe, particularly to see what happens when bubbles are present.

Ideally, a bubble should reduce the voltage in the pickup coil precisely as it reduces the mass flux in the vicinity of the probe. Any effect greater or less is an error, and the probe geometry should be optimized to make this kind of error small.

Tests of Magnetic Flow Measuring Devices

Tests of the magnetic flow-measuring device were continued in an effort to determine a proper coil configuration. Initial tests with a "folded-C" shaped coil, as detailed in the last quarterly report (DOE/ET/13152-4) indicated that the signal output was proportional to the mass flux through the sensing coil (READ coil). However, questions remained as to the effect of iron powder outside of the coils. In addition, other coil configurations were to be considered.

Several series of tests were carried out in an effort to answer these questions. These tests were done with a set of antiparallel WRITE coils with a centered READ coil using the same apparatus described in the previous report. For convenience, the diagrams of the apparatus and coil configurations are reproduced here as Figures 6 and 7. Samples of test results are given below. In all cases, a 1/2-inch I.D. Tygon tube filled with iron powder ($0.316 \text{ lb}_m \text{ iron/ft. of tube}$) was moved through both the READ and WRITE coils at a measured velocity. The particular test conditions and results are as follows:

Figure 6. Calibration assembly.

Folded "C" Configuration

Anti-Parallel Configuration

Figure 7. Coil configuration.

Series I

WRITE Coils: rectangular, 1.25" x 2.75"; 65 turns of #22 wire;
1.5" apart.

READ Coil: centered, parallel to WRITE coils; 1.25" x 1.25";
1000 turns of #34 wire.

Set A: coils surrounded by air.

Current input: 80 amps

Current rise time: 0.68 ms

Voltage drop across WRITE coils + 0.1 Ω resistor:
100 volts

Set B: Coils surrounded by iron powder.

Current input: 80 amps

Current rise time: 1.0 ms

Voltage drop across WRITE coils + resistor: 112 volts.

The results of the tests in Series I are given in Tables 1 and 2 and are depicted in Figure 8.

Series II

WRITE Coils: 1.25" square; 73 turns of #22 wire; 3" apart.

READ Coils: 1.25" square; centered parallel to WRITE coils;
1000 turns of #34 wire.

Set A: Coils surrounded by air.

Current input: 80 amps

Current rise time: 0.52 ms

Voltage drop: 100 volts

Table 1: Results for Series IA. (Coils surrounded by air.)

Motor "RPM"	Tygon tube velocity ft/sec	Iron pdr. mass flow rate inside coils lb _m /sec	Output signal volts
500	0.55	0.17	1.55
700	0.74	0.23	2.4
1000	1.06	0.34	3.2
1500	1.58	0.50	4.5
2000	0.11	0.67	6.00

Table 2: Results for Series IB. (Coils surrounded by iron powder.)

Motor "RPM"	Tygon tube velocity ft/sec	Iron pdr. mass flow rate inside coils lb _m /sec	Output signal volts
500	0.55	0.17	1.90
700	0.74	0.23	2.80
1000	1.06	0.34	3.90
1500	1.58	0.50	5.45
2000	2.11	0.67	7.30

Figure 8. Output signal vs iron powder mass flow rate inside coils for series I.

Set B: Coils surrounded by iron powder.
 Current input: 80 amps
 Current rise time: 0.92 ms
 Voltage drop: 110 volts

The results of the tests in Series II are given in Tables 3 and 4 and are depicted in Figure 9.

Series III

WRITE Coils: 1.25" square; 73 turns of #22 wire; 1.5" apart.
 READ Coil: Rectangular, 1.25" x 1.75"; centered parallel to
 WRITE coils; 1000 turns of #34 wire.

Set A: Coils surrounded by air.
 Current input: 80 amps
 Current rise time: 0.46 ms
 Voltage drop: 100 volts

Set B: Coils surrounded by iron powder.
 Current input: 80 amps
 Current rise time: 0.8 ms
 Voltage drop: 112 volts

The results of the tests in Series III are given in Tables 5 and 6 and are depicted in Figure 10.

The tests designated as Series III show that for that coil configuration, the output signal is unaffected by the media which surrounds the coils, i.e., it makes no difference whether the coils are surrounded by air or iron powder. This is a necessary condition for consistent mass-flow measurements which are independent of the presence of a bubble out-

Table 3: Results for Series IIA. (Coils surrounded by air.)

Motor "RPM"	Tygon tube velocity ft/sec	Iron pdr. mass flow rate inside coils lb _m /sec	Output signal volts
500	0.55	0.17	1.7
700	0.74	0.23	2.1
1000	1.06	0.34	3.2
1500	1.58	0.50	4.4

Table 4: Results for Series IIB. (Coils surrounded by iron powder.)

Motor "RPM"	Tygon tube velocity ft/sec	Iron pdr. mass flow rate inside coils lb _m /sec	Output signal volts
500	0.55	0.17	2.3
700	0.74	0.23	3.0
1000	1.06	0.34	4.0
1500	1.58	0.50	5.5

Figure 9. Output signal vs iron powder mass flow rate inside coils for series II.

Table 5: Results for Series IIIA. (Coils surrounded by air.)

Motor "RPM"	Tygon tube velocity ft/sec	Iron pdr. mass flow rate inside coils lb _m /sec	Output signal volts
500	0.55	0.17	1.2
700	0.74	0.23	1.65
1000	1.06	0.34	2.3
1500	1.58	0.50	3.3
2000	2.11	0.67	4.3

Table 6: Results for Series IIIB. (Coils surrounded by iron powder.)

Motor "RPM"	Tygon tube velocity ft/sec	Iron pdr. mass flow rate inside coils lb _m /sec	Output signal volts
500	0.55	0.17	1.25
700	0.74	0.23	1.7
1000	1.06	0.34	2.3
1500	1.58	0.50	3.4
2000	2.11	0.67	4.4

Figure 10. Output signal vs iron powder mass flow rate inside coils for series III.

side the coils but in close proximity to them. Thus, the output signal represents only the mass flow of iron through the READ coil, and it is unaffected by the presence of iron outside of the coils, moving or stationary. These conclusions are only valid for the configuration designated in Series III of the tests.

The other two series of tests in which the WRITE coils were either further apart (Series II) or larger (rectangular; Series I) did not show positive results. In these cases, the differences between the output signals for the case of coils surrounded by air or coils surrounded by iron were significant. This is apparently caused by the inability to magnetize (saturate) all of the material contained in the region between the two WRITE coils within the limitations of our amplifiers.

In conclusion, the configuration used in Series III seems to achieve the desired results. However, further modifications will be considered to attempt to develop a configuration which does not interfere with solids movement at all (the section of the coils which crosses between the tubes). In addition, the effect of not having the moving iron powder restrained will be investigated (i.e., what happens when the particles can rotate as they will in a fluidized bed?).

PLUME MODEL FOR COAL COMBUSTION

The second quarterly report (DOE/ET/13152-2, March 31, 1980) included a draft of a paper by D. Park on "Modeling of Fluidized Bed Combustors." This work involved the initial development of the "plume model" for combustion. The plume model has now been extended to include the effect of secondary air introduced at the coal feed ports, and an analysis of sulfur capture during combustion carried out in a fluidized bed of limestone. The model is explained in detail, with examples of its application, in Mr. Park's Ph.D. thesis. A copy of the thesis is attached as Appendix I.

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APPENDIX 1

The Plume Model for Large Utility Scale
Atmospheric Fluidized Bed Combustors

by

Dalkeun Park

A THESIS

submitted to

Oregon State University

in partial fulfillment of
the requirements for the
degree of

Doctor of Philosophy

Completed December 1980

Commencement June 1981

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LIST OF SYMBOLS

A, B	- Denote volatiles and oxygen respectively
a, b	- Coefficients defined in equation (4.2)
C, C_A, C_B, C_O	- Gas concentration (mol/m^3)
$\overline{C_{ox}}$	- Average oxygen concentration in the bed (mol/m^3)
D, D_A, D_B	- Lateral gas dispersion coefficient in the bed ($\text{m}^3\text{gas/m bed.s}$)
D_S	- Lateral solid dispersion coefficient in the bed (m^2/s)
D	- Molecular diffusivity of gas (m^2/s)
d_p, d_p, top	- Diameter of particle (m) or (μm)
E	- Exit age distribution
E_x	- Excess air ratio based on the stoichiometric air required for the complete combustion of feed coal
F	- Tracer response to a unit step input
F_0	- Total char feed rate (kg/s)
$F_0(\overline{R}_i)$	- Char feed rate of size $\overline{R}_i$ (kg/s)
F_1	- Char outflow rate (kg/s)
F_2	- Elutriation rate of char (kg/s)
$F_2(\overline{R}_i)$	- Elutriation rate of char of size $\overline{R}_i$ (kg/s)
f_c	- Weight fraction of carbon in char
f_f	- Ratio of carbon remaining in char after devolatilization to total carbon in feed coal
f_p	- Ratio of oxygen needed for the combustion of volatiles in the plume to that for total coal combustion
f_t	- Ratio of transfer air for the coal feed to the total air to the bed

H	- Height of the bed (m)
ΔH_r	- Heat of combustion for carbon to carbon monoxide (J/mol)
ΔH_v	- Heating value of volatiles (J/kg feed coal)
h	- Convective heat transfer rate coefficient ($W/m^2 \cdot K$)
k	- Reaction rate constant for the disappearance of oxygen in the bed ($\frac{m^3 \text{ gas}}{m^3 \text{ bed} \cdot s}$)
k''	- Char combustion rate constant based on the external surface of char $\left\{ \frac{\text{mol carbon}}{(\text{mol } O_2/m^3)(m^2 \text{ char surface})(s)} \right\}$
k _c	- Rate constant for surface reaction rate of char $\left\{ \frac{\text{mol carbon}}{(\text{mol } O_2/m^3)(m^2 \text{ char surface})(s)} \right\}$
k _D	- Rate constant for the devolatilization of coal (s^{-1})
k _H	- Rate constant for the reaction of hydrogen sulfide with limestone ($\frac{m^3 \text{ gas}}{m^3 \text{ bed} \cdot s}$)
k _g	- Gas film mass transfer rate coefficient of oxygen (m/s)
k _s	- Rate constant for the reaction of sulfur dioxide with limestone ($\frac{m^3 \text{ gas}}{m^3 \text{ bed} \cdot s}$)
k _v	- Rate constant for the disappearance of oxygen by the combustion of volatiles in the plumeless model ($\frac{m^3 \text{ gas}}{m^3 \text{ bed} \cdot s}$)
L	- Length of flow path (m)
L ₀ , L ₁ (z)	- Radius of plume; at the bottom of the bed, at height z, respectively (m)
L ₂	- Radius of module for one feed port (m)
n	- Stoichiometric air for the combustion of coal (mol/kg feed coal)
P(r,t)	- Probability density function for a feed coal particle to be at position r, t sec after injected into the bed
$\bar{R}_i$	- Average radius of particles in the i th size interval (m), (μm)

r	- Radial distance from the center of coal feed port, or centerline of the tube (m)
$\hat{r}$	- r/L_2
r_c	- Reaction rate of char (mol carbon/m ² char surface·s)
r_H	- Reaction rate of hydrogen sulfide with limestone (mol/m ³ bed·s)
r_s	- Reaction rate of sulfur dioxide with limestone (mol/m ³ bed·s)
$R(R)$	- Shrinkage rate of particle radius (m/s)
s_0, s	- $L_0/L_2, L_1/L_2$
$\overline{SR}$	- Sulfur retention efficiency of the plume model
$\overline{SRI}$	- Sulfur retention efficiency of the plumeless model I
$\overline{SRII}$	- Sulfur retention efficiency of the plumeless model II
T_b	- Temperature of the bed (K)
T_s	- Surface temperature of a burning char particle (K)
ΔT	- Adiabatic temperature jump above the bed (K)
t	- Time (s)
$\bar{t}, t_o$	- $L/\bar{u}, L/u_o$ (s)
u_f	- Gas velocity in the bed (m/s)
u_o	- Superficial gas velocity in the bed, or maximum velocity of fluid in the tube (m/s)
u_t	- Terminal velocity of an elutriating particle (m/s)
v^*	- Volume of volatiles evolved from coal to form the plume measured at 273K, 101.3 kPa (m ³ /kg feed coal)
W	- Weight of char in the bed (kg)
$W(\bar{R}_i)$	- Weight of char in the i^{th} size interval (kg)
X_b	- Conversion of char in the bed
X_{ce}	- Overall carbon efficiency in the combustor including freeboard section
X_H	- Conversion of hydrogen sulfide in the bed

X_{ox}	- Conversion of oxygen in the bed only
X_v	- Conversion of volatiles in the bed only
x	- Distance from the centerline (m)
Y	- Weight percentage of feed coal smaller than the particle of radius R_i
y, y_B, y_{BT}	- Mol fraction; C/C_0 , C_B/C_0 and $C_{B, bottom}/C_0$
y_H, y_x, y_s	- Mol fraction of hydrogen sulfide, oxygen and sulfur dioxide
y_o	- r_o/R : parameter in Bingham plastic fluid
z	- Vertical distance from the bottom of the bed or axial distance in the tube (m)
$\hat{z}$	- z/H

Greek Letters

α	- Stoichiometric coefficient (mol SO_2 /mol O_2)
β	- Stoichiometric coefficient (mol H_2S /mol O_2)
δ	- Thickness of falling film or half of the distance between two parallel planes (m)
ϵ	- Emissivity of char
θ, θ_o	- Dimensionless time; $t/\bar{t}$, $t_o/\bar{t}$
κ_o	- An elutriation rate constant representative of any size of a given density (s^{-1}), see equation (3.4)
$\kappa(\bar{R}_i)$	- Elutriation constant for particles of size $\bar{R}_i$ (s^{-1})
μ	- Viscosity (kg/m·s)
μ_o	- Parameter in Bingham plastic fluid (kg/m·s)
ν	- Stoichiometric coefficient (mol volatiles/mol O_2)
ρ_c, ρ_g	- Density of char and gas, respectively (kg/m ³)
σ	- Boltzmann coefficient (W/m ² ·K ⁴)

τ	- shear stress ($\text{kg/m}\cdot\text{s}^2$)
τ_0	- Parameter in Bingham plastic fluid ($\text{kg/m}\cdot\text{s}^2$)
Φ	- Fraction of volatiles released inside the plume
Ψ	- Fraction of sulfur devolatilized inside the plume

THE PLUME MODEL FOR LARGE UTILITY SCALE ATMOSPHERIC FLUIDIZED BED COMBUSTOR

CHAPTER I. INTRODUCTION

The atmospheric fluidized bed combustor (AFBC) is currently being considered as an alternative to the pulverized coal combustor for utility scale electric power generation. Even a small AFBC (250 MW) would be enormous by chemical industry standard, consisting of four or five fluidized beds each about 4m by 20m in cross-sectional area, filled to a depth of about 1m with limestone particles and fluidized with air at two to four meters per second. For the distribution of coal, one class of designs calls for coal entering through dozens of feed ports at the bottom of the bed.

A well designed AFBC should:

- minimize the loss of unburned fuel, i.e., maximize combustion efficiency,
- minimize the release of pollutants, i.e., sulfur dioxide, nitrogen oxide and particulates,
- operate with a minimum of excess air to reduce the load on the blower and to maximize thermal efficiency,
- maximize the utilization of limestone for sulfur dioxide retention to minimize the cost on limestone and solid waste disposal problem.

These are competing requirements. To evaluate the tradeoffs involved in different AFBC designs it is necessary to have a model to correlate the variables and to predict the performance of the bed.

In the development of such a model for the AFBC, one must picture clearly the physical and chemical processes in the combustor: the flow of gases and solids in the bed; the devolatilization of coal; the elutriation of unburned char and limestone particles from the bed; the attrition of solids in the bed; the gas-solid reactions and gas-gas reactions within the bed and above the bed as well as heat removal by the submerged heat transfer tubes. A general or "comprehensive" model which incorporates all these features could become extremely complex and difficult to use so a judicious choice of simplification is needed to develop a practical working model.

The AFBC has unique features not found in other applications of fluidized beds. The need for high gas velocities, essential for keeping the bed reasonable in size, requires the use of large particles. At the same time, the immersed tubes in the bed restrict the growth of bubbles therein. Thus, the bed is in either the slow bubble regime or the turbulent-churning flow regime (1), but certainly not in the fast bubble regime for which bubbling bed models were developed and used extensively in the past.

There is so much more limestone than coal in the bed that the physical behavior of the bed is insensitive to the hold-up of coal and is dependent primarily on the limestone and its products (2). This fact allows the fluid dynamics of the bed to be considered independent of coal combustion.

Sulfur retention in the AFBC occurs primarily by the chemical reaction of calcined limestone (CaO) with hydrogen sulfide and sulfur dioxide, products of devolatilization and combustion of coal respectively.

One needs to know how and where in the bed hydrogen sulfide, and sulfur dioxide evolve in order to model their reaction with calcined limestone. As the retention of sulfur consumes only a minute fraction of the inlet oxygen, we can treat the sulfur retention after dealing with the combustion of coal, which dictates the sulfur dioxide formation and local oxygen concentrations.

Chapter II deals with the models on the AFBC published in the literature. The assumptions of the models are tabulated and compared to the observations and checked to see if they are useful for the large utility scale AFBCs.

In Chapter III the plume model is formulated for the combustion of coal. Its calculation results are presented in Chapter IV.

Chapter V deals with sulfur retention. Calculation results are presented and discussed. In Chapter VI examples are given to show how to use the model. In Chapter VII the plume model is summarized and is shown to explain the observed temperature jump above the bed as well as the observed radial variation in concentration of gases in and just above the bed.

Chapter VIII deals with the convective model for residence time distribution of fluids flowing in tubes and pipes. This is not related to the plume model but included in this volume because a substantial part of this development is original and not available elsewhere.

CHAPTER II. MODELS IN THE LITERATURE FOR THE ATMOSPHERIC FLUIDIZED BED COMBUSTOR

Many investigators have published models for the AFBC during the last several years using various assumptions and simplifications (see Table 2.1).

Avedesian and Davidson (3) investigated batch combustion of char in a bench scale fluidized bed. Up to 4.3 grams of carbon, which were devolatilized char or coke, were injected into the bed which was preheated. The diameter of the carbon varied from 0.23 to 2.61 mm. By measuring burn-up time of carbon particles they concluded that the two-film theory for the combustion of carbon particles and two phase model for the fluidization hold in their bed at temperatures around 1173K. The two-film theory assumes the gas-solid reaction of carbon with oxygen to form carbon monoxide on the surface of carbon particle and gas-gas reaction of carbon monoxide to form carbon dioxide are much faster than diffusion of gases. Thus the combustion rate of carbon particle is controlled by diffusion of gases through two films: one is the space between the surface of carbon particle and the thin reaction zone for the oxidation of carbon monoxide to carbon dioxide and the other is from this reaction zone to the bulk gas. Campbell and Davidson (4) did similar work but char was continuously fed this time.

Bethel et al. (18) developed a model to correlate the experimental data but their model is limited to the prediction of sulfur retention.

