FLUIDIZED BED COMBUSTOR MODELING

M. Horio
P. Rengarajan
R. Krishnan
C.Y. Wen

January, 1977

Prepared for National Aeronautics & Space Administration under contract No. NAS3-19725

West Virginia University

College of Engineering

Contract No. NAS3-19725

FLUIDIZED BED COMBUSTOR MODELING

by

M. Horio, P. Rengarajan, R. Krishnan and C. Y. Wen

WEST VIRGINIA UNIVERSITY

prepared for

NATIONAL AERONAUTICS AND SPACE ADMINISTRATION

NASA LEWIS RESEARCH CENTER

CONTRACT NO. NAS3-19725

Bert Phillips, Project Manager

1. Report No.	2. Government Accession No.	3. Recipient's Catalog No.
NAS3-19725		

4. Title and Subtitle	5. Report Date
Fluidized Bed Combustor Modeling	January, 1977
	6. Performing Organization Code

7. Author(s)	8. Performing Organization Report No.
M. Horio, P. Rengarajan, R. Krishnan and C. Y. Wen	
	10. Work Unit No.

9. Performing Organization Name and Address	11. Contract or Grant No.
West Virginia University Morgantown, WV 26506	NAS3-19725
	13. Type of Report and Period Covered

12. Sponsoring Agency Name and Address	14. Sponsoring Agency Code
National Aeronautics and Space Administration Washington, D. C. 20546	

15. Supplementary Notes

Project Manager, Bert Phillips
NASA Lewis Research Center, Cleveland, Ohio

16. Abstract

A general mathematical model for the prediction of performance of a fluidized bed coal combustor (FBC) is developed. The basic elements of the model consists of (a) hydrodynamics of gas and solids in the combustor; (b) description of gas and solids contacting pattern; (c) kinetics of combustion and (d) absorption of SO_2 by limestone in the bed. The model is capable of calculating the combustion efficiency, axial bed temperature profile, carbon hold-up in the bed, oxygen and SO_2 concentrations in the bubble and emulsion phases, sulfur retention efficiency and particulate carry over by elutriation. The effect of bed geometry, excess air, location of heat transfer coils in the bed, calcium to sulfur ratio in the feeds, etc. is examined.

The calculated results are compared with experimental data reported by the National Coal Board, England. Agreement between the calculated results and the observed data are satisfactory in most cases. Recommendations to enhance the accuracy of prediction of the model are suggested.

17. Key Words (Suggested by Author(s))	18. Distribution Statement
Fluidized Bed Coal Combustion	Unclassified - unlimited

19. Security Classif. (of this report)	20. Security Classif. (of this page)	21. No. of Pages	22. Price*
Unclassified	Unclassified	213	

* For sale by the National Technical Information Service, Springfield, Virginia 22161

FOREWORD

The research reported here was conducted in the Department of Chemical Engineering at West Virginia University during the period June, 1975 to December, 1976 and under NASA Contract No. NAS3-19725. The work was done under the management of the NASA Technical Monitor, Dr. Bert Phillips, NASA Lewis Research Center.

ABSTRACT

A general mathematical model for the prediction of performance of a fluidized bed coal combustor (FBC) is developed. The basic elements of the model consists of (a) hydrodynamics of gas and solids in the combustor; (b) description of gas and solids contacting pattern; (c) kinetics of combustion and (d) absorption of SO_2 by limestone in the bed. The model is capable of calculating the combustion efficiency, axial bed temperature profile, carbon hold-up in the bed, oxygen and SO_2 concentrations in the bubble and emulsion phases, sulfur retention efficiency and particulate carry over by elutriation. The effect of bed geometry, excess air, location of heat transfer coils in the bed, calcium to sulfur ratio in the feeds, etc. is examined.

The calculated results are compared with experimental data reported by the National Coal Board, England. Agreement between the calculated results and the observed data are satisfactory in most cases. Recommendations to enhance the accuracy of prediction of the model are suggested.

TABLE OF CONTENTS

LIST OF FIGURES

LIST OF TABLES

Section I

INTRODUCTION

Combustion of coal in a fluidized bed combustor (FBC) takes place in a bed containing coal, char, ash and SO_2 acceptor (limestone or dolomite) and operates at a relatively low temperature (800-900°C). FBC appears to be the most attractive way among the alternative schemes of direct coal combustion to meet near term energy needs of the nation. The high heat transfer coefficient in fluidized bed enables us to have smaller boiler volumes and less heat transfer areas per required combustion load than conventional pulverized coal burning boilers. The low coal char hold up in the bed (1~4 wt.% in carbon) and the presence of solid particles which are inert from pyrolysis or combustion prevents the agglomeration, and caking of coal as well as the smoke generation.

As have been reviewed in several current reports*) a large amount of data from various pilot FBCs have become available concerning the mean volumetric heat release rates, heat transfer coefficients, efficiencies of carbon combustion and sulfur dioxide capture. However, since these experimental tests have concentrated on the feasibility evaluation of FBC and the collection of practical "know-hows", the theoretical examination of these data is far behind the experimental work.

---

*) "National Fluidized Bed Combustion Problem", Vol. III and IV, the MITRE Corp. (1974), and Proc. of the 4th International Conf. on Fluidized Bed Combustion, Mclane, Va (1975).

A great deal of work has been done in Great Britian on study of the performance of FBC not only experimentally but also theoretically. However, only little information has been published. For sulfur dioxide retention by limestone in a fluidized bed combustion Bethell, Gill and Morgan (1973) presented a theoretical model. Horio and Wen (1975a) also formulated a model for the removal of sulfur dioxide by limestone from a FBC. This model considers the hydrodynamics of the fluidizing gas based on the Bubble Assemblage Model (Mori and Wen (1975b).) and treats the variation in limestone reactivity by the population balance technique. Recently as a part of this project Horio and Wen (1976) developed a combustion model to analyze the effect of elutriation on the coal combustion efficiency. In addition, the effect of axial solid mixing on the temperature profile was also examined to explain the temperature nonuniformity and the formation of hot spot observed by Ruth (1975) in the pressurized deep fluidized bed.

In the related field of coal combustion, the combustion of carbon under oxygen lean condition is analyzed by Levenspiel, Kunii and Fitzgerald (1968). They emphasized the important role of the presence of particles within the bubble on the combustion rate. However, this finding seems to be for the oxygen lean case where bubbles are surrounded by carbon particles. In FBC on the other hand, bubbles are surrounded mostly by limestone and excess oxygen is present in the emulsion phase. Despite the development of fluidized bed combustors, there are still many unsolved basic problems. Some of these problems were reviewed by Horio and Wen (1975b). Many hydrodynamic correlations

are not applicable to the range of operation and geometry of FBC. For instance, the bubble size distribution affects the performance of a fluidized bed reactor significantly but the data available are mostly for the case of a non-tapered column without the presence of internals. A general bubble size correlation without presence of internals was given by Mori and Wen (1975a). Recently Rowe (1976) presented a correlation of a different type. However, the behavior of bubbles is likely to change by the presence of internal heat exchange tubes or by the tapering of the bed wall. The knowledge of the bubble behavior for large particle size at very high gas velocity is also uncertain.

The complexity of coal and limestone kinetics is another difficulty of the FBC model development. The devolatilization of coal particles, the effects of temperature and ambient gas composition on the calcination product from limestone and the mechanism of sulfur dioxide-lime reaction are very complicated. The critical problem is whether the reaction kinetic models formulated can be simplified so that they can be incorporated into the hydrodynamic model of FBC and still be accurate enough to describe actual process phenomena.

The objective of this report is to develop a general model of a Fluidized Bed Combustor which can provide a complete simulation of the FBC operation minimizing the use of adjustable parameters. The model must be checked by the experimental data to verify the accuracy. In addition, the study should provide information regarding the areas of experimental or theoretical research needed to improve the understanding of the phenomena and thus the model performance of a FBC.

In order to construct a FBC model the complexity and unknown factors noted above must be examined to assess the level of sophistication needed for the modeling. Based on this consideration, a general model will be formulated. The general model will be simplified into two cases (level I and II) to meet the existing computation capacity of the computer. Program codes corresponding to the simplified models will be presented in the manual. Sample calculations were made and the results are shown in Section X.

Section II

ASSESSMENT OF THE BASIC FACTORS IN FBC MODELING

The following three major aspects of the general modeling of Fluidized Bed Combustors are examined in this section.

1. Hydrodynamics for gas and solids.
2. Description of gas and solids contacting process.
3. Kinetics for combustion and limestone - SO_2 reaction.

1. Hydrodynamics of gas and solids in FBC

1-1. Bubble Size

Bubble size is one of the most critical parameters in Fluidized Bed Reactor Modeling affecting the bubble rising velocity and gas exchange between bubble phase and emulsion phase. The previous measurements are summarized in Table 1. Correlations for the axial distribution of bubble size previously proposed by many investigators are listed in Table 2.

Mori and Wen (1975a) developed a general correlation for the bubble size distribution which can take into consideration the effects of distributor design and tower diameter. The correlation is given by

$$\frac{D_{Bm} - D_B}{D_{Bm} - D_{Bo}} = \exp\ (-0.3\ Z/D_t) \qquad (2\text{-}1)$$

where the maximum bubble diameter D_{Bm} and initial bubble diameter D_{Bo} are given by the following equations:

TABLE 1. SUMMARY OF EXPERIMENTAL CONDITIONS FOR THE BUBBLE DIAMETER IN THE FLUIDIZED BED

B: Bubble cap; T: tuyere; P_e: perforated plate; P_o: porous plate or screen

Investigators	D_t, cm	Solid particles	d_p, cm	u_{mf}, cm/s	u_o/u_{mf}	No. of holes in the distributor, N_D
Werther(1973)	20	Quartz sand	0.0083	1.8	5	P_o
	100					
Chiba(1973)	20	Crushed silica	0.0089	0.5[illegible]	10~39	P_e, 241
			0.0210	2.85	2~8	
Geldart(1971)	30.8	Sand	0.0128	1.2	2.6~7.7	P_e, 3100
Rowe(1972)	30 X 20*	Alumina	0.021	2.54	1.25~2.5	
	30 X 30*	Carbon	0.0296	8.0	1.3~1.7	
		Quartz	0.0135	2.75	2.2~6.6	P_o
	30 X 20*	Ballotini	0.0325	8.0	1.6~2.4	
		Glass powder	0.0268	5.5	1.7~2.7	
Whitehead(1967)	61 X 61*				1.8~6.9	4
	61 X 61*	Silica sand	0.015	2.5	2.8~6.6	T 16
	122 X 122*				3.2~6.2	64
	122 X 122*				2.1~6.3	16
Kunii(1967)	20	M.S.cat.	0.015	2.0	9.5	P_e, 79
	40				1.5~25	P_e, 314
Yasui(1958)		Glass beads	0.0242	7.56	1.5~2.5	
	10.2	Glass beads	0.0175	4.7	1.5~2.7	P_o
		U.O.P.cat.	0.0060	0.418	2~10	
		Coal	0.0450	19.4	1.5~1.75	
Toei(1965)	10 X 10*	Glass beads	0.0137	2.25	1.5~4.0	P_o
Kobayashi	10.0	Crushed silica	0.0210	2.85	2~9.7	P_e, 1850
Miwa(1971)	15.0	Sand	0.016	2.4	3.1~5.2	P_e, 37
Tomita(1971)	21.4					184
	37.8	Sand	0.0202	4.0	4.25	P_e, 575
	59.9					1450
Baumgarten(1960)	7.6	Glass beads	0.0074	0.727	2~84	P_o
Park(1969)			0.0086	0.63	4~10	
	10.0	Conductive coke	0.0156	1.83	1.5~6	
			0.0344	6.8	1.5 3	P_o
Botton(1968)	50	Sand	0.0071	1.0**	2 15	P_e, 78
Fryer(1974)	22.9	Sand	0.0071	1.70	1.47	B 61

*Diameter of a cylinder having same cross-sectional area of the actual bed was used for calculation.
**Gas flow rate through the dense phase reported by Botton (1968).

TABLE 2. SUMMARY OF CORRELATIONS FOR BUBBLE DIAMETER IN FLUIDIZED BEDS

Yasui et al. (1958)	$D_B = 1.6\rho_p d_p \left(\frac{u_o}{u_{mf}} - 1\right)^{0.63} \cdot Z$
Kato and Wen (1969)	$D_B = 1.4\rho_p d_p \left(\frac{u_o}{u_{mf}}\right) Z + D' B_o$
Park et al. (1969)	$D_B = 33.3\, d_p^{1.5} \left(\frac{u_o}{u_{mf}} - 1\right)^{0.77} Z$
Whitehead et al. (1967)	$D_B = 9.76 \left(\frac{u_o}{u_{mf}}\right)^{0.33(0.032Z)^{0.54}}$
Rowe et al. (1972)	$D_B = -A + BZ + C\left(\frac{u_o}{u_{mf}}\right) + DZ\left(\frac{u_o}{u_{mf}}\right) + E\left(\frac{u_o}{u_{mf}}\right)^2$
Geldart (1971)	$D_B = D'_{Bo} + 0.027\,(u_o - u_{mf})^{0.94} Z$
Chiba et al. (1973)	$\dot{D}_B = D_{Bo}'' \{2^{7/6} - 1)\,(Z - Z_{Bo})/ D_{Bo}'' + 1\}^{2/7}$ for $Z < Z_k$*
Mori and Wen (1975)	$\frac{D_{max} - D_B}{D_{max} - D_{Bo}} = e^{-0.3Z/D_t}$
Rowe (1976)	$D_B = (u_o - u_{mf})^{0.5} (Z + Z_o)^{3/4} / g^{1/4}$ **

*Numerical method is used to calculate D_B for $Z > Z_k$

$$D_{Bo}' = (6G/\pi)^{0.4}/g^{0.2} \text{ and } D_{Bo}'' = (6G/\pi k_B)^{0.4}/g^{0.2}$$

where A, B, C, D, E and k_B are constants determined by the properties of the solid particles; Z_{Bo} is the height of the jet above the distributor, (cm); and Z_k is the height from the bottom of the bed where the bubble radius becomes equal to the pitch of the holes in the distributor, (cm). G denotes the volmetric gas flow rate through a nozzle (cm^3/sec)

** Z_o is a constant characterizing a distributor.

$$D_{Bm} = 0.652 \left[A_t (u_o - u_{mf}) \right]^{0.4} \qquad (2\text{-}2)$$

$$D_{Bo} = 0.347 \left\{ A_t (u_o - u_{mf})/n_d \right\}^{0.4} \qquad (2\text{-}3)$$

Equation (2-1) was derived empirically but it can be obtained as a solution of the following differential equation for the case of a non-tapered fluidized bed,

$$\frac{dD_B}{dZ} = \frac{0.3}{D_t} (D_{Bm} - D_B) \qquad (2\text{-}4)$$

$$\text{I.C.} \qquad D_B = D_{Bo} \quad \text{at } Z = 0 \qquad (2\text{-}5)$$

Equation (2-1) can cover the previous data listed in Table 1 within $\pm$ 50 % error. However, all of the data used were from fluidized beds without the presence of bed internals and from beds without tapered wall. No general correlations applicable to beds with tapered geometry and with bed internals have been developed. In spite of the fact that there is no supporting experimental data available, Equations (2-4) and (2-5) are used for the case of tapered beds and the beds with internal tubes in order to maintain the consistency with Equation (2-1). The validity of Equation (2-4) should be examined by future experiments. The maximum bubble size D_{Bm} is a function of the distance from the distribution when the bed is a tapered one. D_{Bm} should also be modified when horizontal cooling tubes are present. This work is left for the second phase study.

1-2. Bubble rising velocity

Table 3 shows the previous investigation of the bubble rising velocity. The available correlations are also listed in the table. The absolute rising velocity of a bubble is affected not only by the

TABLE 3. SUMMARY OF THE MEASUREMENTS AND CORRELATION FOR THE RISING VELOCITY OF A SINGLE BUBBLE

GB = Glass beads
S = Sand
SS = Swede seeds
C = Coke
AC = Alumina Catalyst

Investigators	Bed Size cm	Particle size	Measuring technique	Given Correlation
Davidson et al* (1959)	7.6 ϕ 15.2 X15.2	GB, $\overline{d}_p$ = 150 μ S , $\overline{d}_p$ = 400 μ SS, $\overline{d}_p$ = 170 μ	Capacitance probe	$u_{B_\infty} = 0.71\sqrt{gD_B}$
Harrison & Leung* (1962a)	61.0 x 61.0	S , d_p = 60~150 B.S. Mesh	Capacitance probe	$u_{B_\infty} = 0.64\sqrt{gD_B}$
Rowe & Partridge (1962)	14.0 ϕ	GB, $\overline{d}_p$ = 50 μ	Dissection of the bed	$u_{B_\infty} = 0.60\sqrt{gD_B}$
Toei et al* (1966)	7.6 ϕ 10.0 X 10.0	GB, d_p = 80~100# GB, d_p = 16~24# S , d_p = 80~120# S , d_p = 35~48# pvc , d_p = 80~100#	X-ray Photography and Capacitance probe	$u_{B_\infty} = 0.66\sqrt{gD_B}$
Park et al+ (1969)	10.0 ϕ	C , $\overline{d}_p$ = 344,154, 86 μ	Electro-resistivity probe	$u_{B_\infty} = 0.63\sqrt{gD_B}$
Rowe & Matsuno (1971)	29.5 X 14.4	GB , d_p = 300~400 μ	X-ray Photography	$u_{B_\infty} = 0.64\, g^{1/2} D_B^{0.521}$
Donsi et al (1972)	35.0 ϕ	AC , d_p = 170~350 μ	Photography	$u_{B_\infty} = 0.545\sqrt{gD_B}$

* = Wall correction factor from Uno and Kinter (1956) was used in these works.

+ = The relation $u_{B_\infty} = u_B - (u_o - u_{mf})$ was applied to obtain u_{B_∞}

bubble size but also by the location and sizes of the surrounding bubbles. Therefore, the correlation gives only the average value of the rising velocity. The rising velocity is also affected by the presence of internals, but a general theory has not been developed to take the effect of internals into account. Therefore, in the present model the following form is adopted:

$$u_B = u_o - u_{mf} + K_B \sqrt{gD_B} \qquad (2\text{-}6)$$

1-3. Gas velocity in emulsion phase

The gas velocity in the emulsion phase could become downward at high gas velocity depending on the circulation pattern of particles. The possibility of downward flow was pointed out by Kunii, Yoshida and Hiraki (1967) and was further examined by Fryer and Potter (1975). However, the complete description of the gas flow pattern in emulsion phase has not been clearly established as reviewed by Horio and Wen (1975b).

As long as the gas flow rate in the emulsion phase is much smaller than that in the bubble phase, the calculated conversion may not be affected very much regardless of the gas flow rate assumed in the emulsion phase. That is the reason why it is assumed in the Bubble Assemblage Model (Mori and Wen (1975b)) that the gas flow rate in the emulsion phase is zero.

Therefore, in the present model the gas flow rate is calculated based on the two-phase theory to keep a consistency with hydrodynamic model. This assumption can be easily changed simply by putting a

different value for emulsion phase flow rate. However, if negative flow rate (i.e. downward flow) is assumed, we need to solve the two-point boundary value problem to obtain the gas concentration profile as shown by Fryer and Potter (1975).

1-4. Solids Mixing

The mixing of solids is caused by the motion of bubbles and their wakes as shown by the experimental study of Rowe and Partridge (1965). The effects of bubbling phenomena on solids mixing are classified into two categories, i.e. bulk circulation and local turbulent mixing. The bulk circulation rate due to the lifting of particles by bubbles is usually expressed as (Woollard and Potter (1968)).

upward flow rate of particles

$= (u_o - u_{mf})\ A_t\ f_w\ (1 - \varepsilon_{mf})$ $\quad cm^3/sec$

where f_w is the ratio of the particles volume in the wake of the bubble including the accompanied void space lifted upward by the bubble to the volume of the bubble. Since the area available for the downward flow of solids is $A_t\ \{1 - \varepsilon_B\ (1 + f_w)\}$, the mean residence time of particles in the downward flow is $\{1 - \varepsilon_B\ (1 + f_w)\}L_f / \{f_w\ (u_o - u_{mf})\}$. The mean cycle time for circulation Θ_c is given as the sum of the residence times of upward and downward movements.

$$\Theta_c = L_f\ [\ 1/\bar{u}_B + \{1 - \bar{\varepsilon}_B\ (1 + f_w)\}/\{f_w\ (u_o - u_{mf})\}] \qquad (2\text{-}7)$$

where $\bar{u}_B$ denotes the average rising velocity of the bubble.

The average bubble fraction $\bar{\varepsilon}_B = (L_f - L_{mf})/L_f$ is approximated by

$$\bar{\varepsilon}_B \doteqdot (u_o - u_{mf})/\bar{u}_B \qquad (2\text{-}8)$$

$\bar{U}_B$ can be eliminated from Equation (2-7) by substituting Equation (2-8). Thus, a simple expression for solid cycle time can be obtained as follows:

$$\theta_c = L_{mf}/(u_o - u_{mf})\ f_w \qquad (2\text{-}9)$$

Therefore, the cycle time of solid circulation is nearly as rapid as the passage of the gas (L_f/u_o) except for the case of low gas velocity. Therefore, the assumption of complete mixing is acceptable.

However, for the tapered bed wall or in the presence of the internal tubes or baffles in the bed the cycle time and the solid mixing intensity will be reduced. According to Sutherland (1961) the mixing index from tapered bed is much lower than that from non-tapered bed in the range u_o/u_{mf} = 1.0~1.3. The packing affects the solid mixing drastically as reported by Gabor (1966). It can be expected that in a tapered FBC with many heat exchange tubes, the solid mixing is probably very poor. However, the way to estimate the value of f_w for the case of a fluidized bed with internal tubes has not been established and, therefore, f_w remains an adjustable parameter in the present model. Since the exchange of particles between the wake phase and the emulsion phase is expected to be fast even under the presence of internals, the single phase back-flow cell model is applied to simulate the axial temperature profile. There is a very close resemblance between the present model and the dispersion model. The relationship between the model parameters is given by (see Horio and Wen (1976)).

$$E_Z \doteqdot \frac{(u_o - u_{mf})\ f_w\ \Delta Z}{1 - \varepsilon_B} \qquad (2\text{-}10)$$

where ΔZ is the height of a complete mixing cell in the backflow cell model.

1-5. Elutriation of Char and Fines

It is assumed that the char size before combustion is the same as the size of the coal fed in. The elutriation rate of fine particles is proportional to the concentration of the fines in the bed and the cross-sectional area of the bed for elutriation A_t, therefore,

$$dW_e = A_t \, K^* \cdot \frac{W_c}{W_b} \phi^* \, dy. \quad [g/sec] \tag{2-11}$$

where dW_e is the elutriation rate of coal/char particles whose diameter is between y and y + dy, W_c and W_b are the weight of char and the weight of total bed materials respectively, $\phi^* dy$ denotes the weight fraction of fine based on the total weight of char whose size is between y and y + dy. K^* is the specific elutriation rate constant. The available correlations for K^* are listed in Table 4. However, most of the correlations are not applicable for the size range less than 150 microns. Correlations B, C and D give similar values for K^* in the range greater than 150 microns, but below this size the rate constants of correlations C and D decrease with an increase in particle size. Correlation A is derived in this study based on the experimental data of the saturation carrying capacity for uniform-sized particles reported by Zenz and Weil (1958). Although these data are not the rate of elutriation of fines, the order of magnitude of correlation A is not very much different from other correlations in the range d_c > 150 microns. Comparison of correlations A and B is shown in Figure 1.

In the modeling of FBC, the attention is focused on the effect of freeboard and the presence of bubbles. The concentration of fines decreases exponentially along the height above the bed surface and reaches

TABLE 4 Correlations for elutriation rate constant

A. Zenz and Weil (1958) †

$$\frac{K^*}{\rho_g u_o} = \begin{cases} 5.27 \times 10^{-5} \left(u_o^2/g\, d_p\, \rho_s^2\right)^{1.87} & \dfrac{u_o^2}{g d_p \rho_s^2} \leq 581.8 \\ 4.97 \times 10^{-3} \left(u_o^2/g\, d_p\, \rho_s^2\right)^{1.15} & \dfrac{u_o^2}{g d_p \rho_s^2} \geq 581.8 \end{cases}$$

B. Yagi and Aoji (1955)††

$$\frac{K^* d_p}{\mu} = Fr\, [0.0015\, Re_t^{0.6} + 0.01\, Re_t^{1.2}]$$

C. Wen and Hashinger (1960)

$$\frac{K^*}{\rho_g (u_o - u_t)} = 1.52 \times 10^{-5}\, Fr^{0.5}\, Re_t^{0.725} \left[\frac{\rho_s - \rho_g}{\rho_g}\right]^{1.15}$$

D. Tanaka and Shinohara (1972)

$$\frac{K^*}{\rho_g (u_o - u_t)} = 0.045\, Re_t^{0.3}\, Fr^{0.5} \left(\frac{\rho_s - \rho_g}{\rho_g}\right)^{0.15}$$

†) The equation is fitted by the present authors.

††) The equation is fitted by Leva and Wen (1971)

$Fr \equiv (u_o - u_t)^2/g d_p$, $Re_t \equiv d_p\, u_t\, \rho_g/\mu$

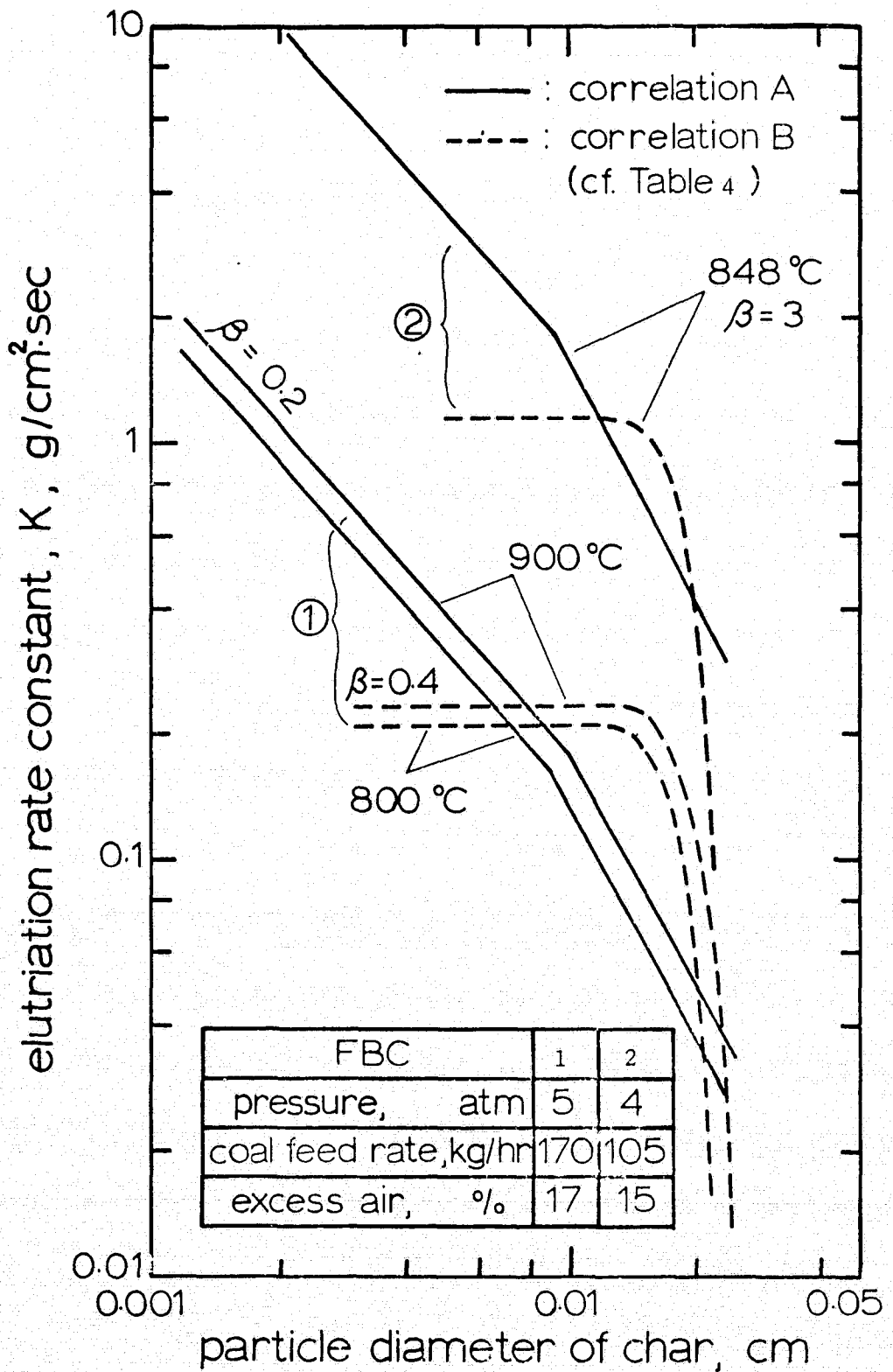


Figure 1. Elutriation rate constant determined by fitting experimental values of carbon combustion efficiency (β is an adjusting parameter multiplied on the correlations.

the equilibrium value at TDH. Large, Martinie and Bergongnore (1976) modified the equation by Zenz and Weil (1958) as follows:

$$F_i = F_{i\infty} + F_{io} \exp(-a_i Z) \qquad (2\text{-}12)$$

where F_i is the fractional entrainment of ith size internal and Z is height from the bed surface. However, the available data are not sufficient to develop correlations for parameters in Equation (2-12) and, therefore, the effect of freeboard is not considered in the present model.

2, Description of Gas and Solid Contacting in FBC

The bubble hydrodynamics, solids mixing and the size distribution of char particles are the major factors in the mathematical formulation of the gas-solid contacting process in a FBC.

The Bubble Assemblage Model can be characterized by the following features:

1. Discrete representation for the axial distribution of process variables, which is convenient for the numerical computation of complex reaction system.

2. The effect of bubble size on the axial gas and solid mixing is considered automatically by setting the compartment height equal to the average bubble diameter at the middle cross section of each compartment.

3. Bubble size is a function of the bed diameter and is axially distributed. It is estimated by applying an empirical correlation.

4. Bubbles and clouds are both combined into the bubble phase. The gas interchange coefficient between the bubble phase and the emulsion phase is a function of the bubble size and distributed axially.

5. The effect of distributor geometry on hydrodynamics is considered by the formulation of a separate jet region from the bubbling region. In the jet region, jet height correlation and initial bubble correlation are used.

6. The gas velocity through the emulsion phase is assumed negligible.

The present FBC model also has most of the features of the Bubble Assemblage Model except items 2 and 6. Since the effect of compartment size distribution is minor in most of the cases, fixed compartment size is used to avoid the complexity in temperature iteration. For the estimation of bubble size Equation (2-6) is applied in the FBC model so that the change in the cross-sectional area can be automatically taken into account.