TABLE 2.1 Models for Fluid Bed Combustors

Model Number and Authors	Year	A	B	C	D	E	F
1. Avedesian & Davidson(3)	(1973)	I	a	I	c	I	No
2. Campbell & Davidson(4)	(1975)	I	a	I	c	I	No
3. Gibbs(5)	(1975)	I	a	I	a	I	Yes
4. Gordon & Amundson(6)	(1976)	I	a	I	c	I&III	No
5. Gordon & co-workers(7)	(1978)	I	a	I	c	III	No
6. Chen & Saxena(8)	(1977)	II	c	I	c	I	Yes
7. Horio & co-workers(9)	(1977)	I	a	I	c	II	Yes
8. Horio & Wen(10)	(1978)						
Rajan & co-workers(11)	(1978)	III	b	II	a	II	Yes
Rajan & Wen(12)	(1980)						
9. Baron & co-workers(13)	(1978)	I	a	I	c	II	Yes
Baron & co-workers(14)	(1977)	I&IV	a&d	I	b	I	Yes
Sarofim & Beer(15)	(1979)	I	a	I	b	II	Yes
10. Fan & co-workers(16)	(1979)	I	a	III	c	I	No
11. Leung and Smith(17)	(1979)	I	a	I	c	II	No

See Table 2.2 for description

TABLE 2.2 Description of Models in Table 2.1

-
- A. Model for Fluidized Bed
- I. Two phase bubbling bed model: bubble phase and emulsion phase.
 - II. Three phase bubbling bed model: bubble, cloud and emulsion phases.
 - III. Compartments in series model: two phases in each compartment.
 - IV. Slow bubble regime model: no distinction made between the bubble phase and the emulsion phase.
- B. Gas Flow Pattern in the Bed
- a. Plug flow in the bubble phase, mixed flow in the emulsion phase.
 - b. Mixed flow in both phases.
 - c. Plug flow in both phases. Gas exchange between two phases is finite.
 - d. Plug flow through the bed. No distinction between phases.
- C. Movement of Solids in the Bed
- I. Well mixed.
 - II. Well mixed in a number of compartments.
 - III. Dispersion of solid is finite. Dispersion coefficient is used for mass balance.
- D. Devolatilization of Feed Coal
- a. Instantaneous devolatilization. Volatiles evolve uniformly across the plane representing coal feed point.
 - b. Devolatilization is slower than mixing of the feed coal. Volatiles evolve uniformly throughout the bed.
 - c. Not considered.
 - d. Devolatilization is instantaneous at the feed point.
- E. Kinetics of Solid Coal Combustion
- I. Film diffusion controlling.
 - II. Both film diffusion and surface reaction influence the rate, but homogenous oxidation of CO to CO₂ is assumed to be very fast.
 - III. Rate of CO oxidation is comparable to that of other reactions.
- F. Is Elutriation Considered?
-

Gibbs (5) proposed a mechanistic model, assuming like others, that coal is fed uniformly to all points on the plane representing the base of the bed. He noted the importance of bubble size that dictates gas exchange rate between the bubble phase and the emulsion phase in the two phase theory of fluidization.

Gordon and Amundson (6) concentrated on the material and energy balance using the bubbling model while ignoring elutriation. They pointed to the possibility of having more than one stable temperature in the bed and the importance of gas exchange coefficient between the bubble phase and the emulsion phase. Their work was extended later (7) but devolatilization of coal was ignored in both these studies.

Horio and Wen (19) developed a model based on the bubble assemblage model but without considering the elutriation of char. Horio and Wen (10) together with Rajan et al. (11) developed a model which accounts for both devolatilization and thermal balance, thus the temperature profile in the bed. This model was extended later (12).

Baron et al. (13) used two phase theory to predict the combustion in AFBCs. They pointed out that surface chemical reaction resistance in the combustion of char may not be ignored. They also noticed that the rising velocity of the bubbles at the bottom of the bed is not faster than the interstitial gas velocity in the emulsion phase to justify the use of the two phase theory (14).

Chen and Saxena (8) presented a model which deals with both the combustion and sulfur retention using the bubbling bed model.

Horio et al. (9) presented a model but their emphasis was on the behavior of carbon monoxide and nitrogen oxide.

All previous models assumed the dispersion of feed coal is very fast. But Fan et al. (16) modeled a shallow bed considering a finite rate of feed coal dispersion and gases in the bed.

Leung and Smith (17) studied the effect of char reactivity on the performance of the combustor using the model of Avedesin and Davidson.

Now let us examine the critical assumptions underlying the models listed in Table 2.1 to see whether they are useful for representing and modeling the large utility scale AFBCs.

Gas Flow in the Bed

As mentioned earlier, AFBCs will be operated in either the slow bubble regime or in the turbulent-churning regime. However, as Table 2.1 shows, most model builders in the past used two phase theories, representative of the fast bubble regime, to describe the flow of gas. The two phase theory was developed specifically for beds of fine particles such as catalytic reactors, and it envisions fast rising bubbles with a captive recirculating vortex of gas with consequent severe gas bypassing. Models of this type might satisfactorily interpret the experimental data from a small bench scale AFBC using fine particles and low gas velocity but they certainly are unsuitable for the understanding of utility scale AFBCs of large particles with their high gas velocities.

Mixing of Solids

It is usually assumed that solids are well mixed in a fluidized

bed. This assumption in effect states that in the time period when the solid particle reacts, it is likely to have wandered a distance at least comparable to the dimension of the bed. This assumption is usually good for small scale experimental fluidized beds. But AFBCs for electric power generation will be so large that multiple coal feed ports will be needed to obtain a relatively uniform distribution of reacting solids in the bed. Current designs call for one feed port for every square meter or so of bed cross-section. Experiments with solids tracers in a one meter square tube-filled bed showed that 10 to 30 seconds are required for tracer particles to move throughout the bed (20). Thus, for reaction times in minutes, the solids can be treated as well mixed; but for reaction times in seconds, the well-mixed assumption is unreasonable.

Entering coal particles devolatilize and then burn as char. If the dispersion of feed coal is much faster than the devolatilization, then each coal particle would have its own tiny diffusion flame while its volatiles evolve and burn. However, if devolatilization is faster than the dispersion from a coal feed port, the volatiles combine to form a large plume of unburned gas rising from the feed port. Since this plume can contain as much as 50% of the heating value of the fuel, it is not something which one can or should ignore.

It is estimated that the time for devolatilization is less than one second for 200 μm particles (21) and less than ten seconds for 3000 μm particles (14). Therefore, one feed point per square meter is not enough to avoid the formation of a plume when coal particles

smaller than 3000 μm are burned.

Some models in the literature simply ignored coal volatiles and others assumed uniform release of volatiles throughout the bed. These simplifications are questionable.

Char combustion is much slower than devolatilization. For example, the time for complete combustion of a 3000 μm particle is about five minutes; for a 300 μm particle, about one minute. Thus compared to the mixing time of particles it is reasonable to consider the char as being well mixed throughout the bed.

For limestone particles, the mean residence time is about one hour or longer so it is reasonable to assume that limestone particles are well mixed throughout the bed.

Carbon Utilization

Unburned fuel can leave the AFBC in three ways: with the spent bed material, as unburned gases, and as elutriated char particles. Results of Babcock and Wilcox (2) and other studies show that the first factor is unimportant since there is negligible char in the exit solids. As for the unburned gases, CO and other combustibles will rapidly burn to near completion above the bed, so this loss is not a significant factor. The most significant loss of unburned fuel, in fact, comes from the elutriation of char particles. Thus, models which ignore the elutriation loss cannot be used for correlating combustion efficiency.

As we can see all the AFBC models consist of submodels dealing with flow patterns, devolatilization of coal, combustion of char,

elutriation etc. Each of these is a very complicated problem and controversy still persists despite a great deal of research work devoted to them.

CHAPTER III. PLUME MODEL FOR COAL COMBUSTION

Because none of the models discussed so far is satisfactory, here we propose a plume model which accounts for the general features of the large scale AFBC.

Assumptions of the Plume Model

The major assumptions of the plume model are as follows:

1. Gas Flow: For beds of large particles having high minimum fluidizing velocity ($0.5 \sim 3$ m/s), the best simple representation for the flow pattern of gas is plug flow.
2. Devolatilization of entering coal particles is instantaneous and occurs at the feed entry ports to give plumes of unburned combustible gases which rise through the bed at the same velocity as the surrounding gases.

This assumption represents the AFBC in which coal is fed from below by entrained air in discrete entry ports. We show later that other methods of coal feed can be treated as special cases of the entry port analysis.

3. Combustion of vapors occurs at the boundary between volatiles and the surrounding oxygen-rich gas. This follows diffusion flame kinetics, the whole plume acting very much like a burning gas flame, with oxygen and combustibles moving to the plume boundary with an effective diffusion (or dispersion) coefficient which can be found by experiment.

4. The volatiles in the plume, which pass through the bed unburned, mix with air just above the bed to burn rapidly to completion.
5. The devolatilized solids are well mixed throughout the bed. They burn everywhere in the bed except in the plume. They maintain a constant density, the ash peeling off as it is formed. Hence, reaction of the char follows shrinking particle kinetics which is first order with respect to oxygen.
6. The bed is uniform in temperature with the exception of isolated char particles which may be much hotter.
7. Large char particles shrink as they burn in the bed and, at any bed condition, a distinct size exists above which no elutriation occurs. Below this size, the chance of elutriation increases progressively as particles shrink.

Figure 3.1 sketches the main features of the bottom-fed coal-burning AFBC.

Combustion of Char, Volatiles and Oxygen in the Bed

Because the main fuel loss in an AFBC is the elutriation of unburned char particles, we concentrate on the combustion of char particles of elutriable size for the prediction of combustion efficiency. Larger particles must burn and shrink down to this size in the bed no matter what the mechanism or kinetics of their combustion actually may be.

The weight of shrinking char solids in a size interval between

Figure 3.1 Sketch of the main features of the plume model for the bottom fed AFBC.

R_i and R_{i+1} in the bed is given by (see reference (22) and (23) for nomenclature, derivation and equations)

$$W(\bar{R}_1) = \frac{F_0(\bar{R}_1)\Delta R_1 - W(\bar{R}_{i+1})R(\bar{R}_{i+1})\left(\frac{\Delta R_1}{\Delta R_{i+1}}\right)}{\frac{F_1}{W}\Delta R_1 - R(\bar{R}_1) + \kappa(\bar{R}_1)\Delta R_1 - \frac{3}{\bar{R}_1}R(\bar{R}_1)\Delta R_1}, \quad (3-1)$$

the total weight of char in the bed by

$$W = \sum_i W(\bar{R}_1),$$

the carryover of unburned char by

$$F_2 = \sum_i W(\bar{R}_1) \kappa(\bar{R}_1), \quad (3-2)$$

and the conversion of char in the bed by

$$X_b = 1 - F_2/F_0 \quad (3-3)$$

Now put $F_1 = 0$, meaning that no unburned carbon leaves in the overflow solids. Also, notice that all the values are for elutriable particles. Particles that are too big to be elutriated can be incorporated into the largest size fraction by adjusting the mass of this fraction accordingly.

Now to calculate F_2 , we need both elutriation and shrinkage rates of particles. For the elutriation rate, $\kappa(\bar{R}_1)$, we use the expression of Colakyan (24), good for any size of solids R_1

$$\kappa(R_1) = \kappa_0 \left(1 - \frac{u_t(R_1)}{u_o}\right)^2 \quad (s^{-1}) \quad (3-4)$$

and for the shrinkage rate, from

$$R(R) \equiv \frac{dR}{dt} = \frac{-12k'' C_{ox}}{\rho_c f_c} \quad (m/s) \quad (3-5)$$

where ρ_c = density of char (kg/m^3)

f_c = mass fraction of carbon in char

$\overline{C_{ox}}$ = average concentration of oxygen in the bed (mol/m^3)

k'' = char combustion rate constant based on the external
surface of char $\frac{\text{mol carbon}}{(\text{mol } O_2/\text{m}^3)(\text{m}^2 \text{ char surface})(\text{s})}$

Thus $k'' \overline{C_{ox}}$ denotes the average combustion rate of char in the bed

($\frac{\text{mol carbon}}{\text{m}^2 \text{ char surface} \cdot \text{s}}$). We have to consider both diffusion and surface

reaction for k'' . Then

$$k'' = \frac{1}{\frac{1}{2k_g} + \frac{1}{k_c}}, \quad \frac{\text{mol carbon}}{(\text{mol } O_2/\text{m}^3)(\text{m}^2 \text{ char surface})(\text{s})} \quad (3.6)$$

where film mass transfer coefficient of oxygen, k_g , can be evaluated using the expression of Ranz and Marshall (25)

$$k_g = \frac{D}{2R} \left[2.0 + 0.6 \left(\frac{2R u_f \rho_g}{\mu} \right)^{1/2} \left(\frac{\rho_g \mu}{D} \right)^{1/3} \right], \quad [\text{m/s}] \quad (3.7)$$

and surface reaction rate constant from Field et al. (26)

$$k_c = 5.96 \times 10^2 T_s \exp \left[\frac{1.8 \times 10^6}{T_s} \right], \quad \left[\frac{\text{mol carbon}}{(\text{mol } O_2/\text{m}^3)(\text{m}^2 \text{ char surface})(\text{s})} \right] \quad (3.8)$$

we assume here that combustion product is CO and oxidation of CO to CO_2 occurs outside the gas film surrounding char. Thus coefficient of 2 appears on the right side of equation (3.6) as one mole of oxygen reacts with two moles of carbon.

The char surface temperature is given by the heat balance

$$h(T_s - T_b) + \epsilon \sigma (T_s^4 - T_b^4) = -r_c (-\Delta H_r) \quad (3.9)$$

T_s and k'' can be obtained by solving equations (3.6), (3.7), (3.8) and (3.9).

It is well known that more than one stable temperature is possible for burning coal particles (Field, et al. (26)). But at what temperature, if there be more than one, are these burning coal particles in the AFBC?

For the modeling of AFBCs we need a simple but useful representation of this behavior. As our concern is for char particles of elutriable size, we concentrate on the combustion of small particles, $< 1\text{mm}$. In addition, if we assume in equation (3.6) that only the homogeneous reaction $\text{CO} + 1/2\text{O}_2 \rightarrow \text{CO}_2$ occurs away from the surface of the particle the energy and mass balance becomes greatly simplified.

In general, we have three different regimes of behavior (see Figure 3.2).

Regime A: Only one high temperature steady state. Here the particle is much hotter than the rest of the bed, the reaction rate is controlled by film diffusion.

Regime B: Here we notice three possible char temperatures X, Y and Z. At X the combustion is slow and reaction controlled, at Z the particle is hot, reaction is fast and diffusion controlled. Point Y is unstable and physically unrealizable. If a particle enters Regime B at high temperature, it settles to point Z.

Regime C: Only one steady state. Here the particle temperature is close to that of the bed, the reaction rate constant is low and the overall combustion rate is slow and chemical reaction controlled.

The regime in which a char particle finds itself depends on the ambient temperature, oxygen concentration, size of particle and the

Figure 3.2 Possible stable temperatures in char combustion.

reactivity of the particle. Since a particle shrinks and moves about the bed into widely different oxygen environments (high at bottom of bed, low at the top, zero in the plume), it experiences frequent changes in regime during its lifetime. This can be conveniently displayed as follows.

First, we evaluate the overall combustion rate of individual particles in a bed at 1116 K. This is shown in Figure 3.3 as a function of oxygen concentration and particle size.

Figure 3.4 is a more useful representation of these results. It shows that Regime A can only be attained for large particles at high oxygen concentration, while Regime C can be found for the entire range of particle size at low oxygen concentrations.

Since coal particles enter the bed cold those smaller than 1mm have no chance of attaining the higher temperature point of Regime B (point Z). However particles larger than 1mm could well enter Regime A (see point 1 of Figure 3.4). These remain at high temperature even when they move to point 2. But they are quenched if they move further into Regime C (point 3). In addition, once quenched, they cannot go back to the higher temperature even when they return to Regime B (from point 4 to point 5). A very few particles may be "lucky" enough to stay in Regime B throughout their lifetimes (from point 1 to point 6), but most do not because the lifetime of particles in the bed is longer than their mixing time and the fraction of bed in Regime C is larger than the fraction in B and A.

Thus, with a bed at 1116 K practically all of the elutriable

Figure 3.3 Reaction rate constant of char as a function of size of coal and oxygen partial pressure.

Figure 3.4 Regimes of char combustion at 1116 K.

particles are at the low stable temperature, close to that of the bed.

But the picture is different at high bed temperature as shown in Figure 3.5. Here, particles in Regime C (point 1) have a good chance of entering Regime A (point 2) thereby experiencing a temperature jump. They then maintain this high temperature even if they enter Regime B (point 3), as long as they do not return to Regime C. Since the fraction of elutriable solids in Regime A is significant, the chance of having hot elutriable solids is not negligible in this bed.

Let us estimate the burn-up time for char at 1116 K. For 300 μm particles k'' is about $0.1 \left(\frac{\text{mol carbon}}{(\text{mol } \text{O}_2/\text{m}^3)(\text{m}^2 \text{ char surface})(\text{s})} \right)$

at $y_{\text{ox}} = 0.1$ from Figure 3.3. Then the rate of particle shrinkage is

$$R(R) = \frac{-12k'' \overline{C_{\text{ox}}}}{\rho_c f_c} = \frac{-(12)(0.1)(1.09 \times 10^{-3})}{(1000)(0.8)} = -1.635 \times 10^{-6} \text{ (m/s)}$$

and burn up time $t = R/R(R) = 150/1.635 = 92 \text{ sec} = 1.5 \text{ min}$

For 3000 μm particles k'' is not shown in Figure 3.3. But if we assume that diffusion controls the combustion rate of char k'' will be about $1 \left(\frac{\text{mol carbon}}{(\text{mol } \text{O}_2/\text{m}^3)(\text{m}^2 \text{ char surface})(\text{s})} \right)$ extrapolated from

Figure 3.3. Then the rate of particle shrinkage rate for this diffusion controlled regime is

$$R(R) = \frac{-(12)(1)(1.09 \times 10^{-3})}{(1000)(0.8)} = -1.635 \times 10^{-5} \text{ (m/s)}.$$

Figure 3.5 Regimes of char combustion at 1228 K.

Thus the time required for the 3000 μm particle to shrink to 1000 μm is

$$t = (1500-500)/(16.35) = 61.2 \text{ sec} = 1 \text{ min}$$

But as shown earlier once shrunk to 1000 μm , the particle has little chance to sustain the diffusion controlled high combustion rate. Therefore it will take several minutes to shrink further to 300 μm .

Calculations also show that k'' does not vary much with particle size and oxygen concentration (Figure 3.3). Therefore, the simple space average concentration for oxygen is used without introducing much error. Notice that first order reaction rate with respect to oxygen is assumed.

The combustion of volatiles determines the average oxygen concentration, $\overline{C_{\text{ox}}}$, encountered by the well-mixed solids within the bed. Let A denote combustible volatiles and B oxygen. Then

Here ν is a stoichiometric coefficient which characterizes the composition of volatiles. This expression assumes that there is no change in the number of moles by reaction. Neglecting axial dispersion, one obtains the following equations by mass balances for oxygen and combustible volatiles:

Inside the Plume

$$\frac{\partial C_A}{\partial z} = \frac{D_A}{u_o r} \frac{\partial}{\partial r} \left(r \frac{\partial C_A}{\partial r} \right) \quad (3-10)$$

$$\text{I.C.} \quad C_A = C_{A0} \text{ for } 0 \leq r < L_0$$

$$\left. \begin{array}{l} \text{B.C.} \quad \frac{\partial C_A}{\partial r} = 0 \text{ at } r = 0 \\ C_A = 0 \text{ at } r = L_1(z) \end{array} \right\} \text{ for all } z > 0$$

Outside the Plume

$$\frac{C_B}{\partial z} = \frac{D_B}{u_o r} \frac{\partial}{\partial r} \left(r \frac{\partial C_B}{\partial r} \right) - \frac{k}{u_o} C_B \quad (3-11)$$

where k is the rate constant for the disappearance of oxygen in the bed based on unit bed volume $\left[\frac{\text{m}^3 \text{ gas}}{\text{m}^3 \text{ bed} \cdot \text{s}} \right]$.

$$\text{I.C.} \quad C_B = C_{B0} \text{ for } L_0 < r \leq L_2$$

$$\left. \begin{array}{l} \text{B.C.} \quad C_B = 0 \text{ at } r = L_1(z) \\ \frac{\partial C_B}{\partial r} = 0 \text{ at } r = L_2 \end{array} \right\} \text{ for all } z > 0$$

On the Plume Surface

$$\left. D_A \frac{\partial C_A}{\partial r} \right|_{r = L_1(z)^-} = -v D_B \left. \frac{\partial C_B}{\partial r} \right|_{r = L_1(z)^+} \quad (3-12)$$

These equations assume that volatiles evolve from a circular region on the bottom of the bed centered on the coal feed port.

The radius of that circle, L_0 , is determined by the amount of volatiles that move upward at the same velocity as the fluidizing air. The radius of the plume at any elevation z is set by Equations (3-10), (3-11) and (3-12). Typical concentration profiles are sketched in Figure 3.6.

We also assume that the gases rise in plug flow with a certain lateral dispersion which is surprisingly small and not too different from that found in a packed bed. We adopt this picture as a result of the experimental studies by Jovanović (27) on the spread of a plume of tracer gas. In essence, he found that the plume of tracer gas meandered about from side to side and that the time-averaged concentration profiles showed a large amount of lateral dispersion. However, the true instantaneous dispersion of gas out from the axis of the meandering plume was much smaller. It is this instantaneous coefficient which is to be used in the above equations for D_A and D_B .

We can simplify the problem by assuming that $D_A = D_B$ because small scale eddy diffusion and not molecular diffusion is the main mechanism for gas dispersion. Applying the classical treatment of Burke and Schumann (28), the concentration of combustible volatiles is treated as a negative oxygen concentration. Oxygen and combustible volatiles move to the flame front (surface of the plume) stoichiometrically so that Equation (3-12) is satisfied. Then C_A , which satisfies Equation (3-10), can be applied to Equation (3-11) if we put $C_A = -vC_B$. Dropping subscripts A and B, combining Equation (3-10) and (3-11), and letting $y = \frac{C}{C_0}$, $\hat{z} = \frac{z}{H}$, and

Figure 3.6 Typical concentration profile of volatiles (A) and oxygen (B) in the vicinity of the plume.

$\hat{r} = \frac{r}{L_2}$, one obtains the dimensionless form

$$\frac{\partial y}{\partial \hat{z}} = \left(\frac{HD}{u_o L_2^2} \right) \frac{\partial}{\partial \hat{r}} \left(\hat{r} \frac{\partial y}{\partial \hat{r}} \right) - \frac{H k}{u_o} y I \quad (3-13)$$

where $I = \begin{cases} 0 & \text{if } y \leq 0 \\ 1 & \text{if } y > 0 \end{cases}$

$$\text{I.C. } y = \begin{cases} -v C_{AO}/C_0 & \text{for } 0 < \hat{r} < s_0 \\ C_{BO}/C_0 & \text{for } s_0 < \hat{r} \leq 1 \end{cases}$$

where $s_0 \equiv L_0/L_2$

B.C. $\frac{\partial y}{\partial \hat{r}} = 0$ at $\hat{r} = 0$ and $\hat{r} = 1$ for all $\hat{z} > 0$.

In this notation the surface of the plume is located where $y = 0$, and the new concentration profile is as shown in Figure 3.7.

We can estimate the values of s_0 and vC_{AO}/C_0 from a mass balance assuming that the ideal gas law holds:

$$s_0 = \left\{ 1 + \frac{(1 + E_x) n (1 - f_t)}{\frac{V^*}{0.0224} + (1 + E_x) n f_t} \right\}^{-0.5} \quad (3.14)$$

$$\frac{vC_{AO}}{C_0} = \left(\frac{C_{BO}}{C_0} \right) \left(\frac{f_p - (1 + E_x) f_t}{1 + E_x} \right) \left(\frac{1 - s_0^2}{s_0^2} \right) \quad (3.15)$$

where n = stoichiometric air for the combustion of coal (mol/kg feed coal)

f_p = ratio of stoichiometric air for the combustion of char to that for total coal combustion

f_t = the ratio of transport air to the total air used

V^* = volume of volatiles released from coal in the plume at

Figure 3.7 Concentration profile of oxygen (+) and volatiles (-) in the vicinity of the plume.

273K, 101.3kPa (m^3/kg feed coal)

E_x = the excess air ratio

If we do not feed coal pneumatically to the combustor the value of f_t is equal to zero. But when air is used as a carrier gas for the transport of coal into the bed its amount can be a significant part of the total air. Thus if the transport air is sufficient to burn all the volatiles from the coal, then there would be no plume of unburned volatiles as all the volatiles are consumed near the feed port. But usually the amount of transport air is insufficient for the complete combustion of volatiles (around 10% of total air in the Babcock and Wilcox pilot plant operation (2)). In this case all the oxygen in the transport air will be quickly consumed near the feed port, thereby lowering the concentration of combustibles in the plume. Transport air also contributes to the size of the plume formed. The excess air ratio, E_x , is related to the excess oxygen (%) at the stack, which people in combustion field use:

$$O_2, \text{ excess at stack (\%)} = \left[0.21 \frac{E_x + (1 - f_p)(1 - X_b)}{1 + E_x} \right] \times 100$$

Thus, for example, if $f_p = 0.4$, $X_b = 0.9$ and $E_x = 0.1$,

$$\begin{aligned} O_2, \text{ excess at stack} &= (0.21) \frac{0.1 + (1 - 0.4)(1 - 0.9)}{1 + 0.1} \times 100 \\ &= 3.05\% \text{ (see Figure 3.8)} \end{aligned}$$

Equation (3-13) is solved to give the mean oxygen concentration in the bed using numerical methods with given initial and boundary conditions (see Appendix A).

The value of k in Equation (9) represents the local oxygen

Figure 3.8 O_2 , excess at stack (%) versus excess air level, E_x .

disappearance rate constant and is constant throughout the bed since char is assumed to be well mixed in the bed. Notice that the value of k is determined by the given bed conditions and feed coal and this value must be found by trial and error.

Solving Equation (9) with an assumed value for k we obtain (at $\hat{z} = 1$) the conversion of volatiles in the bed,

$$X_v = 1 - \frac{2[f_p - f_t(1 + E_x)]}{f_p} \int_0^s \frac{y \hat{r} d\hat{r}}{s_0^2 v C_{A0}/C_0} \quad (3.16)$$

and the conversion of oxygen in the bed,

$$X_{ox} = 1 - 2(1 - f_t) \int_s^1 \frac{y \hat{r} d\hat{r}}{(1 - s_0^2) C_{B0}/C_0} \quad (3.17)$$

Then from an oxygen balance the conversion of char in the bed is

$$X_b = \frac{1}{1 - f_p} [(1 + E_x)X_{ox} - f_p X_v] \quad (3.18)$$

This X_b has to be the same as the one from Equation (3.3).

Thus, using Equations (3.1), (3.2), (3.3), (3.13), (3.16), (3.17) and (3.18), values for k and for the conversion are found by a trial and error procedure.

Combustion Above the Bed

On entering the freeboard region, unburned combustible gases rapidly react with oxygen giving essentially complete combustion within a short distance above the top of the bed. This results in an abrupt temperature jump.

There are also particles in the freeboard which are burning.

Those which do not elutriate are already accounted for in the bed material, those which are elutriating do so much faster than they burn and so their combustion can be ignored. In effect then, the combustion of particles in the freeboard can be included with the combustion in the bed.

Therefore, the overall carbon efficiency is given by

$$X_{ce} = 1 - (1 - X_b) f_f \quad (3.19)$$

where f_f is the ratio of carbon remaining in char after devolatilization to total carbon in the feed coal. Figure 3.9 is a schematic diagram of the calculation scheme for coal combustion in the AFBC.

Figure 3.9 Schematic diagram for the combustion of coal in the AFBC.

CHAPTER IV. RESULTS OF CALCULATIONS

Plume Versus No Plume

For a typical coal of properties shown in Table 4-1, let us first compare the "plume" model with the "plumeless" model. By the "plumeless" model we mean the extreme case where the particles of feed coal disperse uniformly throughout the bed before any devolatilization occurs and where the release of the volatiles and their subsequent combustion is complete before the onset of char combustion. In the "plumeless" model the average oxygen concentration in the bed is given as (see Appendix B)

$$\frac{C_{ox}}{C_{B0}} = \frac{[1 - (1 - X_b)(1 - f_p)]}{(1 + E_x) \ln \left[\frac{(1 + E_x)}{(1 - X_b)(1 - f_p) + E_x} \right]} \quad (4.1)$$

We can now find the char conversion X_b from Equation 4.1 together with Equations (3.1), (3.2) and (3.3), although the procedure again involves trial and error.

The difference in char conversion, thus, in carbon efficiency, between the plumeless and plume model is due to the difference in oxygen concentration in the bed. In the plumeless model, devolatilization is assumed to occur uniformly throughout the bed and all the volatiles burn in the bed. So the average oxygen concentration is always lower than in the case where part of the volatiles enter the freeboard region. Therefore, char conversion in the

TABLE 4.1 Properties of Coal Used for Calculation

Total carbon	73%
Carbon remaining in char after devolatilization	49%
f_f ratio of carbon re- maining in char after devolatilization to total carbon in the feed coal	$\frac{49}{73} = 0.6712$
Volatile matter	43.7%
Volume of volatiles	$0.25 \text{ m}^3/\text{kg of coal}$
Stoichiometric air for the combustion of coal, n	317 mol air/kg coal
Ratio of oxygen needed for the combustion of volatiles in the plume to that of total coal combustion, f_p	0.424
Heating value of coal	31000 kJ/kg coal
Density of char	1000 kg/m^3

plumeless model is always lower than in the plume model and the maximum difference occurs when all the volatiles do not burn in the bed but pass into the freeboard, i.e., $X_v = 0$ (see Figure 4.1).

Figure 4.1 shows char conversions for two cases. The maximum difference is about 8%. But from Equation (3.19), the difference in carbon efficiency becomes

$$\begin{aligned} X_{ce,plume} - X_{ce,plumeless} &= [1 - (1 - X_{b,plume})f_f] - [1 - (1 - X_{b,plumeless})f_f] \\ &= (X_{b,plume} - X_{b,plumeless})f_f \\ &= (0.08)(49/73) \\ &= 0.054 \text{ or } 5.4\% \end{aligned}$$

for the coal of Table 4.1.

It should be noticed, however, that the curves for the plume model approach the curves for the plumeless model as more and more of volatiles in the plume burn in the bed. In practice AFBCs will have X_v close to 1, not to zero, thus the difference in these two models should be small. Therefore we can now estimate char efficiency from equations (3.1), (3.2), (3.3) and (4.1) without considering plumes or equation (3.13).

Single Size Feed

Figures 4.2, 4.3 and 4.4 show the effect of different superficial gas velocities and excess air and elutriation rate constants on char combustion efficiency in an AFBC which is fed different sizes of coal particles whose properties are given in Table 4.1. The bed temperature is 1116 K. These figures all show that char conversion is nearly complete, both for small feed

Figure 4.1 Comparison of char conversion between plumeless and plume model.

Figure 4.2 Conversion of char in the bed as a function of the monosize coal feed and elutriation constant.

Figure 4.3 Conversion of char in the bed as a function of the monosize coal feed and superficial gas velocity in the bed.

Figure 4.4 Conversion of char in the bed as a function of the monosize coal feed and excess air.

particles and large feed particles, while intermediate size particles have lower conversion.

The reason for this somewhat unexpected behavior is as follows. For very small feed particles reaction to completion is more likely than elutriation, hence, high combustion efficiency is obtained. For intermediate sized particles, elutriation is more likely than reaction, hence, the lowered conversion of solids. But for very large feed particles most of the solids are consumed before the particles get down to elutriable size, hence, high combustion efficiency is obtained once again. This calculation shows that there is a critical intermediate size of feed solids which gives minimum char efficiency in the bed.

Feed of Wide Size Distribution

Figures 4.5, 4.6 and 4.7 show char conversion for a feed of wide size distribution which is assumed to be logarithmic:

$$Y = a(2R_i)^b \quad (4.2)$$

where Y is the weight percent of feed smaller than the particle radius (μm)(see Appendix C). Here a is set at 0.1 and b is varied for different values of maximum particle size, $d_{p, \text{top}}$ (μm). This gives

$$b = \ln\left(\frac{100}{a}\right) / \ln(d_{p, \text{top}}) \quad (4.3)$$

where

$$d_{p, \text{top}} \equiv (2) (\text{maximum } R_i)$$

Figure 4.5 Conversion of char in the bed for a feed of logarithmic size distribution as a function of top size of coal feed and elutriation constant.

Figure 4.6 Conversion of char in the bed for a feed of logarithmic size distribution as a function of top size of coal feed and superficial gas velocity in the bed.

Figure 4.7 Conversion of char in the bed for a feed of logarithmic size distribution as a function of top size of coal feed and excess air.

Thus, if $\kappa_0 = 0.05$, $E_x = 0.1$, $u_o = 2$ m/s, $d_{p, \text{top}} = 5000$ μm we get from Figure 4.6 $X_b = 0.94$ and from Equation (3.13) and Table 4.1.

$$\begin{aligned} X_{ce} &= 1 - (1 - X_b)f_f \\ &= 1 - (1 - 0.94)\left(\frac{49}{73}\right) \\ &= 0.96 \text{ or } 96\% \end{aligned}$$

If we increase the gas velocity to $u_o = 4$ m/s, then in the same way

$$X_b = 0.85 \text{ and } X_{ce} = 89.9\%$$

The Plume, the Volatiles and Afterburning

Let us take a close look at the plume. If all the volatiles of the plume burn in the bed i.e., $X_v = 1.0$, the plume will close in the bed (Figure 4.8a), but if not, the plume will stretch to the top of the bed (Figure 4.8b). If the plume is lean in combustibles its diameter will shrink as it rises (Figure 4.8d). But if it is rich in combustibles its diameter will expand at least for the bottom part of the plume (Figure 4.8c) and it can shrink after depleting combustibles depending on the circumstances (Figure 4.8a&b).

Figure 4.9 and 4.10 shows that one parameter, $HD/u_o L_2^2$, which appears in equation (3.13), determines the conversion of volatiles in the bed and that this is insensitive to the conversion of char in the bed and excess air level.

Notice that for a sufficiently large value of $HD/u_o L_2^2$ the volatiles burn completely in the bed and the plume closes and disappears within the bed.

The adiabatic temperature jump above the bed (in the freeboard)

Figure 4.8 Configuration of the plume in the bed.

Figure 4.9 Fraction of volatiles converted in the bed at different char conversion in the bed.

Figure 4.10 Fraction of volatiles converted in the bed at different excess air level.

due to the combustion of remaining volatiles can be calculated from the following equation:

$$\Delta T = \frac{\Delta H_{vol}(1-X_v)}{\bar{c}_p \{0.02896(1+E_x)n+0.9\}} \quad (4.4)$$

where ΔH_{vol} is the heating value of the volatiles from the coal.

For the calculation of ΔH_{vol} the following formula was taken for the calculation basis:

$$\Delta H_{vol} = 30341 f_p, \text{ kJ/kg of feed coal.}$$

The mean specific heat capacity of combustion gas in the freeboard, $\bar{c}_p$, was taken as

$$\bar{c}_p = 0.305 \frac{\text{Btu}}{\text{lb.}^\circ\text{F}} = 1.276 \frac{\text{kJ}}{\text{kg} \cdot \text{K}}$$

for the calculation basis. The number 0.9 which appears in the denominator of equation (4.4) means that 90% of the feed coal goes out of the bed as flue gas. Thus if the feed coal has different heating value or specific heat of combustion gas is different from those values given above, adiabatic temperature jump has to be adjusted accordingly by equation 4.4.

Figure 4.11 shows the adiabatic temperature jump in the freeboard at different levels of char conversion in the bed, or X_b . Figure 4.12 shows the effect of excess air level on the temperature. Notice that temperature jump with less air is higher due to less amount of gas involved.

The effect of transport air is shown in Figure 4.13. Oxygen in the transport air intermixes with volatiles resulting in partial combustion of volatiles at the bottom of the plume. As more transport air is used the adiabatic temperature jump in the freeboard decreases.

FIGURE 1

BLOCK DIAGRAM OF DRIVER AMPLIFIER TO DECREASE DECAY TIME AND CURRENT LEVEL CONTROL.

Figure 2. Recording pulse (a) using a linear voltage amplifier (b) using a current feedback amplifier (c) with "level-switching" circuit.

Figure 3. "H" coil design for magnetic solids velocity measurement.

Figure 4. Typical B-H curve for ferromagnetic material.

Figure 5. Finite difference model for calculating field of magnetized iron.

Figure 6. Calibration assembly.

Folded "C" Configuration

Anti-Parallel Configuration

Figure 7. Coil configuration.

Figure 8. Output signal vs iron powder mass flow rate inside coils for series I.

Figure 9. Output signal vs iron powder mass flow rate inside coils for series II.

Figure 10. Output signal vs iron powder mass flow rate inside coils for series III.

Figure 4.11 Temperature jump above the bed at different char conversion in the bed.

Figure 4.12 Temperature jump above the bed at different excess air level.

Figure 4.13 Temperature jump above the bed as a function of the ratio of transport air to the total air to the bed (f_t).

Thus, if $E_x = 0.1$, $X_b = 0.9$, $H = 1.2$ m, $D = 0.02$ m²/s, $L_2 = 0.5$ m and no transport air is used, then the plume number becomes:

$$HD/u_o L_2^2 = (1.2)(0.02)/(2.4)(0.5)^2 = 0.04$$

From Figure 4.11: $\Delta T = 300$ K.

But if 10% of the total air is used for the transport of coal into the bed then from Figure 4.13: $\Delta T = 180$ K.

Different Types of Coal

So far all the calculations are made for the one type of coal whose properties are shown in Table 4.1. Let us now examine how X_v and ΔT vary with the type of coal. The characteristics of coal, as far as the conversion of volatiles in the bed is concerned, are represented by s_0 and vC_{AO}/C_0 in the initial condition of equation 3.13 as shown in Chapter III.

$$s_0 = \left\{ 1 + \frac{(1+E_x)n(1-f_t)}{\frac{V^*}{0.0224} + (1+E_x)nf_t} \right\}^{-0.5} \quad (3.14)$$

$$\frac{vC_{AO}}{C_0} = (0.21) \left(\frac{f_p - (1+E_x)f_t}{1+E_x} \right) \left(\frac{1-s_0^2}{s_0} \right) \quad (3.15)$$

The value of n varies from coal to coal (180 to 370), but for bituminous coal the variation is smaller (290 to 370). The volume of volatiles, V^* , also varies (0.15 to 0.30). Changing n and V^* causes s_0 , the radius of plume at the bottom of the bed, to vary. But calculations show that X_v is not sensitive to the magnitude of s_0 , though larger s_0 causes X_v to increase slightly. Thus,

doubling or halving V^* or n does not cause X_v to change by much: 2% at maximum, and less as X_v approaches 1.