Gas interchange coefficient is estimated by the following correlation proposed by Kobayashi, Arai and Sunagawa (1967):

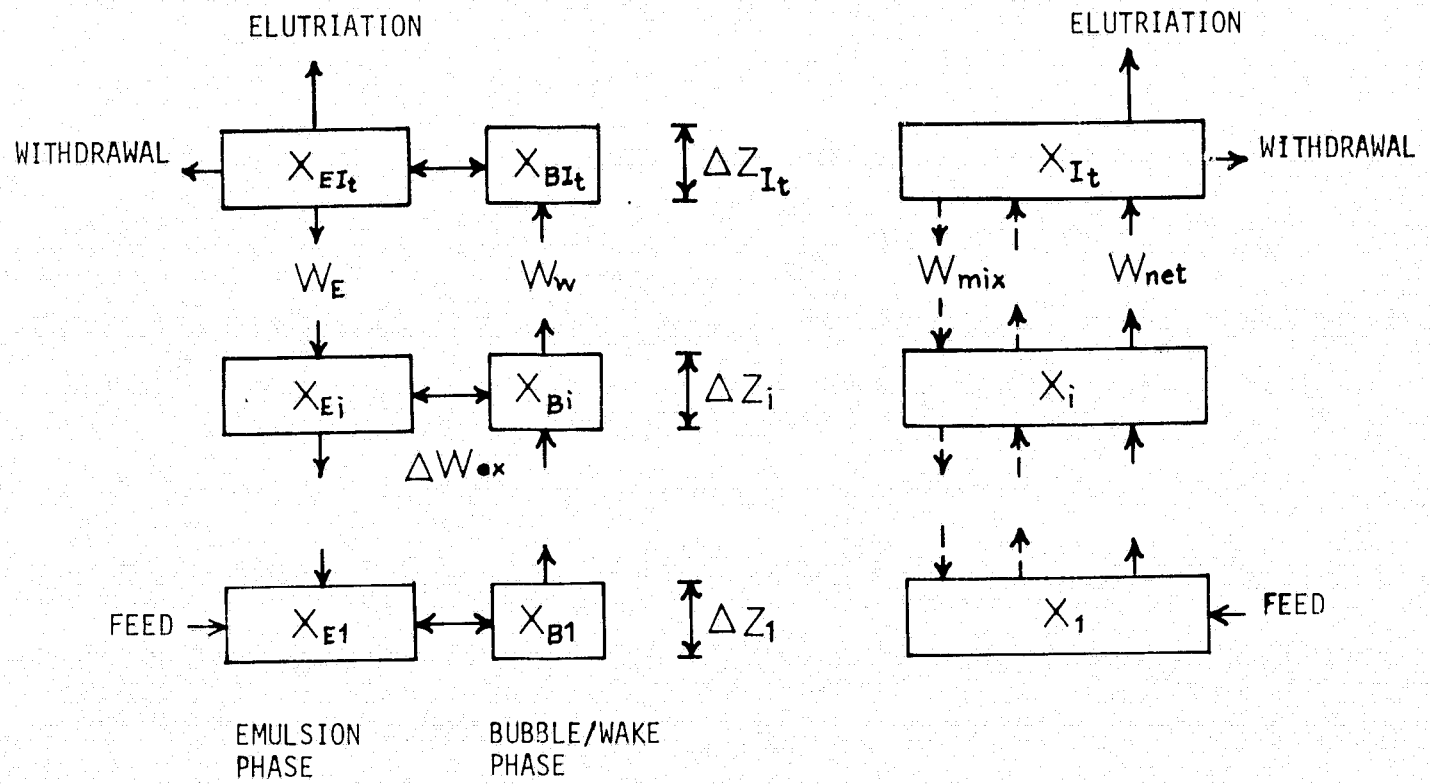
$$K_{BE} = 11/D_B \qquad \text{(C.G.S. Unit)} \qquad (2\text{-}13)$$

The following correlation by Basov et al. is used to estimate the vertical jet height:

$$h_j = \frac{d_p}{0.0007 + 0.556\, d_p} \left\{\frac{A_t}{n_d} (u_o - u_{mf})\right\}^{0.35} \qquad \text{(C.G.S. Unit)} \qquad (2\text{-}14)$$

However, in the case of FBC many distributors have horizontal nozzles and the direct application of Equation (2-14) can result in too large jet height. Therefore, in the case of horizontal jets Equation (2-14) is multiplied by an adjusting coefficient.

In regard to the bulk solid mixing, three models are formulated and tested: (1) complete mixing, (2) single phase backflow cell model, (3) two phase backflow cell model. Figure 2 illustrates the single phase and two phase backflow cell models. Since the solid circulation is usually



(a) Two phase backflow cell model of Ishida and Wen

(b) Single phase backflow cell model (this paper).

W_{min} = upward and downward flow rate of solids (both are equal in magnitude).

Figure 2. Solid mixing models.

very fast in the fluidized bed combustor operation, the simple model based on the assumption of complete mixing is still useful and practical for rough estimation. In the latter two models the same compartment size as that of the gas phase model is used.

The axial variation of the size distribution of char causes the axial distribution of average particle surface area available for combustion. In addition the change in the size distribution of char affects the rate of elutriation. The total surface area of char for combustion can be written as

total surface area of char per unit volume of bed	=	surface area per unit volume of char	$\times$	total volume of char per unit volume of bed

(2-15)

The second term of the right hand side of the above equation is dependent on the bulk solids mixing model and can be calculated from material balance. However, the first term must be determined by population balance for char particles which are shrinking during the course of combustion.

A general model which takes into consideration the variation in the size distribution density function is developed in Section 3. However, because of the numerical difficulties encountered in solving the equations of this model an alternative model is developed which considers only the overall size distribution of char. In this simplified model the axial variation of the total surface area of char per unit volume of bed can still be taken into account by considering the variation of the last term of Equation (2-15) based on the material balance.

The different combination of the gas-phase model, the bulk solids mixing model and the model for the specific surface area of char provides a complete FBC model but of different level of sophistication. Three models of different complexity are developed in this research. The definition of each model can be found in Table 5.

3. Kinetics for coal combustion and limestone - SO_2 reaction

3-1. Coal combustion

The thermal decomposition of coal particles is completed almost instantaneously and produces volatile product and char. The following equations are recommended by Field et al. (1967) to estimate the weight fractions of volatile products.

$$CH_4 = 0.201 - 0.469\ X_{vm} + 0.241\ X_{vm}^2$$
$$H_2 = 0.157 - 0.868\ X_{vm} + 1.338\ X_{vm}^2 \qquad (2\text{-}16)$$
$$CO_2 = 0.135 - 0.900\ X_{vm} + 1.906\ X_{vm}^2$$
$$CO = 0.423 - 2.653\ X_{vm} + 4.845\ X_{vm}^2$$
$$H_2O = 0.409 - 2.389\ X_{vm} + 4.554\ X_{vm}^2$$
$$\text{Tar + Other} = -0.325 + 7.279\ X_{vm} - 12.880\ X_{vm}^2$$

where X_{vm} is the weight fraction of proximate volatile matter of coal on dry ash free (daf) basis. The composition of char produced by rapid heating is different for each system and for each type of coal but no general study is available. Therefore, in this work it is simply assumed that the volatile H, and O are released and react with oxygen instantaneously while carbon, nitrogen and sulphur remain in the char. The release rate of sulphur is assumed to be proportional to the combustion rate of carbon.

TABLE 5 DEFINITION AND PERFORMANCE OF MODELS OF DIFFERENT LEVEL OF SOPHISTICATION

	DEFINITION			PERFORMANCE			
Total model	Gas phase	Bulk solid mixing	Axial variation of char size distribution	Temperature	Volume fraction of char	Surface area of char per unit vol. of char	Reactivity of char = $k_c \lambda_c$
Level I	Not specified*	Complete mixing	Not considered	Uniform	Uniform	Uniform	Uniform
Level II	BAM**	single phase backflow cell model	Not considered	Axially distributed	Axially distributed	Uniform	Axially distributed
Level III	BAM**	Two phase backflow cell model	Two phase backflow cell model	Axially distributed	Axially distributed	Axially distributed	Axially distributed

* Homogeneous complete mixing model and plug flow model are used in calculation, but two phase model can be used in place of them.

** Bubble Assemblage Model

Of course, more realistic bust complicated treatment is possible introducing additional parameters.

The combustion rate of one char particle for a given size is estimated by

$$r_c = \pi d_c^2 k_c C_{O2} \quad [\text{gmole/sec}] \qquad (2\text{-}17)$$

where k_c is the overall rate constant and is given by

$$k_c = 1/(1/k_{cf} + 1/k_{cR}) \qquad (2\text{-}18)$$

where the chemical reaction rate constant k_{cR} is estimated by the following correlation (Field et al. (1967)):

$$k_{cR} = (T/1000) \exp (17.9 - 35{,}700/RT) \qquad (2\text{-}19)$$

The gas film diffusion coefficient, k_{cf}, is estimated assuming the Sherwood Number is equal to 2. Avedesian and Davidson (1973) confirmed by their experimental combustion of char in a fluidized bed of 7.6 cm in diameter that the Sherwood Number is constant (Sh = 1.42) regardless the particle size which was varied from 0.23 to 2.61 mm. The assumed value, Sh = 2, in this model can be changed to other values if necessary but the assumption of a constant Sherwood Number seems reasonable.

3-2. Limestone - SO_2 reaction

The mean residence time of limestone in the bed is long and the circulation rate of solids is rapid enough to assume that the limestone is completely mixed. The assumption of complete mixing is acceptable if the temperature distribution is uniform enough so that there is no dead burning of limestone and no serious effect of temperature history of each particle on the reaction rate. In the present model the average bed volume is used for calculating the rate of limestone - SO_2 reaction.

The reaction rate per limestone particle can be expressed as (Borgwardt (1970))

$$r_{\ell} = \frac{\pi}{6} d_p^3 k_{v\ell} (T, f_{\ell}) C_{SO_2}^m \qquad (2\text{-}20)$$

$$m = 1.088 \doteqdot 1$$

where $k_{v\ell}(T, f_{\ell})$ is overall volumetric reaction rate constant and is a rapidly decreasing function of limestone conversion f_{ℓ}. However, the experimental data are not enough to determine a reliable correlation for $k_{v\ell}$. Therefore, in the present FBC model development a function sub-routine is prepared for the average value of $k_{v\ell}$ in the bed based on the interpolation of available experimental data and population balance for limestone conversion.

Section III

GENERAL MODEL FOR FBC

In this section a general model of FBC is derived. This model is described in the following sequence:

3-1. Reactions

3-2. Reaction rates

3-3. Overall carbon balance

3-4. Overall sulfur balance

3-5. Overall mass balance for gaseous species

3-6. Gas phase model

3-7. Population balance for SO_2 absorption

3-8. Population balance for char combustion, segregation and elutriation

3-9. Heat balance

3-1. Reactions

It is assumed that the calcination of limestone and devolatilization of coal are occurring instantaneously. The following reactions and their reaction rates are considered.

No.	Reaction	Reaction Rate: Per unit vol. of emulsion	Reaction Rate: Per one particle
1	$CaO + SO_2 + 0.5\ O_2 = CaSO_4$	r_1^*	r_1'
2	$CaO + H_2S = CaS + H_2O$	r_2^*	r_2'
3	$C + O_2 = CO_2$	r_3^*	r_3'
4	$C + 0.5\ O_2 = CO$	r_4^*	r_4'
5	$C + H_2O = CO + H_2$	r_5^*	r_5'
6	$S(char) + O_2 = SO_2$	r_6^*	r_6'
7	$S(char) + H_2 = H_2S$	r_7^*	r_7'
8	$N_2\ (char) + \alpha_{nox}\ x'\ O_2 = 2\alpha_{nox}\ NO_{x'} + (1-\alpha_{nox})\ N_2$	r_8^*	r_8'

(3-1)

Let M_g and M_s the vectors of chemical species and at the same time the vectors of molecular weights as follows:

$$M_g \equiv \text{col}\ (M_{gi}) \equiv \text{col}\ (M_{O_2},\ M_{CO_2},\ M_{SO_2},\ M_{H_2O},\ M_{CO}\ M_{H_2S},\ M_{H_2},\ M_{NO_x},\ M_{N_2})$$

$$M_s \equiv \text{col}\ (M_{si}) \equiv \text{col}\ (M_{CaO},\ M_{CaSO_4},\ M_{CaS},\ M_C,\ M_S,\ M_{N_2}) \qquad (3\text{-}2)$$

By using M_g and M_s, Equation (3-1) can be written in one matrix equation as:

$$A\ M_g + B\ M_s = 0 \qquad (3\text{-}3)$$

where A and B are

$$A \equiv \{a_{ij}\} \qquad (3\text{-}4)$$

i \ j	1 (O_2)	2 (CO_2)	3 (SO_2)	4 (H_2O)	5 (CO)	6 (H_2S)	7 (H_2)	8 (NO_x)	9 (N_2)
(1)	-0.5	0	-1	0	0	0	0	0	0
(2)	0	0	0	1	0	-1	0	0	0
(3)	-1	1	0	0	0	0	0	0	0
(4)	-0.5	0	0	0	1	0	0	0	0
(5)	0	0	0	-1	1	0	1	0	0
(6)	-1	0	1	0	0	0	0	0	0
(7)	0	0	0	0	0	1	-1	0	0
(8)	$-\alpha_{nox}$	0	0	0	0	0	0	$2\alpha_{nox}$	$1-\alpha_{nox}$

$$B \equiv \{b_{ij}\} \qquad (3\text{-}5)$$

i \ j	1 (CaO)	2 ($CaSO_4$)	3 (CaS)	4 (C)	5 (S)	6 (N_2)
(1)	-1	1	0	0	0	0
(2)	-1	0	1	0	0	0
(3)	0	0	0	-1	0	0
(4)	0	0	0	-1	0	0
(5)	0	0	0	-1	0	0
(6)	0	0	0	0	-1	0
(7)	0	0	0	0	-1	0
(8)	0	0	0	0	0	-1

Accordingly the gas phase concentration vector C is defined as follows:

$$C = \{C_1, C_2, C_3, C_4, C_5, C_6, C_7, C_8, C_9\} \qquad (3\text{-}6)$$

$$= \{C_{O_2}, C_{CO_2}, C_{SO_2}, C_{H_2O}, C_{CO}, C_{H_2S}, C_{H2}, C_{NO_x}, C_{N_2}\}$$

3-2. Reaction Rates

The reaction rate (positive for production rate) of i th reaction is denoted by

$$r_i^* = \left[\frac{\text{gmol}}{\text{sec}\cdot\text{cm}^3\ \text{(emulsion)}}\right]$$

Here emulsion refers to the dispersed solids. The voidage is assumed to be ε_{mf}.

The formation rate of j th species due to the i th reaction is given by

$$r^*_{gij} = r_i^*\, a_{ij} \qquad \left[\frac{\text{gmol of } (M_{gj} \text{ or } M_{sj})}{\text{sec}\cdot\text{cm}^3\ \text{(emulsion)}}\right] \qquad (3\text{-}7)$$

$$r^*_{sij} = r_i^*\, b_{ij}$$

The total formation rate of each species can, therefore, be obtained as follows:

$$R^*_g = RA = \{\sum_i r_i^*\, a_{ij}\} \qquad (3\text{-}8)$$

$$R^*_s = RB = \{\sum_i r_i^*\, b_{ij}\}$$

where R is defined by

$$R = \{r_i^*\} \qquad (3\text{-}9)$$

The rate of reactions 1 and 2 can be expressed as

$$r_i^* = \rho_{N\ell}\, r_i' \qquad (i = 1 \text{ and } 2) \qquad (3\text{-}10)$$

where $\rho_{N\ell}$ denotes the number of limestone (or dolomite) particles per unit volume of emulsion and the reaction rate for single particle, r_i', is supposed to be written by the first order rate equation regarding the reactant concentration C_3 (SO_2) or C_6 (H_2S) as follows:

$$r_1' = \frac{\pi d_\ell^3}{6} \quad k_{v1} (T, f_\ell, d_\ell) C_3 \tag{3-11}$$

$$r_2' = \frac{\pi d_\ell^3}{6} \quad k_{v2} (T, f_\ell, d_\ell) C_6 \tag{3-12}$$

where k_{v1} and k_{v2} are the overall rate constants.

The rate equations for the reactions 3, 4 and 5 are assumed to be in the following form:

$$r_i^* = \rho_{Nc} \quad r_i' \quad (i = 3, 4 \text{ and } 5) \tag{3-13}$$

where ρ_{Nc} denotes the number of char particles per unit volume of emulsion and the reaction rates for a single char particle, r_i' (i = 3, 4 and 5) are defined as

$$r_3' = \pi d_c^2 k_3 (T, d_c) \quad C_1 \tag{3-14}$$

$$r_4' = \pi d_c^2 k_4 (T, d_c) \quad C_1 \tag{3-15}$$

$$r_5' = \pi d_c^2 k_5 (T, d_c) \quad C_4 \tag{3-16}$$

The rates of reactions 6, 7 and 8 are approximated by

$$r_i^* = \alpha_i (r_3^* + r_4^* + r_5^*) \quad (i = 6, 7 \text{ and } 8) \tag{3-17}$$

where the constants, α_i = (i = 6, 7 and 8), are assumed to be

$$\alpha_6 = \alpha_7 \doteq \left(\frac{X_{Sf}}{M_S} \right) / \left(\frac{X_{Cf}}{M_C} \right) \tag{3-18}$$

$$\alpha_8 \doteq \left(\frac{X_{Nf}}{M_{N2}} \right) / \left(\frac{X_{Cf}}{M_C} \right) \tag{3-19}$$

3-3. Overall Carbon Balance

Figure 3 illustrates the factors contributing to the overall carbon balance.

Let ϕ denote the overall size distribution density function for char particles. The function ϕ is defined so that

ϕ (y) dy = number fraction of char particles whose dimensionless diameter lies in the region between y and y + dy. (3-20)

$$\int_0^1 \phi\ (y)\ dy = 1 \qquad (3\text{-}21)$$

where y is defined as the ratio of char diameter, d_c, to the maximum char diameter in the feed, d_{cm}, namely

$$y = d_c/d_{cm} \qquad (3\text{-}22)$$

An average over the range y = 0~1 for an arbitrary variable A is defined by

$$< A > \equiv \int_0^1 \phi\ (y)\ A\ (y)\ dy \qquad (3\text{-}23)$$

The mean volume of a single char particle in the bed is then expressed as follows:

$$\text{(mean volume of a char particle)} = \frac{\pi}{6} d_{cm}^3\ \psi_v$$

$$\psi_v \equiv < y^3 > = <d_c^3 >/d_{cm}^3$$

From Equations (3-14),(3-15) or (3-16) the average reactivity of char is written as

$$\text{(average reactivity of char)} = \pi\ d_{cm}^2 < y^2\ k_i\ (T, y)> \quad (i = 3\text{~}5) \qquad (3\text{-}24)$$

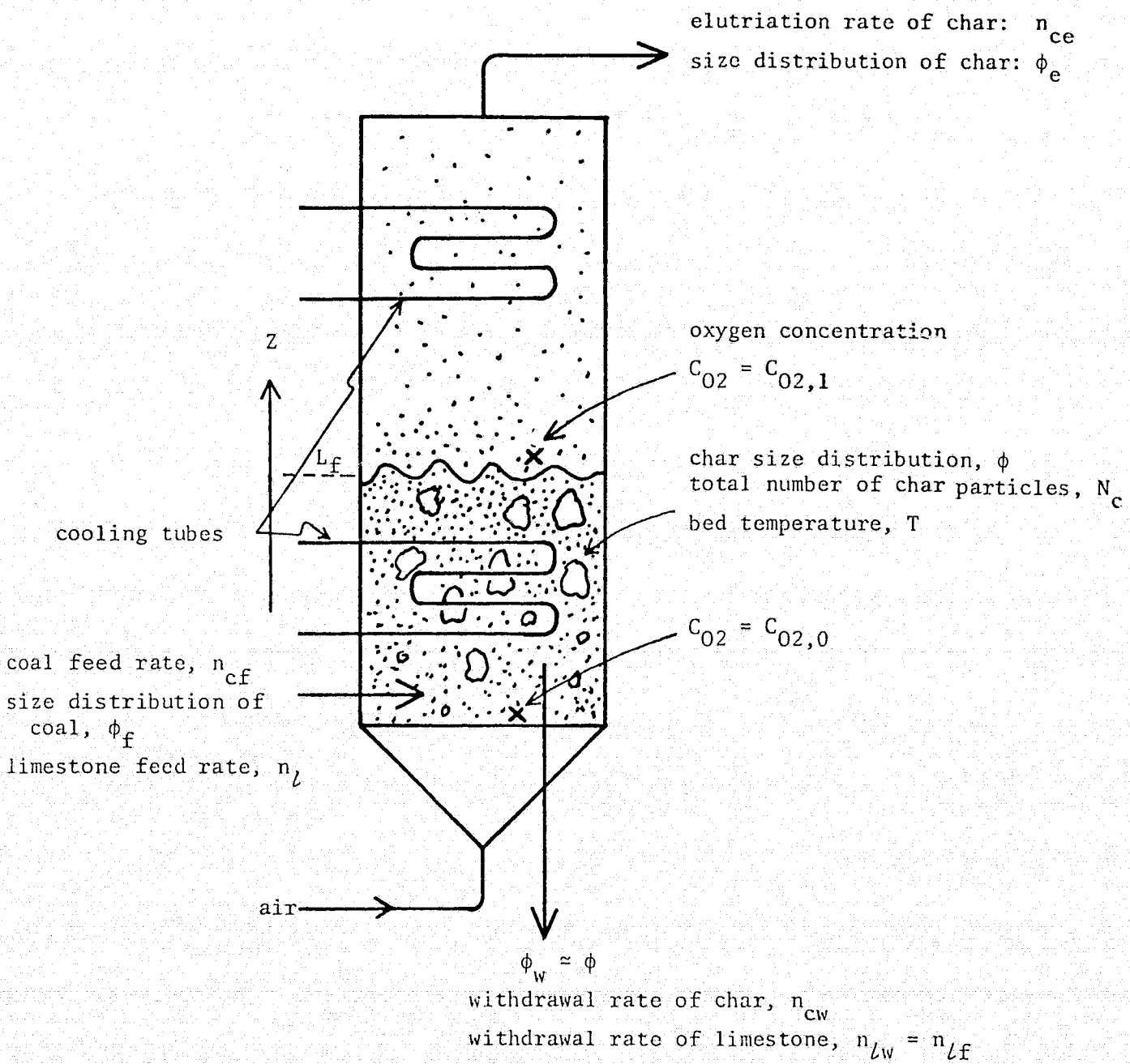


Figure 3. Illustration of the population balance around a fluidized bed combustor. (n: number of particles/sec)

Letting N_c the total number of char particles in the bed, combustion efficiency, η_c, is defined as

$$\eta_c = \frac{M_C N_c \pi d_{cm}^2 \sum_{i=3}^{5} \overline{< k_i y^2 > C_j}}{w_{cf} X_{Cf}} \qquad (3\text{-}25)$$

where

$$j = \begin{cases} 1 & \text{for} \quad i = 3 \text{ or } 4 \\ 4 & \text{for} \quad i = 5 \end{cases}$$

and the bar in Equation (3-25) indicates the space average over the bed.

The overall material balance for carbon in solid phase is derived as

$$w_{cf} X_{Cf} - \frac{\pi}{6} d_{cm}^3 \rho_{ch} X_C n_{cw} \psi_{vw} - \frac{\pi}{6} d_{cm}^3 \rho_{ch} X_C n_{ce} \psi_{ve}$$

(feed) (withdrawal) (elutriation)

$$= M_C N_c \pi d_{cm}^2 \sum_{i=3}^{5} \overline{< k_i y^2 > C_j} \qquad (3\text{-}26)$$

(reaction)

where subscripts f, w and e denote feed, withdrawal and elutriation respectively.

As to the first term of Equation (3-26) the following relation can be written:

$$w_{cf} = \frac{\pi}{6} \; d_{cm}^3 \; \psi_{vf} \; n_{cf} \; \rho_{cf} \qquad (3\text{-}27)$$

Substituting Equations (3-25) and (3-27) into Equation (3-26) we get

$$\eta_c = 1 - \frac{(n_{cw} \psi_{vw} + n_{ce} \psi_{ve}) X_c \; \rho_{ch}}{n_{cf} \; \psi_{vf} \; \rho_{cf} \; X_{cf}} \qquad (3\text{-}28)$$

The elutriation term $n_{ce} \; \psi_{ve}$ is estimated by using the specific elutriation constant K^* as follows (see Appendix V):

$$n_{ce} \; \psi_{ve} = \frac{A_t \; N_c}{W_b} \quad < K^* \; y^3 > \qquad (3\text{-}29)$$

By using Equations (3-28) and (3-29) we obtain the ratio of char particles withdrawal rate to feed rate as,

$$\frac{n_{cw}}{n_{cf}} = \frac{(1 - n_c) \; \psi_{vf}}{\psi_{vw} + \Theta \; \dfrac{A_t}{W_b} < K^* \; y^3 >} \cdot \frac{X_{Cf} \; \rho_{cf}}{X_C \; \rho_{ch}} \qquad (3\text{-}30)$$

where Θ denotes the mean residence time of limestone at the steady state,

$$\Theta \equiv N_\ell / n_{\ell f} = N_c / n_{cw} \qquad (3\text{-}31)$$

From the volume balance Θ is estimated by (see Appendix I)

$$\Theta = \frac{(1 - \varepsilon_{mf}) \; V_{mf}}{w_{\ell f}/\rho_{\ell f} + (\pi/6) \; d_{cm}^3 \; \psi_{vw} \; n_{cw} + (n_c \; w_{cf} \; X_{Af}/\rho_A)(1 - \xi_{Ae})} \qquad (3\text{-}32)$$

where the parameter ξ_{Ae} denotes the ratio of the ash elutriation rate to the total ash formation rate. The numerical value of ξ_{Ae} must be evaluated based on ash elutriation rate constant. In this study, however, ξ_{Ae} is assumed to be 0.5.

3-4. Overall Sulfur Balance

The sulfur balance is derived as follows:

1. (total sulfur in feed gas and formation rate) $= \dfrac{w_{cf}\, X_{Sf}\, \eta_c}{M_S} + F_{mf}\,(y_{SO_2,f} + y_{H_2S,f})$

2. (total sulfur capture rate by adsorbent) $= \dfrac{w_{\ell f}\, X_{\ell Ca}}{M_{Ca}} \cdot \hat{f}_\ell$

where $\hat{f}_\ell$ is the average conversion of adsorbent (limestone or dolomite) in the bed and is defined as

$$\hat{f}_\ell \equiv \int_0^1 \phi_\ell\,(f_\ell)\, f_\ell \, df_\ell \tag{3-33}$$

$\phi_\ell\,(f_\ell)$ is the density function of the distribution of adsorbent conversion and has the feature

$$\int_0^1 \phi_\ell\,(f_\ell)\, df_\ell = 1 \tag{3-34}$$

In addition,

3. (total sulfur capture rate $= N_\ell \dfrac{\pi\, d_\ell^3}{6}\,(\overline{\hat{k}_{v1}\, C_3} + \overline{\hat{k}_{v2}\, C_6})$

where

$$\overline{\hat{k}_{v1}\, C_3} = \frac{1}{L_f} \int_0^{L_f} \left[C_3 \int_0^1 k_{v1}\, \phi_\ell \, df_\ell \right] dZ$$

$$\overline{\hat{k}_{v2}\, C_6} = \frac{1}{L_f} \int_0^{L_f} \left[C_6 \int_0^1 k_{v2}\, \phi_\ell \, df_\ell \right] dZ$$

Defining the sulfur retention efficiency by

$$\eta_S = 1 - \frac{\text{moles } SO_2 \text{ in flue gas}}{\text{moles sulfur input}}$$

We get the following overall relationships on sulfur retention and adsorbent conversion:

$$\eta_S = \frac{[C_a]}{[S]} \hat{f}_\ell \tag{3-35}$$

$$\hat{f}_\ell = \frac{N_\ell M_{Ca} \{ \overline{\hat{k}_{v1} C_3} + \overline{\hat{k}_{v2} C_6} \}}{n_{\ell f} \rho_{\ell f} X_{\ell,Ca}} \tag{3-36}$$

where $[C_a]/[s]$ is the molar ratio of calcium to sulfur.

If we can assume that the temperature profile is almost uniform in the FBC Equation (3-36) can be simplified to the form

$$\hat{f}_\ell = N_\ell M_{Ca} \{ \hat{k}_{v1} (\overline{T}, d_\ell) \overline{C}_3 + \hat{k}_{v2} (\overline{T}, d_\ell) \overline{C}_6 \} / \{ n_{\ell f} \rho_{\ell f} X_{\ell Ca} \} \tag{3-37}$$

3-5. Overall Mass Balance for Gas Phase Species

Theoretical air flow rate required for complete combustion of coal is given as follows:

$$F_{m,th} = (w_{cf} X_{Cf}/M_C y_{O2,f})/A_2 \tag{3-38}$$

where

$$A_2 \equiv (X_{Cf}/M_C)/|(X_{Cf}/M_C) + 0.5 (X_{Hf}/M_{H2}) + (X_{Sf}/M_S) - (X_{Of}/M_{O2})| \tag{3-39}$$

The excess air ratio, EAR, is defined by

$$EAR = F_{mf}/F_{m,th} - 1 \tag{3-40}$$

Neglecting the CH_4 formation, the mole fraction of oxygen at the top of the bed is obtained as follows:

$$y_{O2} = [(1 + EAR)\, y_{O2,f} - \frac{M_C\, y_{O2,f}\, A_2}{X_{Cf}}\{(2 - \xi_{CO})\ \frac{X_{Cf}}{2M_C}\,\eta_c$$

$$+ (1 - \xi_{H2})\ \frac{X_{Hf}}{2M_{H2}} + (1 - \xi_{H2S})\ \frac{X_{Sf}}{M_S} - \frac{X_{Of}}{M_{O2}}\}]$$

$$/\ [\ 1 + EAR + \frac{A_1\ A_2\ M_C\ y_{O2,f}}{X_{cf}} + \frac{w_{\ell f}}{F_{mth}}\ (\frac{X_{\ell Ca}}{M_{Ca}} + \frac{X_{\ell Mg}}{M_{Mg}})\ ] \qquad (3\text{-}41)$$

where

$$\xi_{CO} \equiv \frac{\text{CO formation rate}}{\text{carbon consumption rate}}$$

$$\xi_{H2} \equiv \frac{\text{amount of } H_2 \text{ formed}}{\text{amount of } H_2 \text{ and } H_2O \text{ formed}} \qquad (3\text{-}42)$$

$$\xi_{H2S} \equiv \frac{\text{sulfur release rate in the form of } H_2S}{\text{total sulfur feed rate}}$$

$$A_1 \equiv (X_{Cf}\ \eta_c\ \xi_{CO}/2M_C) + (X_{Of}/M_{O2}) + (1 + \xi_{H2})\ (X_{Hf}/2M_{H2})$$

$$+ (X_{hf}/M_{H2O}) \qquad (3\text{-}43)$$

The outlet concentration of CO_2, CO, H_2, H_2O, SO_2, H_2S and NO_x can then be given as follows:

$$y_{CO2} = \frac{1}{F_m}\ [\ \frac{w_{cf}\ X_{Cf}}{M_C}\ (\ 1 - \xi_{CO})\ \eta_c + W_{\ell f}\ (\frac{X_{\ell Ca}}{M_{Ca}} + \frac{X_{\ell Mg}}{M_{Mg}}) + F_{mf}\ y_{CO2,f}\ ] \qquad (3\text{-}44)$$

$$y_{CO} = \frac{1}{F_m}\ [\ \frac{w_{cf}\ X_{Cf}}{M_C}\ \xi_{CO}\ \eta_c + F_{mf}\ y_{CO,f}\ ] \qquad (3\text{-}45)$$

$$y_{H2} = \frac{1}{F_m}\ [\ \frac{w_{cf}\ X_{Hf}}{M_{H2}} + \frac{w_{cf} X_{hf}}{M_{H_2O}} + F_{mf}\ Y_{hf} + F_{mf}\ Y_{H_2f} + F_{mf}\ Y_{H_2S,f} \qquad (3\text{-}46)$$

$$- \{F_{mf}(Y_{H_2S,f} + Y_{SO_2,f}) + \frac{w_{cf} X_{Sf}}{M_S}\}\ \xi_{H_2S}]\xi_{H_2}$$

$$y_{H_2O} = \frac{1}{F_m}\ [\frac{w_{cf} X_{Hf}}{M_{H_2}} + \frac{w_{cf} X_{hf}}{M_{H_2O}} + F_{mf}\ Y_{hf} + F_{mf}\ Y_{H_2f} + F_{mf}\ Y_{H_2S,f} \qquad (3\text{-}47)$$

$$- \{F_{mf}(Y_{H_2S,f} + Y_{SO_2,f}) + \frac{w_{cf} X_{Sf}}{M_S}\}\ \xi_{H_2S}]\ (1 - \xi_{H_2})$$

ORIGINAL PAGE IS OF POOR QUALITY

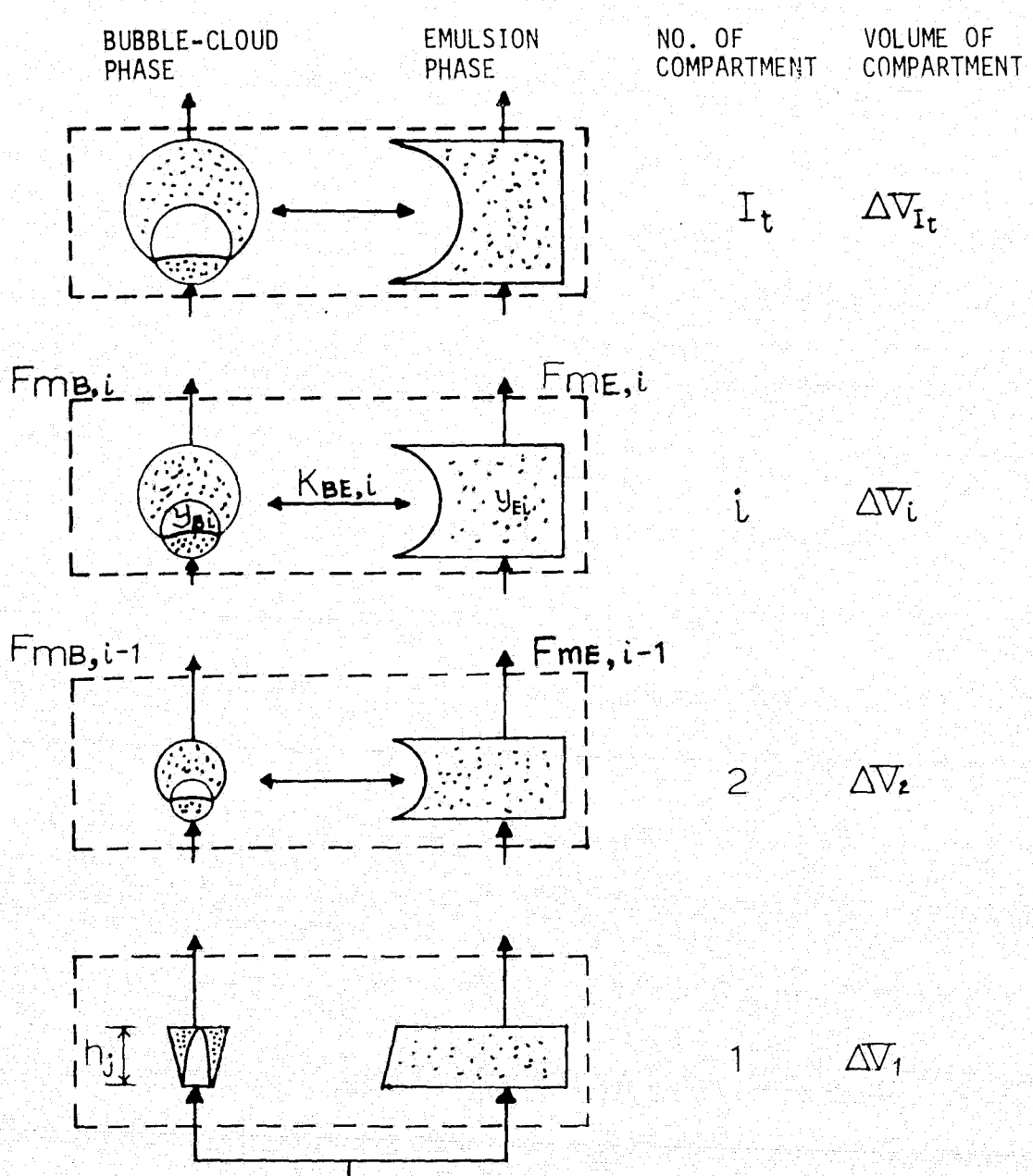


FIGURE 4 SCHEMATIC ILLUSTRATION OF THE GAS PHASE MODEL

$$y_{SO2} = \frac{1 - \eta_S}{F_m} \left[\frac{w_{cf} X_{Sf}}{M_S} + F_{mf} (y_{SO2,f} + y_{H_2S,f}) \right] \quad (3\text{-}48)$$

$$y_{H2S} = \frac{1}{F_m} \left[\frac{w_{cf} X_{Sf}}{M_S} + F_{mf} (y_{H2S,f} + y_{SO_{2,f}}) \right] \xi_{H_2S} \quad (3\text{-}49)$$

total molar flow rate, F_m, is written as:

$$F_m = (1 + EAR) F_{m,th} + A_1 w_{cf} + w_{\ell f} \left(\frac{X_{\ell Ca}}{M_{Ca}} + \frac{X_{\ell Mg}}{M_{Mg}} \right) \quad (3\text{-}50)$$

3-6. Gas-Phase Model

The basic arrangement of a compartment for the gas-phase material balance is illustrated in Figure 4. The reaction rates in bubble-cloud phase and emulsion phase are written in the form,

$$\begin{pmatrix} \text{reaction rate in} \\ \text{bubble-cloud wake} \\ \text{phase} \end{pmatrix} = (\varepsilon_{ci} - \varepsilon_{Bi}) \Delta V_{i,ef} R^*_{gB,i} \quad (3\text{-}51)$$

$$\begin{pmatrix} \text{reaction rate in} \\ \text{emulsion phase} \end{pmatrix} = (1 - \varepsilon_{ci}) \Delta V_{i,ef} R^*_{gE,i} \quad (3\text{-}52)$$

where ε_{ci} is the volume fraction of cloud including bubble. Using Murray's model (Horio and Wen, 1975b).

$$R_{Bi} \equiv \frac{\alpha_{B,i}}{\alpha_{B,i} - 1} \quad (3\text{-}53)$$

$$\alpha_{Bi} \equiv \varepsilon_{mf} u_{B,i} / u_{mf}$$

The bubble fraction, ε_{Bi}, is given by

$$\varepsilon_{B,i} = \{(u_o - u_{mf})/u_B\}_i \qquad (3\text{-}54)$$

and f'_W is the ratio of the volume of wake effectively contacting the bubble phase gas to the volume of the bubble.

In order to express the material balance it is convenient to introduce the mole fraction vectors $y_{B,i}$ and $y_{E,i}$ defined by

$$\begin{aligned} y_{B,i} &= \{y_{Bj,i}\} \qquad (j = 1\sim9) \\ y_{E,i} &= \{y_{Ej,i}\} \qquad (j = 1\sim9) \end{aligned} \qquad (3\text{-}55)$$

where j indicates the name of the gaseous species as already defined by Equation (3-2). A material balance for bubble-cloud phase and emulsion phase can be written as:

$$F_{Bm,i}\ y_{B,i} - F_{Bm,i}\ y_{B,i-1} = (\varepsilon_{ci} - \varepsilon_{bi})\ R^*_{gB,i}\ \Delta V_{i,ef} \qquad (3\text{-}56)$$

(bulk flow out - in) = (formation by reactions)

$$- K_{mBE,i}\ \varepsilon_{B,i}\ \Delta V_{i,ef}(y_{B,i} - y_{E,i}) - F_{mBE,i}\ y_{BE,i}$$

- (gas exchange) - (net flow from bubble phase to emulsion phase)

$$F_{Em,i}\ y_{E,i} - F_{Em,i}\ y_{E,i-1} = (1 - \varepsilon_{ci})\ \Delta V_{i,ef}\ R^*_{E,i}$$

$$- K_{mBE,i}\ \varepsilon_{B,i}\ \Delta V_{i,ef}\ (y_{E,i} - y_{B,i}) + F_{mBE,i}\ y_{BE,i} \qquad (3\text{-}57)$$

The last term of Equation (3-56) or (3-57) is defined as follows:

$$F_{mBE,i}\ y_{BE,i} = \begin{cases} F_{mBE,i}\ y_{B,i} & \text{if } F_{mBE,i} > 0 \\ F_{mBE,i}\ y_{E,i} & \text{if } F_{mBE,i} < 0 \end{cases} \qquad (3\text{-}58)$$

K_{mBE} is the modified gas interchange coefficient and related to K_{BE} by the following equation:

$$K_{mBE,i} = K_{BE,i}/(R\ T_i/P) \qquad (3\text{-}59)$$

3-7. Population Balance for SO_2 Absorption

The assumption of complete mixing of sorbent particles is appropriate for SO_2 absorption process, since the rate of reaction is much slower than the mean circulation cycle of particles. The distribution density function of absorbent conversion, ϕ_ℓ, introduced in section 3-4, therefore, satisfies the population balance equation (see Appendix II).

$$N_\ell \frac{d(\phi_\ell (df_\ell/d\theta)^*)}{df_\ell} = n_{\ell f}\phi_{\ell f} - n_{\ell w}\phi_\ell \qquad (3\text{-}60)$$

where it is assumed that the elutriation of the adsorbent particles is negligible. Assuming no attrition or particle breakdown, we have

$$n_{\ell f} = n_{\ell w} \qquad (3\text{-}61)$$

Substituting the rate equation (3-11) or (3-12) into Equation (3-60), we have the dimensionless equation:

$$\frac{d(\phi_\ell \lambda_\ell)}{df_\ell} = B_\ell (\phi_{\ell f} - \phi_\ell) \qquad (3\text{-}62)$$

where relative reactivity of the adsorbent λ_ℓ is defined by

$$\lambda_\ell (\bar{T}, d_\ell f_\ell) \equiv k_{v1}(\bar{T}, d_\ell, f_\ell)/k_{v1}(\bar{T}, d, 0) \quad (SO_2 \text{ reaction})$$

or (3-63)

$$\lambda_\ell = k_{v2}(\bar{T}, d_\ell, f_\ell)/k_{v2}(\bar{T}, d_\ell, 0) \quad (H_2S \text{ reaction})$$

and the parameter B_ℓ is defined as follows:

$$B_\ell \equiv \begin{cases} \dfrac{n_{\ell f}\rho_{\ell f} X_{\ell Ca}}{N_\ell M_{Ca} k_{v1}(\bar{T}, d_\ell, 0)\bar{C}_3} & (SO_2 \text{ reaction}) \\ \text{or} & (3\text{-}64) \\ \dfrac{n_{\ell f}\rho_{\ell f} X_{\ell Ca}}{N_\ell M_{Ca} k_{v2}(\bar{T}, d_\ell, 0)\bar{C}_6} & (H_2S \text{ reaction}) \end{cases}$$

The solution of Equation (3-62) for the case of fresh limestone feed, namely $\phi_{\ell f} = \delta(f_\ell)$, is given as follows (see Appendix III):

$$\phi_\ell\ (f_\ell, \overline{T}, d_\ell) = \frac{\frac{B_\ell}{\lambda_\ell}\ \exp\ [\ -\ \int_0^{f_\ell} \frac{B_\ell}{\lambda_\ell}\ df_\ell\ ]}{1\ -\ \exp\ [\ -\ \int_0^1 \frac{B_\ell}{\lambda_\ell}\ df_\ell\ ]} \qquad (3\text{-}65)$$

Therefore,

$$\hat{k}_{vi}(\overline{T}, d_\ell) = \int_0^1 k_{vi}\ (\overline{T}, d_\ell, f_\ell)\ \phi_\ell\ df_\ell$$

$$= k_{vi}\ (\overline{T}, d_\ell, 0)\ \int_0^1 \lambda_\ell\ \phi_\ell\ df_\ell$$

$$= k_{vi}\ (\overline{T}, d_\ell, 0)\ \hat{\lambda}_\ell \qquad (3\text{-}66)$$

Using the parameter B_ℓ defined by Equation (3-64), the relation (3-37) can be written in a simple form

$$\hat{f}_\ell = \hat{\lambda}_\ell / B_\ell \qquad (3\text{-}67)$$

where it is assumed that only one of the reactions 1 and 2 is taking place. The reactivity of the adsorbent can be obtained as a function of $\hat{f}_\ell$, $\overline{T}$ and d_ℓ by the following technique:

1. Specify $\overline{T}$ and d_ℓ
2. Specify B_ℓ
3. Obtain $\phi_\ell\ (f_\ell)$ from (3-65) and calculate $\hat{\lambda}_\ell$
4. Obtain $\hat{f}_\ell$ from (3-67)
5. Specify another B_ℓ and repeat 2~4
6. Specify another $\overline{T}$ and d_ℓ and repeat 2~5
7. $\hat{\lambda}_\ell = \hat{\lambda}_\ell\ (\hat{f}_\ell,\ \overline{T},\ d_\ell)$ (3-68)

In order to consider the size distribution of the adsorbent, the distribution density function $\phi_{\ell s}\ (d_\ell)$ is introduced as

$$\begin{pmatrix}\text{number fraction of absorbent particles which have the diameter between } d_\ell \text{ and } d_\ell + d\ (d_\ell)\end{pmatrix} = \phi_{\ell s}\ (d_\ell)\ d(d_\ell)$$

$$\int_0^{d_{max}} \phi_{\ell s}\ (d_\ell)\ d(d_\ell) = 1$$

Thus, the relationship between the average reactivity $\hat{\lambda}_\ell$ and the average conversion of the limestone is obtained in the form

$$< \hat{\lambda}_\ell > \equiv \int_0^{d\ max} \hat{\lambda}_\ell\ (\hat{f}_\ell,\ \overline{T},\ d_\ell)\ \phi_{\ell s}\ (d_\ell)\ d(d_\ell) \qquad (3\text{-}69)$$

3-8 Population balance for char combustion segregation and elutriation

For the combustion of fairly large particles, the rate of solids mixing may become the dominant factor since the segregation of char particles greatly affects the combustion. According to the observation by Avdesian and Davidson (1973) a char particle whose initial size was greater than 1.3 mm burned out in their FBC taking more than 160 seconds. Their results are shown in Figure 5. The superficial gas velocity and the carbon fraction were 38.3 cm/sec and 0.9% respectively. On the other hand, unless the bed internals are present, the circulation cycle, θ_c, is obtained from Equation (2-9) for a bed of L_{mf} = 60 cm as 1.8 sec (f_W = 1 is assumed). Therefore, solids in the bed seem to undergo good circulation to disperse the char particle over the bed.

However, for fine particles in a deep bed the rates of reaction and circulation may be of comparable extent. In this range of particle size elutriation plays an important role in determining the combustion efficiency.

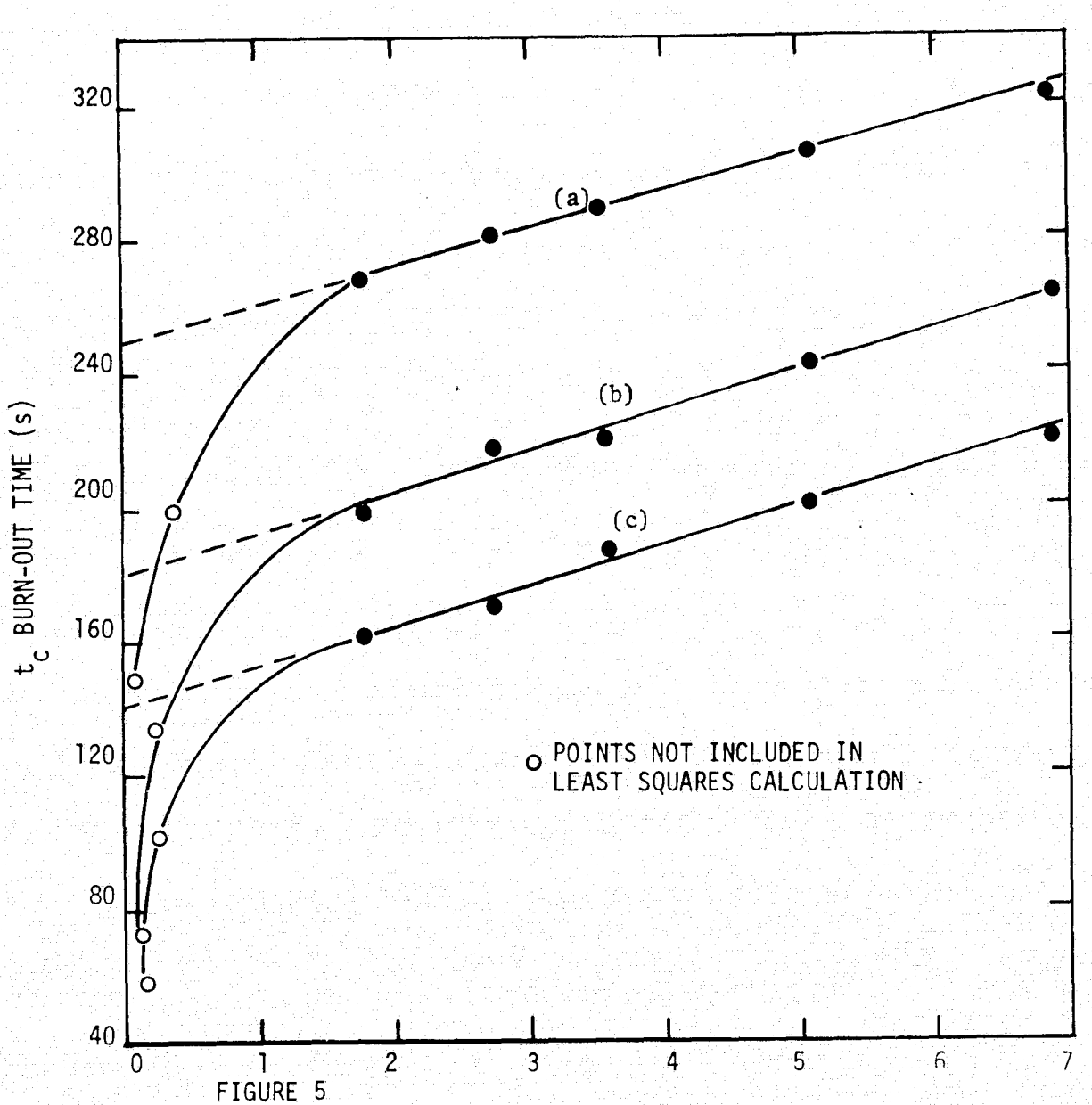


FIGURE 5

(d_i^2) (INITIAL AVERAGE CHAR PARTICLE DIAMETER)^2(mm^2)

d_a = 0.39 mm; m = 3.6g CARBON; U_o = 46 mm/s;
ρ_c = 720 kg CARBON/m^3

(a) U = 214 mm/s; (b) U = 300 mm/s; (c) U = 383 mm/s

-Burn-out time as a function of the initial average char particle diameter (Avdesian and Davidson (1973)).

$$n_{d,i} = \begin{cases} > 0 & \text{if} \quad v_{E,i} < 0 \\ 0 & \text{if} \quad v_{E,i} \geq 0 \end{cases} \qquad i = 2, I_t$$

$$n_{u,i} = \begin{cases} > 0 & \text{if} \quad v_{E,i} > 0 \\ 0 & \text{if} \quad v_{E,i} \leq 0 \end{cases} \qquad i = 2, I_t$$

where $v_{E,i}$ denotes the volumetric flow rate in the cloud-emulsion phase and is positive for upward flow.

From the total number balance of char particles, the initial conditions for $\phi_{B,i}$ and $\phi_{E,i}$ are derived as follows:

$$N_{B,i}\, \phi_{B,i}\, (0)\, (dy/d\theta)^{*}_{B,i,y=0} = n_{BE,i} - n_{EB,i} - n_{B,i-1} + n_{B,i} \qquad (i = 1, I_t) \qquad (3\text{-}74)$$

$$N_{E,i}\, \phi_{E,i}\, (0)\, (dy/d\theta)^{*}_{E,i,y=0} = n_{EB,i} - n_{BE,i} - n_{f,i} - n_{u,i-1} - n_{d,i+1} + n_{u,i} + n_{d,i} + n_{w,i} \qquad (i = 1, I_t) \qquad (3\text{-}75)$$

The functions $\phi_{B,i}$ and $\phi_{E,i}$ also must satisfy the normalization condition,

$$\int_0^1 \phi_{B,i}\, dy = \int_0^1 \phi_{E,i}\, dy = 1 \qquad (3\text{-}76)$$

The assumption of complete mixing in each compartment is expressed by

$$N_{B,i}/\Delta V_{sB,i} = n_{B,i+1}/v_{B,i+1} = n_{BE,i}/v_{BE,i} \qquad (3\text{-}77)$$

$$N_{E,i}/\Delta V_{sE,i} = n_{d,i}/v_{d,i} = n_{u,i+1}/v_{u,i+1} = n_{w,i}/v_{w,i} = n_{EB,i}/v_{EB,i} \qquad (3\text{-}78)$$

where N is the number of char particles in a cell and n is the number flow rate of char particles between cells. The volume of cell, $\Delta V_{sB,i}$ and $\Delta V_{sE,i}$, and the volumetric flow rate of particles including ash and

limestone particles, $v_{B,i}$, $v_{BE,i}$, $v_{EB,i}$, $v_{u,i}$ and $v_{d,i}$ are defined as follows:

$$\Delta V_{sB,i} = \Delta V_{i,ef}\ \varepsilon_{B,i}\ f_W' \tag{3-79}$$

$$\Delta V_{sE,i} = \Delta V_{i,ef}\ \{1 - \varepsilon_{B,i}\ (1 + f_W')\}(1 - \varepsilon_{mf}) \tag{3-80}$$

$$v_{B,i} = (u_o - u_{mf})_i\ A_{t,i}\ f_W\ (1 - \varepsilon_{mf}) \tag{3-81}$$

$$v_{EB,i} = K_{sBE,i}\ \Delta V_{i,ef}\ (1 - \varepsilon_{B,i}) \tag{3-82}$$

$$v_{BE,i} = v_{EB,i} + v_{B,i} - v_{B,i+1} + \varepsilon_{Bi}\ f_W'\ \Delta V_{i,ef} \frac{r^*_{cBi}\ M_C}{X_{Cf}}\ (1/\rho_{cf} - X_{Af}/\rho_A) \tag{3-83}$$

$$v_{u,i} = \begin{cases} v_{E,i} & (\text{if } v_{E,i} > 0) \\ 0 & (\text{if } v_{E,i} \leq 0) \end{cases} \qquad i = 2,\ I_t \tag{3-84}$$

$$v_{d,i} = \begin{cases} v_{E,i} & (\text{if } v_{E,i} < 0) \\ 0 & (\text{if } v_{E,i} \geq 0) \end{cases} \qquad i = 2,\ I_t \tag{3-85}$$

From a volume balance for the i th level

$$v_{E,i} = v_{net,i} - v_{B,i} \tag{3-86}$$

The overall volume balance for the i th compartment gives

$$v_{net,i+1} = v_{net,i} + v_{B,i} - v_{B,i+1} + v_{f,i} - v_{w,i} - \frac{\Delta V_i M_C}{X_{Cf}}\ \{(\varepsilon_{Wi} - f_W'\ \varepsilon_{B,i})\ r^*_{cB,i} + (1 - \varepsilon_{W,i} - \varepsilon_{B,i}) r^*_{cE,i}\}\ \chi\ (1/\rho_{cf} - X_{Af}/\rho_A) \tag{3-87}$$

In Equations (3-83) and (3-87) ρ_A denotes the density of ash particles formed after combustion, and $r^*_{cB,i}$ and $r^*_{cE,i}$ are defined as

$$\left.\begin{aligned} r^*_{cB,i} &\equiv r^*_{3B,i} + r^*_{4B,i} + r^*_{5B,i} \\ r^*_{cE,i} &\equiv r^*_{3E,i} + r^*_{4E,i} + r^*_{5E,i} \end{aligned}\right\} \tag{3-88}$$

The particle exchange coefficient, $K_{sBE,i}$ in Equation (3-82) is a parameter proportional to $(1/D_B)$ as reported by Kobayashi, Chiba and Ihara (1971).

The following relations are the boundary conditions for the bottom and top compartments.

$$v_{u,1} = v_{d,1} = v_{B,1} = 0 \tag{3-89}$$

$$v_{u,I_t+1} = v_e \tag{3-90}$$

$$v_{B,I_t+1} = v_{d,I_t+1} = 0$$

where v_e is the total volumetric elutriation rate including ash particles.

The shrinking rate of a single char particle $(dy/d\theta)^*$ in Equations (3-70) and (3-71) is given:

$$(dy/d\theta)^*_{B,i} = -\frac{2\,M_C}{\rho_{ch}\,X_C\,d_{cm}}\,(k_3\,\overline{C}_1 + k_4\,\overline{C}_1 + k_5\,\overline{C}_4)_{B,i} \tag{3-91}$$

$$(dy/d\theta)^*_{E,i} = -\frac{2\,M_C}{\rho_{ch}\,X_C\,d_{cm}}\,(k_3\,\overline{C}_1 + k_4\,\overline{C}_1 + k_5\,\overline{C}_4)_{E,i} \tag{3-92}$$

These equations are adequate to determine the axial distribution of size distribution function ϕ_B and ϕ_E for the given temperature and gas phase concentration.

The system described by the population balance equations (3-70) and (3-71), overall number balance (3-74) and (3-75) and the integral constraints (3-76) also satifies the material balance as proven in Appendix IV. However, it is convenient to develop material balance equations, when we need to device a steadily converging numerical algorithm.

For the weight fraction of carbon in the solids of the i th cell we have the following material balance equations:

(bubble-wake phase)

$$w_{B,i-1}\, x_{B,i-1} + w_{EB,i}\, x_{E,i} = (w_{B,i} + w_{BE,i})\, x_{B,i} + \Delta V_i\, \varepsilon_{B,i}\, f'_W\, r^*_{cB,i}\, M_C \qquad (3\text{-}93)$$

(cloud-emulsion phase)

$$w_{d,i+1}\, x_{E,i+1} + w_{u,i-1}\, x_{E,i-1} + w_{BE,i}\, x_{B,i} + w_{f,i}\, x_{f,i} = (w_{d,i} + w_{u,i} + w_{EB,i} + w_{w,i})\, x_{E,i} + \Delta V_i \{(\varepsilon_{c,i} - \varepsilon_{B,i}\, f'_{W,i})\, r^*_{cB,i} + (1 - \varepsilon_{c,i} - \varepsilon_{tube,i})\, r^*_{cE,i}\}\, M_C \qquad (3\text{-}94)$$

where

$$\left.\begin{aligned} w_{B,i} &= v_{B,i}\, \rho_{sB,i} \\ w_{E,i} &= v_{E,i}\, \rho_{sE,i} \\ w_{BE,i} &= v_{BE,i}\, \rho_{sB,i} \\ w_{EB,i} &= v_{EB,i}\, \rho_{sE,i} \\ w_{u,i} &= v_{u,i}\, \rho_{sE,i-1} \\ w_{d,i} &= v_{d,i}\, \rho_{sE,i} \end{aligned}\right\} \qquad (3\text{-}95)$$

and correspondingly

$$\left.\begin{aligned} w_{u,1} &= w_{d,1} = w_{B,1} = 0 \\ w_{u,I_t+1} &= v_{u,I_t+1}\, \rho_{E,i} \\ w_{B,I_t+1} &= w_{d,I_t+1} = 0 \end{aligned}\right\} \qquad (3\text{-}95)$$

The two phase backflow cell model illustrated in Figure 2 is applied to FBC to simulate the process of char combustion, circulation and elutriation in Level III.

The size distribution density function of char particles in bubble-wake phase $\phi_{B,i}$ and in cloud-emulsion phase $\phi_{E,i}$ satisfies the following population balance equations (see Appendix II)

$$N_{B,i} \frac{d\left[\phi_{B,i}(dy/d\theta)^{*}_{BW,i}\right]}{dy} = n_{EB,i}\,\phi_{E,i} + n_{B,i-1}\,\phi_{B,i-1} - (n_{BE,i} + n_{B,i})\phi_{B,i} \qquad (i = 2, I_t - 1) \qquad (3\text{-}70)$$

$$N_{E,i} \frac{d\left[\phi_{E,i}\,(dy/d\theta)^{*}_{CE,i}\right]}{dy} = n_{BE,i}\,\phi_{B,i} - n_{EB,i}\phi_{E,i} + n_{f,i}\,\phi_{f,i} + n_{u,i}\,\phi_{E,i-1} + n_{d,i+1}\,\phi_{E,i+1} - (n_{u,i} + n_{d,i} + n_{w,i})\phi_{E,i} \qquad (i = 2, I_t - 1) \qquad (3\text{-}71)$$

For $i = I_t$ (top compartment)

$$N_{B,i} \frac{d\left[\phi_{B,i}\,(dy/d\theta)^{*}_{BW,i}\right]}{dy} = n_{EB,i}\,\phi_{E,i} + n_{B,i-1}\,\phi_{B,i-1} - (n_{BE,i}+n_{B,i})\phi_{B,i}$$

$$N_{E,i} \frac{d\left[\phi_{E,i}\,(dy/d\theta)^{*}_{CE,i}\right]}{dy} = n_{BE,i}\,\phi_{B,i} - n_{EB,i}\,\phi_{E,i} + n_{f,i}\,\phi_{f,i} + n_{u,i-1}\,\phi_{E,i-1} - n_e\,\phi_e - (n_{d,i} + n_{w,i})\phi_{E,i} \qquad (3\text{-}72)$$

For $i = 1$ (bottom compartment)

$$N_{B,i} \frac{d\left[\phi_{B,i}\,(dy/d\theta)^{*}_{BW,i}\right]}{dy} = n_{EB,i}\,\phi_{E,i} - (n_{BE,i} + n_{B,i})\,\phi_{B,i}$$

$$N_{E,i} \frac{d\left[\phi_{E,i}\,(dy/d\theta)^{*}_{CE,i}\right]}{dy} = n_{BE,i}\,\phi_{B,i} - n_{EB,i}\,\phi_{E,i} + n_{f,i}\,\phi_{f,i} + n_{d,i+1}\,\phi_{E,i+1} - (n_{u,i} + n_{w,i})\phi_{E,i} \qquad (3\text{-}73)$$

3-9 Heat Balance

Assuming that the temperature differences between gas and solids and between the solids in cloud, in wake and in emulsion phases are negligible the following equations are derived for axial temperature distribution:

$$c_s \{(S_i - 1)\, w_{net,i} + w_{mix,i}\}\, T_{i+1}$$

(heat flow in from (i+1)th cell)

$$-[c_s\{S_i\, w_{net,i} + (S_{i-1} - 1)\, w_{net,i-1} + w_{mix,i} + w_{mix,i-1} + w_{wi}\} + c_{gm,i}\, F_{gm}]\, T_i$$

(heat flow out from ith cell)

$$+[c_s\, (S_{i-1}\, w_{net,i-1} + w_{mix,i-1}) + c_{gm,i-1}\, F_{gm}]\, T_{i-1}$$

(heat flow in from i-1th cell)

$$+ r^*_{ci} M_C \Delta V_{i,ef}\, (q_c/X_{Cf}) - w_{\ell f}\, q_\ell\, \Delta V_{i,ef}\, (1 - \varepsilon_{Bi})/V_{mf,ef}$$

(heat generated by combustion) (heat consumed by calcination of limestone)

$$+ w_{fi} c_{sfi} T_{fi} = U_i a_{HEi} \Delta V_i \quad (T_i - T_{wi}) \qquad (3\text{-}96)$$

(sensible heat accompanied by solids feed) (heat recovered by cooling tubes)

where

$$S_i = \begin{cases} 0 & \text{if } w_{net,i} \leq 0 \\ 1 & \text{if } w_{net,i} > 0 \end{cases} \qquad (3\text{-}97)$$

The reaction rate r^*_{ci} in Equation (3-96) is defined by

$$r^*_{c,i} = (\varepsilon_{c,i} - \varepsilon_{B,i})\, r^*_{cB,i} + (1 - \varepsilon_{c,i} - \varepsilon_{tube,i})\, r^*_{cE,i} \qquad (3\text{-}98)$$

The net flow rate, $w_{net,i}$ and the backflow rate, w_{mix}, is calculated by

$$w_{net,i} - w_{net,i-1} = w_{f,i}\,(1 - X_{vf,i}) - w_{w,i} - r^*_{c,i}\, M_c \Delta V_i \qquad (3\text{-}99)$$

$$w_{mix} = (u_o - u_{mf})\, A_t f_W \rho_s\, (1 - \varepsilon_{mf}) \qquad (3\text{-}100)$$

For calculating reaction rates, the temperature of char particles, T_c, is treated separately from bed temperature, T, assuming a temperature difference exists between char particles and the surrounding gas and taking the following heat balance:

$$\frac{2\lambda'}{d_c}\,(T_c - T) + \varepsilon'\sigma\,(T_c^4 - T^4) = r_c\,(T_c)\, M_C q_c / X_{Cf}\, \pi d_p^2 \qquad (3\text{-}101)$$

where ε' is the emissivity of particles, λ' is the thermal conductivity of the gas surrounding char particles and σ is the Stefan-Boltzman constant.