But, on the other hand, X_v is strongly dependent on f_p , which is the measure of amount of combustible volatiles released to form the plume. Figure 4.14 and Figure 4.15 show that X_v is high when the plume has but a small amount of combustibles (low f_p).

The calculation basis for these figures is summarized below:

$$f_t = 0.0$$

$$n = 330.0 \text{ (mol air/kg feed coal)}$$

$$X_b = 0.9$$

$$V^* = 0.7f_p \text{ m}^3/\text{kg feed coal, except for } f_p = 0.96, \text{ in which case } V^* = 0.07.$$

The difference between Figure 4.14 and Figure 4.15 is in excess air level; 0.1 for Figure 4.14 and 0.2 for Figure 4.15, respectively. The effect of excess air level on X_v is insignificant at small X_v , but becomes somewhat important as X_v approaches 1. Figure 4.16 shows the adiabatic temperature jump above the bed which is calculated from X_v values given in Figure 4.14 and Figure 4.15.

Figure 4.17 and Figure 4.18 show volatiles conversion in the bed and temperature jump above the bed at different values of X_v , but this time 10% of total air to the bed is used for the transport of feed coal into the bed ($f_t = 0.1$).

Incomplete Devolatilization of Coal in the Plume

So far we assumed that all the volatiles are released at the feed port. Now we will examine the case where the dispersion of

Figure 4.14 Conversion of volatiles in the bed as a function of the ratio of the oxygen needed for the combustion of volatiles in the plume to that for total coal combustion, f_p , with 10% of excess air but without transport air.

Figure 4.15 Conversion of volatiles in the bed as a function of the ratio of oxygen needed for the combustion of volatiles in the plume to that for total coal combustion, f_p , with 20% excess air but without transport air.

Figure 4.16 Temperature jump above the bed as a function of the ratio of oxygen needed for the combustion of volatiles in the plume to that for total coal combustion, f_p , but without transport air.

Figure 4.17 Conversion of volatiles in the bed as a function of the ratio of oxygen needed for the combustion of volatiles in the plume to that for total coal combustion with 10% excess air and 10% transport air.

Figure 4.18 Temperature jump above the bed as a function of the ratio of oxygen needed for the combustion of volatiles in the plume to that for total coal combustion, f_p , with 10% excess air and 10% transport air.

feed coal competes with the devolatilization. For this we have to know the kinetics of the devolatilization and the kinetics of dispersion of feed coal in the bed, both of which are not fully predictable unfortunately. Therefore we will limit our study to the simple picture to elucidate the competition of these two processes.

For the devolatilization of feed coal in the bed we assume first order kinetics:

$$\frac{dV}{dt} = k_D V = k_D V^* e^{-k_D t}$$

where k_D is the rate constant (s), and V^* is the maximum amount of volatiles.

For the dispersion of feed coal away from the feed port we assume a simple two dimensional diffusion model which ignores vertical movement. Notice that vertical position of coal particles is relatively unimportant because volatiles from those coal particles inside the plume contribute to the plume regardless of their vertical position. Then the probability of a feed coal particle to be inside the plume at time t after injected into the bed is the same as the probability of a particle to be within distance L_0 in one dimensional random motion:

$$\int_0^{L_0} 2\pi r P(r,t) dr = \int_0^{L_0} P(x,t) dx = \text{erf}\left[\frac{L_0}{\sqrt{4D_s t}}\right] \quad (4.5)$$

where P is a probability density function and D_s is the solid dispersion coefficient.

Then the fraction of volatiles released inside the plume is given as

$$\phi = \int_0^{\infty} k_D e^{-k_D t} \operatorname{erf} \left[\frac{L_2}{\sqrt{4D_s t}} \right] dt$$

Here we assume that coal particles from other feed ports do not contribute to the plume. This is reasonable if the devolatilization is very fast or if the feed ports are far from each other. Let $x \equiv k_D t$, then

$$\phi = \int_0^{\infty} e^{-x} \operatorname{erf} \left[0.5 s_0 \left(\frac{L_2^2 k_D}{D_s} \right)^{1/2} x^{1/2} \right] dx \quad (4.6)$$

Thus ϕ depends on only on parameter, $L_2^2 k_D / D_s$, but still it has to satisfy another equation:

$$s_0 = \left\{ 1 + \frac{(1+E_x)n(1-f_t)}{\frac{\phi V^*}{0.0224} + (1+E_x)nf_t} \right\}^{-1/2} \quad (4.7)$$

which is the modified version of equation 3.14. Note that we can calculate ϕ and s_0 using equation (4.6) and equation (4.7) with given values for $L_2^2 k_D / D_s$ and other parameters in equation (4.7).

Figure 4.19 shows the effect of f_t and $L_2^2 k_D / D_s$ on ϕ , the fraction of volatiles released inside the plume. For the calculation properties of coal in Table 4.1 were used. Figure 4.19 shows that ϕ increases with f_t and $L_2^2 k_D / D_s$. This is quite natural because an increase in these parameters increases the size of the plume. ϕ is also found to be insensitive to the variation of E_x and n . For the low values of $L_2^2 k_D / D_s$ ϕ is very low (figure 4.19). Thus if dispersion of feed coal is much faster than devolatilization, or

Figure 4.19 Fraction of volatiles released in the plume as a function of transport air, f_t .

D_s is much bigger than k_D , there would be very small amount of volatiles in the plume. In the extreme case ϕ goes to zero and the plume model reduces to the plumeless model.

Figure 4.20 shows the remarkable effect of ϕ on X_v , the conversion volatiles in the bed. If only a small fraction of volatiles join the plume the rest will evolve outside the plume and burn completely there resulting high overall X_v . Figure 4.21 shows the adiabatic temperature jump above the bed which is based on Figure 4.20. Notice that the effect of feed port spacing does not follow the line of constant ϕ . If we increase the spacing, L_2 , ϕ will increase as shown in Figure 4.19. Thus, if $f_t = 0.1$, $E_x = 0.1$, $X_b = 0.9$, $L_2^2 k_D / D_s = 10$ and $HD/u_0 L_2^2 = 0.01$,

$$\phi = 0.67 \text{ from Figure 4.19,}$$

and $\Delta T = 200 \text{ K}$ from Figure 4.21.

But if we double the spacing,

$$L_2^2 k_D / D_s = 40 \text{ and } HD/u_0 L_2^2 = 0.0025,$$

then, $\phi = 0.9$ from Figure 4.19

and $\Delta T = 460 \text{ K}$ from Figure 4.21.

Figure 4.20 Conversion of volatiles in the bed as a function of the fraction of volatiles released inside the plume.

Figure 4.21 Temperature jump above the bed as a function of the fraction of volatiles released inside the plume.

CHAPTER V. SULFUR RETENTION FROM THE PLUME MODEL

In order to predict sulfur retention in the AFBC we have to know how the sulfur in coal releases and reacts with limestone particles in the bed. In this chapter we will look at the behavior of sulfur during devolatilization and combustion of coal and the reaction of limestone with sulfur dioxide and hydrogen sulfide. Then we will develop two kinds of plumeless models as well as the plume model for sulfur retention. Calculation results will be illustrated and discussed.

Sulfur in Coal

Sulfur in coal occurs in various forms: pyritic, organic and as sulfates. The total sulfur in coal varies in the range of 0.1 - 10% (29) although in most cases it is between 1 and 3%. Pyritic sulfur which occurs in coal as discrete particles is a heavy mineral with specific gravity of about 5, compared to coal which has a maximum specific gravity of only 1.7. The pyritic content of most coals can be reduced significantly with coal preparation methods of size reduction and gravimetric separation.

Organic sulfur, which is an integral part of the coal matrix and which generally cannot be removed by direct physical separation, comprises from 30% to 70% of the total sulfur in the most coals.

The sulfate sulfur content is normally an oxidation product which is water-soluble and can be removed readily during coal cleaning. Sulfate sulfur contents are usually less than 0.05% in fresh coal but

increases when the coal is exposed to air.

During the pyrolysis of coal some of sulfur devolatilizes and the proportion of devolatilized sulfur depends on several factors (30); rank of coal, mineral matter in the coal, etc. Peet et al. (31) found a linear relation between weight loss of the coal and loss of original total sulfur for high organic sulfur coal. Maa et al. (32) reported that sulfur removal from the coal was 59% after pyrolysis under nitrogen. Although the composition of this devolatilized sulfur can vary depending on the conditions of pyrolysis it is presumed that hydrogen sulfide is the main component in the reducing environment.

For the plume model this devolatilization has a significant meaning: a portion of sulfur in the feed coal devolatilizes and becomes part of the plume while the char retains the rest. The sulfur remaining in the char reacts with oxygen to form sulfur dioxide as char burns in the oxidizing zone. The volatile sulfur in the plume reacts with oxygen to form sulfur dioxide on the plume surface like other combustibles in the plume. However the volatile sulfur in the plume also reacts with limestone particles as another way of sulfur retention. The remaining volatile sulfur in the plume goes to the freeboard and burns there to give more sulfur dioxide.

The limestone particles are first calcined and then react with sulfur dioxide in the oxidizing zone. They also react with hydrogen sulfide in the reducing zone:

The time required for the calcination of limestone is much shorter than the mean residence time of the limestone particles in the bed, so it is assumed that all the limestone particles are already calcined when they react with sulfur dioxide and/or hydrogen sulfide. Finally the calcium sulfide formed reacts readily with oxygen to form calcium sulfate.

Past Studies on the Reaction of CaO with SO₂ and H₂S

The reaction of SO₂ with CaO decreases with the increasing conversion of CaO and virtually stops well below the complete conversion. The problem is further complicated because the reaction rate depends on the origin and type of parent rock. The condition of calcination also influences the reaction behavior. One of the reasons for the complicated problem is the change of solid volume during the reaction. The particles become more porous as they lose mass by calcination but they regain more mass and become even less porous during sulfation.

Sulfation product CaSO₄ plugs the pores in the particles and impedes the approach of gas reactant to the surface of unreacted CaO. Borgwardt (33) reported that the first order reaction of sulfur dioxide with calcined limestone was the predominant resistance limiting the rate of sulfur dioxide sorption and that the activation

energy ranged between 8.1 and 18.1 kcal/mol depending on the type of limestone. Borgwardt and Harvey (34) concluded that the intrinsic reaction rate constant of limestone derived from different carbonate rocks with sulfur dioxide is approximately the same when evaluated on the basis of surface area at zero conversion. They also reported that the porosity of the rock and grain size are important for the sulfation capacity.

Pigford and Sliger (35) developed a kinetic model for the reaction of sulfur dioxide with calcium oxide assuming the reaction rate is governed by two diffusional processes: the diffusion of SO_2 through the pores in the limestone particle and the diffusion of SO_2 through a layer of CaSO_4 . Thus their model requires knowing the values of two diffusion rate constants as well as the pore structure and surface area of the limestone particle.

Wen and Ishida (36) developed a similar model but they included chemical reaction rate in addition to two diffusion rates, and they calculated the reaction rate constant based on the surface area. Their activation energy for the chemical reaction was 17.5 kcal/mol.

Hartman and Coughlin (37) reported a model to relate the maximum possible conversion of CaO in limestone to CaSO_4 with the properties of limestone such as porosity. Later (38) they developed a model to simulate the progress of conversion with time. Hartman (39) also studied the effect of SO_2 concentration and particle size on the conversion and the maximum conversion is dependent on the SO_2 concentration level. Hartman et al. also studied the effect of porosity of the calcium carbonates (40) and temperature (41) on the

reactivity of CaO with SO_2 .

Yang et al. (42) reported that the reaction of CaO in half calcined dolomite with SO_2 is first order with respect to SO_2 and 0.22 order with respect to O_2 in the presence of water vapor and that water vapor concentration does not affect reaction rate. Yang et al. (43) found that four percent by weight of Fe_2O_3 physically mixed with CaO approximately doubles the reaction rate and coal ash also catalyzes the sulfation reaction. They also found that the reaction order with respect to SO_2 depends on the SO_2 concentration level.

Fieldes et al. (44) reported that the maximum conversion of limestone particles in a fluidized bed of hot sand was influenced by the concentration of O_2 and SO_2 in the inlet gas, concluding that SO_3 is important intermediate in the sulfation reaction.

During the thermogravimetric study of the sulfation of limestone and dolomite O'Neill et al. (45) observed that sample size and gas flow rate strongly influence the kinetics, and that the carbon dioxide pressure in which the stone is originally calcined is the dominant influence on the sulfation reaction.

Unlike the case with SO_2 the published data on the reaction with H_2S is rather scant. Squires et al. (46,47) studied the reaction of H_2S with calcined dolomite in processes for the gasification of coal where this reaction is very important to scrub the product gas of H_2S . They reported that the reaction occurs homogeneously throughout the solid and is first order with respect to unreacted calcium oxide and hydrogen sulfide. Ruth et al. (48) reported

their study on the reaction of half calcined dolomite with H_2S at elevated pressure (20 atm).

Habashi and Mikhail (49) reported on the kinetics of the reaction and estimated the activation energy to be 3.3 to 4.5 kcal/mol.

Schreiber and Petrie (50) studied the effect of carbon monoxide on the reaction and found no significant effect of carbon monoxide concentration up to 35 percent by volume. They also reported that the reaction is 0.85 order with respect to hydrogen sulfide for calcined dolomite and first order for calcined calcium carbonate. The activation energy was reported as 10 kcal/mol.

Attar and Dupuis (51) reported that diffusion controls the reaction of calcite and dolomite with H_2S at 700 °C and gas film mass transfer controlling around 780 °C. They also reported the oxidation of sulfide ion S^{2-} to the sulfate SO_4^{2-} results in "breaking" of the sulfate layer since the molar volume of sulfate ion is larger than that of sulfide ion.

Assumptions of the Plume Model For Sulfur Retention

For the sulfur retention model the following assumptions are made in addition to those already made for the combustion model.

1. The volatile sulfur compounds (assumed to be hydrogen sulfide) react with oxygen instantaneously to form sulfur dioxide at the plume surface.
2. The reaction of hydrogen sulfide with limestone particles is first order with respect to hydrogen sulfide.

3. The reaction of sulfur dioxide with limestone is first order with respect to sulfur dioxide and zeroth order to oxygen. Sulfur dioxide does not react in the reductive environment (inside the plume).
4. All other reactions involving sulfur compounds are much slower than those mentioned above.

Formulation of Sulfur Release and Retention in
the Bed for the Plume Model

For the plume model we need the reaction rate for hydrogen sulfide retention

$$-r_H = k_H C_{H_2S} \frac{\text{mol}}{\text{m}^3 \text{ bed} \cdot \text{s}} \quad (5.4)$$

and for sulfur dioxide retention

$$-r_S = k_S C_{SO_2} \frac{\text{mol}}{\text{m}^3 \text{ bed} \cdot \text{s}} \quad (5.5)$$

Both the reaction expressions are based on a unit of bed volume. Therefore k_H and k_S have dimension of ($\text{m}^3 \text{ gas}/\text{m}^3 \cdot \text{bed} \cdot \text{s}$) and are dependent on the concentration of calcium oxide in the bed. With these reactions we can set up mass balance equations for sulfur dioxide and hydrogen sulfide similar to equation (3.13). Thus for H_2S (inside the plume only)

$$\frac{\partial y_H}{\partial \hat{z}} = \frac{HD}{u_o L_2^2} \frac{\partial}{\partial \hat{r}} \left(\hat{r} \frac{\partial y_H}{\partial \hat{r}} \right) - \frac{H}{u_o} k_H y_H \quad (5.6)$$

$$I.C \quad y_H = y_{H0} \text{ at } \hat{z} = 0$$

$$B.C \quad \left. \begin{aligned} \frac{\partial y_H}{\partial \hat{r}} &= 0 \text{ at } \hat{r} = 0 \\ y_H &= 0 \text{ at } \hat{r} = s(\hat{z}) \end{aligned} \right\} \text{ for all } 0 < \hat{z} < 1$$

where y_H = mol fraction of hydrogen sulfide

$$y_{H0} = \frac{31.2 f_s \Psi [1 - (1+E_x) f_t / f_p]}{\frac{V^*}{0.0224} + n f_t (1+E_x)} \quad (\text{see Appendix D})$$

f_s = weigh fraction of sulfur in the feed coal

Ψ = fraction of sulfur in the feed coal which devolatilizes and enters the plume

for SO_2 (outside AND inside the plume)

$$\frac{\partial y_s}{\partial \hat{z}} = \frac{HD}{u_o L_2^2} \frac{\partial}{\partial \hat{r}} \left(\hat{r} \frac{\partial y_s}{\partial \hat{r}} \right) + I \frac{H}{u_o} (\alpha k_y - k_s y_s) \quad (5.7)$$

$$I.C \quad y_s = \begin{cases} y_{S0} = \frac{31.2 f_s \Psi (1+E_x) f_t / f_p}{\frac{V^*}{0.224} + n f_t (1+E_x)} & \text{for } 0 \leq \hat{r} < s_0 \\ 0 & \text{for } s_0 < \hat{r} < 1 \end{cases}$$

$$B.C \quad \frac{\partial y_s}{\partial \hat{r}} = 0 \text{ at } \hat{r} = 0 \text{ and } \hat{r} = 1$$

$$\left. \frac{\partial y_s}{\partial \hat{r}} \right|_{\hat{r} = s^-} - \left. \frac{\partial y_s}{\partial \hat{r}} \right|_{\hat{r} = s^+} = \left. \frac{\partial y_H}{\partial \hat{r}} \right|_s$$

where $y_s \equiv$ mol fraction of sulfur dioxide.

$$\alpha \equiv \frac{31.2(1-\Psi)}{n(1-f_p)(0.21)} \quad (\text{see Appendix D})$$

Equations (5.4) and (5.5) can be solved using numerical methods with given initial and boundary conditions (see Appendix A).

Let us now take a sulfur balance on the basis of 1 kg of feed coal.

A. In the Feed Coal:

$$1000 \frac{f_s}{32.06} = 31.2 f_s \text{ mol sulfur/kg feed coal}$$

of which $\begin{cases} 31.2 f_s & \text{will go into the volatiles, and} \\ 31.2 f_s (1-\Psi) & \text{will remain in char.} \end{cases}$

B. Sulfur in the elutriating char:

$$31.2 f_s (1-\Psi)(1-X_b)$$

C. Sulfur dioxide at the top of the bed:

$$\bar{y}_s \Big|_{\hat{z}=1} \cdot \left[n(1+E_x) + \frac{V^*}{0.0224} \right]$$

where $\bar{y}_s \Big|_{\hat{z}=1} \equiv$ the average value of y_s at the top of the bed.

D. Sulfur dioxide from the combustion of volatiles in the freeboard.

$$31.2 f_s \cdot \Psi(1-X_H)$$

where X_H is conversion of volatile sulfur in the bed,

$$X_H \equiv 1 - \frac{[1-(1+E_x)f_t/f_p]}{y_{H0} \cdot S_0^2} \int_0^{s(1)} 2\pi y_H \hat{r} dr.$$

Note that $X_H = 0$ if $s(1) = 0$, i.e., the plume closes inside the bed

or $X_v = 1$.