Section IV

LEVEL I MODEL FOR FBC

The general model defined in Section 3 is simplified by imposing the assumption of complete mixing for solids.

In this case the size distribution of char particles withdrawn from the bed is the same as that of char particles in the bed. Therefore,

$$\psi_{vw} = \psi_v$$

$$\phi_w = \phi$$

Instead of the equations introduced in 3-8 the following simple equation can be used to obtain the size distribution of char:

$$N_c \frac{d\phi R^*}{dy} + n_{cw}\,\phi = n_{cf}\,\phi_f - n_{ce}\,\phi_e \qquad (4\text{-}1)$$

where

$$R^* \equiv (dy/d\theta)^* = -2M_C r_c^* / (\pi d_c^2\, d_{cm}\, \rho_{ch}\, X_c) \qquad (4\text{-}2)$$

$$r_c^* \equiv \Sigma r_{ci}^*\ \Delta V_i / \Sigma\, \Delta V_i \doteq (N_c/V_{mf})\pi d_c^2\, k_{c0}\, \lambda_c\,(y)\, \overline{C}_{O2} \qquad (4\text{-}3)$$

where $\lambda_c\,(y)$ is the relative reactivity of char. Neglecting reaction 5,

$$k_{c0}\,\lambda_c(y) = k_3\, k_x \qquad (4\text{-}4)$$

The solution of the differential equation (4-1) under the constraint

$$\int_0^1 \phi(y)\, dy = 1$$

is obtained as follows:

$$\phi \frac{Y(y)}{\lambda_c(y)}\ [C_c - B_{cf} Z_f(y)] \qquad (4\text{-}5)$$

where

$$Y(y) \equiv \exp\ [B_{cw} \int_0^y \frac{1 + (\Theta A_t/W_b)K^*}{\lambda_c}\ dy] \qquad (4\text{-}6)$$

$$Z_f(y) = \int_0^y (\phi_f/Y)\, dy \tag{4-7}$$

$$C_c = 1 + B_{cf} \int_0^1 [Y(y) Z_f(y)/\lambda_c(y)]dy / \int_0^1 [Y(y)/\lambda_c(y)]dy \tag{4-8}$$

$$B_{cw} = \frac{d_{cm}\, \rho_{ch}\, X_C}{2\, M_C\, \Theta\, \overline{k_{c0}\, C_{02}}} \tag{4-9}$$

$$B_{cf} = B_{cw} \frac{n_{cf}}{n_{cw}} \tag{4-10}$$

According to the definition of B_{cw}, we obtain the following relation from Equations (3-26), (3-27) and (3-31):

$$B_{cw} = \frac{3 < \lambda_c\, y^2 > (1 - \eta_c)}{\left(\psi_v + \frac{A_t\, \Theta}{W_b} < K^* y^3 >\right) \eta_c} \tag{4-11}$$

The gas phase model shown in Section 3-6 gives a solution for the exit oxygen concentration in the form

$$C_{02,1} = f_1(N_c < \lambda_c\, y^2 > \pi d_{cm}^2,\ k_{c0},\ L_f,\ u_o,\ u_{mf},\ C_{02,0} \ldots) \tag{4-12}$$

The form of the function, f_1, is dependent on the assumptions for the gas hydrodynamics in the FBC. The first term enclosed in the parentheses of Equation (4-12) is part of the coefficients in the reaction rate equation and $C_{02,0}$ represents the concentration of oxygen above the distributor plate.

On the other hand, the overall material balance for oxygen in the gas phase is given by

$$F_m\, (y_{02,0} - y_{02,1}) = N_c < \lambda_c\, y^2 > \pi d_{cm}^2\, \overline{k_{c0}\, C_{02}} \tag{4-13}$$

From Equations (3-25), (3-26) and (3-27) the outlet oxygen concentration can be related to the combustion efficiency as follows:

$$y_{O2,1} = y_{O2,0} - \frac{w_{cf}\, X_{Cf}}{M_C\, F_m}\, \eta_c \qquad (4\text{-}14)$$

Using Equations (4-12), (4-13) and (4-14), we can obtain the following relationship between η_c and $\overline{k_{c0}\, C_{O2}}$ where the term $N_c < \lambda_c\, y^2 >$ and $C_{O2,1}$ are already eliminated.

$$f_2(\overline{k_{c0}\, C_{O2}},\ \eta_c,\ L_f,\ u_o,\ u_{mf},\ C_{O2,0} \ldots) = 0 \qquad (4\text{-}15)$$

where f_2 is a function dependent on the assumptions for fluidized bed hydrodynamics.

If we can assume that the gas phase is completely mixed Equation (4-15) can be simplified as

$$\overline{k_{c0}\, y_{O2}} = \overline{k}_{c0}\, [\, y_{O2,f}\, F_{mf}/F_m - w_{cf}\, X_{Cf}\, \eta_c/M_C\, F_m] \qquad (4\text{-}15)'$$

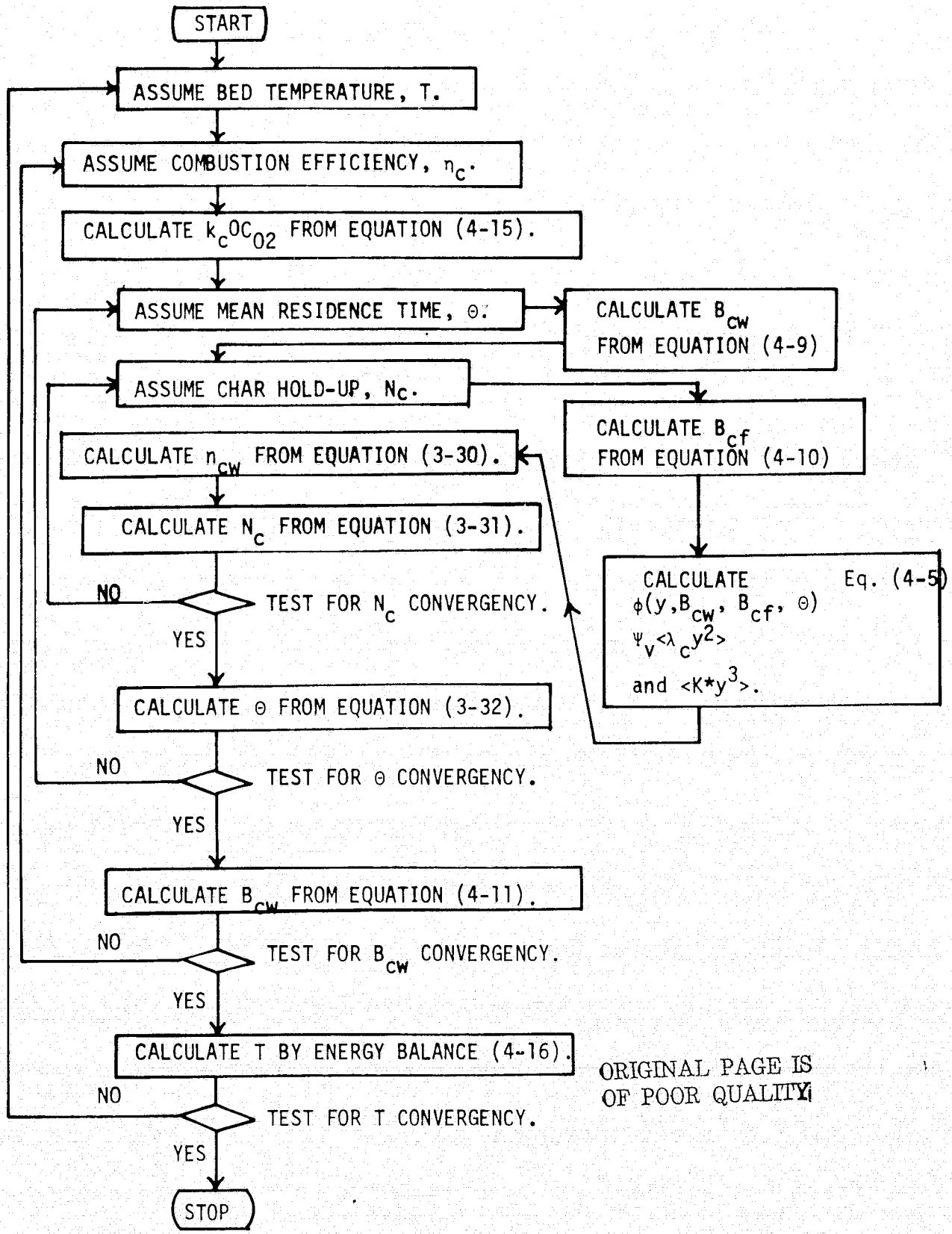
In the case of plug flow we obtain

$$\overline{k_{c0}\, y_{O2}} = \overline{k}_{c0}\, \left[\, \frac{w_{cf}\, X_{Cf}\, \eta_c}{M_C\, F_m}\, \right] / \ln \left[\, \frac{1}{1 - \dfrac{w_{cf}\, X_{Cf}\, \eta_c}{M_C\, F_{mf}\, y_{O2,f}}}\, \right] \qquad (4\text{-}15)''$$

For shallow fluidized bed combustors Equation (4-15)' is preferred compared with Equation (4-15)''. In such cases as in the gas phase model presented in Section 3-6, it may be too complicated to obtain the term $\overline{k_{c0}\, y_{O2}}$ analytically and numerical solution by iteration technique becomes necessary.

By an overall heat balance, the bed temperature $\overline{T}$ is obtained as

$$\overline{T} = \frac{\begin{bmatrix} c_{gmf}\, F_{mf}\, T_{gt} + c_{cf}\, w_{cf}\, T_{cf} + c_{\ell f}\, w_{\ell f}\, T_{\ell f} \\ + q_c\, w_{cf}\, (1 - \eta_c) - q_\ell\, w_{\ell f} + U\, A_{HE}\, \overline{T}_w \end{bmatrix}}{\begin{bmatrix} c_{gm}\, F_m + c_{ch}\, w_{cf}\, (X_{Cf} + X_{Af})(1 - \eta_c) \\ + c_A\, w_{cf}\, X_{Af}\, \eta_c + U\, A_{HE} \end{bmatrix}} \qquad (4\text{-}16)$$



ORIGINAL PAGE IS
OF POOR QUALITY

FIGURE 6. FLOW DIAGRAM FOR THE COMPUTATION OF COMBUSTION EFFICIENCY.

The algorithm for the computation of Level I model is shown in Figure 6.

The purpose of developing this Level I model is to compute the size distribution of char particles and to estimate the loss of carbon resulting from elutriation of fines. As already discussed previously the assumption of complete mixing is acceptable for the modeling of FBC, unless the solids mixing is so restricted by the presence of the internals.

Section V

V. LEVEL II MODEL FOR FBC

The major objective of the development of the Level II model is to predict the effect of axial solids mixing on the temperature profile and on the distribution of char particles along the bed axis.

The following assumptions are made:

(1). The density functions of char particle size distribution in the bubble phase $\phi_{B,i}$ and in the emulsion phase $\phi_{E,i}$ ($i = 1\sim I_t$) are approximately equal to each other and, therefore, the mean diameter of char is uniform throughout the bed.

(2). The difference between the weight fractions of char in the bubble phase and the emulsion phase is negligible. However, an axial distribution of carbon exists which can be designated by the carbon weight fraction in the bed, x.

The equations introduced in Sections 3-1~7 and Section 3-9 may still hold even the above assumptions are made. Because of the assumption (1), equations for ϕ derived in Section IV are used, instead of equations for $\phi_{B,i}$ and $\phi_{E,i}$ derived in Section 3-8. In place of Equations (3-93)~(3-95) the following equation is obtained for the weight fraction of carbon, x_i:

$$\begin{aligned}
&\{(S_i - 1)w_{net,i} + w_{mix,i}\} x_{i+1} \\
&-\{S_i\, w_{net,i} + (S_{i-1} - 1)w_{net,i-1} + w_{mix,i} + w_{mix,i-1} + w_{wi}\}x_i \\
&+\{S_{i-1}\, w_{net,i-1} + w_{mix,i-1}\}\, x_{i-1} \qquad (5\text{-}1) \\
&= r^*_{ci}\, \Delta V_{i,ef}\, M_C - w_{fi} x_{fi}
\end{aligned}$$

The net flow rate, $w_{net,i}$, can be obtained from Equation (3-99).

In the present programming of the Level II model further simplifications are made. The additional assumptions are:

(3). In oxygen rich operation reactions 2 and 7 can be neglected.

(4). In fuel rich operation reactions 1 and 6 can be neglected.

(5). Reactions 5 and 8 can be neglected.

(6). Oxygen consumption for reaction 1 is neglected. Equations (3-56) and (3-57) are used to solve oxygen and sulfur dioxide balances.

Letting $Y_{B \text{ or } E,i}$ denote the mole fraction of oxygen, equations (3-56) and (3-57) become,

$$F_{Bm,i}Y_{Bi} - F_{Bm,i-1}Y_{B,i-1} + (1 - 0.5\ \xi_{CO})\ r^{*}_{cB,i}\Delta V_i\ \varepsilon_{W,i} = K_{BE,i}(P/RT_i)\ \Delta V_i \varepsilon_{B,i}\ (Y_{E,i}-Y_{B,i}) \tag{5-2}$$

$$F_{Em,i}Y_{E,i} - F_{Em,i-1}Y_{E,i-1} + (1 - 0.5\ \xi_{CO})\ r^{*}_{cE,i}\ \Delta V_i \times(1 - \varepsilon_{W,i} - \varepsilon_{B,i} - \varepsilon_{tube,i}) = K_{BE,i}(P/RT_i)\ \Delta V_i \varepsilon_{B,i}\ (Y_{B,i} - Y_{E,i}) \tag{5-3}$$

Let $Y'_{B \text{ or } E,i}$ designates either mole fraction of sulfur dioxide or hydrogen sulfide, depending on the case, we get

$$F_{Bm,i}\ Y'_{B,i} - F_{Bm,i-1}\ Y'_{B,i-1} + \Delta V_i\ \varepsilon_{W,i}(r^{*}_{\ell B,i} - \frac{X_{Sf}}{X_{Cf}}\ r^{*}_{cB,i}) = K_{BE,i}\ (P/RT_i)\ \Delta V_i\ \varepsilon_{B,i}\ (Y'_{E,i} - Y'_{B,i}) \tag{5-4}$$

$$F_{Em,i}\, Y'_{Ei} - F_{Em,i-1}\, Y_{E,i-1} + \Delta V_i (1 - \varepsilon_{W,i} - \varepsilon_{B,i} - \varepsilon_{tube,i}) \times \left(r^*_{\ell E,i} - \frac{X_{Sf}}{X_{Cf}}\, r^*_{cE,i}\right) \qquad (5\text{-}5)$$

$$= K_{BE,i}(P/RT_i)\, \Delta V_i\, \varepsilon_{B,i}\, (Y'_{B,i} - Y'_{E,i})$$

where the term $(X_{Sf}/X_{Cf})\, r^*_{c\,B \text{ or } E,i}$ denotes the generation rate of SO_2 or H_2S.

The equations applied for calculation are:

[Gas phase concentration]

Oxygen:	Equations (5-2)* and (5-3)*
Sulfur dioxide or hydrogen sulfide:	Equations (5-4)* and (5-5)*
Other species:	Equations (3-44)~(3-47)

[Axial distribution of char concentration]

Equations (5-1)*, (3-99)*

[Axial distribution of temperature]

Equation (3-96)*

[Reactivity of sulfur adsorbent]

Equations (3-35), (3-65), (3-67) and (3-68)

[Average reactivity of char]

Equations (4-5) and (3-24)

where the equations marked by the symbol, *, have the following boundary conditions:

1). For Equations (5-2) and (5-3)

$$Y_{E,0} = Y_{B,0} = y_{O2,f}\, F_{mf}/F_m$$

2). For Equations (5-4) and (5-5)

$$Y'_{E,0} = Y'_{B,0} = y_{SO2,f} F_{mf}/F_m$$

$$\text{of } y_{H2S,f} F_{mf}/F_m$$

3) For Equations (5-1), (3-99) and (3-96)

$$w_{net,1} = 0$$

$$w_{net,I_t+1} = w_e$$

$$w_{mix,1} = 0$$

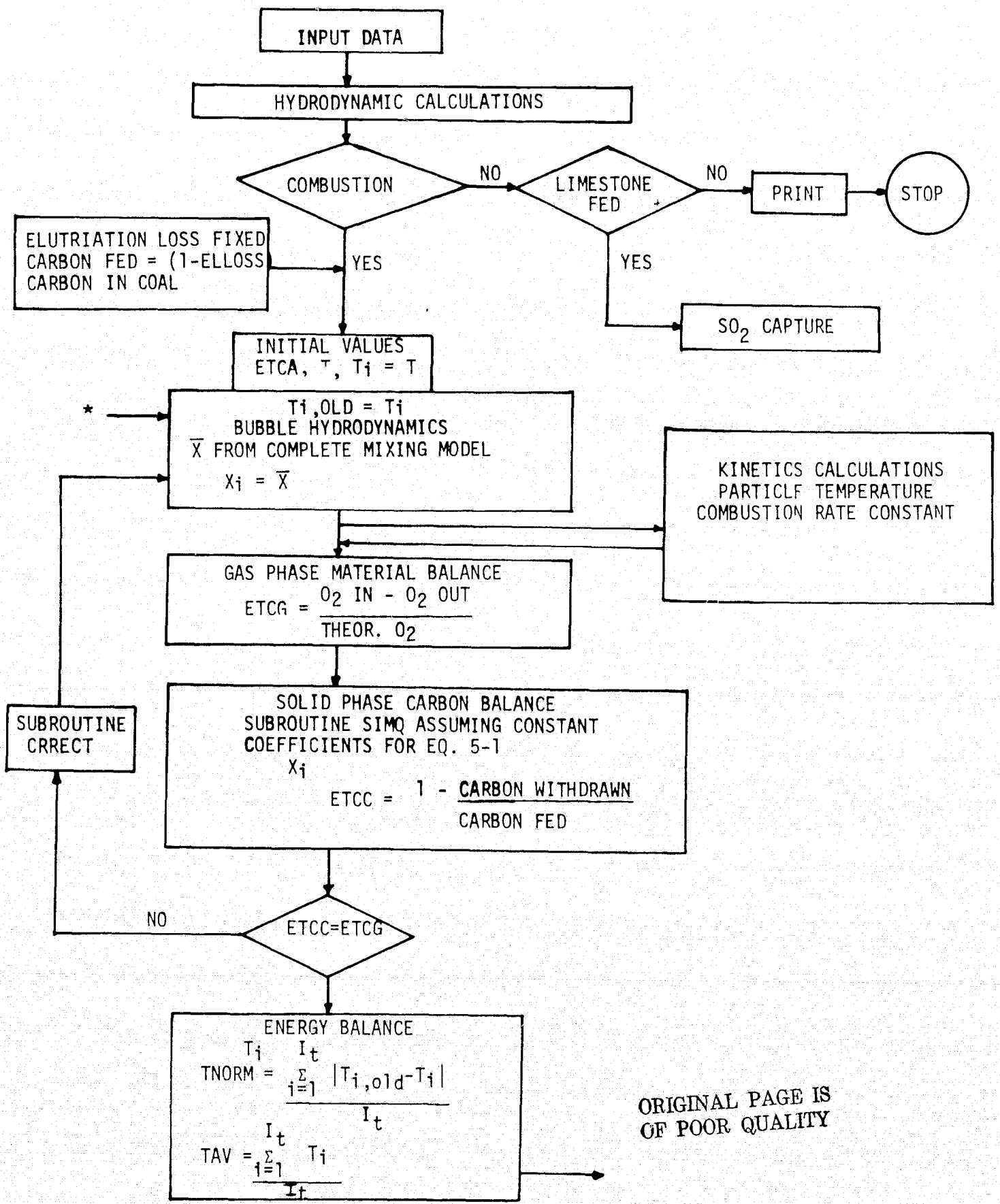
$$w_{mix,1} = 0$$

4) For Equation (3-96)

$$T_o = T_{gf}$$

$$c_{gm0} = c_{gmf}$$

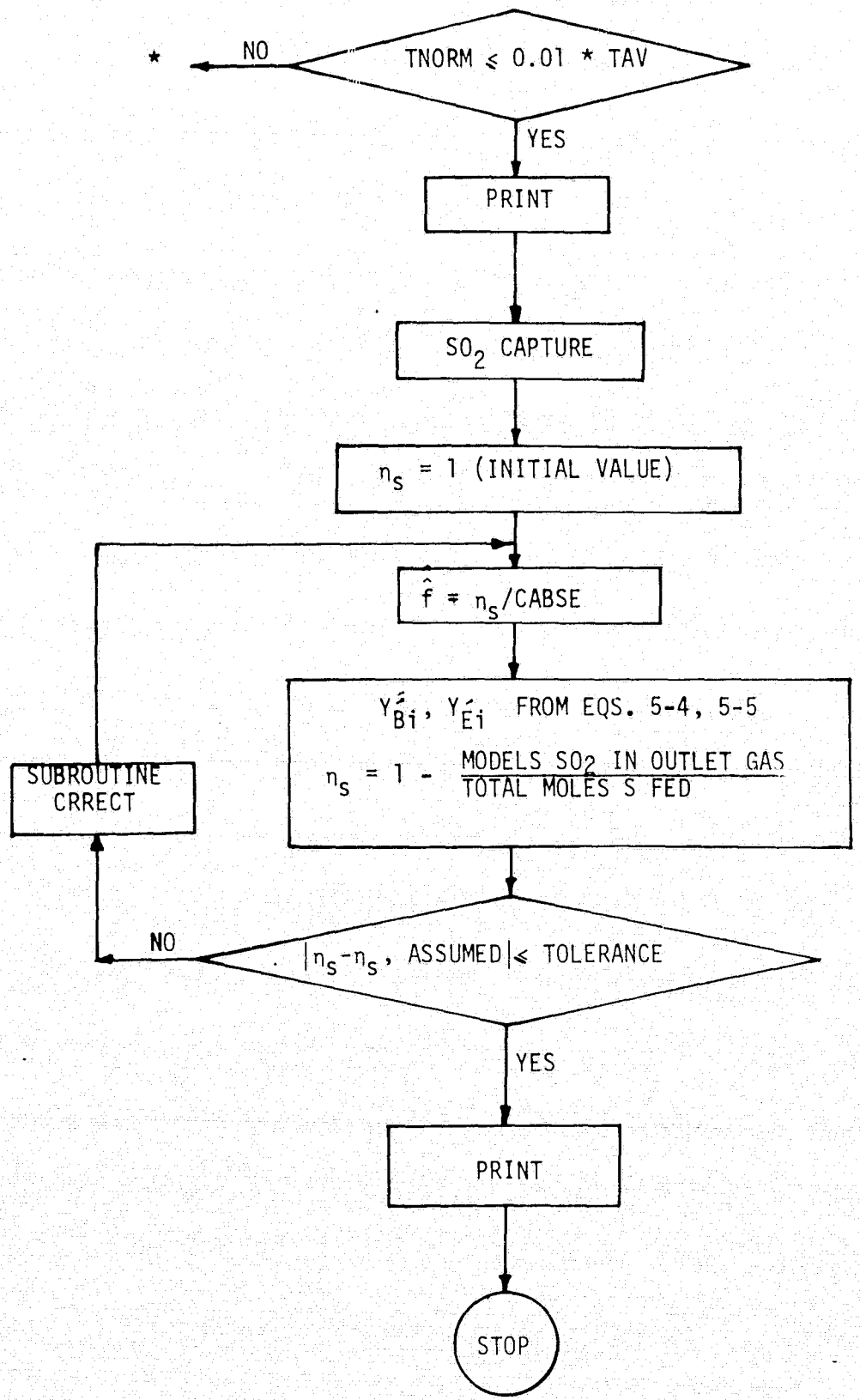
The system involves a diffusion (i.e. backflow) term and nonlinear reaction terms. Therefore, iteration is necessary to solve the equations. The flow diagram illustrating the iteration procedure is shown in Figure 7.



ORIGINAL PAGE IS
OF POOR QUALITY

FIGURE 7 FLOW DIAGRAM FOR LEVEL II MODEL

FIGURE 7 (CONTINUED)



Section VI

LISTS OF LEVEL I AND II COMPUTER PROGRAMS

6-1. LEVEL I PROGRAM

```
C
C
C
C
C     A MODEL FOR COMBUSTION AND ELUTRITIATION BEHAVIORS
C     OF A FLUIDIZED BED COMBUSTOR        M. HORIO   1976
C
C
C     MOLECULAR WEIGHT
0001        REAL  MC,MH2,MS,MO2,MN2,MH2O,MCA,MAIR
0002        DATA  MC,MH2,MS,MO2,MN2,MH2O,MCA,MAIR/12.,2.,32.,32.,28.,18.,
           140.09,28.8/
0003        DIMENSION DP0(35),DPF(35),DP(201),FRACT(35)
0004        DIMENSION PHIFW(201),PHIW(201),PHIFW(201)
           1,DPF0(35),FRACT0(35)
0005        COMMON Y(201),DY(200),PHIF(201),PHI(201),AKE(201),AKEI(201),YY(201
           1),ZF(201),CC,ALAMV,ALAMA,EC,WBED,AT
           2,ALAM(201),ALAMI(201)
C
C     PARAMETERS ASSUMED
C
0006        DATA NDP,PASH,PHCASH,EPTCM/1,0.5,1.4,0.1E-6/
C     NDP: NUMBER OF SUBDIVISION OF AN INTERVAL OF DP0
C     PASH: FRACTION OF ASH ELUTRIATED
C     EPTCM: TOLERANCE LIMIT OF ETC ITERATION
C
C     CONTANTS
C
0007        EPTCM=0.1E-4
C   ***   IELUTR 1=ZENZ, 2=YAGI, 3=OTHERS
0008        IELUTR=3
0009        IELUTR=2
0010        IELUTR=1
0011        IMODEL =2                                                    PLUG
0012        IMODEL =1                                                    CM
0013        BETA=1.
0014        DR=10.
0015        ANDP=NDP
0016        EMF=0.5
0017        G=980.1
0018        RHOC=1.4
C           LIMESTONE    NO. 1359
0019        RHOLS=2.4
0020        XLCA=0.392
0021        RHOLCA=RHOLS*XLCA
0022        RHOL=RHOLCA
0023        XG00=0.21
0024        RG=32.05
0025        DATA DPF,FRACT/70*0.0/
0026        DATA DP0/0.002,0.0043,0.0061,0.0088,0.0104,0.0124,0.0147,0.0175,
           10.0208,0.0246,0.0295,0.0351,0.0417,0.0495,0.0589,0.0701,0.0833,
           20.0991,0.1166,0.1387,0.1651,0.1981,0.2362,0.2794,0.3327,0.3962,
           30.4699,0.5613,0.7,0.8,0.9,1.0,1.5,2.0,2.0/
C
C     INPUT 1 NAME AND PROPERTIES OF COAL
C
0027      5 READ(5,1000) NAM1,NAM2,XCF,XCV,XH,XS,XC,XN,XW,N
0028        NO=N
0029        XA=1.-XCF-XCV-XH-XS-XC-XN
0030        XC=XCF+XCV
0031        READ(5,1001) (DPF(I),I=1,N)
0032        READ(5,1001) (FRACT(I),I=1,N)
0033        RHOP=RHOC*(1.-XCV-XH-XS-XC-XN)
0034        DCM=DPF(N)
C
C     OUT PUT 1 NAME AND PROPERTIES OF COAL
C
0035        WRITE(6,2000) NAM1,NAM2,XCF,XCV,XH,XS,XC,XN,XW,(DPF(I),FRACT(I),I=
           11,N)
0036        DPP=DPF(1)
0037        DPAV=DPF(1)/2.
0038        SUM=0.
0039        DO 6 I=1,N
0040        IF(I.NE.1) DPAV=(DPF(I)+DPF(I-1))*0.5
0041        FRACT(I)=FRACT(I)/DPAV**3
0042        SUM=SUM+FRACT(I)
```

```
0043              6 CONTINUE
                C
                C     CALCULATION OF NUMBER FRACTION FROM WEIGHT FRACTION
                C
0044                  DO 7 I=1,N
0045                  FRACT(I)=FRACT(I)*DPF(N)/(DDP*SUM)
0046                  DPF0(I)=DPF(I)
0047                  FRACT0(I)=FRACT(I)
0048                  IF(I.EQ.N) GO TO 7
0049                  DDP=DPF(I+1)-DPF(I)
0050              7 CONTINUE
                C
                C     INPUT 2 OPERATING CONDITIONS
                C
0051             10 READ(5,1001) WCOAL,CABS,EXAIR,UO,P,TK,DT,HLMF,DPL,UMF
0052                  IF(TK.EQ.0.) GO TO 5
                C
                C     PREPARATORY CALCULATION
                C
0053                  AT=3.1416*0.25*DT**2
0054                  AK1=17.90-35.7/(0.001986*TK)
0055                  AK=EXP(AK1)*TK/1000.
0056                  VISC=3.72E-5*TK**0.676
0057                  D=4.26*(TK/1800.)**1.75/P
0058                  RHOG=MAIR*P/(RG*TK)
                C
                C     THEORETICAL AIR FLOW RATE FMTH (MOLE/SEC)
                C
0059                  A2=1./((XH/MH2*0.5+XS/MS-XC/MO2)*MC/XC+1.)
0060                  A1=XH/MH2*0.5+XC/MO2+XN/MN2+XW/MH2O
0061                  ALF0=A1
0062                  ALF1=A1*A2*MC/XC
0063                  ALF2=A2
0064                  FMTH=WCOAL*XC/(MC*A2*XG00)
0065                  IF(EXAIR.EQ.0.)EXAIR=(P*UO*AT/(RG*TK*WCOAL)-A1)*A2*MC*XG00/XC-1.
0066                  FMO=(1.+EXAIR)*FMTH+A1*WCOAL
0067                  IF(UO.EQ.0.)UO=FMO*RG*TK/(P*AT)
                C
                C     CALCULATION OF HYDRODYNAMIC PARAMETERS
                C
0068                  UMF=(VISC/DPL/RHOG)*(SQRT(33.7**2+0.040E*DPL**3*RHOG*(RHOL-RHOG)*G
                     1/VISC/VISC)-33.7)
0069                  UB=0.71*SQRT(G*DB)
0070                  US=0.35*SQRT(G*DT)
0071                  IF(UB.GT.US)UB=US
0072                  UB=UB+UO-UMF
0073                  EB=(UO-UMF)/UB
0074                  DPCR=SQRT(18.*UO*VISC/((RHOP-RHOG)*G))
0075                  RE=DPCR*UO*RHOG/VISC
0076                  IF(RE.LE.5.76) GO TO 12
0077                  RE=RE/DPCR
0078                  DPCR=(56.25*RHOG*VISC/(((RHOP-RHOG)*G)**2))**0.33333*UO
0079                  RE=RE*DPCR
0080                  IF(RE.LE.540.) GO TO 12
0081                  DPCR =UO**2*RHOG/((RHOP-RHOG)*3.1*G)
0082             12 CONTINUE
                C
                C     OUT PUT 2
                C
0083                  WRITE(6,2004)IFLUTR,BETA,IMODEL,DB,EB
                C
                C     CALCULATION OF THE SIZE DISTRIBUTION
                C     DENSITY FUNCTION OF COAL PARTICLES FED TO THE BED , PHIF (I)
                C
0084                  INDX=0
0085                  N=NO
0086                  DO 11 I=1,N
0087                  DPF(I)=DPF0(I)
0088                  FRACT(I)=FRACT0(I)
0089             11 CONTINUE
0090                  DO 14 I=1,N
0091                  IF(INDX.EQ.0.AND.DPF(I).EG.DPCR) INDX=1
0092                  IF(DPF(I).LE.DPCR) GO TO 14
0093                  IF(INDX.EQ.1) GO TO 14
0094                  IF(INDX.EQ.2) GO TO 13
0095                  A=DPF(I+1)
```

```
      B=FRACT(I+1)
      DPF(I+1)=DPF(I)
      DPF(I)=DPCR
      FRACT(I+1)=FRACT(I)
      INDX=2
      GO TO 14
   13 CONTINUE
      A1=DPF(I+1)
      B1=FRACT(I+1)
      DPF(I+1)=A
      FRACT(I+1)=B
      A=A1
      B=B1
   14 CONTINUE
      IF(INDX.EQ.2) N=N+1
      D=FLOAT(NDP)
      DDP=DPO(1)
      DP(1)=0.
      PHIF(1)=0.
      K=1
      L=2
      DO 20 I=1,34
      DO 18 J=1,NDP
      A=FLOAT(NDP-J)*DDP/D
      DP(L)=DPO(I)-A
      IF(DP(L).GT.DPF(K)) GO TO 15
      PHIF(L)=FRACT(K)
      IF (DP(L).EQ.DPF(K)) K=K+1
      GO TO 17
   15 CONTINUE
      XX=DP(L)
      DP(L)=DPF(K)
      DP(L+1)=XX
      PHIF(L)=FRACT(K)
      IF(K.EQ.N) GO TO 21
      L=L+1
      K=K+1
      PHIF(L)=FRACT(K)
   17 IF(K.EQ.N+1) GO TO 21
      L=L+1
   18 CONTINUE
      DDP=DPO(I+1)-DPO(I)
   20 CONTINUE
   21 CONTINUE
C
C     CALCULATION OF THE REACTIVITIES OF CHAR PARTICLE , ALAM(I) AND
C     ELUTRIATION RATE CONSTANT, AKE(I)
      DY(1)=0.
      Y(1)=0.
      SUM1=0.
      ALAM(1)=ACTIV(Y(1),DCM,RHOG,VISC,D,AK,UO)
      ALENAX=(1.-EMF)*RHOL*UO
      AKE(1)=0.
      DO [illegible]
      Y([illegible])=[illegible]/DCM
      ALAM([illegible])=ACTIV(Y(I),DCM,RHOG,VISC,D,AK,UO)
      DY(I)=Y(I)-Y(I-1)
      SUM1=PHIF(I)*DY(I)+SUM1
      UTF=[illegible]REEFV(DP(I),RHOP,RHOG,VISC)
      AKE(I)=0.
      IF(UO.LE.UTF)GO TO 23
      GO TO (121,122,123),IELUTR
  121 CONTINUE
      A=UO**2/(RHOP**2*DP(I)*G)
      IF(A.LT.501.8)AKE(I)=A**1.866*RHOG*UO*5.269E-5
      IF(A.GE.501.8)AKE(I)=A**1.152*RHOG*UO*4.973E-3
      GO TO 124
  122 CONTINUE
      RET=DP(I)*UTF*RHOG/VISC
      FR=(UO-UTF)**2/(G*DP(I))
      XX=RET**0.6
      AKE(I)=(0.0015+0.01*XX)*XX*FR*VISC/DP(I)
      GO TO 124
  123 CONTINUE
      AKE(I)=1.52E-5*(UO-UTF)**2*RHOG/SQRT(G*DP(I))*(DP(I)*UTF*RHOG/
     1VISC)**0.725*((RHOP-RHOG)/RHOG)**1.15
```

WENGMASS

ORIGINAL PAGE IS
OF POOR QUALITY

ORIGINAL PAGE IS
OF POOR QUALITY

```
0168          124 CONTINUE
0169              AKE(1)=BETA*AKE(1)
0170              IF(AKE(1).GT.AKEMAX)AKE(1)=AKEMAX
0171              DO 22 I=2,L
0172              JL=I+L-1
0173              IF(AKE(JL).LT.AKE(I))AKE(JL)=AKE(I)
0174           22 CONTINUE
0175           23 CONTINUE
0176              AKEI(1)=0.
0177              ALAMI(1)=0.
0178              DO 30 I=2,L
0179              AKEI(I)=(AKE(I-1)/ALAM(I-1)+AKE(I)/ALAM(I))*0.5*DY(I)+AKEI(I-1)
0180              ALAMI(I)=(1./ALAM(I-1)+1./ALAM(I))*0.5*DY(I)+ALAMI(I-1)
0181           30 CONTINUE
0182              PHITTL=SUM1
0183              SUM=0.
0184              SUM1=0.
0185              A=0.
0186              B=0.
0187              DO 32 I=2,L
0188              PHIF(I)=PHIF(I)/PHITTL
0189              BB=Y(I)**2*PHIF(I)
0190              AA=Y(I)*BB
0191              SUM=(A+AA)*DY(I-1)*0.5+SUM
0192              SUM1=(B+BB)*DY(I-1)*0.5+SUM
0193              A=AA
0194              B=BB
0195           32 CONTINUE
0196              ALAMVF=SUM
0197              ALAMAF=SUM1
0198              WRITE(6,3006)SUM1,ALAMVF
0199         3006 FORMAT(' SUM1=',E12.4,'  ALAMVF=',E12.4)
                C
                C     OUT PUT 3 AND  4
                C
0200              VCF=WCOAL/RHOC
0201              WLS=CABS*WCOAL*XS*MCA/MS
0202              VLS=WLS/RHOLCA
0203              VMF=HLMF*AT
0204              THETM=VMF*(1.-EMF)/VLS
0205              TH1=WCOAL*XA*(1.-PASH)/(RHOASH*VLS)
0206              ETHMAX=THETM*0.0001
0207              WBED=THETM*WLS
0208              WRITE(6,2001) WCOAL,WLS,CABS,EXAIR,FMO,UO,P,TK,DT,HLMF,AK,DPCR,
                 1VCF,VLS,THETM,ALAMVF,ANDP,PASH,RHOASH,EETCM,ETHMAX
0209              A1=ALF0
0210              A2=ALF2
0211              DTH=-THETM*0.25
0212              DETC=-0.05
0213              INDETC=0
0214              ETC=1.+EXAIR
0215              IF(ETC.GT.1.0)ETC=1.
0216              DETC=-0.24999999
0217              DETC=-0.05
0218              DETC=-0.1
0219              EC=0.0
                C
                C     ITERATION OF ETC (COMBUSTION EFFICIENCY) STATES FROM HERE
                C
0220              VCW=0.
0221              BC1=0.
                C
                C     ITERATION LOOP FOR ETC,UP TO "500 CONTINUE"
                C
0222              DO 500 IETC=1,30
0223              IF(ETC.LE.0.) GO TO 501
0224              INDTH=0
0225              THET=THETM/(1.+TH1*ETC)
                C
                C     ITERATION LOOP FOR THET , UP TO "200 CONTINUE "
                C
0226              DO 200 ITHET=1,30
0227              IF (THET.EQ.0.)THET=0.0001
0228              IF(THET.LE.0.) GO TO 201
0229              XINF=EXAIR/(EXAIR+ALF2)
0230              COXO=(EXAIR+ALF2)*P/(((1.+EXAIR)/XGOO+ALF1)*RG*TK)
```

```
0231              GO TO (41,42),IMODEL
0232           41 CONTINUE
0233              COXAV=((1.-XINF)*(1.-ETC)+XINF)*COX0                          /  CM
0234              GO TO 45
0235           42 CONTINUE
0236              COXAV=-(1.-XINF)*ETC/ALOG(1.-(1.-XINF)*ETC)                   PLUG
0237              COXAV=COXAV*COX0
0238           45 CONTINUE
0239              BC=DCM*RHOC*XC/(2.*MC*AK*THET*COXAV)
0240              IF(ETC.EQ.1.) GO TO 210
0241              INDBC1=0.
0242              BC1=0.
0243              DBC1=100.
                C
                C     ITERATION FOR BC1 , UP TO "50 CONTINUE "
                C
0244              DO 50 IBC1=1,20
0245              BC10=BC1
0246              EBMAX=ABS(BC1)*0.00005
0247              CALL POP(BC,BC1,THET,L)
0248              A=(ALAMV+THET*EC)/((1.-ETC)*ALAMVF)
0249              EBC1=BC*A-BC1
                C
                C     CORRECTION OF BC 1
                C
0250              CALL CRRECT(IBC1,INDBC1,DBC1,BC11,BC12,BC1,EBC11,EBC12,EBC1,EBMAX)
0251              IF(INDBC1.EQ.2)GO TO 51
0252              IF(INDBC1.EQ.1.AND.ABS(BC1-BC10).LT.EBMAX)GO TO 51
0253           50 CONTINUE
0254              WRITE(6,3010)BC,BC1,THET,CC,ALAMA,ALAMV,EC
0255           51 CONTINUE
0256              VCW=(1.-ETC)*VCF*ALAMV/(ALAMV+THET*EC)
0257              THETA=THETM/(1.+VCW/VLS+TH1*ETC)
0258              WBED=(VCW*RHOP+VLS*RHOL+TH1*VLS*ETC*RHOASH)*THET
0259              EE=THET-THETA
0260              THE=THET
                C     CORRECTION OF THET
0261              CALL CRRECT(ITHET,INDTH,DTH,THET1,THET2,THE,EE1,EE2,EE,ETHMAX)
0262              XX=ABS(THET-THE)
0263              IF(XX.LE.ETHMAX) GO TO 210
0264              THET=THE
0265              IF(INDTH.EQ.2) GO TO 210
0266          200 CONTINUE
0267          201 CONTINUE
0268              WRITE(6,3000)
0269          210 CONTINUE
0270              BBC=0.
0271              IF(ETC.EQ.1.) GO TO 212
0272              BBC=(1.-ETC)*3.*ALAMA/((ALAMV+THET*EC)*ETC)
0273          212 E=(BC-BBC)/(BC+BBC)*2.
0274              ETCOLD=ETC
                C
                C     CORRECTION OF ETC
                C
0275              CALL CRRECT(IETC,INDETC,DETC,ETC1,ETC2,ETC,E1,E2,E,EETCM)
0276              XX=ABS(ETC-ETCOLD)
0277              IF(XX.LE.0.1E-4) GO TO 510
0278              IF (INDETC.EQ.2) GO TO 510
0279              ELOSS=1.-ETC-VCW/VCF
0280              XGO=((1.-ETC)*A2+EXAIR)*XGOO/(A1+EXAIR)
0281              HCHAR=THET*VCW*RHOP
0282              HCARBN=THET*VCW*RHOC*XCF
0283              HRC=HCARBN/WBED
0284          500 CONTINUE
0285          501 CONTINUE
0286              WRITE(6,3001)
0287          510 CONTINUE
0288              A1=AT/(WBED*EC)
0289              YA1=0.
0290              YB1=0.
0291              YC1=0.
0292              PHIFW(1)=0.
0293              PHIW(1)=0.
0294              PHIEW(1)=0.
0295              DO 520 I=2,L
0296              YA2=YA1
```

```
0297                YB2=YB1
0298                YC2=YC1
0299                YA1=DP(I)**3*PHIF(I)/ALAMVF
0300                YB1=DP(I)**3*PHI(I)/ALAMV
0301                YC1=DP(I)**3*A1*AKE(I)*PHI(I)
0302                PHIFW(I)=(YA1+YA2)*DY(I)*0.5+PHIFW(I-1)
0303                PHIW(I)=(YB1+YB2)*DY(I)*0.5+PHIW(I-1)
0304                PHIEW(I)=(YC1+YC2)*DY(I)*0.5+PHIEW(I-1)
0305             520 CONTINUE
0306                DO 530 I=2,L
0307                PHIFW(I)=PHIFW(I)/PHIFW(L)
0308                PHIW(I) =PHIW(I) /PHIW(L)
0309                PHIEW(I)=PHIEW(I)/PHIEW(L)
0310             530 CONTINUE
0311                ELOSS=1.-ETC-VCW/VCF
0312                XGO=((1.-ETC)*A2+EXAIR)*XGOO/(A1+EXAIR)
0313                HCHAR=THET*VCW*RHOP
0314                HCARBN=THET*VCW*RHOC*XCF
0315                HRC=HCARBN/WBED
                 C
                 C      OUT PUT 5 (RESULTS)
                 C
0316                WRITE(6,2000) NAM1,NAM2,XCF,XCV,XH,XS,XO,XN,XW,(DPF(I),FRACT(I),I=
                   11,N)
0317                WRITE(6,2004)IELUTR,BETA,IMODEL,CB,EB
0318                WRITE(6,2001) WCOAL,WLS,CABS,EXAIR,FMO,UO,P,TK,DT,HLMF,AK,DPCR,
                   1VCF,VLS,THETM,ALAMVF,ANDP,PASH,RHOASH,EETCM,ETHMAX
0319                WRITE(6,2002) ETC,XGO,THET,BC,BC1,VCW,VCF,VLS,HCHAR,WBED,HRC,EC,
                   1ELOSS,ALAMV,ALAMA
0320                WRITE(6,2003)(Y(I),DP(I),PHIF(I),PHI(I),PHIFW(I),PHIW(I),PHIEW(I),
                   1AKE(I),ALAM(I),I=1,L)
0321                WRITE(6,3005)
0322             790 CONTINUE
0323             800 CONTINUE
0324                GO TO 10
0325            1000 FORMAT(2A4,7F8.0,I4)
0326            1001 FORMAT(10F8.0)
0327            2000 FORMAT(1H1,///10X,'FBC CALCULATION'//10X,'EFFECT OF ELUTRIATION
                   1ON COMBUSTION EFFICIENCY'//,1X,2A4,1X,'COMPOSITION OF COAL',7F10.4
                   2,/(2E12.4))
0328            2001 FORMAT(/' WCOAL,WLS,CABS,EXAIR,FMO,UO,P,TK,DT,HLMF'/10E12.4//' AK,
                   1DPCR,VCF,VLS,THETM,ALAMVF,NDP,PASH,RHOASH'/9E12.4//' EETCM,ETHMAX'
                   2,(2E12.4))
0329            2002 FORMAT(/' ETC,XGO,THET,BC,BC1'/5E12.4//' VCW,VCF,VLS,HCHAR,WBED,
                   1HRC,EC,ELOSS,ALAMV,ALAMA'/10E12.4/)
0330            2003 FORMAT(/'      Y          DP          PHIF          PHI          PHIFW
                   1          PHIW          PHIEW          AKE          ALAM'/(9E12.4))
0331            2004 FORMAT('  ELUTRIATION CORRELATION : NO.',I2,' BETA=',F10.5/
                   1/'  GAS PHASE MODEL : NO.',I2,'  DB,EB=',F10.1,F10.5/)
0332            3000 FORMAT(/' THET HAS NOT CONVERGED.'/)
0333            3001 FORMAT(/' ETC HAS NOT CONVERGED.'/)
0334            3005 FORMAT(1H1)
0335            3010 FORMAT(/' POP *****',2X,7E11.3)
0336                END
```

```
0001                SUBROUTINE CRRECT(I,INDX,DX,X1,X2,XNEW,E1,E2,E,EMAX)
                C       I: NUMBER OF THIS TRIAL, 1 FOR FIRST TRIAL
                C       INDX: INDEX OF THE TRIAL LEVEL
                C       INDX=0: JUST PROCEEDING
                C       INDX=1: THE ROOT HAS BEEN CAUGHT BETWEEN X1 AND X2
                C       INDX=2: THE ITERATION HAS CONVERGED
0002                    IF (ABS(E).GT.EMAX) GO TO 5
0003                    INDX=2
0004                    RETURN
0005                  5 CONTINUE
0006                    IF(INDX.EQ.1) GO TO 100
0007                    X2=XNEW
0008                    E2=E
0009                    IF(I.EQ.1) GO TO 10
0010                    IF(E1*E2.LE.0.)INDX=1
0011                    IF(INDX.EQ.1)GO TO 150
0012                 10 X1=X2
0013                    E1=E2
0014                    XNEW=XNEW+DX
0015                    RETURN
0016                100 CONTINUE
0017                    IF(E1*E.LT.0.) GO TO 110
0018                    E1=E
0019                    X1=XNEW
0020                    GO TO 150
0021                110 E2=E
0022                    X2=XNEW
0023                150 CONTINUE
0024                    XNEW=(X1-X2)*E2/(E2-E1)+X2
0025                    RETURN
0026                    END
```

```
0001                SUBROUTINE POP(BC,BC1,THET,L)
                C
                C       THIS SUBROUTINE
                C
                C       CALCULATES THE SIZE DISTRIBUTION DENSITY FUNCTION
                C       PHI (I) AND SECOND AND THIRD MOMENTS AND AVERAGE VALUE OF
                C       (ELUTRIATION CONSTANT * PARTICLE VOLUME)
                C       FOR GIVEN BC, BC1 AND THET.
0002                COMMON Y(201),DY(200),PHIF(201),PHI(201),AKE(201),AKEI(201),YY(201
                   1),ZF(201),CC,ALAMV,ALAMA,EC,WBED,AT
                   2,ALAM(201),ALAMI(201)
0003                ZF(1)=0.
0004                SUM1=0.
0005                SUM2=0.
0006                X1=0.
0007                DO 100 I=1,L
0008                A=(ALAMI(I)+THET*AKEI(I)*AT/WBED)*BC
0009                IF(A.LT.0.1E-30)A=0.0
0010                YY(I)=EXP(A)
0011                X2=X1
0012                IF(I.EQ.1)GO TO 100
0013                ZF(I)=(1./YY(I)+1./YY(I-1))*0.5*PHIF(I)*DY(I)+ZF(I-1)
0014                X1=YY(I)*ZF(I)/ALAM(I)
0015                SUM1=(YY(I)/ALAM(I)+YY(I-1)/ALAM(I-1))*0.5*DY(I)+SUM1
0016                SUM2=(X1+X2)*0.5*DY(I)+SUM2
0017            100 CONTINUE
0018                CC=(1.+BC1*SUM2)/SUM1
0019                SUM1=0.
0020                SUM2=0.
0021                SUM3=0.
0022                A11=0.
0023                A21=0.
0024                A31=0.
0025                DO 200 I=1,L
0026                A12=A11
0027                A22=A21
0028                A32=A31
0029                PHI(I)=(-BC1*ZF(I)+CC)*YY(I)/ALAM(I)
0030                A11=PHI(I)*Y(I)**2
0031                A21=A11*Y(I)
0032                A31=A21*AKE(I)
0033                SUM1=(A11+A12)*0.5*DY(I)+SUM1
0034                SUM2=(A21+A22)*0.5*DY(I)+SUM2
0035                SUM3=(A31+A32)*0.5*DY(I)+SUM3
0036            200 CONTINUE
0037                ALAMA=SUM1
0038                ALAMV=SUM2
0039                EC=SUM3*AT/WBED
0040                RETURN
0041                END
```

```
0001            FUNCTION ACTIV (Y,DCM,RHOG,VISC,D,AK,UO)
                C
                C       REACTIVITY OF CHAR
                C       AS A FUNCTION OF PARTICLE SIZE,
                C       GAS VELOCITY AND TEMPERATURE
                C
0002                    DP=Y*DCM
0003                    IF(DP.LE.0.00001)DP=0.00001
0004                    SC3=(VISC/(RHOG*D))**0.3333
0005                    REP=UO*RHOG*DP/VISC
0006                    A1=0.1
0007                    SHP=REP**1.2*A1*SC3
0008                    SHP=2.
0009                    AKF=SHP*D/DP
0010                    ACTIV=1./(AK/AKF+1.)
0011                    RETURN
0012                    END
```

```
0001                FUNCTION FREEFV(DP,RHOP,RHOG,VISC)
                C
                C       CALCULATION OF TERMINAL VELOCITY UT
                C         FREE FALL VELOCITY
0002                    G=980.1
0003                    UT=(RHOP-RHOG)*G*DP*DP/(18.*VISC)
0004                    RET=UT*RHOG*DP/VISC
0005                    IF(RET.LE.5.76)GO TO 40
0006                    UT=(((RHOP-RHOG)*G)**2*4./(225.*RHOG*VISC))**0.33333*DP
0007                    RET=UT*RHOG*DP/VISC
0008                    IF(RET.LE.540.)GO TO 40
0009                    UT=SQRT((RHOP-RHOG)*3.1*G*DP/RHOG)
0010                40  FREEFV=UT
0011                    RETURN
0012                    END
```