Then the sulfur retention efficiency based on released sulfur in the combustor is defined as

$$\overline{SR} = 1 - \frac{(C) + (D)}{(A) - (B)} \quad (5.8)$$

Figure 5.1 schematically shows the sulfur flow in the AFBC.

Mol fraction of sulfur dioxide is given by sulfur balance.

-Total mol of combustion gas

$$n(1+E_x) + \frac{V^*}{0.0224} \quad (\text{mol/kg feed coal})$$

-Total sulfur released (mol/kg feed coal)

$$31.2 f_s - 31.2 f_s (1-\psi)(1-X_b) = 31.2 f_s [1 - (1-\psi)(1-X_b)]$$

-Total sulfur in flue gas

$$31.2 f_s [1 - (1-\psi)(1-X_b)] \{1 - \overline{SR}\}$$

-mol fraction of sulfur in flue gas

$$y_{s, \text{ flue}} = \frac{31.2 f_s [1 - (1-\psi)(1-X_b)] (1 - \overline{SR})}{n(1+E_x) + \frac{V^*}{0.0224}} \quad (5.9)$$

Plumeless Models

Now let us develop the plumeless model to see if the plumeless model can be used instead of the plume model which would be more complicated. Here we can think of two different cases for the plumeless model: plumeless model I is the case where volatile sulfur is released and reacts with oxygen to sulfur dioxide uniformly throughout the bed, and plumeless model II is the case where all the volatiles are released and burn at the bottom of the bed, which is actually the limit as $HD/u_o L_2^2$ approaches infinite.

Figure 5.1 Schematic diagram for the release of sulfur from the coal and subsequent retention of the sulfur in the bed.

Plumeless Model I

From the mass balance

for oxygen (see Appendix D)

$$y_B = (0.21 + k_v/k) e^{-\frac{kH}{u_o} \hat{z}} - k_v/k$$

$$\text{where } k_v = 0.21 \frac{u_o}{H} \frac{f_p}{1+E_x}, \quad \frac{m^3 \text{ gas}}{m^3 \text{ bed} \cdot s} \quad (5.10)$$

for SO₂

$$\frac{\partial y_s}{\partial \hat{z}} = \alpha k \frac{H}{u_o} y_B - k_s \frac{H}{u_o} y_s + \beta k_v \frac{H}{u_o} \quad (5.11)$$

$$\text{I.C. } y_s = 0 \text{ at } \hat{z} = 0$$

$$\text{where } \beta \equiv \frac{31.2 f_s \Psi}{0.21 n f_p} \quad (\text{see Appendix D})$$

By solving equation (5.11) with equation (5.10), we obtain

$$y_s = \frac{\alpha k (0.21 + k_v/k)}{k_s - k} \left(e^{-\frac{kH}{u_o} \hat{z}} - e^{-\frac{k_s H}{u_o} \hat{z}} \right) + (\beta - \alpha) k_v/k_s (1 - e^{-\frac{k_s H}{u_o} \hat{z}}) \quad (5.12)$$

At the top of the bed, $\hat{z} = 1$

$$y_{BT} = (0.21 + k_v/k) e^{-\frac{kH}{u_o}} - k_v/k$$

Thus

$$\frac{k_H}{u_o} = \ln \left\{ \frac{0.21 + k_v/k}{y_{BT} + k_v/k} \right\} \quad (5.13)$$

From the definition of X_b and oxygen balance

$$y_{BT} = 0.21 \frac{E_x + (1-f_p)(1-X_b)}{1 + E_x} \quad (5.14)$$

Therefore we can calculate kH/u_o and k_v by trial and error using equations (5.11), (5.13) and (5.14) with given values for f_p , E_x and X_b . Then the sulfur retention efficiency of the plumeless model I is given as

$$\begin{aligned} \overline{SRI} = 1 - \frac{(1+E_x)/0.21}{1 - (1-X_b)(1-\psi)} & \left\{ \frac{1-\psi}{1-f_p} \frac{k(0.21 + k_v/k)}{k_s - k} \left(e^{-\frac{kH}{u_o}} - e^{-\frac{k_s H}{u_o}} \right) \right. \\ & \left. + \frac{\psi}{f_p} - \frac{1-\psi}{1-f_p} \frac{k_v}{k_s} \right\} 1 - e^{-\frac{k_s H}{u_o}} \end{aligned} \quad (5.15)$$

with known values for E_x , X_b , ψ , f_p , $k_s H/u_o$, $k_v H/u_o$ and kH/u_o .

Plumeless Model II

From the mass balance

$$\begin{aligned} & \text{for oxygen} \\ y_B = 0.21 \frac{1+E_x-f_p}{1+E_x} e^{-\frac{kH}{u_o} \hat{z}} \end{aligned} \quad (5.16)$$

for SO_2

$$\frac{\partial y_s}{\partial \hat{z}} = \alpha k \frac{H}{u_o} y_B - \frac{k_s H}{u_o} y_s \quad (5.17)$$

$$\text{I.C.} \quad y_s = \frac{31.2 f_s \psi}{n f_p} = 0.21\beta$$

By solving equation (5.17) with equation (5.16), we obtain

$$y_s = 0.21 \left(\frac{1+E_x - f_p}{1+E_x} \right) \left(\frac{\alpha k}{k_s - k} \right) \left(e^{-k \frac{H}{u_o} \hat{z}} - e^{-k_s \frac{H}{u_o} \hat{z}} \right) + 0.21\beta e^{-k_s \frac{H}{u_o} \hat{z}} \quad (5.18)$$

Thus at the top of the bed

$$\begin{aligned} y_{BT} &= 0.21 \frac{1+E_x - f_p}{1+E_x} e^{-k \frac{H}{u_o}} \\ &= 0.21 \frac{E_x + (1-f_p)(1-X_b)}{1+E_x} \quad (\text{equation 5.14}) \end{aligned}$$

$$\text{or } k \frac{H}{u_o} = \ln \frac{1+E_x - f_p}{E_x + (1-f_p)(1-X_b)} \quad (5.19)$$

Then the sulfur retention efficiency of the plumeless model II is given as

$$\begin{aligned} \text{SR II} &= 1 - \frac{1}{1-(1-X_b)(1-\psi)} \left\{ \psi e^{-k_s \frac{H}{u_o}} + \frac{1-\psi}{(1-f_p)} (1+E_x - f_p) \frac{k}{k_s - k} \right. \\ &\quad \left. X(e^{-k \frac{H}{u_o}} - e^{-k_s \frac{H}{u_o}}) \right\} \quad (5.20) \end{aligned}$$

with given values for E_x , X_b , ψ , f_p and $k_s H/u_o$. Note that kH/u_o is fixed by equation (5.19).

Calculation of Sulfur Retention Efficiency

For the calculation of sulfur retention efficiency, $\overline{SR}$, for the plume model we need the values of the following parameters:

1. Properties of the feed coal

$$n, V^*, f_p, f_s, \psi$$

2. Design and operating conditions of the bed

$$f_t, \frac{HD}{u_o L^2}, \frac{H}{u_o}$$

3. Reaction constants

$$k, k_S, k_H$$

Of these parameters all were used for the combustion modeling except f_s, ψ, k_H and k_S . Now let us examine the range of values for these parameters.

f_s : 0.001 to 0.1. If all other parameters are fixed the sulfur retention efficiency is independent of this value because we assume that the chemical reaction rates are first order with respect to sulfur or sulfur compounds.

ψ : 0 to 1 Depends on the specific type of coal and the devolatilization of environment.

k_S and k_H : Dependent on the origin and condition of limestone as well as its conversion. There are kinetics data published in the literature but we have to convert the reaction rate constants to the unit defined by equations

(5.4) and (5.5).

One easy way of obtaining reaction rate of calcium oxide with sulfur dioxide is measuring weight change of a fixed amount of calcium oxide sample when they are exposed to a stream of gases with fixed composition. The amount of calcium oxide is chosen to be very small compared to the gas flow rate so that gas composition does not change but the weight of solid changes with time as calcium oxide converts to calcium sulfide or calcium sulfate.

But in the AFBC the situation is opposite. Here gas composition does change as gases move upward, but composition of solid does not change with time at steady state and uniform throughout the bed because we assume that solid particles are well mixed in the bed for sulfur retention reactions.

Therefore we have to know the concentration of calcium oxide in both the experimental unit and the operating AFBC to convert the kinetic data from experiment to the rate constants defined by equations (5.4) and (5.5). The concentration of calcium oxide in the AFBC can vary widely depending on the operating condition but let us take the following as the basis for the estimation of reaction rate constants:

voidage of bed:	65%
density of solid:	3110 kg/m ³ solid
weight fraction of calcium in solid:	0.43 kg Ca/kg solid
molecular weight of Ca:	40
average conversion of calcium oxide in bed:	35%

Then concentration of calcium oxide in the bed is given as

$$(CaO) = (3110)(1 - 0.65)(0.43)(1000/40)$$

$$= 11700 \text{ mol CaO/m}^3 \text{ bed}$$

Note that here concentration of calcium oxide, (CaO), is the total concentration, reacted and unreacted.

1. Borgwardt (33) reported kinetic data on the reaction (5.2) for limestone at 10% conversion, 870°C.

$$\text{rate} = 3 \times 10^{-5} \text{ mol SO}_2 / \text{g stone} \cdot \text{s}$$

Concentration of SO₂ was 3000 ppm (2.9×10^{-8} mol/cc).

Thus

$$k_S = 3 \times 10^{-5} \frac{\text{mol SO}_2}{\text{g stone} \cdot \text{s}} \frac{1}{2.9 \times 10^{-2} \frac{\text{mol SO}_2}{\text{m}^3 \text{ gas}}} \frac{3110 \times 10^3 \times (1-0.65) \frac{\text{g stone}}{\text{m}^3 \text{ bed}}}{\text{m}^3 \text{ bed} \cdot \text{s}}$$

$$= 1126 \frac{\text{m}^3 \text{ gas}}{\text{m}^3 \text{ bed} \cdot \text{s}}$$

2. O'Neill et al. (52) reported kinetic data on the reaction (5.2) at 22% conversion of CaO, 871°C.

$$\text{rate} = 1.1 \times 10^{-1} \frac{\text{kg SO}_3 \text{ absorbed}}{\text{kg stone} \cdot \text{s} \cdot \frac{\text{kg SO}_2}{\text{m}^3 \text{ gas}}}$$

$$= (1.1 \times 10^{-1}) \left(\frac{64}{80} \right) \frac{\text{mol SO}_3 \text{ absorbed}}{\text{kg stone} \cdot \text{s} \cdot \frac{\text{mol SO}_3}{\text{m}^3 \text{ gas}}}$$

Thus

$$k_S = (1.1 \times 10^{-1}) \left(\frac{64}{80} \right) \frac{\text{mol SO}_3 \text{ absorbed}}{\text{kg stone} \cdot \text{s}} \times 3110 \times (1 - 0.65) \frac{\text{kg stone}}{\text{m}^3 \text{ bed}}$$

$$= 95.8 \frac{\text{m}^3 \text{ gas}}{\text{m}^3 \text{ bed} \cdot \text{s}}$$

3. Pell et al. (47) reported kinetic data on reaction (5.3) using calcined dolomite at 800°C ($y_H = 3 \times 10^{-3}$)

$$\text{rate} = 4 \times 10^{-4} \text{ s}^{-1}$$

Thus

$$k_H = (4 \times 10^{-4} \text{ s}^{-1}) \frac{1}{3.41 \times 10^{-2} \frac{\text{mol H}_2\text{S}}{\text{m}^3 \text{ gas}}} 11700 \frac{\text{mol CaO}}{\text{m}^3 \text{ bed}}$$

$$= 137 \frac{\text{m}^3 \text{ gas}}{\text{m}^3 \text{ bed} \cdot \text{s}}$$

4. Schreiber and Petrie (50) reported kinetic data on the reaction using calcium carbonate at 700°C.

$$\text{rate constant} = 1.5 \times 10^{-4} (\text{H}_2\text{S}) \text{ s}^{-1}$$

where (H_2S) is mol percent of H_2S .

Thus

$$k_H = 1.5 \times 10^{-4} \left(\frac{1}{\text{mol} \% \cdot \text{s}} \right) 100 \left(\frac{\text{mol} \%}{\text{mol}} \right) 11700 \left(\frac{\text{mol}}{\text{m}^3 \text{ bed}} \right)$$

$$= 175.5 \frac{\text{m}^3 \text{ gas}}{\text{m}^3 \text{ bed} \cdot \text{s}}$$

They reported the apparent activation energy to be 10 kcal/mol.

Therefore at 800°C

$$k_H = 14 \exp \left[\frac{10,000}{1.987} \left(\frac{1}{973} - \frac{1}{1073} \right) \right]$$

$$= 284.6 \frac{\text{m}^3 \text{ gas}}{\text{m}^3 \text{ bed} \cdot \text{s}}$$

Author	k_H or k_S	T	Conversion of CaO
Borgwardt (1970)	$k_S = 1126$	870°C	10%
O'Neill et al. (1976)	$k_S = 95.8$	871°C	22%
Pell et al. (1971)	$k_H = 137$	800°C	unspecified
Schreiber and Petrie (1978)	$k_H = 285$	800°C	unspecified

Reaction rate of CaO with SO₂ decrease sharply with increasing conversion of CaO to CaSO₄. Westinghouse data (52) shows the reaction rate decreases 100 times as the conversion increases from zero to 35%.

Simon and Rawlins (53) analyzed the experimental data of the reaction of CaO with SO₂ and H₂S and reported that chemical reaction of CaO with H₂S is nearly the same as that of with SO₂ though CaO utilization with H₂S is higher than SO₂.

The conversion level of CaO to CaSO₄ in the bed is directly related to the ratio of feed rate of calcium to that of sulfur in coal. Thus if we use just the stoichiometric amount of limestone for the removal of sulfur 50% sulfur retention efficiency means the average conversion of limestone in the bed is 50%. But if we

use three times of stoichiometric amount, 30% conversion of limestone will give sulfur retention efficiency of 90%. Thus with given coal feed higher ratio of Ca to S feed ratio will give higher sulfur retention efficiency by lowering limestone conversion level in the bed, i.e., raising reaction rate constants k_s and k_H .

Results of Calculation for the Plumeless Models

Figure 5.2 shows the effect of $k_s \frac{H}{u_o}$ on sulfur retention efficiency for the plumeless model. Curve I is for $\overline{SRI}$ and II for $\overline{SRII}$. Here $\overline{SRII}$ is always higher than $\overline{SRI}$ because SO_2 from the combustion of volatiles in the case of $\overline{SRII}$ has a longer residence time, hence reaction time, in the bed. Figure 5.3 shows the effect of ψ on $\overline{SRI}$. With smaller amount of sulfur in the plume $\overline{SRI}$ becomes larger. Figure 5.4 shows quite the opposite trend for the case of $\overline{SRII}$. In both cases the effects of E_x , X_b and f_p were very small.

Results of Calculation for the Plume Model

For the AFBC with plumes typical concentration profiles of sulfur dioxide and hydrogen sulfide are shown in Figure 5.5a and Figure 5.5b. Figure 5.5a is for the case where transport air is used for the feed of coal into the bed and Figure 5.5b is for the case of no transport air. If transport air is used, partial combustion of H_2S occurs in the plume and the concentration of SO_2 can be high inside the plume at the bottom of the bed. On the other hand if no transport air is used the concentration of SO_2 is zero inside and outside of the plume at the bottom of the bed. The

Figure 5.2 Sulfur retention efficiency of the plumeless model I and II.

Figure 5.3 , Sulfur retention efficiency for the plumeless model I at three different volatile sulfur fraction.

Figure 5.4 Sulfur retention efficiency for the plumeless model II at three different volatile sulfur fraction.

Figure 5.5 Concentration profiles of sulfur dioxide and hydrogen sulfide in the AFBC with plume.

concentration of H_2S decreases as gases move upward due to absorption by limestone particles and by combustion at the plume boundary. SO_2 concentration increases for a while as gases move upward due to the combustion of H_2S and char to form SO_2 , but it decreases sooner or later as limestone particles absorb more SO_2 than produced. But the absorption of SO_2 occurs only outside of the plume thus resulting higher concentration of SO_2 inside the plume and much lower concentration outside the plume. Figure 5.5a and Figure 5.5b show a significant lateral variation in SO_2 concentration in the bed with plumes.

Figure 5.6 to 5.13 show sulfur retention efficiency, $\overline{SR}$, for the plume model. Notice that we need two different reaction rate coefficients, k_S and k_H for sulfur dioxide and hydrogen sulfide, respectively.

Figure 5.6 shows the modest effect of $HD/u_o L_o^2$, thus of X_v , on the sulfur retention efficiency, $\overline{SR}$, at various values of $k_S H/u_o$. Figure 5.7 shows the effect of Ψ on $\overline{SR}$ is similar to case of $\overline{SRI}$.

Figure 5.8 shows the effect of $k_H H/u_o$ on the sulfur retention efficiency. Obviously $\overline{SR}$ is lower at lower values of $k_H H/u_o$ but there is a limit on what the reaction of H_2S with CaO can contribute to the overall sulfur retention efficiency. Broken lines denote $\overline{SRI}$ and $\overline{SRII}$ for the same $k_S H/u_o$ from Figure 5.3 and Figure 5.4. Notice that $\overline{SRII}$ is a kind of upper limit for $\overline{SR}$ with the values given in the figure. For low values of $HD/u_o L_o^2$ conversion of volatiles in the bed is low and relative role H_2S retention is important. But for high values of $HD/u_o L_o^2$ conversion of volatiles in the bed is high

Figure 5.6 Sulfur retention efficiency at different reactivity of limestone with SO_2 and H_2S .

Figure 5.7 Sulfur retention efficiency at three different volatile sulfur fractions.

Figure 5.8 Sulfur retention efficiency at different reactivity of limestone with H_2S (high reactivity with SO_2).

Figure 5.9 Sulfur retention efficiency at different reactivity of limestone with H_2S (low reactivity with SO_2).

Figure 5.10 Sulfur retention efficiency at different amount of transport air (reactivity of limestone with SO_2 is high).

Figure 5.11 Sulfur retention efficiency at different amount of transport air (reactivity of limestone is low with SO_2 , but high with H_2S).

Figure 5.12 Sulfur retention efficiency at different ratio of oxygen needed for the combustion of volatiles in the plume to that for total coal combustion, f_p (reactivity of limestone is high with SO_2).

Figure 5.13 Sulfur retention efficiency at different ratio of oxygen needed for the combustion of volatiles in the plume to that for total coal combustion, f_p (reactivity of limestone is low with SO_2 , but high with H_2S).

and the H_2S not yet absorbed by limestone burns in the bed and SO_2 from that combustion has a chance of being absorbed by limestone anyway. Thus even for the case of no reaction between H_2S and limestone the sulfur retention at high $HD/u_o L_2^2$ is comparable to that of high reactivity between H_2S and limestone. At very high values of $HD/u_o L_2^2$ ($X_v = 1$) most of volatiles burn near the bottom of the bed and in this case $\overline{SR}$ is close to $\overline{SR_{II}}$ which is based on the assumption that all the volatiles burn at the bottom of the bed (the plume closes in the bed). But Figure 5.9 shows that this is not the case if the reactivity of limestone with SO_2 is low (i.e., conversion of CaO to $CaSO_4$ is not high). Due to the low reactivity of the limestone a significant portion of SO_2 from the combustion of volatile sulfur is not absorbed in the bed, thus making the combustion of the volatiles in the bed less important. But if the limestone is very reactive with H_2S sulfur retention efficiency can be much higher than $\overline{SR_{II}}$ as volatile sulfur (H_2S) is absorbed by the limestone without being converted to SO_2 which is not readily absorbed by the limestone.