6-2. LEVEL II PROGRAM

```
$JOB
C-----------------------------------------------------------------------
C-----------------------------------------------------------------------
C
C              A GENERAL MODEL OF FLUIDIZED COMBUSTOR
C
C                          PROGRAMMED BY
C
C                    M. MORIO  AND  P. PENGARAJAN
C
C                                AT
C
C                    WEST VIRGINIA UNIVERSITY    (AUG.,1976)
C
C
C
C
C-----------------------------------------------------------------------
1       REAL MC,MH2,MS,MO2,MN2,MH2O,MSO2,MH2S,MCC,MCO2,MCACO3,MCAO,MCASO4
       1,MMGCO3,MMGO,MAIR ,MGAS
2       COMMON ZHE(46),AHE(46),PV(46),PH(46),ZF(46),FFC(46),
       1FFAD(46),ZDIS(46),FD(46),AHEAV(101),ETUBE(101),DB(46),MFEED,MDIS
3       COMMON /HYMAIN/ UO(46),UMF(46),H(46),AT(46),DT(46),T(101),X(46),
       1YE(46),FPB(46),EPC(46),DVBB(46),DVBBEF(46),DBAV(46),UB(46),HLMF,
       2HLF,VMF,EMO,EMF,UF,PF,TF,RG,G,MGAS,DPFIX,DPFLU,DPDIS,DPP,RHOCAD,
       3EMF,YB(46),PAV,HCR,AKBE(46),BEDVOL,EFFVOL,SOLVOL,TETUBE,ICR,IFBC
4       COMMON /GEN/ Z(101),DVBEFF(101),ZB(46),ATB(46),PI,DZAV,MTB,MT,M1,M
5       COMMON/LEMAIN/AND,DNZL,DTHICK,FW
6       DIMENSION ALFA(46),BETA(46),GAMA(46),DELT(46),UHE(101),
       1WMIX(46),WNET(46),WFC(46),WFAD(46),WD(46),S(46),TW(46),
       2DPADF(20),DPCF(20),FRACTA(20),FRACTC(20),XGF(8),XGO(8),AG(8,2),
       3YBO(46),YFO(46),SRELB(46),SRELE(46),ZAVG(46),TPB(46),TPF(46),
       4RP(46),RPB(46),RPF(46),TOLD(46),AAA(2116),BBB(46),FEM(46),FBM(46)
7       NAMELIST / DPCF / HLMF,VMF,HLF,PAV,TAV,TWAV,UHEAV,WCOAL,WAD,WCAD,
      *CABS,UF,TF,PF,EXAIR,XGF,GZCO,GZH2S,GZH2,IGNITE,MGAS,EMTH,EMF,EMO,
      $RHOCAD,RHOCH
      */DPCF1/ ICR,IFBC,HCR,HLF,HLMF,VMF,BEDVOL,EFFVOL,SOLVOL,TETUBE,
      *HAREA,QTRANS,QVOL,QAREA,WELT,CELU,CLOSS,WDIS
8       DATA MC,MH2,MS,MO2,MN2,MH2O,MSO2,MH2S,MCO,MCO2,MCACO3,MCAO,MCASO4
       1,MMGCO3,MMGO,MAIR
       1/12.,2.,32.,32.,28.,18.,64.,34.,28.,44.,100.1,56.08,136.14,84.32
       2,40.31,28.8/
9       DATA AAA,BBB/2162*0./
10      EMF = 0.5
11      RG = 82.05
12      G  =  980.1
13      PI = 3.141593
14      DATA RHOC,RHOASH,RHOAD/1.4,1.4,2.4/
15      ETUBE(1)=0.
16      FPB(1)=0.
17      FPC(1)=0.
18      DBAV(1)=0.
19      UB(1)=0.
20      DVBB(1)=0.
21      AHEAV(1)=0.
22      DATA HAREA,QTRANS,QVOL,QAREA /4*0.0/
C
C-----------------------------------------------------------------------
C           SOLID DENSITY       G/CM**3
C-----------------------------------------------------------------------
C      RHOC             RHOASH           RHOAD
C      COAL             ASH              LIMESTONE OR DOLOMITE
C-----------------------------------------------------------------------
C     RHOCH             RHOCAD
C      CHAR             CALCINED ADDITIVES
C-----------------------------------------------------------------------
C
23      DATA CADF,CCF,CGMF/0.198,0.193,6.79/
C-----------------------------------------------------------------------
C         HEAT CAPACITY OF FEED MATERIALS AT 25 DEG "
C          CADF,CCF  :  CAL/( G * DEG ),   CGMF  :  CAL/( MOL * DEG)
C-----------------------------------------------------------------------
C
24      CALL DESIGN
C       =============
C       MAIN OUTPUT 1       ( CF. SUBROUTINE DESIGN )
C       =============
```

```
C                                                                       76.
C       SIZE DISTRIBUTION OF LIMESTONE OR DOLOMITE PARTICLES            77.
C                                                                       78.
C       NDPAD : TOTAL NUMBER OF SIZE INTERVALS                          79.
C       DPADF : UPPER BOUND OF EACH SIZE INTERVAL                       80.
C      FRACTA : WEIGHT FRACTION                                         81.
C                                                                       82.
25          READ(5,1000) NDPAD                                          83.
26          READ(5,1001)(DPADF(I),I=1,NDPAD)                            84.
27          READ(5,1001)(FRACTA(I),I=1,NDPAD)                           85.
28          SUM = FRACTA(1)*2.0 / DPADF(1)                              86.
29          DPADR = FRACTA(1)*0.5*DPADF(1)                              87.
30                                    DO 10 I = 2,NDPAD                 88.
31          DPBAR = (DPADF(I) + DPADF(I-1)) * 0.5                       89.
32          SUM = FRACTA(I) / DPBAR + SUM                               90.
33          DPADR = FRACTA(I) * DPBAR + DPADR                           91.
34    10                              CONTINUE                          92.
35          DPADH=1./SUM                                                93.
C                                                                       94.
C       DPADH : SURFACE VOLUME MEAN DIAMETER FOR HYDRODYNAMIC CALCULATION 95.
C       DPADR : WEIGHT MEAN DIAMETER FOR REACTION RATE CALCULATION      96.
C                                                                       97.
36          DPB=DPADH                                                   98.
C                                                                       99.
C       DPB : AVERAGE PARTICLE SIZE OF BED PARTICLES                   100.
C                                                                      101.
C       COMPOSITON OF ADDITIVES                                        102.
C                                                                      103.
37          READ(5,1010)NAMEL1,NAMEL2,XCACO3,XMGCO3                    104.
C                                                                      105.
C      COMPOSITION AND NET HEATING VALUE OF COAL                       106.
C                                                                      107.
38          READ(5,1010)NAMEC1,NAMEC2,XCF,XCV,XH,XS,XO,XN,XW,QCOAL     108.
39          XC=XCF+XCV                                                 109.
40          XA=1.-XC-XH-XS-XO-XN                                       110.
41          QCOALC=QCOAL                                               111.
42          ETCP=0.0                                                   112.
C                                                                      113.
C       ------------------------------------------------------------   114.
C       XCF  : FIXED CARBON                                            115.
C       XCV  : VOLATILE CARBON                                         116.
C       XH   : HYDROGEN                                                117.
C       XS   : SULPHUR                                                 118.
C       XO   : OXYGEN                                                  119.
C       XN   : NITROGEN                                                120.
C       XW   : MOISTURE                                                121.
C       ----------------  DRY BASIS ----------------------              122.
C       QCOAL : CAL/GRAM                                               123.
C                                                                      124.
C                                                                      125.
C       SIZE DISTRIBUTION OF COAL                                      126.
C                                                                      127.
C                                                                      128.
43          READ(5,1000)NDPC                                           129.
44          READ(5,1001)(DPCF(I),I=1,NDPC)                             130.
45          READ(5,1001)(FRACTC(I),I=1,NDPC)                           131.
46          DP2=0.                                                     132.
47          SUM = 0.0                                                  133.
48                                    DO 20 I=1,NDPC                   134.
49          DP1=DP2                                                    135.
50          DP2=DPCF(I)                                                136.
51          SUM = FRACTC(I)*2.0/(DP1+DP2) + SUM                        137.
52       20                           CONTINUE                         138.
53          DCF = 1.0/SUM                                              139.
54          DCAV = (3.0/4.0) * DCF                                     140.
C                                                                      141.
C       DCF : SURFACE VOLUME MEAN DIAMETER OF COAL FEED                142.
C                                                                      143.
C       OPERATING CONDITIONS 1 (BED CONDITION)                         144.
C                                                                      145.
55          READ(5,1020)HLMF,VMF,HLF,PAV,TAV,TWAV,UHEAV                146.
C                                                                      147.
C       OPERATING CONDITION 2 (SOLIDS AND GAS FEEDS)                   148.
C                                                                      149.
56          READ(5,1021)WCOAL,WAD,CABS,UF,TF,PF,EXAIR,(XGF(I),I=1,7),  150.
           1GZCO,GZH2S,GZH2                                            151.
```

```
      IF (TF .EQ. 0.0) TF = 298.0                                          152.
      T(1) = TF                                                            153.
C                                                                          154.
C     XGF (I) : FEED GAS COMPOSITION (MOLE FRACTION)                       155.
C-------------------------------------------------------------------------156.
C        I      1       2       3       4       5       6       7       8 157.
C      XGF =  O2      CO2     SO2     H2O     CO      H2S     H2      N2  158.
C-------------------------------------------------------------------------159.
C                                                                          160.
C     GZCO,GZH2S,GZH2 --- USED ONLY FOR FUEL RICH CASE                     161.
C      GZCO : (CO FORMATION RATE)/(CARBON COMBUSTION RATE)                 162.
C      GZH2S : (H2S FORMATION RATE)/(SULPHUR FEED RATE)                    163.
C      GZH2 : (H2FORMATION RATE FROM COAL)/(H2+H2O FROM COAL)              164.
C                                                                          165.
C      QCOALC : HEAT OF COMPLETE COMBUSTION  CAL/G  (COAL)                 166.
C      QCOAL : HEAT OF INCOMPLETE COMBUSTION   CAL/G(COAL)                 167.
C                                                                          168.
      QCOAL=QCOALC-67636.*GZCO*XC/MC                                       169.
      READ(5,1000)IGNITE                                                   170.
      IF(WCOAL.EQ.0.)IGNITE=0                                              171.
      TSF=298.                                                             172.
C-------------------------------------------------                         173.
C     IGNITE        0          1                                           174.
C              NO COMBUSTION   COMBUSTION                                  175.
C-------------------------------------------------                         176.
      XGF(8) = 1.-XGF(1)-XGF(2)-XGF(3)-XGF(4)-XGF(5)-XGF(6)-XGF(7)         177.
      MGAS =  XGF(1)*MO2+XGF(2)*MCO2+XGF(3)*MSO2+XGF(4)*MH2O+XGF(5)*MCO    178.
     1 +XGF(6)*MH2S+XGF(7)*MH2+XGF(8)*MN2                                  179.
      A2=1./((XH*0.5/MH2+XS/MS-XO/MO2)*MC/XC+1.)                           180.
      FMTH=WCOAL*XC/(MC*XGF(1)*A2)*(1.-XW)                                 181.
      FMF=FMTH*(1.+EXAIR)                                                  182.
      IF(UF.GT.0.)FMF=UF*ATB(1)*PF/(RG*TF)                                 183.
      IF (UF.EQ.0.0) UF = FMF*RG*TF/(PF*ATB(1))                            184.
      EXAIR=1.E5                                                           185.
      IF(FMTH.LE.0.0001)GO TO 22                                           186.
      EXAIR=FMF/FMTH-1.                                                    187.
   22 CONTINUE                                                             188.
      IF(FMF.LT.0.0001)STOP                                                189.
      A1=(XC*GZCO*0.5/MC+XO/MO2+(1.+GZH2)*XH*0.5/MH2)*(1.-XW)+XW/MH2O      190.
      FMO=FMF+A1*WCOAL                                                     191.
      AN = 2.9E-8 * EXAIR ** 0.449                                         192.
C                                                                          193.
C      FMO : AVERAGE FLOW RATE OF GAS IN THE BED          MOLE/SEC         194.
C                                                                          195.
      AG(1,1)=FMF*XGF(1)/FMO-((1.-GZH2)*XH*0.5/MH2+(1.-GZH2S)*XS/MS-XO/    196.
     1MO2)*WCOAL/FMO*(1.-XW)                                               197.
      AG(1,2)=-(GZCO*XC*0.5/MC+(1.-GZCO)*XC/MC)*WCOAL/FMO*(1.-XW)          198.
      AG(2,1)=FMF*XGF(2)/FMO                                               199.
      AG(2,2)=(1.-GZCO)*WCOAL*XC*(1.-XW)/(MC*FMO)                          200.
      AG(3,1)=(WCOAL*(1.-XW)*XS/MS+FMF*(XGF(3)+XGF(6)))/FMO                201.
      AG(4,1)=(WCOAL*(XH*(1.-XW)/MH2+XW/MH2O)+FMF*(XGF(4)+XGF(6)+XGF(7))   202.
     $-(FMF*(XGF(6)+XGF(3))+WCOAL*(1.-XW)*XS/MS)*GZH2S)*(1.-GZH2)/FMO      203.
      AG(5,1)=FMF*XGF(5)/FMO                                               204.
      AG(5,2)=GZCO*WCOAL*XC*(1.-XW)/(MC*FMO)                               205.
      AG(6,1)=AG(3,1)*GZH2S                                                206.
      AG(7,1)=AG(4,1)*GZH2/(1.-GZH2)                                       207.
C                                                                          208.
C      RHOCH : DENSITY OF CHAR                                             209.
C     RHOCAD : DENSITY OF CALCINED ADDITIVE                                210.
      RHOCH = (1.-XH-XO)*RHOC                                              211.
      IF(IGNITE.EQ.0)RHOCH=RHOC                                            212.
      RHOCAD = (XCACO3*MCAD/MCACO3+XMGCO3*MMGO/MMGCO3+1.-XCACO3-XMGCO3)    213.
     1*RHOAD                                                               214.
      IF(IGNITE.EQ.0)RHOCAD=RHOAD                                          215.
      IF(CABS.EQ.0..AND.WAD.GT.0.)                                         216.
     1CABS=WAD*XCACO3/MCACO3/(WCOAL*(1.-XW)*XS/MS+(XGF(3)+XGF(6))*FMF)     217.
      IF(CABS.GT.0..AND.WAD.EQ.0.)                                         218.
     1WAD=CABS*(WCOAL*(1.-XW)*XS/MS+(XGF(3)+XGF(6))*FMF)/(XCACO3/MCACO3)   219.
      WCAD=WAD*RHOCAD/RHOAD                                                220.
      RHOGAS=PAV*MGAS/(RG*TAV)                                             221.
      VISC=3.72E-6*(TAV**0.676)                                            222.
C      =============                                                       223.
C     MAIN OUTPUT 2                                                        224.
C      =============                                                       225.
      WRITE (6,2000) NAMEL1,NAMEL2,XCACO3,XMGCO3,(DPADF(I),FRACTA(I),      226.
     *I = 1,NDPAD)                                                         227.
```

```
 98          WRITE(6,2010) DPADH,DPADR                                                228.
 99          WRITE(6,2020) NAMEC1,NAMEC2,XCF,XCV,XH,XS,XO,XN,XA,XW,QCOAL,QCOALC       229.
100          WRITE (6,2030) ( DPCF(I),FRACTC(I), I = 1 , NDPC )                       230.
101          WRITE (6,2040) DCF,DCAV                                                  231.
102          WRITE (6,OPCF)                                                           232.
103                                    DO 25 I=1,46                                   233.
104          TW(I)=TWAV                                                               234.
105          UHE(I)=UHFAV                                                             235.
106       25                           CONTINUE                                      236.
107          ZAVG(1) = 0.0                                                            237.
108          X(1) = 0.0                                                               238.
109          DATA RR(1),RRB(1),RRE(1)/3*0.0/                                          239.
110                                    DO 30 I=2,MT                                   240.
111     •    T(I)=TAV                                                                 241.
112       30                           CONTINUE                                      242.
          C    ****************************************                              243.
          C    INITIAL BUBBLE HYDRODYNAMIC CALCULATION                               244.
113          IF (HLF .EQ. 0.0 .AND. VMF .EQ. 0.0) VMF = VOLUME(HLMF)                  245.
114          CALL HYDRO                                                               246.
115                                   DO 611 I=2,M1                                   247.
116          ZAVG(I) = ( H(I) + H(I-1) ) * .5                                         248.
117       611                          CONTINUE                                      249.
          C    ****************************************                              250.
118          IF(IGNITE.EQ.1)GO TO 41                                                  251.
119          ETC=0.                                                                   252.
120          YAV=XGF(1)                                                               253.
121          XAV=WCOAL*XC/(WCOAL+WAD)*(1.-XW)                                         254.
122          FMO=FMF                                                                  255.
123          IF (WAD.EQ.0.0 .AND. IGNITE .EQ. 0) GO TO 900                            256.
          C    ********************************************************************* 257.
          C    FOR CONDITIONS  A  &  B , NO COAL COMBUSTION. IGNITION IS ZERO        258.
          C    WHEN NO IGNITION, TEMP ITERATION,ENERGY BALANCE,MASS BALANCE          259.
          C    CALCULATIONS  SKIPPED.                                                260.
          C    ********************************************************************* 261.
124          YB(1) = YAV                                                              262.
125          YE(1) = YB(1)                                                            263.
126          FEM(1) = UMF(1) * AT(1) * PAV / (RG*T(2))                                264.
127          FBM(1) = FMO - FEM(1)                                                    265.
128                                   DO 115 I = 2 , 46                               266.
129          RRB(I) =0.0                                                              267.
130          RRE(I) = 0.0                                                             268.
131          YB(I)=YAV                                                                269.
132          YE(I)=YAV                                                                270.
133          X(I)=XAV                                                                 271.
134          IF (I .GT. M1) GO TO 115                                                 272.
135          FEM(I) = UMF(I)*AT(I)*(1.0-ETUBE(I))*PAV / (RG*T(I))                     273.
136          FBM(I) = FMO - FEM(I)                                                    274.
137          IF (UO(I) .LE. UMF(I)) FEM(I) = 0.0                                      275.
138       115                          CONTINUE                                      276.
139          IF (IGNITE .EQ. 0) GO TO 630                                             277.
140       41 CONTINUE                                                                 278.
          C                                                                          279.
          C     QCLCN   : HEAT CONSUMED BY CALCINATION.   THIS HEAT CONSUMPTION IS   280.
          C     DISTRIBUTED UNIFORMLY TO EACH COMPT. HAVING TEMP.>900 KELVIN.        281.
          C     QIN     : SENCIBLE HEAT CARRIED IN BY THE FEED SOLIDS AND GAS.       282.
          C                                                                          283.
141          QIN = (CADF*WAD+CCF*WCOAL)*(TSF-273.) + CGMF*FMF*(TF-273.)               284.
142          QCLCN=(42500.0*XCACO3/MCACO3 + 23810.0*XMGCO3/MMGCO3) * WAD              285.
143          CGM=6.8+0.5E-3*(TAV-273.)                                                286.
144          CS=0.215                                                                 287.
145          ELLOSS = 0.07                                                            288.
146          IF (IFBC .GT. 0) ELLOSS = 0.0                                            289.
147          CELU = WCOAL * XC * ELLOSS*(1.-XW)                                       290.
148          WELT = CELU / 0.25                                                       291.
149          TAV=1200.                                                                292.
150          A4 = WCOAL *XC *(1.-XW)*(1.-ELLOSS)/(FMO*MC)                             293.
151          AMODF = 10.0 * RHOCAD * (1.0 - EMF) / (RHOCH * DCF)                      294.
          C                                                                          295.
          C      PREPARATORY STATEMENTS FOR THE WHOLE ITERATION.                     296.
          C                                                                          297.
152          ETCA = 0.9975                                                            298.
153          YAV = FMF*XGF(1)/FMO - A4*ETCA*(1.-0.5*GZCO)                             299.
154                                   DO 130 I = 2,46                                 300.
155          T(I) = TAV                                                               301.
156          YB(I)=YAV                                                                302.
157          YE(I)=YAV                                                                303.
```

```
      130                              CONTINUE
      C      BOUDARY CONDITION OF OXYGEN CONCENTRATION
      C
            YBO(1)=AG(1,1)+AG(1,2)*ETCP
            YEO(1)=YBO(1)
            YB(1)=YBO(1)
            YE(1)=YEO(1)
            M1OLD = M1
      C
      C      FROM HERE TO THE STATEMENT NO.600 : TEMPERATURE ITERATION LOOP
      C
                                       DO 600  ITRIAL = 1,30
            CALL HYDRO
                                       DO 150 I=1,M1
            IF (I.EQ.1) FEM(I)=UMF(I)*AT(I) *(1.0-ETUBE(I)) *PAV/(RG*T(2))
            IF (I.NE.1) FEM(I) = UMF(I)*AT(I)*(1.0-ETUBE(I))*PAV/(RG*T(I))
            IF(UO(I).LE.UMF(I)) FEM(I) = FMO
            FBM(I)=FMO-FEM(I)
      150                              CONTINUE
            IF(ITRIAL.NE.1.AND.M1.EQ.M1OLD)GO TO 170
            J1=1
                                       DO 56 I=2,M1
            WFC(I)=0.
            WFAD(I)=0.
            J2=J1
            IF(J1.GT.MFEED)GO TO 56
                                       DO 55 J=J1,MFEED
            IF(ZF(J).GT.H(I))GO TO 55
            WFC(I)=WCOAL*FFC(J)*(XA+(1.0-ETCP)*XC)*(1.-XW)+WFC(I)
            WFAD(I)=WFAD(I)+WCAD*FFAD(J)
            J2=J+1
       55                              CONTINUE
            J1=J2
       56                              CONTINUE
            IF(J1.GT.MFEED)GO TO 58
                                       DO 57 J=J1,MFEED
            WFC(M1)=WFC(M1)+WCOAL*FFC(J)*(XA+(1.0-ETCP)*XC)*(1.-XW)
            WFAD(M1)=WFAD(M1)+WCAD*FFAD(J)
       57                              CONTINUE
       58 CONTINUE
      170 CONTINUE
                                      DO 133 I=2,M1
            TOLD(I)=T(I)
      133                              CONTINUE
      C
      C      FROM THE STATEMENT NO. 200 TO 300 : ITERATION OF MATERIAL BALANCE
      C      BASED ON THE GIVEN TEMPERATURE PROFILE. GAUSS SEIDEL METHOD
      C
      200 CONTINUE
            INDEX = 0
            DETC = -0.05
            EETCM = 0.01
                                       DO 201 NT = 1,30
      199   CONTINUE
            WNET1=WCAD+WCOAL*(XA+XC*(1.0-ETCA)*(1.-ELLOSS))*(1.-XW)
            XAVIC=WCOAL*XC*(1.-ETCA)*(1.-XW)*(1.-ELLOSS)/WNET1
                                       DO 1 I = 1,M1
      1     X(I) = XAVIC
      C       GENB AND GENE : GENERATION RATE OF OXYGEN
            GENE=0.
            GENB=0.
            TCRATE = 0.0
                                       DO 235 I=2,M1
            CALL AKK(AKB,T(I),PAV,DCAV,TPB(I),YB(I),RG)
            TAVB=(T(I)+TPB(I))/2.
            CALL AKK(AKE,T(I),PAV,DCAV,TPE(I),YE(I),RG)
            TAVE=(T(I)+TPE(I))/2.
            I1=I-1
            AM=AMODF*X(I)
            CALL GPHASE (AKB,AKE,AM,PAV,RG,ETUBE(I),EPB(I),EPC(I),
           1AKBE(I),DVBB(I),FBM(I1),FEM(I1),FBM(I),FEM(I),T(I),TAVB,TAVE,YB(I1
           2),YE(I1),YB(I),YE(I),GENB,GENE)
            A1 = DVBB(I)*MC
            RRB(I) = A1*AM*(PAV/RG)*(EPC(I)-EPB(I))*YB(I)*AKB/TAVB
            RRE(I) = A1*AM*(PAV/RG)*(1.-EPC(I)-ETUBE(I))*YE(I)*AKE/TAVE
            RR(I)=(RRB(I)+RRE(I))/X(I)
```

```
222           TCRATE = TCRATE + RRB(I) + RRE(I)                                  380.
      C*      WRITE (6,202)  I,RRB(I),RRE(I),RR(I),YB(I),YE(I)                   381.
      C*202 FORMAT ('0',' I,RRB(I),RRE(I),RR(I),YB(I),YE(I)  = ',T50,I5,5X,     382.
      C*    1 1P5E12.4)                                                          383.
      C*      WRITE (6,203) TPB(I),TPE(I),T(I),X(I),ETCA                         384.
      C*203 FORMAT ('0',' TPB(I),TPE(I),T(I),X(I),ETCA = ',T60,1P5E12.4)         385.
      C*      WRITE (6,204)  WFC(I),WFAD(I),AKB,AKE                              386.
      C*204 FORMAT('0',' WFC(I),WFAD(I),AKB,AKE  = ',T60,1P4E12.4)               387.
223   235                              CONTINUE                                   388.
224           ETCG=FMF*XGF(1)+WCOAL*(1.-XW)*XO/MO2-FBM(M1)*YB(M1)-FEM(M1)*YF(M1) 389.
225           ETCG = ETCG/(FMTH*XGF(1)*(1.-ELLOSS))                              390.
      C*      WRITE (6,205) ETCG,TCRATE                                          391.
      C*205 FORMAT ('0',50X,'ETCG  =  ',F6.4,20X,'TCRATE  =  ',F7.3,/)           392.
226           IF ( NT .NE. 1) GO TO 215                                          393.
227           IF ( ETCG . LT . ETCA .OR. ETCG .GE. 1.0 ) GO TO 215               394.
228           ETCA = ETCG                                                        395.
229           GO TO 199                                                          396.
230   215     CONTINUE                                                           397.
      C                                                                        398.
      C       DEFENCE FOR CONTRADICTON BETWEEN GAS AND SOLID MATERIAL BALANCE   399.
      C                                                                        400.
231           TCAR = WCOAL*(1.-XW)*XC*(1.-ELLOSS)                                401.
232           IF (TCRATE .LE. TCAR) GO TO 241                                    402.
233                                DO 212 I = 2,M1                               403.
234           RRB(I) = RRB(I) * TCAR / TCRATE                                    404.
235           RRE(I) = RRE(I) * TCAR / TCRATE                                    405.
236           RR(I)  = ( RRB(I)+RRE(I) ) / X(I)                                  406.
237           BB = AKBF(I) * DVBB(I) * EPB(I) * PAV / (RG * T(I))                407.
238           IF (BB.EQ.0.) YB(I) = 0.0                                          408.
239           BB1 = FEM(I-1) * YE(I-1) - RRE(I)/MC                               409.
240           BB2 = BB1*BB/(BB+FEM(I)) -RRB(I)/MC + FBM(I-1) * YB(I-1)           410.
241           IF (BB .NE. 0.0) YB(I) = BB2 / ( FBM(I)+FEM(I)*BB/(BB+FEM(I)) )    411.
242           YE(I) = ( YB(I)*BB+BB1)/(BB+FEM(I))                                412.
243   212     CONTINUE                                                           413.
      C*      WRITE (6,230)                                                      414.
      C*230 FORMAT ('0',T9,'I',T24,'RRB(I)',T46,'RRE(I)',T68,'RR(I)',           415.
      C*    1T90,'YB(I)',T112,'YF(I)',/)                                         416.
      C*      WRITE (6,240) (I,RRB(I),RRE(I),RR(I),YB(I),YF(I),I=2,M1)           417.
      C*240 FORMAT (I10,1P5E22.4)                                              418.
244           ETCG=FMF*XGF(1)+WCOAL*(1.-XW)*XC/MO2-FBM(M1)*YB(M1)-FEM(M1)*YE(M1) 419.
245           ETCG = ETCG/(FMTH*XGF(1)*(1.-ELLOSS))                              420.
246           IF (ETCG .GT. 1.0) ETCG = 0.999                                    421.
      C*      WRITE (6,205) ETCG,TCAR                                            422.
247   241     CONTINUE                                                           423.
248     250   CONTINUE                                                           424.
249           WMIX(1)=0.                                                         425.
250           WNET(1)=0.                                                         426.
251           WDIS=(XA+(1.-ETCG)*XC)*WCOAL*(1.-XW)+WCAD-WELT                     427.
252           IF (WDIS .LT.0.0) WDIS = 0.0                                       428.
253           J1=1                                                               429.
254                                DO 61 I=2,M1                                  430.
255           WD(I)=0.                                                           431.
256           J2=J1                                                              432.
257           IF(J1.GT.MDIS)GO TO 61                                             433.
258                                DO 60 J=J1,MDIS                               434.
259           IF(ZDIS(J).GT.H(I))GO TO 60                                        435.
260           WD(I)=WD(I)+WDIS*FD(J)                                             436.
261           J2=J+1                                                             437.
262        60                              CONTINUE                              438.
263           J1=J2                                                              439.
264        61                              CONTINUE                              440.
265           IF(J1.GT.MDIS)GO TO 63                                             441.
266                                DO 62 J=J1,MDIS                               442.
267           WD(M1)=WD(M1)+WDIS*FD(J)                                           443.
268        62                              CONTINUE                              444.
269        63 CONTINUE                                                           445.
      C                                                                        446.
      C       WMIX : UP- AND DOWN-WARD SOLID MIXING FLOW WHICH IS SUPERPOSED ON 447.
      C              FLOW OF SOLIDS.     G/SEC                                 448.
      C       WNET(I) : NET FLOW RATE OF SOLID FROM THE TOP OF I-TH COMPARTMENT. 449.
      C              POSITIVE VALUE MEANS THE UPWARD FLOW.                      450.
270                                DO 255 I=2,M1                                 451.
271           WNET(I)=WNET(I-1)+WFC(I)+WFAD(I)-WD(I)-RR(I)*X(I)                  452.
272           S(I)=0.                                                            453.
273           IF(WNET(I).GT.0.)S(I)=1.                                           454.
274           WMIX(I)=AT(I)*(1.0-ETUBE(I))*(UO(I)-UMF(I))*(1.-EMF)*RHOCAD*FW     455.
```

```
      IF(WMIX(I).LT.0.)WMIX(I)=0.                                          456.
  255 CONTINUE                                                             457.
      WMIX(M1)=0.                                                          458.
C                                                                          459.
C     CARBON CONCENTRATION CALCULATION.                                    460.
C                                                                          461.
      MM=M*M                                                               462.
                              DO 411 I=1,MM                                463.
  411 AAA(I)=0.                                                            464.
                              DO 412 I=1,M                                 465.
  412 BBB(I)=0.                                                            466.
      AAA(1)=-RR(2)-WMIX(2)-WNET(2)*S(2)-WD(2)                             467.
      AAA(M1)=WMIX(2)+(S(2)-1.)*WNET(2)                                    468.
      AAA(MM)=-RR(M1)-WMIX(M)-S(M1)*WNET(M1)-(S(M)-1.)*WNET(M)-WD(M1)      469.
      AAA(MM-M)=S(M)*WNET(M)+WMIX(M)                                       470.
      A1=(1.0-ETCP)*XC/(XA+(1.0-ETCP)*XC)                                  471.
                              DO 413 I=1,M                                 472.
      I1=I+1                                                               473.
      IF (WFC(I1) .NE. 0.0 .OR. WFAD(I1) .NE. 0.0)                         474.
     *BBB(I)=-WFC(I1)*A1/(WFC(I1)+WFAD(I1))                                475.
  413                         CONTINUE                                     476.
      M0=M-1                                                               477.
                              DO 270 I=2,M0                                478.
      II=(I-1)*M+I                                                         479.
      I1=I+1                                                               480.
      AAA(II)=-RR(I1)-WMIX(I1)-WMIX(I)-S(I1)*WNET(I1)-(S(I)-1.)*WNET(I)    481.
     1-WD(I1)                                                              482.
      AAA(II-M)=S(I)*WNET(I)+WMIX(I)                                       483.
      AAA(II+M)=(S(I1)-1.)*WNET(I1)+WMIX(I1)                               484.
  270 CONTINUE                                                             485.
      CALL SIMQ(AAA,BBB,M,KS)                                              486.
      SUM=0.                                                               487.
      SUM2=0.                                                              488.
                              DO 280 I=1,M                                 489.
      X(I+1) = BBB(I)                                                      490.
      SUM2=SUM2+X(I+1)                                                     491.
  280 CONTINUE                                                             492.
      XAV=SUM2/FLOAT(M)                                                    493.
      SUM=0.                                                               494.
                              DO 285 I=2,M1                                495.
      SUM=WD(I)*X(I)+SUM                                                   496.
  285                         CONTINUE                                     497.
      CLOSS = SUM - CFLU                                                   498.
      ETCC = 1.0 - SUM / ( WCOAL * XC * (1.-XW) *(1.-ELLOSS) )             499.
C*                            DO 220 I = 2,M1                            500.
C*    WRITE (6,206) I,WD(I),WNET(I),X(I),ETCC,XAV                        501.
C*206 FORMAT ('0','   THIS IS AFTER MATERIAL BALANCE CALCULATIONS',/,     502.
C*   1'    I,WD(I),WNET(I),X(I),ETCC,XAV    =' ,I5O,I5,5X,1P5E12.4)      503.
C*220                         CONTINUE                                     504.
      EE = ETCC - ETCG                                                     505.
      CALL CRRECT (NT,INDEX,DETC,ETC1,ETC2,ETCA,E1,E2,EE,EETCM)            506.
      IF (INDEX .EQ. 2) GO TO 211                                          507.
  201                         CONTINUE                                     508.
      WRITE (6,3400)                                                       509.
 3400 FORMAT ('0',10X,' ETCA HAS NOT CONVERGED. S.NO.  =  3400',/)         510.
  211 CONTINUE                                                             511.
      SUM=0.                                                               512.
      ETC = 1. - CLOSS / ( WCOAL * XC * (1.-XW))                           513.
                              DO 290 I=2,M1                                514.
      SUM=RR(I)*X(I)+SUM                                                   515.
  290 CONTINUE                                                             516.
C                                                                          517.
C  THE DEFINITION OF RR(I) IS CHANGED FOR TEMPERATURE CALCULATIONS.        518.
C  RR(I)=(HEAT GENERATION RATE- HEAT CONSUMPTION RATE) IN THE              519.
C  ITH COMPARTMENT.                                                        520.
C                                                                          521.
      IQC=0                                                                522.
                              DO 291 I=2,M1                                523.
      IF (T(I)-900.) 291,291,292                                           524.
  292 IQC=IQC+1                                                            525.
  291 CONTINUE                                                             526.
      DQCAL = 0.0                                                          527.
      IF (IQC .GT. 0) DQCAL = QCLCN/FLOAT(IQC)                             528.
                              DO 295 I=2,M1                                529.
      AQCAL=1.                                                             530.
      IF (T(I).LE.900.) AQCAL=0.                                           531.
```

```
336           RR(I)=RR(I)*X(I)/SUM*QCOAL*WCOAL*ETC-DQCAL*AQCAL                  532.
337       295 CONTINUE                                                          533.
338       300 CONTINUE                                                          534.
          C                                                                     535.
          C       CALCULATION OF TEMPERATURE                                    536.
          C                                                                     537.
339           A1= CADF*WAD/WCAD                                                 538.
340           A2= CCF/(XA+(1.0-ETCP)*XC)                                        539.
341           A3=CGM*FMO                                                        540.
342           ALFA(2)=(WNET(2)*S(2)+WMIX(2)+WD(2))*CS+A3+UHE(2)*AHEAV(2)*DVBB(2) 541.
343           BETA(2)=((S(2)-1.)*WNET(2)+WMIX(2))*CS                            542.
344           GAMA(2)=0.                                                        543.
345           DELT(2)=RR(2)+CGMF*FMF*(TF-273.)+(A1*WFAD(2)+A2*WFC(2))*(TSF-273.) 544.
             1+UHE(2)*AHEAV(2)*DVBB(2)*(TW(2)-273.)                             545.
346                                   DO 310 I=3,M                              546.
347           I1=I-1                                                            547.
348           ALFA(I)=(WNET(I)*S(I)+(S(I1)-1.)*WNET(I1)+WMIX(I)+WMIX(I1)+WD(I))  548.
             1*CS+A3+UHE(I)*AHEAV(I)*DVBB(I)                                    549.
349           BETA(I)=((S(I)-1.)*WNET(I)+WMIX(I))*CS                            550.
350           GAMA(I)=(S(I1)*WNET(I1)+WMIX(I1))*CS+A3                           551.
351           DELT(I)=RR(I)+(A1*WFAD(I)+A2*WFC(I))*(TSF-273.)+UHE(I)*AHEAV(I)*  552.
             1DVBB(I)*(TW(I)-273.)                                              553.
352       310                         CONTINUE                                554.
353           ALFA(M1)=((S(M)-1.)*WNET(M)+WMIX(M)+WD(M1))*CS+A3                 555.
             1+UHE(M1)*AHEAV(M1)*DVBB(M1)                                       556.
354           BETA(M1)=0.                                                       557.
355           GAMA(M1)=(S(M)*WNET(M)+WMIX(M))*CS+A3                             558.
356           DELT(M1)=RR(M1)+(A1*WFAD(M1)+A2*WFC(M1))*(TSF-273.)               559.
             1+UHE(M1)*AHEAV(M1)*DVBB(M1)*(TW(M1)-273.)                         560.
          C                                                                     561.
          C  TEMPERATURE SOLUTION BY SIMQ                                       562.
357                                   DO 501 I=1,MM                             563.
358       501 AAA(I)=0.                                                         564.
359                                   DO 502 I=1,M                              565.
360       502 BBB(I)=DELT(I+1)                                                  566.
361           AAA(1)=ALFA(2)                                                    567.
362           AAA(M1)= -BETA(2)                                                 568.
363           AAA(MM)= ALFA(M1)                                                 569.
364           AAA(MM-M)=-GAMA(M1)                                               570.
365                                   DO 503 I=2,MO                             571.
366           II=(I-1)*M+I                                                      572.
367           AAA(II)=ALFA(I+1)                                                 573.
368           AAA(II-M)=-GAMA(I+1)                                              574.
369           AAA(II+M)=-BETA(I+1)                                              575.
370       503 CONTINUE                                                          576.
371           CALL SIMQ(AAA,BBB,M,KS)                                           577.
372           TNORM=0.                                                          578.
373           TAV=0.                                                            579.
374                                   DO 504 I=2,M1                             580.
375           T(I)=BBB(I-1)+273.                                                581.
          C*        WRITE (6,207) I,T(I)                                      582.
          C*207 FORMAT ('0','*** AFTER ENERGY BALANCE ***. I,T(I)  = ',I55,F12.2) 583.
376           TAV=TAV+T(I)                                                      584.
377           TNORM=TNORM+ABS(T(I)-TOLD(I))                                     585.
378       504 CONTINUE                                                          586.
379           TAV=TAV/FLOAT(M)                                                  587.
380           TNORM=TNORM/FLOAT(M)                                              588.
381       360 CONTINUE                                                          589.
          C*        WRITE (6,208) TNORM                                       590.
          C*208 FORMAT ('0', 50X,'TNORM = ',T60,F5.1)                         591.
382           IF(TNORM.LT.0.01*TAV) GO TO 610                                   592.
383           M1OLD = M1                                                        593.
384       600                         CONTINUE                                594.
385           WRITE (6, 3003)                                                   595.
386       3003 FORMAT('0',10X,'GAUSS SEIDEL TEMPERATURE TRIAL HAS NOT CONVERGED. 596.
             1 S.NO. = 3003',/)                                                 597.
387       610 CONTINUE                                                          598.
388                                   DO 620 I = 2,M1                           599.
389           A1 = AHEAV(I) * DVBB(I)                                           600.
390           HAREA = HAREA + A1                                                601.
391           QTRANS = UHE(I) * A1 * ( T(I)-TW(I) ) + QTRANS                    602.
392           RR(I) = RR(I) / DVBBEF(I)                                         603.
393           ZAVG(I) = ( H(I-1) + H(I) ) * 0.5                                 604.
394       620                         CONTINUE                                605.
395           QVOL = QTRANS/BEDVOL                                              606.
396           IF (HAREA .NE. 0.0) QAREA = QTRANS/HAREA                          607.
```

```
      TPB(1)=T(1)                                                       608.
      TPE(1)=T(1)                                                       609.
      TAV=TAV-273.                                                      610.
                                    DO 612 I=1,M1                       611.
      T(I)=T(I)-273.                                                    612.
      TPB(I)=TPB(I)-273.                                                613.
      TPE(I)=TPE(I)-273.                                                614.
  612 CONTINUE                                                          615.
C      =============                                                    616.
C      MAIN OUTPUT 3                                                    617.
C      =============                                                    618.
      WRITE(6,2001)ETC,XAV,TAV,ITRIAL,(I,YB(I),YE(I),X(I),H(I),T(I)     619.
     1  ,ZAVG(I),TPB(I),TPE(I),WNET(I),RR(I),I=1,M1)                    620.
      TAV=TAV+273.                                                      621.
C                                                                       622.
  630 CONTINUE                                                          623.
C          CALCULATION OF SO2 REDUCTION                                 624.
C                                                                       625.
      IF (IGNITE.EQ.0) TCRATE = 0.0                                     626.
                                    DO 710 I=2,M1                       627.
      YBO(I)=YB(I)                                                      628.
      YEO(I)=YE(I)                                                      629.
      YB(I)=0.                                                          630.
      YE(I)=0.                                                          631.
  710                               CONTINUE                            632.
      FTS=1.                                                            633.
      A1=WCOAL*XS/MS*FLOAT(IGNITE)*(1.-XW)                              634.
      DENOM=(XGF(3)+XGF(6))*FMF+A1                                      635.
      IF (DENOM . LE. 1.E-6) GO TO 810                                  636.
      CABSE=WAD*XCACO3/MCACO3/DENOM                                     637.
C                                                                       638.
C       CABSE : EFFECTIVE RATIO OF CA TO S(ACTIVE) IN THE FEEDS         639.
C                                                                       640.
                                    DO 711 I=2,M1                       641.
      SRELB(I)=0.                                                       642.
      SRELF(I)=0.                                                       643.
      IF (TCRATE .LE. 0.) GO TO 711                                     644.
      SRELB(I) = RRB(I)/TCRATE*A1                                       645.
      SRELF(I) = RRF(I)/TCRATE*A1                                       646.
  711                               CONTINUE                            647.
      SRELB(1)=0.                                                       648.
      SRELF(1)=0.                                                       649.
      YB(1)=(XGF(3)+XGF(6))*FMF/FMO                                     650.
      YE(1)=YB(1)                                                       651.
      ETS=1.                                                            652.
      DETS=-0.1                                                         653.
      EETSM=0.0005                                                      654.
      INDX=0.                                                           655.
      A2=0.                                                             656.
      IF(WAD.GT.0.)A2=1.                                                657.
                                    DO 800 ITRY=1,30                    658.
      FS=ETS/CABSE                                                      659.
C                                                                       660.
C       FS : FRACTIONAL CONVERSION OF ADDITIVE                          661.
C                                                                       662.
      AK0=AKAD(FS,DPADR,TAV)*A2                                         663.
C                                                                       664.
C   IF THE RESIDENCE TIME OF SOLIDS AT THE TOP COMPARTMENT IS TOO SMALL 665.
C     AND UO IS SMALLER THAN UMF IN THIS COMPARTMENT, IT IS ASSUMED     666.
C     LIME IS INACTIVE FOR SO2 ADSORPTION.                              667.
C                                                                       668.
      A3=1.                                                             669.
      IF(UO(M1).GT.UMF(M1))GO TO 730                                    670.
      THET = VMF*(1.-EMF)*RHOCAD/WCAD                                   671.
      IF(VMF*(1.-EMF)*RHOCAD.GT.WNET(M)*THET*5.)A3=0.                   672.
  730 CONTINUE                                                          673.
                                    DO 740 I=2,M1                       674.
      I1=I-1                                                            675.
      AK=AK0                                                            676.
      IF(I.EQ.M1)AK=AK0*A3                                              677.
      AM=(1.-EMF)                                                       678.
      CALL GPHASE(AK,AK,AM,PAV,RG,ETUBE(I),FPB(I),EPC(I),               679.
     1AKBE(I),DVBB(I),FBM(I1),FEM(I1),FBM(I),FEM(I),T(I),T(I),T(I),     680.
     2YB(I1),YE(I1),YB(I),YE(I),SRELB(I),SRELF(I))                      681.
  740                               CONTINUE                            682.
      ETSC=1.-(FBM(M1)*YB(M1)+FEM(M1)*YE(M1))/DENOM                     683.
```

```
      EE=ETS-ETSC
      CALL CRRECT(ITRY,INDX,DETS,ETS1,ETS2,ETS,E1,E2,EE,EETSM)
      IF(INDX.EQ.2)GO TO 810
  800                              CONTINUE
      WRITE(6,3500)
 3500 FORMAT('0',10X,'   ETS HAS NOT CONVERGED. S.NO.  =  3500',/)
  810 CONTINUE
C      =============
C      MAIN OUTPUT 4
C      =============
      WRITE(6,2005)ETS,FS,CABS,CABSE
     1,(H(I),ZAVG(I),YB(I),YE(I),SRELB(I),SRELF(I),I=2,M1)
      XGO(1)=( FBM(M1)*YBO(M1)+FEM(M1)*YEO(M1) ) / FMO
      XGO(2)=AG(2,1)+AG(2,2)*ETC+WAD*(XCACO3/MCACO3+XMGCO3/MMGCO3)
      XGO(3)=( FBM(M1)*YB(M1)+FEM(M1)*YE(M1) ) / FMO
      XGO(4)=AG(4,1)
      XGO(5)=AG(5,1)+AG(5,2)*ETC
      XGO(6)=AG(6,1)
      XGO(7)=AG(7,1)
      ANOX = AN * WCOAL * (1.-ETC) * QCOAL / FMO
      WRITE(6,2006) (XGO(I),I=1,7),ANOX
  900 CONTINUE
      IF (VMF.EQ.0.0) VMF = SOLVOL
      IF (HLMF .EQ. 0.0) HLMF = HEIGHT(VMF)
      IF (HLF .EQ. 0.0) HLF = H(M1)
C
C     PRESSURE DROP CALCULATION
C
C     ******************************************
C     ALL THE PRESSURE DROP GIVEN IN CM OF WATER
C     ******************************************
C
C     PRESSURE DROP CALCULATIONS ACROSS THE DISTRIBUTOR
C
      TEMP = (T(1)+T(2)) * 0.5
      RHOFG = PF * MGAS / (RG*TEMP)
      UOR = FMF * RG * TEMP/ PF /(AND*0.25*PI*DNZL**2)
      DPDIS = ( UOR/0.6 ) **2 * RHOFG / (2.0*G)
      WRITE (6,2050) DPDIS
C
C     PRESSURE DROP CALCULATIONS IN THE FLUCIZIED BED SECTION
C
      WRITE (6,2051)
      N1 = M1
      IF (IFBC .GT. 0) N1 = M1 - 1
                                  DO 920 I = 2,N1
      DPFLU     = (1.0-EMF)*(1.0-EPB(I))*(H(I)-H(I-1)) * RHOCAD
      WRITE (6,2052) I, DPFLU
  920 CONTINUE
      IF (IFBC .EQ.0) GO TO 930
C
C     PRESSURE DROP CALCULATIONS IN THE FIXED BED SECTION
C
      E1 = ( H(M1) - H(M1-1) ) / G
      E2 = ( 1.0 - EMF )  / EMF ** 3
      DPFIX = E1 * ( 150.0 * ( 1.0 - EMF ) * E2 * VISC * UO(M1)
     1 / DPB ** 2 + 1.75 * E2 * RHOGAS * UO(M1)**2/DPB)
  930 CONTINUE
      IF ( IFBC .EQ. 0 ) DPFIX = 0.0
      WRITE (6,2053) DPFIX
      WRITE (6,OPCF1)
      WRITE(6,2060)
                                  DO 910 I = 2,M1
      WRITE(6,2070) I,H(I),ZAVG(I),DBAV(I),UB(I),EPB(I),EPC(I),UO(I),
     1UMF(I)
  910                              CONTINUE
 1000 FORMAT(I10)
 1001 FORMAT(8F10.0)
 1010 FORMAT(2A4/(8F10.0))
 1020 FORMAT(8F10.0)
 1021 FORMAT(8F10.0)
 2000 FORMAT ('0',1X,2A4,10X,'XCACO3 = ',F6.3,10X,'XMGCO3 = ',F6.3/'0',
     *T41,'DPADF , CM',T81,'WT.FRACTION',/,'0',(T41,F8.4,T81,F8.4))
 2001 FORMAT(//10X,'RESULTS ,ALL TEMPERATURES IN CENTIGRADE'//
     *' ETC,XAV,TAV,ITRIAL,=',3E12.4,I4//
     12X,'I',6X,'YB',10X,'YE',10X,'X',11X,'Z',11X,'T',10X,'ZAVG'
```

```
     2,10X,'TPB',10X,'TPE',7X,'WNET',9X,'RR'/(I4,1P10E12.4))
2005  FORMAT(//' (ETS,FS,CABS,CABSE)='/10X,4E12.4//7X,'HT.',10X,'ZAVG',
     110X,'YB',10X,'YE',10X,'SRELB',9X,'SRELE'/(1P6E13.4))
2006  FORMAT(/' OUTLET GAS CONCENTRATION' .//5X,'O2',10X,'CO2',9X,'SO2',
     19X,'H2O',9X,'CO',10X,'H2S',9X,'H2',10X,'NOX'//8E12.4//)
2010  FORMAT ('0',5X,'SURFACE VOLUME MEAN DIA. = DPADH = ',F10.4,3X,'CM'
     *,5X,'WEIGHT MEAN DIA. = DPADR = ',F10.4,3X,'CM',/)
2020  FORMAT ('0',1X,2A4,3X,'XCF = ',F5.3,3X,'XCV = ',F5.3,3X,'XH = ',
     *F5.3,3X,'XS = ',F5.3,3X,'XO = ',F5.3,3X,'XN = ',F5.3,3X,'XA = ',
     $F5.3,3X,'XW = ',F5.3,/,11X,'QCOAL = ',F8.2,3X,'CALS/GM',10X,
      'QCOALC = ',F8.2,3X,'CALS/GM',/)
2030  FORMAT ('0',T41,'DPCF , CM',T81,'WT.FRACTION'/'0',(T41,F8.4,T81,
     *F8.4))
2040  FORMAT('0',T21,'SURFACE VOL MEAN DIA OF COAL FEED = DCF = ',F10.4,
     *3X,'CM',5X,'DCAV = ',F10.4,/)
2050  FORMAT ('0',40X,'PRESSURE DROP ACROSS THE DISTRIBUTOR = ',1PE11.4)
2051  FORMAT ('0',20X,'COMP.NO',13X,'PRESSURE DROP IN THE BED',/)
2052  FORMAT (20X,I5,20X,1PE11.4)
2053  FORMAT ('0',40X,'PRESSURE DROP IN THE FIXED BED SECTION = ',1PE11.
     *4)
2060  FORMAT ('0',3X,'I',3X,'HEIGHT',6X,'ZAVG',3X,'AV.BUBBLE DIA',6X,
     1'BUBBLE VEL.',4X,'BUBBLE FRAC.',5X,'CLOUD FRAC.',6X,'SUP.VELOCITY'
     2,5X,'MIN.FLU.VEL.',/)
2070  FORMAT (I5,F8.3,2X,F8.3,6(3X,1PE12.4,2X))
10000 STOP
      END

      SUBROUTINE AKK(AKR,T,P,DC,TP,YO2,RG)
C
C  THIS COMPUTES REACTION RATE AKR, AND PARTICLE TEMP. TP
C
      EM=0.5
      SIGM=1.36E-12
      SHP=2.
      INDX=0
      DTS=100.
      TP=T
      ETSMAX=0.05
                                  DO 100 I=1,30
      AKS=EXP(17.9-35.7/(.001986*TP))*TP/1000.
      TAV=(T+TP)*.5
      D=4.26*(TAV/1800.)**1.75/P
      COND=0.5659E-04+1.07E-07*TAV
      AKF=SHP*D/DC
      AKR=1./(1./AKS+1./AKF)
      ETS=TP-T-AKR*P*YO2*7900./((2.0*COND/DC+(((TP+T)*TP
     *    +T**2)*TP+T**3)*EM*SIGM)*RG*TAV)
      CALL CRRECT(I,INDX,DTS,TP1,TP2,TP,E1,E2,ETS,ETSMAX)
      IF (INDX.EQ.2) GO TO 110
  100 CONTINUE
      WRITE (6, 4000)
 4000 FORMAT ('0',10X,'TP CALCULATION HAS NOT CONVERGED. S.NO.=4000',/)
  110 CONTINUE
      RETURN
      END

      SUBROUTINE CRRECT(I,INDX,DX,X1,X2,XNEW,E1,E2,E,EMAX)
C     I: NUMBER OF THIS TRIAL, 1 FOR FIRST TRIAL
C     INDX: INDEX OF THE TRIAL LEVEL
C     INDX=0: JUST PROCEEDING
C     INDX=1: THE ROOT HAS BEEN CAUGHT BETWEEN X1 AND X2
C     INDX=2: THE ITERATION HAS CONVERGED
      IF (ABS(E).GT.EMAX) GO TO 5
      INDX=2
      RETURN
    5 CONTINUE
      IF(INDX.EQ.1) GO TO 100
      X2=XNEW
      E2=E
      IF(I.EQ.1) GO TO 10
      IF(E1*E2.LE.0.)INDX=1
      IF(INDX.EQ.1)GO TO 150
   10 X1=X2
      E1=E2
```

```
      XNEW=XNEW+DX                                                      832.
      RETURN                                                            833.
  100 CONTINUE                                                          834.
      IF(E1*E.LT.0.) GO TO 110                                          835.
      E1=E                                                              836.
      X1=XNEW                                                           837.
      GO TO 150                                                         838.
  110 E2=E                                                              839.
      X2=XNEW                                                           840.
  150 CONTINUE                                                          841.
      XNEW=(X1-X2)*E2/(E2-E1)+X2                                        842.
      RETURN                                                            843.
      END                                                               844.

      SUBROUTINE SIMQ(A,B,N,KS)                                         845.
      DIMENSION A(2116),B(46)                                           846.
C                                                                       847.
C     FORWARD SOLUTION                                                  848.
C                                                                       849.
      TOL=0.0                                                           850.
      KS=0                                                              851.
      JJ=-N                                                             852.
                                    DO 65 J=1,N                         853.
      JY=J+1                                                            854.
      JJ=JJ+N+1                                                         855.
      BIGA=0.                                                           856.
      IT=JJ-J                                                           857.
                                    DO 30 I=J,N                         858.
C                                                                       859.
C     SEARCH FOR MAXIMUM COEFFICIENT IN COLUMN                          860.
C                                                                       861.
      IJ=IT+I                                                           862.
      IF( ABS(BIGA) - ABS(A(IJ)))20,30,30                               863.
   20 BIGA=A(IJ)                                                        864.
      IMAX=I                                                            865.
   30 CONTINUE                                                          866.
C                                                                       867.
C     TEST FOR PIVOT LESS THAN TOLERANCE ( SINGULAR MATRIX )            868.
C                                                                       869.
      IF( ABS(BIGA) - TOL) 35,35,40                                     870.
   35 KS=1                                                              871.
      WRITE(6,100) KS                                                   872.
  100 FORMAT(/' NO SOLUTION','   KS=',I2)                              873.
      STOP                                                              874.
C                                                                       875.
C     INTERCHANGE ROWS IF NECESSARY                                     876.
C                                                                       877.
   40 I1=J+N*(J-2)                                                      878.
      IT=IMAX-J                                                         879.
                                    DO 50 K=J,N                         880.
      I1=I1+N                                                           881.
      I2=I1+IT                                                          882.
      SAVE=A(I1)                                                        883.
      A(I1)=A(I2)                                                       884.
      A(I2)=SAVE                                                        885.
C                                                                       886.
C     DIVIDE EQUATION BY LEADING COEFFICIENT                            887.
C                                                                       888.
   50 A(I1)=A(I1)/BIGA                                                  889.
      SAVE=B(IMAX)                                                      890.
      B(IMAX)=B(J)                                                      891.
      B(J)=SAVE/BIGA                                                    892.
C                                                                       893.
C     ELIMINATE NEXT VARIABLE                                           894.
C                                                                       895.
      IF( J - N) 55,70,55                                               896.
   55 IQS=N*(J-1)                                                       897.
                                    DO 65 IX=JY,N                       898.
      IXJ=IQS+IX                                                        899.
      IT=J-IX                                                           900.
                                    DO 60 JX=JY,N                       901.
      IXJX=N*(JX-1)+IX                                                  902.
      JJX=IXJX+IT                                                       903.
   60 A(IXJX)=A(IXJX)-(A(IXJ)*A(JJX))                                   904.
   65 B(IX)=B(IX)-B(J)*A(IXJ)                                           905.
```

```
C                                                                       906.
C     BACK SOLUTION                                                     907.
C                                                                       908.
      70 NY=N-1                                                         909.
         IT=N*N                                                         910.
                                      DO 80 J=1,NY                      911.
         IA=IT-J                                                        912.
         IB=N-J                                                         913.
         IC=N                                                           914.
                                      DO 80 K=1,J                       915.
         B(IB)=B(IB)-A(IA)*B(IC)                                        916.
         IA=IA-N                                                        917.
      80 IC=IC-1                                                        918.
         RETURN                                                         919.
         END                                                            920.

         SUBROUTINE GPHASE(AKB,AKE,AM,PAV,RG,ETUBE,EPB,EPC,AKBE,DVBB,FBM0,  921.
        *FEM0,FBM,FEM,T,TB,TE,YB0,YE0,YB1,YE1,GENB,GENE)                922.
         D1= ((1.-ETUBE-EPC)*AM*AKE/TE+AKBE*EPB/T)*PAV/RG*DVBB+FEM      923.
         ALF=AKBE*EPB*DVBB*PAV/(D1*RG*T)                                924.
         D2 = FBM+ALF*FEM+((EPC-EPB)*AKB/TB+                            925.
        1ALF*(1.0-EPC-ETUBE)*AKE/TE)*DVBB*AM*PAV/RG                     926.
         IF (D2 .EQ. 0.0) YB1 = 0.0                                     927.
         IF (D2 .NE. 0.0) YB1=(FBM0*YB0+GENB+ALF*FEM0*YE0)/D2           928.
         YE1=(YE0*FEM0+GENE)/D1+ALF*YB1                                 929.
         RETURN                                                         930.
         END                                                            931.

         FUNCTION AKAD(FS,DP,T)                                         932.
         DIMENSION FB(13),RR(13),RB(13),RC(13)                          933.
         DATA FB/0.0,0.05,0.1,0.2,0.3,0.4,0.5,0.6,0.7,0.8,0.9,0.95,1.0/ 934.
         DATA RR/1.0,0.22,0.075,0.00105,0.00040,0.00022,0.00015,0.00011, 935.
        10.00007,0.00004,0.00002,0.00001,1.E-10/                        936.
         DATA RB/1.0,0.6,0.39,0.165,0.03,0.0071,0.0036,0.00225,0.00145, 937.
        1 0.00089,0.00042,0.00017,1.0E-10/                              938.
         DATA RC/1.0,0.75,0.63,0.45,0.33,0.21,0.115,0.05,0.019,0.0072,  939.
        1 0.0028,0.0012,1.0E-10/                                        940.
         DP1=0.13                                                       941.
         DP2=0.025                                                      942.
         DP3=0.0096                                                     943.
         IF( DP .GE. DP2 ) XXX=ALOG(DP/DP2)/ALOG(DP1/DP2)               944.
         IF( DP .LT. DP2) XXX=ALOG(DP/DP3)/ALOG(DP2/DP3)                945.
         ALIME=0.0                                                      946.
         AKAD = 0.0                                                     947.
         IF( FS .GE. 1.0) RETURN                                        948.
                                      DO 10 I=2,13                      949.
         N=I                                                            950.
         IF( FS .LE. FB(I) ) GO TO 11                                   951.
      10 CONTINUE                                                       952.
      11 CONTINUE                                                       953.
         N1=N-1                                                         954.
         A=(FS-FB(N1))/(FB(N)-FB(N1))                                   955.
         IF( DP .LT. DP2) GO TO 12                                      956.
         R1=(RR(N)/RR(N1))**A*RR(N1)                                    957.
         R2=(RB(N)/RB(N1))**A*RB(N1)                                    958.
         GO TO 13                                                       959.
      12 CONTINUE                                                       960.
         R1=(RB(N)/RB(N1))**A*RB(N1)                                    961.
         R2=(RC(N)/RC(N1))**A*RC(N1)                                    962.
      13 CONTINUE                                                       963.
         ALIME=(R1/R2)**XXX*R2                                          964.
         IF( ALIME .GT. 1.0) ALIME=1.0                                  965.
         TSG = T                                                        966.
         IF (T .LT. 1100) TSG = 1100.0                                  967.
         SG = -193.75*TSG + 2.75E05                                     968.
         AKAD = 490.0*EXP(-17500.0/1.987/T)* SG * ALIME                 969.
C*       WRITE (6,20) AKAD                                              970.
C*20     FORMAT ('0',50X,'AKAD = ',1PE12.4)                             971.
         RETURN                                                         972.
         END                                                            973.

         SUBROUTINE DESIGN                                              974.
         COMMON ZHE(46),AHE(46),PV(46),PH(46),ZF(46),FFC(46),           975.
```

```
     1FFAD(46),ZDIS(46),FD(46),AHEAV(101),ETUBE(101),DB(46),MFEED,MDIS    976.
672   COMMON /DEHYD/ DBED(101),ABED(101),DTUBEI(101),                     977.
     1PHI(101),PVI(101),DVB(101),                                         978.
     2IARRNG(101)                                                         979.
673   COMMON /GEN/ Z(101),DVBEFF(101),ZB(46),ATB(46),PI,DZAV,MTB,MT,M1,M 980.
674   COMMON/DEMAIN/AND,DNZL,DTHICK,FW                                    981.
675   DIMENSION DTUBE(46),IARR(46)                                        982.
      C                                                                   983.
      C     AXIAL VARIATION OF BED CROSS SECTION                          984.
      C                                                                   985.
676   READ (5,1000) A1,A2,A3,A4                                           986.
677   READ (5,1001) MTB,(ZB(J),ATB(J), J = 1, MTB)                        987.
      C                                                                   988.
      C     IARRNG        1              2              3          4      989.
      C     1 -----   VERTICAL TRIANGULAR ARRANGEMENT                     990.
      C     2 -----   VERTICAL RECTANGULAR ARRANGEMENT                   991.
      C     3 -----   HORIZONTAL INLINE ARRANGEMENT                      992.
      C     4 -----   HORIZONTAL STAGGERED ARRANGEMENT                   993.
      C                                                                   994.
      C                                                                   995.
      C     HEAT EXCHANGE TUBES                                           996.
678   READ (5,1002) MTHE,(ZHE(J+1),AHE(J),DTUBE(J),PV(J),PH(J),          997.
     1IARR(J), J = 1,MTHE)                                                998.
      C                                                                   999.
      C     LOCATION OF FEED AND DISCHARGE                               1000.
679   READ (5,1001) MFEED,(ZF(J),FFC(J),FFAD(J), J = 1,MFEED)             1001.
      C                                                                  1002.
680   READ (5,1001) MDIS,(ZDIS(J),FD(J), J = 1,MDIS)                     1003.
      C                                                                  1004.
      C     DISTRIBUTOR                                                  1005.
      C                                                                  1006.
681   READ (5,1003) AND , DNZL , DTHICK                                  1007.
682                           DO 100 J = 1, MTHE                         1008.
683   IF (AHE(J) .GT. 0.0) GO TO 100                                     1009.
684   IF (DTUBE(J) .EQ. 0.0) GO TO 100                                   1010.
685   AHE(J) = PI * DTUBE(J) / (PH(J)*PV(J))                             1011.
686 100                     CONTINUE                                     1012.
      C                                                                  1013.
      C     CONDITION FOR COMPUTING AVERAGE CELL SIZE                    1014.
      C                                                                  1015.
687   READ (5,1003) DZAV,FW                                              1016.
688   N = IFIX (ZB(MTB)/DZAV)                                            1017.
689   IF (ZB(MTB) - FLOAT(N) * DZAV .GT. 0.1 * DZAV) N = N + 1           1018.
690   IF (N .LT. (101)*1) GO TO 25                                       1019.
691   WRITE (6,2020) N                                                   1020.
692 2020  FORMAT ('0',20X,'ARRAY SIZE FOR Z TOO SMALL. N > (101). TRACE DZAV1021.
     1 IN SUBROUTINE DESIGN. MAKE SURE N < Z ARRAY SIZE. N = ',I5 )     1022.
693   STOP                                                               1023.
694 25    CONTINUE                                                       1024.
695   WRITE (6,2000) A1,A2,A3,A4                                         1025.
696   WRITE (6,2001)                                                     1026.
697   WRITE (6,2002) (ZB(J),ATB(J), J = 1,MTB)                           1027.
698   WRITE (6,2003)                                                     1028.
699   WRITE (6,2004) (ZHE(J+1),AHE(J),DTUBE(J),PV(J),PH(J),IARR(J),      1029.
     1J = 1,MTHE)                                                       1030.
700   WRITE (6,2005)                                                     1031.
701   WRITE (6,2006) (ZF(J),FFC(J),FFAD(J), J = 1,MFEED)                 1032.
702   WRITE (6,2007)                                                     1033.
703   WRITE (6,2008) (ZDIS(J),FD(J), J = 1,MDIS)                         1034.
704   WRITE (6,2009) AND,DNZL,DTHICK,DZAV,FW                             1035.
      C                                                                  1036.
      C     SPECIFIC HEAT EXCHANGE AREA CALCULATION FOR EACH COMPARTMENT 1037.
      C                                                                  1038.
705   Z(1) = ZB(1)                                                       1039.
706   ABED(1) = ATB(1)                                                   1040.
707   DBED(1) = SQRT(4.0 * ABED(1) / PI)                                 1041.
708   DVB(1) = 0.0                                                       1042.
709   DVBEFF(1) = 0.0                                                    1043.
710   ZHE(1) = 0.0                                                       1044.
711   IARRNG(1) = 0                                                      1045.
712                           DO 10 I = 1,N                              1046.
713   Z(I+1) = Z(I) + DZAV                                               1047.
714   IF (I .EQ. N) Z(I+1) = ZB(MTB)                                     1048.
715                           DO 20 J = 1,MTHE                           1049.
716   IF ( ZHE(J) .LE. Z(I) .AND. ZHE(J+1) .GE. Z(I+1) ) GO TO 30        1050.
717   IF ( ZHE(J) .LE. Z(I+1) .AND. ZHE(J+1) .LT. Z(I+1) ) GO TO 20      1051.
```

```
      DENOM = Z(I+1) - Z(I)                                                  1052.
      F1 = ( Z(I+1) - ZHE(J) ) / DENOM                                       1053.
      F2 = ( ZHE(J) - Z(I) ) / DENOM                                         1054.
      AHEAV(I+1) = F1 * AHE(J) + F2 * AHE(J-1)                               1055.
      DTUBEI(I+1) = F1 * DTUBE(J) + F2 * DTUBE(J-1)                          1056.
      PVI(I+1) = F1 * PV(J) + F2 * PV(J-1)                                   1057.
      PHI(I+1) = F1 * PH(J) + F2 * PH(J-1)                                   1058.
      GO TO 40                                                               1059.
30    AHEAV(I+1) = AHE(J)                                                    1060.
      DTUBEI(I+1) = DTUBE(J)                                                 1061.
      PVI(I+1) = PV(J)                                                       1062.
      PHI(I+1) = PH(J)                                                       1063.
40    IARRNG(I+1) = IARR(J)                                                  1064.
      GO TO 50                                                               1065.
20                              CONTINUE                                     1066.
50    CONTINUE                                                               1067.
C                                                                            1068.
C     CELL VOL CALCULATION                                                   1069.
C                                                                            1070.
      CALL AREA ( Z(I+1),DBED(I+1),ABED(I+1) )                               1071.
      DVB(I+1) = 0.5 * (ABED(I+1)+ABED(I)) * (Z(I+1)-Z(I))                   1072.
C                                                                            1073.
C      EFFECTIVE CELL VOLUME EXCLUDING THE VOLUME OCCUPIED BY THE            1074.
C      HEAT EXCHANGE TUBES                                                   1075.
C                                                                            1076.
      DVBEFF(I+1) = DVB(I+1) * (1.0 - 0.25 * AHEAV(I+1) * DTUBEI(I+1))       1077.
C                                                                            1078.
C      TUBE VOLUME FRACTION                                                  1079.
C                                                                            1080.
      ETUBE(I+1) = 1.0 - DVBEFF(I+1) / DVB(I+1)                              1081.
10                              CONTINUE                                     1082.
      WRITE (6,2010)                                                         1083.
      M1 = N+1                                                               1084.
      MT = M1                                                                1085.
                                DO 60 I = 2 , M1                             1086.
      WRITE (6,2012) I,Z(I),DVB(I),DVBEFF(I),ETUBE(I),AHEAV(I),              1087.
     1DTUBEI(I),PVI(I),PHI(I),IARRNG(I)                                      1088.
60                              CONTINUE                                     1089.
      WRITE (6,2011)                                                         1090.
                                DO 70  I = 1,M1                              1091.
      WRITE (6,2013) I,Z(I),DBED(I),ABED(I)                                  1092.
70                              CONTINUE                                     1093.
1000  FORMAT (4A4)                                                           1094.
1001  FORMAT (I10/(8F10.0))                                                  1095.
1002  FORMAT (I10/(5F10.0,I10))                                              1096.
1003  FORMAT (8F10.0)                                                        1097.
2000  FORMAT ('1',20X,4A4,//)                                                1098.
2001  FORMAT ('0',T41,'HT.ABOVE DISTRIBUTOR,CM',T81,'CROSS SECTIONAL ',      1099.
     1'AREA OF BED,SQ.CM.',/)                                                1100.
2002  FORMAT (T49,F8.4,T96,F10.3)                                            1101.
2003  FORMAT ('0',T6,'HEIGHT,CM',T20,'SP.HEAT TRANS.AREA,SQ.CM/CU.CM',       1102.
     1T58,'DIA.OF TUBES,CM',T78,'VER.PITCH,CM',T95,'HOR.PITCH,CM',           1103.
     2T113,'TUBES ARRNGT',/)                                                 1104.
2004  FORMAT (T8,F6.2,T33,F8.4,T62,F6.3,T82,F6.3,T99,F6.3,T118,I2)           1105.
2005  FORMAT ('0',T21,'SOLIDS FEED LEVEL',T51,'FRACTION COAL FED',           1106.
     1T81,'FRACTION LIMESTONE FED',/)                                        1107.
2006  FORMAT (T27,F6.2,T58,F6.4,T88,F6.4)                                    1108.
2007  FORMAT ('0',T21,'SOLIDS DISCHARGE LEVEL',T51,'FRACTION DISCHARGED'     1109.
     1,/)                                                                    1110.
2008  FORMAT (T29,F6.2,T58,F6.4)                                             1111.
2009  FORMAT ('0', T12,'NO.OF DISTRIBUTOR HOLES ',T40,'=',T45,F7.1,/,        1112.
     1'0',T12,'NOZZLE DIAMETER ',T40,'=',T45,F7.4,3X,'CM'/'0',T12,           1113.
     2'DISTRIBUTOR THICKNESS ',T40,'=',T45,F7.4,3X,'CM',/,'0',T12,           1114.
     3'AVERAGE CELL SIZE =  DZAV ',T40,'=',T45,F8.3,3X,'CM',/,'0',T12,       1115.
     4'FW',T40,'=',T45,F6.3)                                                 1116.
2010  FORMAT ('0',T5,'NO.',T10,'HEIGHT',T20,'CELL VOLUME',T35,'CELL EFF.     1117.
     1VOL.',T50,'TUBE VOL.FR.',T62,'SP.HE.AREA',T75,'TUBE DIA.',T87,         1118.
     2'VER.PITCH',T100,'HOR.PITCH',T114,'TURE ARRNGT',/)                     1119.
2012  FORMAT (T3,I3,T10,F6.2,T18,1PE12.4,T33,1PE12.4,T50,1PE10.3,T62,        1120.
     *1PE10.3,T75,1PE10.3,T87,1PE10.3,T100,1PE10.3,T116,I3)                  1121.
2011  FORMAT ('0',T10,'COMPT.NO.',T25,'HEIGHT',T42,'BED DIA.',T55,           1122.
     1'BED C/S AREA',/)                                                      1123.
2013  FORMAT (T12,I3,T25,F6.2,T40,1PE10.3,T55,1PE10.3)                       1124.
      RETURN                                                                 1125.
      END                                                                    1126.
```

```
      SUBROUTINE HYDRO                                                  1127.
      REAL MGAS                                                         1128.
      COMMON ZHE(46),AHE(46),PV(46),PH(46),ZF(46),FFC(46),              1129.
     1FFAD(46),ZDIS(46),FD(46),AHEAV(101),ETUBE(101),DB(46),MFEED,MDIS  1130.
      COMMON /DEHYD/ DBED(101),ABED(101),DTUBEI(101),                   1131.
     1PHI(101),PVI(101),DVB(101),                                       1132.
     2IARRNG(101)                                                       1133.
      COMMON/DEMAIN/AND,DNZL,DTHICK,FW                                  1134.
      COMMON /HYMAIN/ UO(46),UMF(46),H(46),AT(46),DT(46),T(101),X(46),  1135.
     1YE(46),EPB(46),EPC(46),DVFB(46),DVBBEF(46),DBAV(46),UB(46),HLMF,  1136.
     2HLF,VMF,FMO,FMF,UF,PF,TF,RG,G,MGAS,DPFIX,DPFLU,DPDIS,DPB,RHOCAD,  1137.
     3EMF,YB(46),PAV,HCR,AKBE(46),BEDVOL,EFFVOL,SOLVOL,TETUBE,ICR,IFBC  1138.
      COMMON /GEN/ Z(101),DVBEFF(101),ZB(46),ATB(46),PI,DZAV,MTB,MT,M1,M1139.
C                                                                       1140.
C     CALCULATION OF BUBBLE HYDRODYNAMICS                               1141.
C                                                                       1142.
      I=0                                                               1143.
      SUM=0.0                                                           1144.
      SUMEFF=0.0                                                        1145.
      BEDVOL = 0.0                                                      1146.
      SUMV = 0.0                                                        1147.
      ICR = 0                                                           1148.
      HCR = 0.0                                                         1149.
      IFBC = 0                                                          1150.
      DTUBEI(1) = 0.0                                                   1151.
15    I = I + 1                                                         1152.
13    IF (I .LE. M1) GO TO 5                                            1153.
      T(I) = T(M1)                                                      1154.
      X(I) = X(M1)                                                      1155.
      YB(I) = YB(M1)                                                    1156.
      YE(I) = YE(M1)                                                    1157.
C                                                                       1158.
C     CALCULATION OF MINIMUM FLUIDIZING VELOCITY                        1159.
C                                                                       1160.
5     CONTINUE                                                          1161.
      IF (IFBC .GT. 0) GO TO 11                                         1162.
      H(I) = Z(I)                                                       1163.
      DT(I) = DBED(I)                                                   1164.
      AT(I) = ABED(I)                                                   1165.
      DVB(I) = DVB(I)                                                   1166.
      DVBBEF(I) = DVBEFF(I)                                             1167.
11    CONTINUE                                                          1168.
      TEMP = T(I)                                                       1169.
      IF (I .EQ. 1) TEMP = T(2)                                         1170.
12    RHOGAS = PAV * MGAS / (RG*TEMP)                                   1171.
      VISC = 3.72E-6 * TEMP **0.676                                     1172.
C                                                                       1173.
C     UMF(I) --- MIN.FLUIDIZING VEL. AT THE H(I) LEVEL ABOVE THE        1174.
C     DISTRIBUTOR                                                       1175.
      A1 =  33.7**2 + 0.0408 * (DPB/VISC)                               1176.
     1 **2 * DPB * G * (RHOCAD - RHOGAS) * RHOGAS                       1177.
      UMF(I) = VISC/(DPB*RHOGAS) * ( SQRT(A1) - 33.7 )                  1178.
      IF (I .GT. 1) GO TO 16                                            1179.
      UO(1) = FMF * MGAS /RHOGAS/AT(1)                                  1180.
      DB(1) = 0.347 * ( AT(1) * (UO(1)-UMF(1))/AND ) **0.4              1181.
      GO TO 15                                                          1182.
C                                                                       1183.
C     UO(I) --- SUPERFICIAL GAS VEL. AT H(I) LEVEL ABOVE DISTRIBUTOR    1184.
16    UO(I) = FMO * RG * T(I) / (PAV*AT(I)*(1.0-ETUBE(I)))              1185.
      IF (IFBC .GT. 0) GO TO 125                                        1186.
      IF (ABS(UO(I)-UMF(I)) .LE. 0.01 * UMF(I)) GO TO 18                1187.
      IF (UO(I) .LT. UMF(I)) GO TO 10                                   1188.
      GO TO 17                                                          1189.
C                                                                       1190.
C     ICR --- INDICATOR FOR THE CRITICAL HEIGHT WHERE UO = UMF          1191.
C                                                                       1192.
18    ICR = 1                                                           1193.
C                                                                       1194.
C     BUBBLE SIZE CALCULATIONS                                          1195.
17    DBMAX = 0.652 * (AT(I) *(1.0-ETUBE(I)) * ABS(UO(I)-UMF(I)))**0.4  1196.
      IF (DBMAX .LT. PHI(I)) GO TO 8                                    1197.
      IF (IARRNG(I) .GT. 2 .AND. PHI(I) .GE. 0.5*DB(I-1)) DBMAX=PHI(I)  1198.
8     DB(I) = DBMAX - (DBMAX-DB(I-1)) * EXP(-0.3 * (H(I)-H(I-1))/DT(I)) 1199.
      DBAV(I) = 0.5 * ( DB(I) + DB(I-1) )                               1200.
      AKBE(I) = 11.0 / DBAV(I)                                          1201.
C                                                                       1202.
```

```
      C     CALCULATIONS FOR UBR --- BUBBLE RISING VEL.AT MIN.FLUDIZATION,      1203.
      C                          UBS --- BUBBLE VEL. AT SLUGGING CONDITIONS,     1204.
      C                          UB ---- ABS.BUBBLE RISING VELOCITY,             1205.
      C                          EPB --- BUBBLE FRATION,                         1206.
      C                          EPC --- CLOUD FRACTION                          1207.
      C                                                                          1208.
  821       UBR = 0.711 * SQRT ( G * DBAV(I) )                                   1209.
  822       UBS = 0.355 * SQRT ( G * (DT(I)+DT(I-1)) / 2.0 )                     1210.
  823       IF (UBR .GT. UBS) UBR = UBS                                          1211.
  824       UOAV = 0.5 * ( UO(I) + UO(I-1) )                                     1212.
  825       UMFAV = 0.5 * ( UMF(I) + UMF(I-1) )                                  1213.
  826       UB(I) = UOAV - UMFAV + UBR                                           1214.
  827       EPB(I) = ( UOAV - UMFAV ) / UB(I)*(1.0-ETUBF(I))                     1215.
  828       ALFB = EMF * UB(I) / UMFAV                                           1216.
  829       EPC(I) = EPB(I) * ALFB / ( ALFB - 1.0 )                              1217.
  830       IF (EPB(I) .GT. 0.7) EPB(I) = 0.7                                    1218.
  831       IF (EPC (I) .GT. (0.99 - ETUBE(I)) ) EPC(I) = 0.99 - ETUBE(I)        1219.
  832       BEDVOL = BEDVOL + DVBB(I)                                            1220.
  833       SUMV = SUMV + DVBBEF(I)                                              1221.
  834       SOLVOL = DVBBEF(I) - DVBB(I) * EPB(I)                                1222.
  835       SUMEFF = SUMEFF + SOLVOL                                             1223.
  836       SUM = SUM + SOLVOL / ( 0.5 * (AT(I)+AT(I-1)) )                       1224.
  837       IF (ICR .GT. 0) GO TO 35                                             1225.
  838       IF (HLF .NE. 0.0) GO TO 20                                           1226.
      C                                                                          1227.
      C     TEST FOR CONVERGENCY                                                 1228.
      C                                                                          1229.
  839       IF (ABS(SUMEFF-VMF) .LT. 0.01*VMF) GO TO 125                         1230.
  840       IF (SUMEFF .LT. VMF) GO TO 15                                        1231.
  841       VOL = SUMV-(SUMEFF-VMF) * (1.0 - ETUBE(I)) / (1.0-EPB(I)-ETUBE(I))   1232.
  842       H(I) = HEIGHT(VOL)                                                   1233.
  843       CALL AREA ( H(I), DT(I), AT(I) )                                     1234.
  844       SUMV = SUMV - DVBBEF(I)                                              1235.
  845       SUMEFF = SUMEFF - SOLVOL                                             1236.
  846       SUM = SUM - SOLVOL / (0.5*(AT(I) + AT(I-1)))                         1237.
  847   26  DVBB(I) = 0.5 * ( AT(I) + AT(I-1) ) * ( H(I) - H(I-1) )             1238.
  848       DVBBEF(I) = DVBB(I) * ( 1.0 - 0.25 * AHEAV(I) * DTUBEI(I) )          1239.
  849       GO TO 16                                                             1240.
  850   20  CONTINUE                                                             1241.
      C                                                                          1242.
      C     TEST FOR CONVERGENCY                                                 1243.
  851       IF (ABS(H(I)-HLF) .LE. 1.0E-3*HLF) GO TO 125                         1244.
  852       IF (ABS(H(I)-HLF) .LE. 0.25 * (H(I)-H(I-1))) GO TO 50                1245.
  853       IF (H(I) .LT. HLF) GO TO 15                                          1246.
  854   50  H(I) = HLF                                                           1247.
  855       BEDVOL = BEDVOL - DVBB(I)                                            1248.
  856       SUMV = SUMV - DVBBEF(I)                                              1249.
  857       SUMEFF = SUMEFF - SOLVOL                                             1250.
  858       SUM = SUM - SOLVOL / (0.5*(AT(I) + AT(I-1)))                         1251.
  859       CALL AREA ( H(I), DT(I), AT(I) )                                     1252.
  860       DVBB(I) = 0.5 * ( AT(I) + AT(I-1) ) * ( H(I) - H(I-1) )             1253.
  861       DVBBEF(I) = DVBB(I) * ( 1.0 - 0.25 * AHEAV(I) * DTUBEI(I) )          1254.
  862       GO TO 16                                                             1255.
  863   10  UO(I) = UMF(I)                                                      1256.
  864       AT(I) = EMO * RG * T(I) / ( PAV * UO (I) * (1.0-ETUBE(I))  )         1257.
  865       CALL HEATI ( AT(I), DT(I), H(I) )                                    1258.
  866       ICR = 1                                                              1259.
  867       DVBB(I) = 0.5 * ( AT(I) + AT(I-1) ) * ( H(I) - H(I-1) )             1260.
  868       DVBBEF(I) = DVBB(I) * ( 1.0 - 0.25 * AHEAV(I) * DTUBEI(I) )          1261.
  869       GO TO 17                                                             1262.
  870   35  CONTINUE                                                             1263.
  871       HCR = H(I)                                                           1264.
  872       IF (ABS(H(I)-HLF) .LE. 1.0E-3*HLF) GO TO 125                         1265.
  873       IF ( ABS(VMF-SUMEFF) .LE. 0.01 * VMF ) GO TO 125                     1266.
  874       I = I + 1                                                            1267.
  875       DBAV(I) = 0.0                                                        1268.
  876       UB(I) = 0.0                                                          1269.
  877       AKBE(I) = 1000.0                                                     1270.
  878       EPB(I) = 0.0                                                         1271.
  879       EPC(I) = 0.0                                                         1272.
  880       IF (VMF .EQ. 0.0) GO TO 45                                           1273.
      C                                                                          1274.
      C     FIXED BED CONDITIONS                                                 1275.
      C                                                                          1276.
  881       VOL = SUMV + ( VMF - SUMEFF )                                        1277.
  882       H(I) = HEIGHT(VOL)                                                   1278.
```

```
      CONTINUE                                                          1279.
      IF (VMF .EQ. 0.0) H(I) = HLF                                      1280.
      CALL AREA ( H(I), DT(I), AT(I) )                                  1281.
      DVBB(I) = 0.5*(AT(I)+AT(I-1))*(H(I)-H(I-1))                       1282.
      DVBBEF(I) = DVBB(I)*(1.0 -0.25*AHEAV(I)*DTUBEI(I))                1283.
      BEDVOL = BEDVOL + DVBB(I)                                         1284.
      SUMV = SUMV + DVBBEF(I)                                           1285.
      SUMEFF = SUMEFF + DVBBEF(I)                                       1286.
      SUM = SUM + DVBBEF(I) / (0.5*(AT(I)+AT(I-1)))                     1287.
      IFBC = 1                                                          1288.
      GO TO 13                                                          1289.
125   M1 = I                                                            1290.
      TETUBE = 1.0 - SUMV/BEDVOL                                        1291.
      EFFVOL = SUMV                                                     1292.
      SOLVOL = SUMEFF                                                   1293.
      M = M1 - 1                                                        1294.
C*    WRITE(6,206)                                                      1295.
C*                                  DO 910 I = 2,M1                   1296.
C*    WRITE(6,207) I,H(I),DBAV(I),UB(I),EPB(I),EPC(I),UO(I),UMF(I)      1297.
C*910                               CONTINUE                          1298.
C*206 FORMAT ('0',3X,'I',3X,'HEIGHT',3X,'AV.BUBBLE DIA',6X,'BUBBLE VEL.'1299.
C*   1,4X,'BUBBLE FRAC.',5X,'CLOUD FRAC.',6X,'SUP.VELOCITY',5X,         1300.
C*   2'MIN.FLU.VEL.',/)                                                 1301.
C*207 FORMAT (I5,F8.3,6(3X,1PE12.4,2X))                                 1302.
      RETURN                                                            1303.
      END                                                               1304.

      SUBROUTINE AREA ( ZI, DTI, ATI )                                  1305.
      COMMON /GEN/ Z(101),DVBEFF(101),ZB(46),ATB(46),PI,DZAV,MTB,MT,M1,M1306.
C                                                                       1307.
C     CALCULATION OF THE CROSS SECTIONAL AREA GIVEN THE HEIGHT ABOVE    1308.
C     THE DISTRIBUTOR                                                   1309.
C                                                                       1310.
                                    DO 10 J = 1 , MTB                   1311.
      IF ( ZI .GT. ZB(J) ) GO TO 10                                     1312.
      RJM1 = SQRT ( ATB(J-1) / PI )                                     1313.
      A = ( ZI - ZB(J-1) ) / ( ZB(J) - ZB(J-1) )                        1314.
      B = SQRT ( ATB(J) / ATB(J-1) ) - 1.0                              1315.
      RI = ( 1.0 + A * B ) * RJM1                                       1316.
      DTI = 2.0 * RI                                                    1317.
      ATI = PI * RI ** 2                                                1318.
      GO TO 20                                                          1319.
10                                  CONTINUE                            1320.
20    CONTINUE                                                          1321.
      RETURN                                                            1322.
      END                                                               1323.

      SUBROUTINE HEATI ( ATI, DTI, ZI )                                 1324.
      COMMON /GEN/ Z(101),DVBEFF(101),ZB(46),ATB(46),PI,DZAV,MTB,MT,M1,M1325.
C                                                                       1326.
C     CALCULATION OF THE HEIGHT GIVEN THE CROSS SECTIONAL AREA          1327.
C                                                                       1328.
      RI = SQRT ( ATI / PI )                                            1329.
      DTI = 2.0 * RI                                                    1330.
                                    DO 10 J = 1 , MTB                   1331.
      IF ( ATI .GT. ATB(J) ) GO TO 10                                   1332.
      A = SQRT ( ATI / ATB(J-1) ) - 1.0                                 1333.
      B = SQRT ( ATB(J) / ATB(J-1) ) - 1.0                              1334.
      C = ZB(J) - ZB(J-1)                                               1335.
      ZI = ZB(J-1) + A * C / B                                          1336.
      GO TO 20                                                          1337.
10                                  CONTINUE                            1338.
20    CONTINUE                                                          1339.
      RETURN                                                            1340.
      END                                                               1341.

      FUNCTION HEIGHT (VV)                                              1342.
      COMMON /GEN/ Z(101),DVBEFF(101),ZB(46),ATB(46),PI,DZAV,MTB,MT,M1,M1343.
C                                                                       1344.
C     CALCULATION OF THE HEIGHT GIVEN THE EFFECTIVE VOLUME OF THE BED   1345.
C     (EXCLUDING THE VOLUME OCCUPIED BY THE TUBES)                      1346.
C                                                                       1347.
      H = 0.0                                                           1348.
```