Figure 5.10 and Figure 5.11 show the effect of transport air on the sulfur retention efficiency. The introduction of transport air reduces the $\overline{SR}$ significantly when the conversion of volatiles in the bed is low but its effect diminishes at high conversion of volatiles in the bed. Figure 5.12 and Figure 5.13 show the effect of f_p on $\overline{SR}$ is similar to that of transport air. Thus we can see that if the plume is lean in combustible sulfur, then retention is low at low conversion of volatiles in the bed. But at high conversion

of volatiles in the bed its effect is much smaller and can show the opposite trend (see Figure 5.12).

CHAPTER VI. A COMPREHENSIVE ILLUSTRATION

In this chapter we will show how to use the model. The operating conditions of the bed are adopted from the data of the Babcock and Wilcox company's pilot plant scale AFBC (2):

Height of the bed, $h = 1.2\text{m}$

Superficial gas velocity, $u_o = 2.6\text{m/s}$

Cross-sectional area of the bed $= 1.81 \times 1.81 \text{ m}^2$

Number of feed ports at the bottom of the bed $= 1 \text{ or } 4$

Temperature of the bed $= 1550^\circ\text{F}$

Part 1 Carbon efficiency

Let us choose a coal feed which has a logarithmic size distribution with top particle size, $3500 \mu\text{m}$. Then, by equation (4.2)

$$b = \ln\left(\frac{100}{0.1}\right) / \ln(3500) = 0.8465.$$

<u>$2R_1 (\mu\text{m}) \quad Y = (0.1)(2R_1)^{0.8465}$</u>			<u>B & W Data (Test 6-1)</u>
6350	100		100
4570	100		99.1
2380	72.2		92.9
1190	40.1		42.5
595	22.3		22.3
297	12.4		11.5
149	6.9		6.0
74	3.8		3.3
44	2.5		2.2 ($X_{ce} = 91.7\%$)

On the right is shown one of B & W data for comparison. For the other properties of coal we will use the values in Table 4.1 unless

otherwise specified.

(1-A) If $u_o = 2\text{m/s}$, $\kappa_o = 0.05\text{ s}^{-1}$, $E_x = 0.1$ and $d_{p, \text{top}} = 3500\text{ }\mu\text{m}$

$$X_b = 0.93 \text{ from Figure 4.6}$$

$$\begin{aligned} X_{ce} &= 1 - (1 - X_b)f_f \\ &= 1 - (1 - 0.93)(0.6712) \\ &= 0.953 \text{ or } 95.3\% \end{aligned}$$

(1-B) If we double the superficial gas velocity, $u_o = 4\text{m/s}$, and

$$\kappa_o = 0.05\text{ s}^{-1}, E_x = 0.1, d_{p, \text{top}} = 3500\text{ }\mu\text{m}$$

$$X_b = 0.85 \text{ from Figure 4.6}$$

$$\begin{aligned} X_{ce} &= 1 - (1 - 0.85)(0.6712) \\ &= 0.899 \text{ or } 89.9\% \end{aligned}$$

(1-C) The elutriation rate constant κ_o is doubled to 0.1 s^{-1} .

$$u_o = 2\text{m/s}, E_x = 0.1, d_{p, \text{top}} = 3500\text{ }\mu\text{m}$$

$$X_b = 0.9 \text{ from Figure 4.5}$$

$$\begin{aligned} X_{ce} &= 1 - (0.9)(0.6712) \\ &= 0.933 \text{ or } 93.3\% \end{aligned}$$

(1-D) Top size of coal feed is decreased to $1000\text{ }\mu\text{m}$.

$$u_o = 2\text{m/s}, E_x = 0.1, \kappa_o = 0.05\text{ s}^{-1}, d_{p, \text{top}} = 1000\text{ }\mu\text{m}.$$

$$X_b = 0.82 \text{ from Figure 4.6}$$

$$\begin{aligned} X_{ce} &= 1 - (0.82)(0.6712) \\ &= 0.879 \text{ or } 87.9\%. \end{aligned}$$

Part 2 Conversion of Volatiles in the Bed, X_v , and the
Adiabatic Temperature Jump above the Bed, ΔT

As a base case for these examples take the following values

$$u_o = 2.6 \text{ m/s}$$

$$H = 1.2 \text{ m}$$

$$E_x = 0.1$$

$$X_b = 0.9 \quad (X_{ce} = 0.933)$$

$$L_2 = 0.5642 \quad (\text{One feed port per square meter of the bed} \\ \text{cross-sectional area: } \pi L_2^2 = 1)$$

$$D = 0.01 \text{ m}^2/\text{s} \quad (\text{from reference 27})$$

$$n = 330 \text{ mol air/kg feed coal}$$

$$f_p = 0.2$$

$$V^* = 0.7 f_p = (0.7)(0.2) = 0.14 \text{ m}^3/\text{kg feed coal}$$

$$\Delta H_{vol} = 30341 f_p = (30341)(0.2) = 6068 \text{ kJ/kg feed coal}$$

$$\overline{c_p} = 1.276 \text{ kJ/kg}\cdot\text{K}$$

Thus the maximum possible temperature jump above the bed

$$\begin{aligned} \Delta T_{\max} &= \frac{\Delta H_{vol}}{\overline{c_p} \{0.02896(1+E_x)n+0.9\}} \\ &= \frac{6068}{(1.276)[0.02896(1+0.1)(330)+0.9]} \\ &= 417 \text{ K} \end{aligned}$$

$$\begin{aligned} \text{If } X_v &= 0.5, \quad \Delta T = \Delta T_{\max}(1-X_v) \\ &= (417)(1-0.5) = 209\text{K} \end{aligned}$$

$$\text{value of plume group, } \frac{HD}{u_o L_2^2} = \frac{(1.2)(0.01)}{(2.6)(0.5692)^2} = 1.45 \times 10^{-2}$$

(2.A) No transport air is used, $f_t = 0$.

From equation (3.14)

$$s_0 = \left\{ 1 + \frac{(1+E_x)n(1-f_t)}{\frac{V^*}{0.0224} + (1+E_x)nf_t} \right\}^{-0.5} = \left\{ 1 + \frac{(1+0.1)(330)(1-0)}{\frac{0.14}{0.0224} + (1+0.1)(330)(0)} \right\}^{-0.5}$$

$$= 0.130$$

Thus the radius of the plume at the base

$$L_0 = s_0 L_2 = (0.13)(0.5642) = 0.0734 \text{ m}$$

$$\frac{HD}{u_0 L_2^2} = 1.45 \times 10^{-2}, f_p = 0.2$$

From Figure 4.14 $X_v = 0.54$

From Figure 4.16

$$\Delta T = 190K$$

(2.B) If $E_x = 0.2$ instead of 0.1 (all else the same)

$$s_0 = \left\{ 1 + \frac{(1+0.2)(330)(1-0)}{\frac{0.14}{0.0224} + (1+0.2)(330)(0)} \right\}^{-0.5} = 0.1246$$

$$L_0 = (0.1246)(0.5642) = 0.0703 \text{ m}$$

$$X_v = 0.6 \text{ from Figure 4.15}$$

$$\Delta T = 150K \text{ from Figure 4.16}$$

(2.C) If 10% transport air is used.

$$f_t = 0.1, E_x = 0.1, \frac{HD}{u_o L_2^2} = 1.45 \times 10^{-2}$$

$$s_0 = \left\{ 1 + \frac{(1+0.1)(330)(1-0.1)}{\frac{0.14}{0.0224} + (1+0.1)(330)(0.1)} \right\}^{-0.5} = 0.3395$$

$$L_0 = (0.3395)(0.5642) = 0.1915 \text{ m}$$

$$X_v = 0.86 \text{ from Figure 4.17}$$

$$\Delta T = 60K \text{ from Figure 4.18}$$

(2.D) The number of feed ports are reduced to one feed port for every four square meter bed cross-sectional area. Thus

$$L_2 = 1.128 \text{ m}$$

$$\frac{HD}{u_o L_2^2} = \frac{(1.2)(0.01)}{(2.6)(1.128)^2} = 3.63 \times 10^{-3}$$

If $E_x = 0.1$, $f_t = 0.1$, then $s_0 = 0.3395$ from (2.C)

$$L_0 = (0.3395)(1.128) = 0.383 \text{ m}$$

$$X_v = 0.72 \text{ from Figure 4.17}$$

$$\Delta T = 120K \text{ from Figure 4.18}$$

(2.E) Now the height of the bed is doubled to 2.4m, all else as in the base case.

$$\frac{HD}{u_o L_2^2} = \frac{(2.4)(0.01)}{(2.6)(1.128)^2} = 7.26 \times 10^{-3}$$

$$X_v = 0.77 \text{ from Figure 4.17}$$

$$\Delta T = 90K \text{ from Figure 4.18}$$

For a different type of coal:

$$f_p = 0.424, v^* = 0.25 \text{ m}^3/\text{kg feed coal}$$

$$n = 317 \text{ mol air/kg feed coal}$$

$$(2.F) \text{ If } f_t = 0, E_x = 0.1, \frac{HD}{u_o L_2^2} = 1.45 \times 10^{-2}$$

$$X_v = 0.4 \text{ from Figure 4.9}$$

$$\Delta T = 560\text{K from Figure 4.10}$$

$$(2.G) \text{ If } f_t = 0.2, E_x = 0.1, \frac{HD}{u_o L_2^2} = 1.45 \times 10^{-2}$$

$$\Delta T = 210\text{K from Figure 4.13}$$

Now for incomplete devolatilization in the plume, all else as in (2.F).

$$(2.H) \text{ If } f_t = 0.1, \frac{HD}{u_o L_2^2} = 1.45 \times 10^{-2}, L_2^2 k_D / D_s = 10$$

$$\phi = 0.67 \text{ from Figure 4.19}$$

$$X_v = 0.82 \text{ from Figure 4.20}$$

$$\Delta T = 170\text{K from Figure 4.21}$$

$$(2.I) \text{ If } L_2 \text{ is doubled, all else as in (2.F)}$$

$$\frac{L_2^2 k_D}{D_s} = 40, \frac{HD}{u_o L_2^2} = 3.63 \times 10^{-2}$$

$$\phi = 0.9 \text{ from Figure 4.19}$$

$$X_v = 0.5 \text{ from Figure 4.20}$$

$$\Delta T = 460\text{K from Figure 4.21}$$

Part 3. Sulfur Retention Efficiency

For the calculation of sulfur retention efficiency the following values are chosen as the base case.

$$f_s = 0.04$$

$$f_p = 0.424$$

$$V^* = 0.25 \text{ m}^3/\text{kg coal}$$

$$n = 317 \text{ mol air/kg feed coal}$$

$$H = 1.2 \text{ m}$$

$$u_o = 2.6 \text{ m/s}$$

$$L_2 = 0.5642 \text{ m}$$

$$D = 0.01 \text{ m}^2/\text{s}$$

$$X_b = 0.9$$

$$E_x = 0.1$$

$$f_t = 0$$

(3.A) If $\Psi = 0.5$, $k_s = 4$, $k_H = k_s$ then $k_s \frac{H}{u_o} = (4) \left(\frac{1.2}{2.6} \right) = 1.85$.

$$\overline{\text{SR}} = 0.66 \text{ from Figure 5.6}$$

(3.B) If we apply plumeless models ($k_s \frac{u_o}{H} = 1.85$, $\Psi = 0.5$)

$$\overline{\text{SRI}} = 0.6$$

from Figure 5.3

$$\overline{\text{SRII}} = 0.75$$

(3.C) If k_s and k_H are increased to 8.67.

$$k_s \frac{H}{u_o} = (8.67) \left(\frac{1.2}{2.6} \right) = 4$$

$$\overline{\text{SR}} = 0.84 \text{ from Figure 5.6}$$

(3.D) If H is reduced to 0.6 m, $\frac{HD}{u_o L_2^2} = 0.725 \times 10^{-3}$

and $k_S \frac{H}{u_o} = 2$, $k_H \frac{H}{u_o} = 2$

$\overline{SR} = 0.7$ from Figure 5.6

(3.E) If $\Psi = 0$, i.e. no sulfur devolatilizes in the plume and

$k_S \frac{H}{u_o} = 4$, $\frac{HD}{u_o L_2^2} = 1.45 \times 10^{-2}$

$\overline{SR} = 0.89$ from Figure 5.7

(3.F) $\Psi = 0.5$. But if $k_S = 2.17$, $k_H = 21.7$

$k_S \frac{H}{u_o} = (2.17) \left(\frac{1.2}{2.6} \right) = 1$

$k_H \frac{H}{u_o} = (21.7) \left(\frac{1.2}{2.6} \right) = 10$

Then from Figure 5.9 $\overline{SR} = 0.6$

So far $f_t = 0$ and $f_p = 0.424$. But

(3.G) if $f_t = 0.1$ and $k_S \frac{H}{u_o} = 1$, $k_H \frac{H}{u_o} = 10$, $f_p = 0.424$

$\overline{SR} = 0.56$ from Figure 5.11

(3.H) if $f_t = 0.1$, $k_S \frac{H}{u_o} = 10$, $f_p = 0.2$,

$\overline{SR} = 0.47$ from Figure 5.13

(3.I) Let us now calculate the mol fraction of SO_2 in flue gas for (3.F) using equation (5.9).

$$f_s = 0.04$$

$$\psi = 0.5$$

$$X_b = 0.9$$

$$\overline{\text{SR}} = 0.67$$

$$\begin{aligned} y_{\text{S, flue}} &= \frac{31.2 f_s [1 - (1 - \psi)(1 - X_b)](1 - \overline{\text{SR}})}{n(1 + E_x) + \frac{V^*}{0.0224}} \\ &= \frac{(31.2)(0.04)[1 - (1 - 0.5)(1 - 0.9)](1 - 0.67)}{317(1 + 0.1) + \frac{0.25}{0.0224}} \\ &= 1.087 \times 10^{-3} \quad \text{or} \quad 1087 \text{ ppm} \end{aligned}$$

CHAPTER VII. DISCUSSION AND CONCLUSION OF THE PLUME MODEL

The plume model is developed here to represent large utility scale AFBCs with large particles in which air-entrained coal enters in a number of feed ports. It assumes that the volatiles are rapidly released from the coal at the feed ports to rise as plumes of combustible vapors.

Calculations show that there is little difference between the plume model and "plumeless model" in the prediction of carbon efficiency of the combustor. This enables us to use the plumeless model, which is much easier to use, for the calculation of carbon efficiency of the combustor. Graphs have been prepared (Figure 4.2-4.4) to display the predictions of this model for narrow size cuts of a typical coal feed (Table 4.1). For a given coal feed, the carbon efficiency depends only on the superficial gas velocity in the bed, the excess air and the elutriation rate constant. These figures show that the lowest carbon conversion always comes with an intermediate size of feed coal.

A logarithmic size distribution is picked to illustrate char conversion for a feed of wide size distribution (Figure 4.5 to 4.7). Low conversion with an intermediate top particle size, $d_{p, \text{top}}$, means that this feed has much coal particles of intermediate size with lowest conversion. Also, the shape of curves can be different if the feed coal size distribution is quite different from logarithmic. However, conversion of char can be predicted for a feed of any size distribution by solving equations (3.1), (3.2), (3.3) and (4.1)

for each slice of the size distribution.

All aspects of plume behavior, whether it breaks the surface of the bed, the temperature jump above the bed, concentration variation across the bed, etc. are all governed by the dimensionless group, $HD/u_0 L_2^2$, which accounts primarily for the spacing of feed ports in the bed (Figure 4.8 to 4.21). As an example Figure 4.7 shows the doubling the distance between feed ports lowers the conversion of volatiles in the bed from 90% to about 50%.

The effect of transport air on the adiabatic temperature jump in the freeboard is shown in Figure 4.13. Thus, one can see that the transport air reduces temperature jump in the freeboard.

So far all the calculations and graphs are for one type of coal (Table 1). Figures 4.14 to 4.18 generalize these predictions for the different types of coal, the main factor in characterizing coal type being the ratio of oxygen needed for the combustion of volatiles in the plume to that for total coal combustion, f_p .

Now for large particles not all the volatiles may be released while the coal particles remain in the plume. Figure 4.19 shows the fraction of volatiles released in the plume for the simplified situation: first order kinetics for the devolatilization and simple two dimensional diffusion for the dispersion of feed coal particles. This figure shows the spacing between the feed ports is a very important factor. Figure 4.20 and Figure 4.21 show the conversion of volatiles in the bed and the temperature jump above the bed for incomplete devolatilization in the plume. Examining Figures 4.13, 4.16, 4.18 and 4.21 we see that the effect of transport air, the

ratio of oxygen needed for the combustion of volatiles in the plume to that for total coal combustion and the fraction of volatiles released in the plume is similar. Notice that all these three factors f_t , f_p and ϕ are a measure of how rich or how lean the plume is in combustibles. Also notice that the conversion of volatiles in Figure 4.20 does not follow constant ϕ lines when we change the spacing between the feed ports, in the case of incomplete devolatilization in the plume. Increase in the spacing increases the fraction of volatiles released in the plume.

Figures 5.2 to 5.5 show sulfur retention efficiency for the two different plumeless models. The plumeless model I is for the case where volatiles are released uniformly throughout the bed and plumeless model II is for the case where all the volatiles are released at the bottom of the bed. Figures show that the plumeless model II always gives higher sulfur retention efficiency because more time is available for sulfur to react with limestone particles in the bed. Plumeless model I is the limit when devolatilization is much slower than the dispersion of feed coal, and plumeless model II represents the extreme where there are an infinite number of feed ports while devolatilization is still infinitely fast.

Now for the plume model typical concentration profiles of sulfur dioxide and hydrogen sulfide are shown in Figure 5.5. In order to calculate sulfur retention efficiency we need two different kinds of kinetics data: reaction of limestone particles with sulfur dioxide AND hydrogen sulfide. Figures 5.6 to 5.13 show that sulfur retention efficiency depends on the dimensionless group, $HD/u_o L_2^2$.

more or less. This means that the sulfur retention efficiency depends on the conversion level of volatiles in the bed. One other factor is the fraction of sulfur which is released during devolatilization of coal. Although this effect on sulfur retention efficiency is not dramatic (Figures 5.3, 5.4 and 5.7) it has to be considered in the modeling.

Figures 5.7 to 5.9 demonstrate the dominant effect of the reactivity of limestone on the sulfur retention efficiency. But the effect of transport air and the ratio of oxygen needed for the combustion of volatiles in the plume to that for total coal combustion on the sulfur retention efficiency also cannot be ignored. We see that at high conversion level of volatiles in the bed the effect of these two parameters diminish. All these lead to the importance of relative magnitude of hydrogen sulfide concentration in the plume coupled with the reactivity of limestone with hydrogen sulfide compared to the sulfur dioxide concentration coupled with the reactivity of limestone with sulfur dioxide. Thus if hydrogen sulfide concentration is high in the plume at the bottom of the bed and the reactivity of limestone with it is high but not with sulfur dioxide, the existence of plumes in the bed enhances the sulfur retention efficiency. But if conversion of volatiles in the bed is high a large fraction of hydrogen sulfide is converted to sulfur dioxide at the plume boundary thus reducing the role of hydrogen sulfide reaction with limestone.

But if the reactivity of limestone is low with hydrogen sulfide compared with sulfur dioxide or only a small fraction of sulfur in

the feed coal devolatilizes the existence of plumes in the bed does not help sulfur retention in the bed by much. Introduction of transport air lowers hydrogen sulfide concentration in the plume at the bottom of the bed thus contributes negatively to the sulfur retention.

The unique feature of the plume model is that it naturally explains that there exist radial variations of gas concentration in the bed. Models published in the literature in the past are one dimensional: they consider only the vertical variation or radial variation only. But the plume model gives a three dimensional picture of the bed using cylindrical coordinate. The plume model also implies that there are regions in the bed which are in a reducing environment, that these plumes are devoid of oxygen, are not stationary but fluctuate like the plumes from smoke stacks.

The plume model also predicts a temperature jump above the bed which rises with increasing spacing of feed ports. This was indeed observed in the Babcock and Wilcox pilot plant studies.

For the sulfur retention efficiency the plume model tells us the importance of the devolatilization of sulfur and its subsequent behavior.

CONCLUSIONS OF THE PLUME MODEL

- For the prediction of carbon efficiency the plumeless model can be used instead of the plume model.
- The plume model has to be used to predict temperature jump above the bed and to know the extent of reducing zone in the bed.
- The spacing between feed ports and the amount of volatiles released from feed coal are the dominant factors determining the conversion of volatiles in the bed.
- The plume model has to be used for the prediction of sulfur retention efficiency.
- The devolatilization of sulfur and the reaction of H_2S with limestone are important factors in the sulfur retention.

APPENDIX A. Numerical Solution for Partial Differential Equations in the Plume Model

The plume model has three partial differential equations:

- equation (3.13) for oxygen and combustible volatiles,
- equation (5.6) for hydrogen sulfide, and
- equation (5.7) for sulfur dioxide.

We have to solve equation (3.13) first because we need information on the concentration of oxygen and the location of plume boundary to solve equation (5.6) and (5.7) for the calculation of sulfur retention efficiency.

The Crank-Nicolson Method is used for the finite difference approximation of partial differential equations:

$$\frac{\partial y}{\partial z} \doteq \frac{1}{\Delta z} (y_{i,j+1} - y_{i,j})$$

$$\frac{\partial^2 y}{\partial \hat{r}^2} \doteq \frac{1}{2(\Delta \hat{r})^2} (y_{i+1,j+1} - 2y_{i,j+1} + y_{i-1,j+1} + y_{i+1,j} - 2y_{i,j} + y_{i-1,j})$$

$$\frac{\partial y}{\partial \hat{r} \partial \hat{r}} \doteq \frac{1}{4(\Delta \hat{r})^2 (i-1)} (y_{i+1,j+1} - y_{i-1,j+1} + y_{i+1,j} - y_{i-1,j})$$

$$y \doteq \frac{1}{2} (y_{i,j+1} + y_{i,j})$$

Substituting these approximations into equations (3.13), (5.6), (5.7) and boundary conditions we obtain a tridiagonal matrices which relate $y_{i,j+1}$ to $y_{i,j}$. Figure A.1 shows the flow chart for the calculation procedure and Figure A.2 shows the Fortran code.

Figure A1. Flow chart for the calculation of the plume model.

```

C
PROGRAM CONSUL INPUT, OUTPUT, IAF6=OUTPUT, IAIT5=INPUT)
COMMON/RESUL/S,XVOL,XOXY,XCOAL,K1,K2,R1,R2,KLM,SPR
COMMON/PROP/COALM,VOLAT,F1,F2,F3,EXA,FL,5X0,FXS
5 COMMON/FFF/F(260),N,N,HOUR,XK0,XK2,XK3,VIN,OXIN,MM,KK,DR
DATA R1,N/0.1,998/
DATA FL,F1,R1,N/1.0,0.5759,0.1,998/
READ(5,555)F2,COALM,VOLAT,EXA
555 FORMAT(IX,4F10.4)
10 1 READ(5,60)M;F3,5X0,FXS
IF(N.LE.1)GO TO 79
CALL INITI
2 READ(5,65)HOUR,XK0
IF(XK0.LE.0.0)GO TO 1
15 READ(5,70)XK2,XK3
3 CALL HAERA
GO TO 2
60 FORMAT(IX,I3,3F10.4)
65 FORMAT(IX,2F10.4)
20 70 FORMAT(2E10.4)
99 STOP
END

C
SUBROUTINE INITI
COMMON/FFF/F(260),N,N,HOUR,XK0,XK2,XK3,VIN,OXIN,MM,KK,DR
COMMON/TRANS/K20,R20,VS(260),XS(260),FS(260),DRR,XVOL0
5 COMMON/PROP/COALM,VOLAT,F1,F2,F3,EXA,FL,5X0,FXS
COMMON/RESUL/S,XVOL,XOXY,XCOAL,K1,K2,R1,R2,KLM,SPR
COMMON/ENL/FHS,S4,ASO2,AHS,RSO2,RSVOL,SM4
EXN=(1.0+EXA)*COALM
MM=N-1
10 DR=1.0/FLOAT(MM)
DR0=1.0+DR
DRDR=DR+DR
C LOCATION OF S0
XVOL=(1.0+EXA)*F3/((1.0-F2)*F1)
15 IF(XVOL.GE.1.0)GO TO 99
A1=VOLAT*FL/22.4*EXN*F3
S=(1.0+EXN*(1.0-F3)/A1)*(1.0-F2)
CNU=COALM*FL*(1.0-F2)*0.21*(1.0-XVOL)/A1
XVOL=PL+XVOL

20 C
XVOL0=XVOL
CNU0=CNU
K1=FIX(S+DR0)
K2=K1+1
IF(K2.GE.N)RETURN
K20=K2
RR=0.015
RC=1.0/RR
DO 10 I=1,N
30 F(I)=0.5/FLOAT(I-1)
XS(I)=0.0
FS(I)=0.0
RR=FLOAT(I-1)*RR
IF(RP.GT.S-RR)GO TO 2
35 VS(I)=CNU0
GO TO 10
2 IF(RR.GT.S)GO TO 3
VS(I)=(RR-(S-RR))*RC
VS(I)=CNU0*(1.0-VS(I)+VS(I))
GO TO 10
40 3 IF(RP.GT.S+RR)GO TO 5
VS(I)=(RR-(S+RR))*RC
VS(I)=0.21*(1.0-VS(I)+VS(I))
GO TO 10
45 5 VS(I)=0.21
10 CONTINUE
SX=S+DR0
R2=SX-FLOAT(K1)
IF(R2.LT.1.0E-10)R2=1.0E-10
50 IF(1.0-R2.LT.1.0E-10)R2=1.0-1.0E-10
R20=R2
KK=K1+2
VOL=0.0
DO 20 I=2,K1
55 20 VOL=VOL+VS(I)*FLOAT(I-1)
VOL=VOL+VOL+VS(K2)*(FLOAT(K1)+R2*(FLOAT(K1)+0.5+R2))
C
VIN=S+S*CNU0/(DRDR*(PL-XVOL))
OXIN=(1.0-S*S)*0.21/(DRDR*(1.0-F3))
FACT1=VIN*(PL-XVOL)/VOL
40 OXY=0.0
FE2=KK+1
DO 30 I=K2,M
30 OXY=OXY+VS(I)*FLOAT(I-1)

```

Figure A2. Fortran code for equations (3.13), (5.6) and (5.7).

```

65   OXY=OXY+OXY-VS(M)+FLOAT(MM)+VS(MK)+(FLOAT(K2)+C1.0-
    * R2)+(FLOAT(K2)-3.5*(C1.0-R2))
    VOL=0.0
    FACT2=OXY*(1.0-F3)*OXY
70   35  VS(1)=VS(1)+FACT1
    DO 40 I=KK,M
    40  VS(1)=VS(1)+FACT2
    WRITE(6,101)COALM,VOLAT,F1,F2,F3,PL,M,FXB,XVOL,ENH,FACT1
101  FORMAT(1X,*,COALM,VOLAT,F1,F2,F3,PL,*,4F8.4,2F6.2/1X,15,4
    >>> E11.4)
75   IF(XVOL.GE.1.0)RETURN
    S4=32.06*(EXM+VOLAT*PL/22.4)/SX0
    RS02=SX0*FIXS*0.14853/(COALM*F2)
    RSVOL=SX0*(1.0-FIXS)+0.14853/(COALM*(1.0-F2))
80   SH4=32.06*EXM/SX0
    YHS=(1.0-FIXS)*SX0*(1.0-XVOL)/(32.06*A1)
    YS02=(1.0-FIXS)*SX0*XVOL/(32.06*A1)
    YHS1=FACT1*YHS
    DO 510 I=1,K2
    510  XS(I)=YS02
    RR=FLOAT(1-I)*DZ
    IF(RR.GT.5-RR)GO TO 505
    ES(I)=YHS1
    GO TO 510
90   505  TPR=(RR-(5-RR))*R2
    TPR=1.0-TPR+TPR
    ES(I)=YHS1+TPR
    510  CONTINUE
    FHS=YHS+S*S
95   WRITE(6,690)YHS,YS02,SX0,FIXS
690  FORMAT(1X,*,YHS,YS02,SX0,FIXS,*,4F11.4)
    RETURN
99  WRITE(6,199)
199  FORMAT(1X,*,NO COMBUSTIBLE IN THE FLAME)
104  RETURN
    END

```

```

C   SUBROUTINE IMERA
    COMMON/EROP/COALM,VOLAT,F1,F2,F3,EXA,PL,SX0,FIXS
    COMMON/VUXY/U(260),V(260),X(260),E(260)
5   COMMON/FFF/F(260),N,M,HDUR,YK0,YK2,XK3,VIN,OXIN,MN,KX,DR
    COMMON/RESUL/S,XVOL,XOXY,XCOAL,K1,K2,R1,R2,KLM,SRR
    COMMON/PQS/F,90,Q1,Q2,R3,HP
    COMMON/SUL/FHS,S4,AS02,AHS,RS02,RSVOL,SN4
    COMMON/TRANS/R20,R20,VS(260),XS(260),ES(260),DRDR,XVOLD
10  IF(XVOLD.GE.1.0)RETURN
    RDH=HDUR/DRDR
    DZ=0.4704*DEFDR/SORT(HDUR)
    K2=K20
    R2=R20
15  K1=K2
    DO 190 I=1,M
    V(I)=VS(I)
    F(I)=ES(I)
190  X(I)=XS(I)
    X(M+1)=0.0
20  CSTAR=0.0
    KLM=0
    ZZ=0.0
    VOUNT=0
25  DO 410 J=7,N
    ZOLD=ZZ
    ZZ=ZZ+DZ
    IF(ZZ.LE.1.0)GO TO 44
    DZ=1.0-ZOLD
    ZZ=1.0
30  44  P=DZ*RDH
    HP=0.5*P
    GO=XK0+DZ
    CALL PCRA
35  CALL TRIPAG(-1,H)
    CALL CONCUM
    IF(KLM.LE.0)GO TO 55
    IF(VLN.GT.5)GO TO 755
    DZ=DZ/ARG(SRR1)
    ZZ=ZOLD+DZ
    GO TO 44
55  CSTAR=CSTAR+DZ*XOXY

```

```

45      IF(K2.LY.1)GO TO 555
      IF(K2.EQ.K1)KOUNT=KOUNT+1
      IF(K2.NE.K1)KOUNT=0
555     R1=RSO2*OD
          D2=XK2*OZ
          R5=XK3*OZ
50      CALL SULFU(1)
          IF(XCOAL.GE.1.0)GO TO 11
          IF(Z7.GE.1.0)GO TO 11
          IF(K2.GT.2)GO TO 57
          DZ=DZ+DZ+DZ+DZ
55      GO TO 9
57      IF(KOUNT.1.1.2)GO TO 7
          KOUNT=0
          DZ=1.5*OZ
          GO TO 9
60      7 IF(K2.GT.K1)GO TO 8
          DZ=DZ+(1.0-2.0/FLOAT(K2-K1+3))
          GO TO 410
          8 DZ=DZ+(1.0-2.0/FLOAT(K2-K1+1))
          9 IF(DZ.GT.0.025) DZ=0.025
65      410 CONTINUE
          11 JEND=J
          ZFIN=ZZ
          CSTAR=CSTAR/ZFIN
          CSTAR=0.21*(1.0-CSTAR)
          CEFF=1.0-(1.0-XCOAL)*F1
          DEX=0.21*(EXA+F2*(1.0-XCOAL))/(1.0*EXA)
          WRITE(6,100)JEND,ZFIN,S,CSTAR,DEX,HTMR
100     FORMAT(/2X,15,2F8.4,2F11.4,3X,E11.4)
          WRITE(6,202)XVOL,XCOAL,XOXY,CEFF
75     202 FORMAT(5X,4E12.4)
          CALL SULCON
          XHS=1.0-AHS+DRDR/THS
          ASO2=ASO2+DRDR
          S21=FIXS*(1.0-XCOAL)
          S11=(1.0-FIXS)*(1.0-XVOL)+(1.0-XHS)
          S41=S4+ASO2
          SSS=ASO2/S41
          XSA=1.0-(S31+S41)
          XSR=1.0-(S31+S41)/(1.0-S21)
          SFLUE=(1.0+S31/S41)*ASO2
85     WRITE(6,647)XSA,XSR,SFLUE,XHS,ASO2,SSS
647     FORMAT(1X,3E11.4,3X,1E11.4)

```

```

          XKV=0.21*(1.0-F2)/(1.0*EXA)
          OOUT=0.21*(F2*(1.0-XCOAL)+EXA)/(1.0*EXA)
90      CALL XKSEA(XKV,OOUT,XKN)
          IF(XK2.GT.0.0)GO TO 650
          ASON=RSO2*(0.21*XKV/XKN)+(1.0-EXP(-XKN))*(RVOL-RSO2)
          *XKV
          GO TO 653
          650 XK2=XK2*XK2
          95 AAA=RSO2*XKN*(0.21*XKV/XKN)/(XK2-XKN)
          RRR=(RVOL-RSO2)*XKV/XK2
          ASON=-(AAA+RRR)*EXP(-XK2)+RRR+AAA*EXP(-XKN)
          653 S41=ASON+SN4
          SSS=ASON/S41
          100 XSA=1.0-(S41+S21)
          XSR=1.0-S41/(1.0-S21)
          B1=0.21*(F2*EXA)/(1.0*EXA)
          R2=SKD*(1.0-FIXS)/(32.06*COALN*(1.0*EXA))
          XKN=ALOG((EXA+F2)/(EXA+F2*(1.0-XCOAL)))
          105 S41=RSO2*XKN+R1/(XK2-XKN)
          S41=S41*EXP(-XKN)+(R2-S41)*EXP(-XK2)
          S41=S41+SN4
          XSC=1.0-S41/(1.0-S21)
          WRITE(6,657)XSA,XSR,ASON,SSS,XSC
          110 657 FORMAT(3X,4E11.4,3X,E11.4)
          RETURN
          755 WRITE(6,777)J,SBR
          777 FORMAT(/3X,*J,5HR*,2F11.4)
          RETURN
          115 END

```

```

SUBROUTINE TRIDAG(TCON,MK)
COMMON/ABCD/A(260),R(260),C(260),U(260)
COMMON/VUXY/V(260),W(260),X(260),E(260)
DIMENSION BETA(260),T(260),GAN(260)
5  BETA(1)=R(1)
   GAN(1)=D(1)/BETA(1)
   DO 10 I=2,MK
     BETA(I)=R(I)-A(I)*C(I-1)/BETA(I-1)
10  GAN(I)=(D(I)-A(I)*GAN(I-1))/BETA(I)
   T(MK)=GAN(MK)
   MM=MK-1
   DO 20 J=1,MM
     I=MM-J
20  T(I)=GAN(I)-C(I)*T(I+1)/BETA(I)
   IF(TCON)1,3,2
   1 DO 30 I=1,MK
     V(I)=T(I)
     RETURN
   2 DO 40 I=1,MK
     X(I)=T(I)
     RETURN
   3 DO 50 I=1,MK
     E(I)=T(I)
50  RETURN
25  END

```

```

SUBROUTINE DCRA
COMMON/PDS/P,QQ,Q1,Q2,RS,HP
COMMON/RESUL/S,XVOL,XOXY,XCOAL,K1,K2,R1,R2,KLM,SRR
COMMON/FFF/F(260),M,M,HDUR,XK0,XK2,XK3,VIN,OXIN,MM,KK,DR
COMMON/ABCD/A(260),R(260),C(260),D(260)
COMMON/VUXY/V(260),W(260),X(260),E(260)
IF(KLM.NE.0)GO TO 3
DO 2 I=1,M
10 2  W(I)=V(I)
   3  C(I)=-P-P
   R(I)=1.0*P*P
   B(I)=W(I)+(P+P)*(U(2)-U(1))
   DO 33 I=2,MM
     A(I)=HP*(F(I)-1.0)
15  R(I)=1.0*P
     C(I)=-A(I)-P
33  D(I)=W(I)+HP*(U(I+1)-U(I))
   U(I)=U(I-1)+C(I)*B(I+1)-U(I-1)
25  11)

```

```

A(M)=-P
20  B(M)=1.0*P
   D(M)=W(M)+P*(U(M-1)-U(M))
   JS=KK
   IF(K1.GT.K2)JS=K1+1
   DO 35 I=JS,M
     R(I)=B(I)+QQ
25  D(I)=D(I)-QQ*W(I)
   RETURN
END

```

```

C
SUBROUTINE CONCOM
COMMON/VUXY/V(260),W(260),X(260),E(260)
COMMON/RESUL/S,XVOL,XOXY,XCOAL,K1,K2,R1,R2,KLM,SRR
5  COMMON/FFF/F(260),M,M,HDUR,XK0,XK2,XK3,VIN,OXIN,MM,KK,DR
COMMON/FROP/COALM,VOLAT,F1,F2,F3,EXA,PL,SXO,FI,XS
OXY=0.0
IF(K1.LT.1)GO TO 70
DO 10 I=1,M
10  IF(V(I).GE.0.0)GO TO 11
   IP=M
   WRITE(6,100)
100  FORMAT(/IX,*S=1.0*)
   RETURN
15  11 IP=I-1
   IF(IP.LE.0)GO TO 12
   FPR=V(IP)/(V(IP+1)-V(IP))
12  IF(IAPS(K2-IP).LT.2)GO TO 20
   IF(K2.LE.2)GO TO 20
   KLM=KLM+1
   SRR=FLOAT(IP-K2)
   RETURN
20  K1=K2
   K2=IP
   R1=R2
25  IF(K2.LT.2)GO TO 70
   R2= FOR
   S=(FLOAF(K2-1)+R2)*DP
   IF(R2.LT.1.0E-10)R2=1.0E-10
   IF(1.0-R2).LT.1.0E-10)R2=1.0-1.0E-10
   VOL=0.0
30  IF(IP.LE.2)GO TO 77