C-8

```
      SUM = 0.0                                                          1349.
                                    DO 100 I = 2 , MT                    1350.
      SUM = SUM + DVBEFF(I)                                              1351.
      H = H + DZAV                                                       1352.
      IF ( SUM .LT. VV )  GO TO 100                                      1353.
      H = ( VV - SUM ) * DZAV / DVBEFF(I) + H                            1354.
      GO TO 110                                                          1355.
  100                               CONTINUE                             1356.
  110 CONTINUE                                                           1357.
      HEIGHT = H                                                         1358.
      RETURN                                                             1359.
      END                                                                1360.

      FUNCTION VOLUME (ZZ)                                               1361.
      COMMON /GEN/ Z(101),DVBEFF(101),ZB(46),ATB(46),PI,DZAV,MTB,MT,M1,M1362.
C                                                                        1363.
C     CALCULATON OF THE EFFECTIVE VOLUME OF THE BED GIVEN THE HEIGHT     1364.
C                                                                        1365.
      N = IFIX (ZZ/DZAV)+1                                               1366.
      IF ( ZZ - FLOAT(N-1) * DZAV .GT. 0.01 * DZAV ) N = N + 1           1367.
      SUM = 0.0                                                          1368.
                                    DO 100 I = 2 , N                     1369.
      SUM = SUM + DVBEFF(I)                                              1370.
      IF ( I .LT. N ) GO TO 100                                          1371.
      A = 1.0 - ( ZZ - Z(N) ) / DZAV                                     1372.
      SUM = SUM - DVBEFF(I) * A                                          1373.
  100                               CONTINUE                             1374.
      VOLUME = SUM                                                       1375.
      RETURN                                                             1376.
      END                                                                1377.

      $ENTRY                                                             1378.
```