```



```

      IIP=IP-1
      DO 25 I=2,IIP
35    25 VOL=VOL+V(I)*FLOAT(I-1)
      VOL=VOL+VOL+V(IP)*(FLOAT(IIP)+R2*(FLOAT(IIP)+0.5+R2))
      XVOL=1.0-VOL/VIN
      KK=IP+1
      IF2=IP+2
40    DO 30 I=IF2,M
      30 OXY=OXY+V(I)*FLOAT(I-1)
      OXY=OXY+OXY-V(M)*FLOAT(M-1)+V(KK)*(FLOAT(IP)+(1.0
      *FPR)*(FLOAT(IP)-0.5*(1.0-R2)))
      GO TO 77
45    70 XVOL=1.0
      S=0.0
      K2=0
      R2=0.0
      35 DO 76 I=2,M
      76 OXY=OXY+V(I)*FLOAT(I-1)
      OXY=OXY+OXY-V(M)*FLOAT(M-1)
      77 XOXY=1.0-OXY/OXIN
      XCOAL=(XOXY*(1.0+ETA)-(1.0-F2)+XVOM)/F2
      KLM=0
55    RETURN
      END

```

```

      SUBROUTINE XKSEA(A,R,YKH)
      F(X)=ALOG(10.21+A/X)/(R+A/X)
      X1=1.0
      Y1=F(X1)
5    Y2=Y1
      Y2=F(X2)
      DO 10 J=1,20
      X1=(X1+Y2-X2+Y1)/(X1-X2+Y2-Y1)
      Y1=F(X1)
10    IF(ABS(X1/Y1-1.0).LT.0.001)GO TO 11
      X1=X2
      Y1=Y2
      X2=X1
10    Y2=Y1
15    WRITE(6,100)
100  FORMAT(1X,'X1,Y1,NOT CONVERGED')
11    XKH=Y1
      RETURN
      END

```

```

      SUBROUTINE SIFU(J)
      COMMON/RESUL/S,XVOL,XOXY,XCOAL,K1,K2,R1,R2,KLM,SRR
      COMMON/FFF/F(260),N,N,HOUR,XK0,XK2,XK3,VIN,OXIN,MH,KK,DR
      COMMON/VUXY/V(260),U(260),X(260),E(260)
      COMMON/FOS/P,00,01,02,R5,RP
      COMMON/CS12/C1,C2,C3,C4,C5,C6,C7,C8,61,62,63,64,65,H1,H2

```

```

1    H3,H4,H5,NCON
      MK=M
      IF(K1.LE.1)GO TO 9
      IF(K2.GE.2)MK=MK+1
      G1=1.0-R1
      G2=1.0/G1
      G3=1.0/(1.0+R1)
      G4=1.0/(2.0-R1)
      G5=1.0/R1
      IF(K2.LE.1)GO TO 9
      H1=1.0-R2
      H2=1.0/H1
      H3=1.0/(1.0+R2)
      H4=1.0/(2.0-R2)
      H5=1.0/R2
      C1=P+H3*(R2+F(K2)-1.0)
      C2=P+H4+H2*(F(KK)-1.0)
25    C3=1.0+P+R5
      C4=1.0+H3+P*(1.0+H5+F(K2)+(H5-R2))
      C6=1.0+P+H4*(1.0+H2+F(KK)+(H1-H2))
      C7=-H5+P+H3*(1.0+F(K2))
      C8=-H4+P*(1.0+F(KK)+H1)
      IF(K2-K1)1,2,3
30    1 NCON=-1
      GO TO 9
      2 NCON=0
      GO TO 9
      3 NCON=1
      9 C5=1.0+P+R2
      IF(K2.LT.2)GO TO 70
      CALL COEFF(J,0)
      CALL TRIDAG(0,K2)
40    IF(K2.GE.K1)GO TO 70
      JS=KK
      DO 60 I=JS,K1
      60 F(I)=0.0
      70 CALL COEFF(I,1)
      CALL TRIDAG(I,MK)
45    RETURN
      END

```

```

SUBROUTINE COEFF(J,NAP)
COMMON/ARCB/A(260),B(260),C(260),D(260)
COMMON/VUXY/V(260),U(260),X(260),E(260)
5 COMMON/CS12/C1,C2,C3,C4,C5,C6,C7,C8,C1,C2,R1,R2,C3,C4,C5,H1,H2

1 H3,H4,H5,NCON
COMMON/POS/P,00,01,02,05,HP
COMMON/FFF/F(260),M,N,IMUR,XK0,XK2,XK3,VIN,OXIN,MH,KK,DR
COMMON/RESUL/S,XV0,XDX,XCOA1,K1,K2,R1,R2,RLM,SR
10 IF(NAP.GT.0)GO TO 90
C 0 - H2S 1 - S02
R(1)=C3*P
D(1)=(P+P)*E(2)+(1.0-P-PS)*F(1)
IF(K2.LE.2)GO TO 15
15 JE=K2-1
DO 10 I=2,JE
A(I)=HP*(F(I)-1.0)
B(I)=C3
C(I)=-A(I)-P
20 10 D(I)=1/2,I)
IF(NCON.LT.1)GO TO 15
D(K1)=(1.0-PS)*E(K1)+P*G3+(-E(V1)+G5-E(K1)+E(K1-1)+
1 F(K1)+(R1+(E(K1)-E(K1-1))-E(K1)+G5))
15 A(K2)=C
B(K2)=C4*PS
IF(NCON)20,30,40
30 D(K2)=(1.0-PS)*E(K2)+G3*P+(-E(K2)+G5-F(H2)+E(K2-1)+
1 P(K2)+(R1+(E(K2)-E(K2-1))-E(K2)+G5))
RETURN
40 D(K2)=0.0
RETURN
20 D(K2)=1/2,K2)
RETURN
C
35 90 IF(K2.GT.1)GO TO 300
IF(K1.GT.1)GO TO 200
B(1)=CS*P
D(1)=X(1)+(F(1)+X(2)-X(1))*T(4,1)
DO 110 I=2,MH
40 A(I)=HP*(F(I)-1.0)
B(I)=C5
C(I)=-A(I)-P
110 D(I)=T(3,I)+T(4,1)

```

```

D(N)=T(9,N)+T(4,N)
45 GO TO 290
C
200 R(1)=1.0
C(1)=0.0
D(1)=X(1)
50 A(2)=-HP*G3
B(2)=1.0+(P+P)*G3
C(2)=-P*(P+P)*G3
D(2)=X(1)
DO 210 I=3,MH
55 A(I)=HP*(F(I)-1.0)
B(I)=C5
C(I)=-A(I)-P
210 D(I)=T(7,I+1)+T(5,I+1)
D(N)=T(9,N+1)+T(5,N+1)
60 290 A(N)=-P
B(N)=C5
RETURN
C
300 R(1)=1.0+P*P
D(1)=X(1)+(P+P)*X(2)-X(1)
65 IF(K2.LT.3)GO TO 320
JE=K2-1
IF(NCON.EQ.1)JE=K2-2
IF(JE.LT.2)GO TO 320
70 DO 310 I=2,JE
A(I)=HP*(F(I)-1.0)
B(I)=1.0*P
C(I)=-A(I)-P
310 D(I)=T(3,I)
75 320 IF(NCON.EQ.1)GO TO 321
A(K2)=P*(R2+R2)*F(K2)-1.0)/(1.0+R2+R2)
B(K2)=1.0*P*(1.0+H5+F(K2)+(H5-R2-R2))/(1.0+R2+R2)
C(K2)=-H5*P*(1.0+F(K2))/(1.0+R2+R2)
321 A(KK)=-H5
ALP=1.0+0.5/(FLOAT(K2-1)+0.5+R2)
ALP=ALP*ALP
B(KK)=H5+H2*ALP
C(KK)=-H2*ALP
D(KK)=H5+E(K2)
85 IF(NCON.LT.0)GO TO 500
A(K2+2)=P*(F(KK)-1.0)+H2/(3.0-R2-R2)
B(K2+2)=1.0*P*(1.0+H2+F(KK)+(H1+H1-H2))/(3.0-R2-R2)
C(K2+2)=-P*(1.0+F(KK)+(H1+H1))/(3.0-R2-R2)
IF(NCON)500,330,400

```

```

90 330 D(K2)=X(K2)+F/(1.0+R1+R1)*((X(KK)-X(K2))*G5-X(K2)+X(K2-1
    ))
    1 +F(K2)*((X(K2)-X(K2-1))*R1+R1)+(X(KK)-X(K2))*G5))
    D(K2+2)=T(6,K2+2)+T(5,K2+2)
335 JS=K2+3
340 IF(JS.E1.N)GO TO 900
95 DO 350 I=JS,N
    A(I)=HP*(F(I-1)-1.0)
    R(I)=C5
    C(I)=-P-A(I)
350 D(I)=T(7,I)+T(5,I)
100 GO TO 900
C
400 A(K2-1)=T(1,K2-1)
    R(K2-1)=1.0+P
    C(K2-1)=-A(K2-1)*P
105 D(K2-1)=X(K2-1)+F/(1.0+R1+R1)*((X(K2)-X(K2-1))*G5-X(K2-1
    ))+X(K2-2)
    1 +F(K2-1)*((X(K2-1)-X(K2-2))*R1+R1)+(X(K2)-X(K2-1))*G
    5))
    D(K2+2)=T(7,K2+2)+T(5,K2+2)
    TR1=G1/(G1+R2)
    IF(J.E0.2)TR1=0.0
110 TR2=1.0-TR1
    A(K2)=(TR2+TR2)*F+(TR2+R2)*F(K2)-1.0)/(1.0+R2+R2)
    C(K2)=(TR2+TR2)*(-H5)+F*(1.0+P(K2))/(1.0+P2+R2)-TR1
    R(K2)=1.0+P/(1.0+R2+R2)*(TR2+TR2)+(1.0+H5+F(K2))*H5-R2
    ))
    D(K2)=TR2*X(K2)
115 GO TO 335
C
500 D(K2)=T(3,K2)
    TR2=H1/(R1+H1)
    TR1=1.0-TR2
120 A(K2+2)=(TR2+TR2)*P*(F(KK)-1.0)+H2/(3.0-R2-R2)
    R(K2+2)=1.0-TR1+P/(3.0-R2-R2)*(TR2+TR2)+(1.0+H2+F(KK))*
    ))
    H1+H1-H2))
    C(K2+2)=(TR2+TR2)*(-P)*(1.0+F(KK)*(H1+H1))/(3.0-P2-R2)
    D(K2+2)=TR2*X(K1+1)
    A(K1+2)=T(1,K1+1)
125 R(K1+2)=C5
    C(K1+2)=-A(K1+2)-P
    D(K1+2)=T(6,K1+2)+T(5,K1+2)
    JS=K1+3
    GO TO 340

```

```

130 900 A(H+1)=-P
    R(H+1)=C5
    D(H+1)=T(9,H+1)+T(5,H+1)
    RETURN
END

C
FUNCTION T(I,J)
COMMON/VVXY/V(260),U(260),X(260),E(260)
COMMON/CS12/C1,C2,C3,C4,C5,C6,C7,C8,G1,G2,G3,G4,G5,H1,H2
    ))
5 1 H3,H4,H5,NCON
COMMON/PNS/P,00,01,02,05,HP
COMMON/FFF/F(260),M,N,HDIR,XK0,XK2,XK3,UTN,OXIN,MN,KK,DR
COMMON/RESUL/S,XVOL,XOXY,XCOAL,K1,K2,R1,R2,K1N,SRR
GO TO 11,2,3,4,5,6,7,8,9),1
10 1 T=HP*(F(J)-1.0)
    RETURN
2 T=(1.0-BS)*E(J)+HP*(E(J+1)-E(J)-E(J)+E(J-1)+F(J)+E(J+1)
    1 -E(J-1)))
    RETURN
15 3 T=X(J)+HP*(X(J+1)-X(J)-X(J)+X(J-1)+F(J)+(X(J+1)-X(J-1)))
    RETURN
4 T=D1*(V(J)+U(J))-02*X(J)
    RETURN
5 T=D1*(V(J-1)+U(J-1))-02*X(J)
20 RETURN
6 T=X(J)+P*(X(J+1)-X(J)-(X(J)-X(J-1))*02+F(J-1)+(2.0
    1 -R1-R1)*(X(J+1)-X(J))+(X(J)-X(J-1))*02))/(3.0-R1-R1)
    RETURN
7 T=X(J)+HP*(X(J+1)-X(J)-X(J)+X(J-1)+F(J-1)+(X(J+1)-X(J-1)
    ))
25 RETURN
8 T=X(J)+P/(1.0+R1+R1)*((X(J+1)-X(J))+G5-(X(J)-X(J-1))
    1 +F(J))*((X(J+1)-X(J))+G5*(X(J)-X(J-1))*(R1+R1)))
    RETURN
9 T=X(J)+X(J-1)-X(J)*P
30 RETURN
END

```

```

      SUBROUTINE SULCON
      COMMON/SUL/FHS,S4,AS02,AHS,R02,R0VOL,SN4
      COMMON/EFF/F(260),M,N,HDP,R,XI0,XK2,XK3,V0N,0XT0,MH,KK,DR
5     COMMON/UXY/V(260),U(260),X(260),F(260)
      COMMON/RESUL/S,XVOL,XOXY,XCOAL,K1,K2,R1,R2,R1M,SRR
      AHS=0.0
      AS02=0.0
      IF(R2.LE.1)GO TO 103
10    DO 537 I=2,K2
      537  AHS=AHS+E(I)*FLOAT(I-1)
      AHS=AHS-AHS-E(K2)*FLOAT(K2-1)*(1.0-R2)
      DO 520 I=2,K2
      520  AS02=AS02+X(I)*FLOAT(I-1)
15    XI=X(K2)*(1.0-R2)+X(K2-2)*R2
      AS02=AS02+AS02*(FLOAT(K2-1)+R2)+X(KK)-XI)*R2
      I
      +X(KK)-XI)*(1.0-R2))
      RSUM=0.0
      JS=K2+2
20    JE=N+1
      DO 530 I=JS,JE
      530  RSUM=RSUM+X(I)*FLOAT(I-1)
      AS02=RSUM+RSUM+AS02-X(N+1)*FLOAT(MH)
      RETURN
25  103 DO 124 I=2,N
      124  AS02=AS02+X(I)*FLOAT(I-1)
      AS02=AS02+AS02-X(N)*FLOAT(MH)
      RETURN
      FNN

```

APPENDIX B. Derivation of Equation 4.1; Average Oxygen Concentration in the Bed for the Plumeless Model

By plumeless model we mean the extreme case where particles of the feed coal disperse uniformly throughout the bed before any devolatilization occurs. In this case oxygen concentration does not decrease exponentially with the height of the bed, because we assume that volatiles evolve and burn uniformly throughout the bed (see equations 5.7 and 5.9). But for the convenience of calculations the oxygen concentration in the bed is assumed to decrease exponentially with the height within the bed. In this case average concentration is given by the logarithmic mean of the concentration at the bottom of the bed and that of at the top of the bed:

$$C_{B, \text{ bottom}} = C_{B0}$$

$$C_{B, \text{ top}} = C_{B0} [E_x + (1-X_b)(1-f_p)] / (1+E_x)$$

$$\begin{aligned} \overline{C}_{ox} &= \frac{C_{B, \text{ bottom}} - C_{B, \text{ top}}}{\ln \frac{C_{B, \text{ bottom}}}{C_{B, \text{ top}}}} \\ &= \frac{C_{B0} [1 - (1-X_b)(1-f_p)]}{(1 + E_x) \ln \left[\frac{1 + f_p}{E_x + (1-X_b)(1-f_p)} \right]} \end{aligned}$$

This average concentration is slightly smaller than the true average concentration.

APPENDIX C. Logarithmic Size Distribution

One simple approximation to the size distribution of crushed coal particles is a logarithmic function:

$$Y = a (2R)^b \quad (4.2)$$

We can obtain size distribution function by differentiation of the above equation,

$$P(d_p) = \frac{d}{d(d_p)} \left(\frac{Y}{100} \right) = \frac{ab}{100} d_p^{b-1} \quad (\mu\text{m}^{-1})$$

Figure C.1 shows the $P(d_p)$ vs d_p .

Figure C1. Logarithmic size distribution.

APPENDIX D.. Derivation of y_{HO} , y_{SO} and α

At the bottom of the bed the amount of volatiles and transport air is

$$\frac{V^*}{0.0224} + n f_t (1+E_x), \text{ mol/kg feed coal}$$

Due to the partial combustion of volatiles by the oxygen in transport air SO_2 can form inside the plume. The fraction of volatiles burned with transport air is

$$(1+E_x) f_t / f_p$$

Then the mol fraction of H_2S in the plume at the bottom of the bed is

$$y_{HO} = \frac{\frac{1000}{32.06} f_s \Psi \frac{\text{mol volatiles}}{\text{kg coal}} \left[1 - (1+E_x) f_t / f_p \right]}{\frac{V^*}{0.0224} + n f_t (1+E_x) \frac{\text{mol gas}}{\text{kg coal}}}$$

Likewise the mol fraction of SO_2 inside the plume is

$$y_{SO} = \frac{\frac{1000}{32.06} f_s (1-\Psi) (1+E_x) f_t / f_p}{\frac{V^*}{0.0224} + n f_t (1+E_x)}$$

Outside the plume sulfur dioxide forms as char burns. For the combustion of char from 1 kg of feed coal $n(1-f_p)$ mol of air is needed, and $(1000/32.06) f_s (1-\Psi)$ mol of SO_2 is formed by that combustion. Thus for 1 mol of oxygen the amount of SO_2 formed is

$$\frac{\frac{1000}{32.06} f_s (1-\Psi)}{n(1-f_p)(0.21)} \equiv \alpha, \quad \frac{\text{mol } SO_2 \text{ formed}}{\text{mol } O_2 \text{ consumed}}$$

APPENDIX E. The Plumeless Model I for Sulfur Retention

In the plumeless model we assume that volatiles are released and burn uniformly throughout the bed. We have to consider two different ways of consumption: one is for the combustion of char, the other for volatiles. Thus

$$\frac{\partial y_B}{\partial z} = -\frac{kH}{u_o} y_B - \frac{Hk_v}{u_o}$$

where k_v is the rate constant of oxygen consumption rate for volatiles ($\frac{\text{m}^3 \text{ gas}}{\text{m}^3 \text{ bed} \cdot \text{s}}$). Note that this is actually a zeroth order rate constant multiplied by reference concentration C_0 .

By integration and the initial condition of $y_B = 0.21$ at $\hat{z} = 0$ we obtain

$$y_B = (0.21 + k_v/k) e^{-\frac{kH\hat{z}}{u_o}} - k_v/k.$$

From the oxygen balance the fraction oxygen consumed for volatiles is $f_p/(1+E_x)$. Thus

$$k_v \frac{H}{u_o} = 0.21 \frac{f_p}{1+E_x}$$

$$\text{or } k_v = \frac{0.21 u_o f_p}{H(1+E_x)}$$

For the combustion of volatiles from 1 kg of feed of air is needed, and $(1000/32.06) \cdot f_s \cdot \psi$ mol of SO_2 is formed for 1 mol of oxygen the amount of SO_2 is formed is

$$\frac{\frac{1000}{32.06} f_s \psi}{0.21 \cdot n \cdot f_p} = \beta \quad \frac{\text{mol SO}_2 \text{ formed}}{\text{mol O}_2 \text{ consumed}}$$