Section VII

MANUAL OF LEVEL I COMPUTER PROGRAM

7-1. Description of the Main Program

The FBC computation is initiated from the section between ISN (i.e. internal statement number) 1 and 26. Elutriation correlation and gas-phase mixing model are chosen following the rule,

IELUTR = 1 Correlation A

IELUTR = 2 Correlation B

IMODEL = 1 Homogeneous complete mixing

IMODEL = 2 Homogeneous plug flow

The elutriation rate calculated from the correlations chosen above is multiplied by adjusting parameter BETA before the use for calculation.

The statements from ISN 42 through 50 are for the input data of coal properties, i.e. name, composition and particle size distribution. In the section between ISN 36 and 50 the weight fraction is converted into number fraction mainly by the statement at ISN 41. Than at ISN 45 the size distribution density function is obtained and substituted into FRACT(I).

The operating conditions are fed to the program at ISN 51. The basic parameters which are derived from the operating conditions are calculated by the statements up to ISN 73.

From ISN 74 to ISN 82 the critical particle diameter DPCR is calculated by solving the equation,

$$u_t\ (DPCR) = u_o$$

From ISN 84 to ISN 91 a new grid is introduced at the point d_c = DPCR and FRACT(I) vs DPF(I) relation is modified. Then from ISN 92 to 139 the value of size distribution density function for the coal particle PHIF(L) corresponding to each interval of DP(L) ~ DP(L + 1) is found from the FRACT(k) vs DPI(k) relationship. The value of DPO is defined by the preceding data statement based on the Tyler standard mesh opening. The series DP is almost the same as the series DPO except that DP includes the critical diameter DPCR as one of the grids.

The reactivity of char, ALAM, elutriation rate constant, AKE, and the dimensionless diameter of char particle, Y, are evaluated from ISN 140 ~ ISN 176. Where AKE MAX is for the maximum allowable value of elutriation rate constant.

The integrations

$$\int_0^{y_i} (1/\lambda_c)\, dy \quad \text{and} \quad \int_0^{y_i} (K^*/\lambda_c)\, dy$$

are performed between ISN 177 and 182 and stored in ALAMI AND AKEI.

By the DO loop 32 the second and third moments of the feed size distribution are calculated.

From ISN 210 the iteration to determine η_c (= ETC), Θ (= THET) and B_{cf} (= BC1)is prepared. The iteration scheme is basically the same as the one illustrated in Figure . Instead of using N and n_w for iteration parameters Θ and B_{cf} are used.

ETC iteration is started from

$$\text{ETC} = \begin{cases} 1 & \text{if EXAIR} \geq 0 \\ 1 + \text{EXAIR} & \text{if EXAIR} < 0 \end{cases}$$

The interval for changing ETC should, therefore, be negative. DO loop 500 is for ETC iteration. DO loop 200 is for THET iteration. The average oxygen concentration $\overline{C_{O2}}$ (= COXAV) is calculated by the specified model in the section ISN 231 - ISN 239 so that the parameter B_{cw} (= BC) can be calculated at ISN 240.

From ISN 242 to ISN 256 the calculation to determine B_{cf} (= BC1) is performed. Subrontine CRRECT is called to correct the assumed value of BC1. EBC1 is the difference between the two values of B_{cf} assumed and calculated.

Then the new value of Θ, THETA, is calculated at ISN 258 and the difference of assumed values and calculated values, EE, is examined by CRRECT subroutine.

The new value of B_{cw} is obtained at ISN 273 and the difference, E, of this value and the previous value of B_{cw} is taken so that E is used for the criterion for ETC iteration. The new assumption for ETC is given again by the CRRECT subroutine.

The statements from ISN 289~ISN 311 are devoted to the transformation of number density functions PHIF, PHI and PHIE into the density functions based on weight fraction, PHIFW, PHIW and PHIEW. Total elutriation loss, ELOSS, oxygen mole fraction at the outlet, XGO, total amount of char in the bed, HCHAR, total amount of carbon in the bed, HCARBN, and the weight fraction of carbon in the bed, HRC, are calculated and printed out.

In this program the temperature iteration and bubble hydrodynamics calculations have not been included, but combining with Level II program all of the necessary information can be available.

The relationships between the main program and sub-programs are shown in Figure 8.

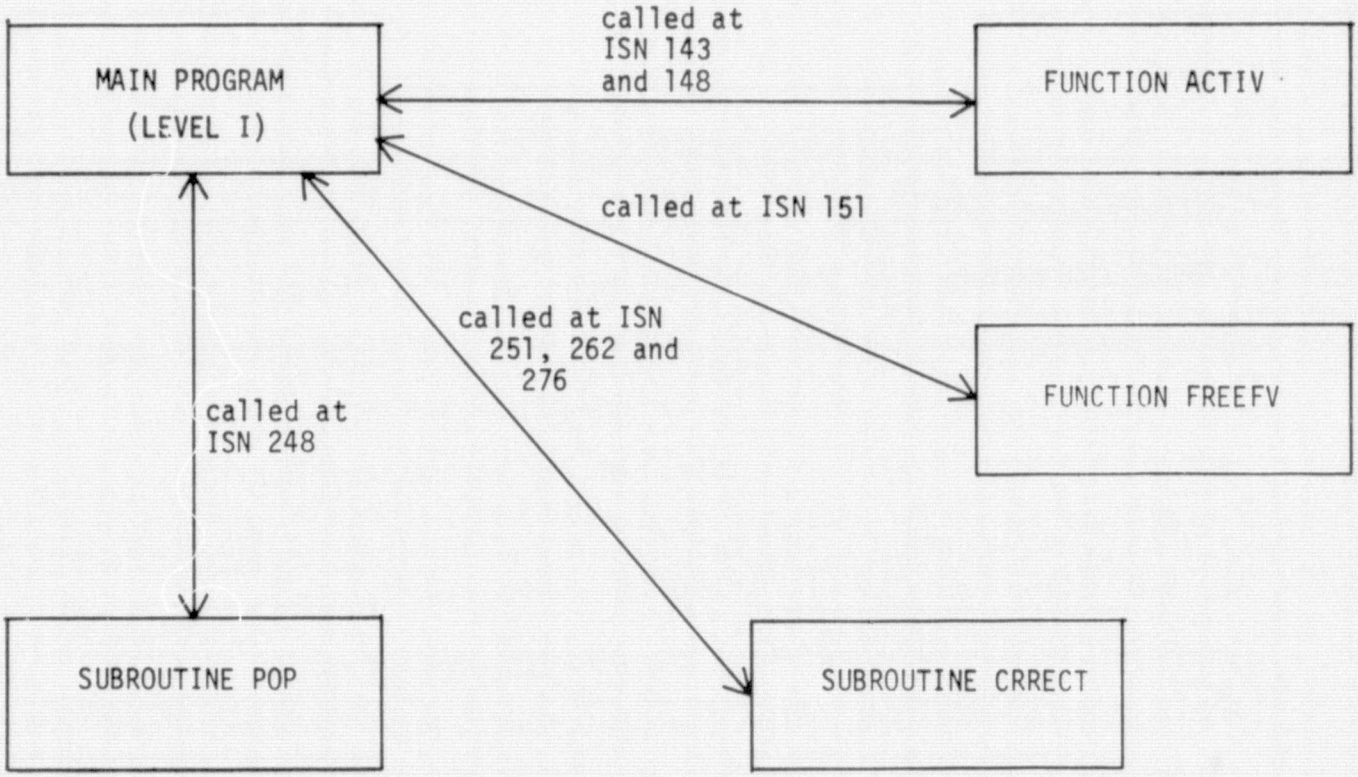


FIGURE 8. STRUCTURAL ILLUSTRATION OF LEVEL I PROGRAM

7-2. Input to the Program

The input data of Level I program is shown in the following table. The INTEGER variables are right justified. If the 4th card is a blank card the execution returns to the 1st READ statement.

TABLE 6

	Column	Variable	Example	Type
Card 1	1-4	NAM1	PITT	Alphanumeric
	4-8	NAM2	S	Characters
	9-16	SCF	0.504	REAL
	17-24	XCV	0.222	REAL
	25-32	XH	0.046	REAL
	33-40	XS	0.027	REAL
	41-48	XO	0.042	REAL
	49-56	XN	0.014	REAL
	57-64	XW	0.013	REAL
	65-68	N	9	INTEGER
Card 2	1-8	DPF(1)	0.002	REAL
	9-16	DPF(2)	0.0045	REAL
	17-24	DPF(3)	0.0066	REAL
	25-32	DPF(4)	0.0125	REAL
	33-40	DPF(5)	0.025	REAL
	41-48	DPF(6)	0.05	REAL
	49-56	DPF(7)	0.1	REAL
	57-64	DPF(8)	0.168	REAL
	65-72	DPF(9)	0.3175	REAL
Card 3	1-8	FRACT(1)	0.0	REAL
	9-16	FRACT(2)	0.075	REAL
	17-24	FRACT(3)	0.031	REAL
	25-32	FRACT(4)	0.088	REAL
	33-40	FRACT(5)	0.129	REAL
	41-48	FRACT(6)	0.212	REAL
	49-56	FRACT(7)	0.344	REAL
	57-64	FRACT(8)	0.119	REAL
	65-72	FRACT(9)	0.002	REAL
Card 4	1-8	WCOAL	29.2	REAL
	9-16	CABS	2.2	REAL
	17-24	EXAIR	0.13	REAL
	25-32	UO	0.0	REAL
	33-40	P	4.0	REAL
	41-48	TK	1121.0	REAL
	49-56	DT	73.0	REAL
	57-64	HLMF	33.5	REAL
	65-72	DPL	0.168	REAL
	73-80	UMF	70.0	REAL

7-3. Output of the Program

The output of a typical run of Level I program is following.

FBC CALCULATION

EFFECT OF ELUTRIATION ON COMBUSTION EFFICIENCY

PITTS COMPOSITION OF COAL 0.5040 0.2220 0.0460 0.0270 0.0420 0.0140 0.0130

0.2000E-02	0.0
0.4500E-02	0.1114E 03
0.6600E-02	0.1100E 02
0.1250E-01	0.2182E 01
0.2285E-01	0.1995E 00
0.2500E-01	0.1995E 00
0.5000E-01	0.2049E-01
0.1003E 00	0.2053E-02
0.1680E 00	0.9278E-04
0.3175E 00	0.1192E-06

ELUTRIATION CORRELATION : NO. 1 BETA= 1.00000

GAS PHASE MODEL : NO. 1 DB,EB= 10.0 0.29962

WCOAL,WLS,CABS,EXAIR,FMC,UO,P,TK,DT,HLMF

0.2920E 02 0.2172E 01 0.2200E 01 0.6000E-01 0.1095E 02 0.6017E 02 0.4000E 01 0.1121E 04 0.7300E 02 0.3350E 02

AK,DPCR,VCF,VLS,THETM,ALAMVF,NDP,PASH,RHOASH

0.7233E 01 0.2285E-01 0.2086E 02 0.2309E 01 0.3036E 05 0.2131E-04 0.1000E 01 0.5000E 00 0.1400E 01

FETCM,ETHMAX 0.1000E-04 0.3036E 01

ETC,XGO,THET,BC,BCI

0.9291E 00 0.5332E-07 0.1859E 05 0.1005E 00 0.1701E 03

VCW,VCF,VLS,HCHAR,WBED, HRC,FC,ELOSS,ALAMV,ALAMA

0.8210E-01 0.2086E 02 0.2309E 01 0.1386E 04 0.7832E 05 0.1375E-01 0.1131E-06 0.6694E-01 0.1236E-03 0.7792E-03

Y	DP	PHIF	PHI	PHIFW	PHIW	PHIEW	AKE	ALAM
0.0	0.0	0.0	0.2006E 02	0.0	0.0	0.0	0.2709E 01	0.1000E 01
0.6299E-02	0.2000E-02	0.0	0.9523E 02	0.0	0.6064E-03	0.8692E-01	0.2709E 01	0.9928E 00
0.1354E-01	0.4300E-02	0.1114E 03	0.2391E 02	0.5154E-01	0.3044E-02	0.2901E 00	0.1121E 01	0.9847E 00
0.1417E-01	0.4500E-02	0.1114E 03	0.1297E 02	0.6116E-01	0.3289E-02	0.3044E 00	0.1064E 01	0.9840E 00
0.1921E-01	0.6100E-02	0.1100E 02	0.7717E 01	0.1124E 00	0.5157E-02	0.3910E 00	0.7496E 00	0.9784E 00
0.2079E-01	0.6600E-02	0.1100E 02	0.5399E 01	0.1195E 00	0.5814E-02	0.4161E 00	0.6846E 00	0.9767E 00
0.2772E-01	0.8800E-02	0.2182E 01	0.4598E 01	0.1454E 00	0.9916E-02	0.5300E 00	0.4456E 00	0.9692E 00
0.3276E-01	0.1040E-01	0.2182E 01	0.3414E 01	0.1614E 00	0.1436E-01	0.6192E 00	0.3262E 00	0.9638E 00
0.3906E-01	0.1240E-01	0.2182E 01	0.1397E 01	0.1949E 00	0.1953E-01	0.6984E 00	0.2350E 00	0.9571E 00
0.3937E-01	0.1250E-01	0.2182E 01	0.1285E 01	0.1970E 00	0.1974E-01	0.7009E 00	0.2315E 00	0.9567E 00
0.4630E-01	0.1470E-01	0.1995E 00	0.1215E 01	0.2243E 00	0.2532E-01	0.7584E 00	0.1710E 00	0.9495E 00
0.5512E-01	0.1750E-01	0.1995E 00	0.1051E 01	0.2363E 00	0.3589E-01	0.8384E 00	0.1235E 00	0.9405E 00
0.6551E-01	0.2080E-01	0.1995E 00	0.7839E 00	0.2602E 00	0.5255E-01	0.9306E 00	0.8950E-01	0.9300E 00
0.7196E-01	0.2285E-01	0.1995E 00	0.5884E 00	0.2819E 00	0.6402E-01	0.9806E 00	0.7511E-01	0.9237E 00
0.7748E-01	0.2460E-01	0.1995E 00	0.3991E 00	0.3056E 00	0.7305E-01	0.1000E 01	0.0	0.9183E 00
0.7874E-01	0.2500E-01	0.1995E 00	0.3532E 00	0.3118E 00	0.7488E-01	0.1000E 01	0.0	0.9171E 00
0.9291E-01	0.2950E-01	0.2049E-01	0.3052E 00	0.3533E 00	0.9879E-01	0.1000E 01	0.0	0.9036E 00
0.1106E 00	0.3510E-01	0.2049E-01	0.2431E 00	0.3733E 00	0.1397E 00	0.1000E 01	0.0	0.8874E 00
0.1313E 00	0.4170E-01	0.2049E-01	0.1653E 00	0.4129E 00	0.1988E 00	0.1000E 01	0.0	0.8690E 00
0.1559E 00	0.4950E-01	0.2049E-01	0.7005E-01	0.4913E 00	0.2623E 00	0.1000E 01	0.0	0.8482E 00
0.1575E 00	0.5000E-01	0.2049E-01	0.6490E-01	0.4977E 00	0.2657E 00	0.1000E 01	0.0	0.8469E 00
0.1855E 00	0.5890E-01	0.2053E-02	0.5605E-01	0.5648E 00	0.3350E 00	0.1000E 01	0.0	0.8244E 00
0.2208E 00	0.7010E-01	0.2053E-02	0.4316E-01	0.5968E 00	0.4523E 00	0.1000E 01	0.0	0.7977E 00
0.2624E 00	0.8330E-01	0.2053E-02	0.2742E-01	0.6600E 00	0.6136E 00	0.1000E 01	0.0	0.7685E 00
0.3121E 00	0.9910E-01	0.2053E-02	0.4116E-02	0.7874E 00	0.7385E 00	0.1000E 01	0.0	0.7362E 00
0.3159E 00	0.1003E 00	0.2053E-02	0.4132E-02	0.7998E 00	0.7424E 00	0.1000E 01	0.0	0.7338E 00
0.3679E 00	0.1168E 00	0.9278E-04	0.4344E-02	0.8925E 00	0.8152E 00	0.1000E 01	0.0	0.7030E 00
0.4400E 00	0.1397E 00	0.9278E-04	0.2323E-02	0.9157E 00	0.9360E 00	0.1000E 01	0.0	0.6643E 00
0.5200E 00	0.1651E 00	0.9278E-04	0.0	0.9589E 00	0.1000E 01	0.1000E 01	0.0	0.6261E 00
0.5291E 00	0.1680E 00	0.9278E-04	0.0	0.9661E 00	0.1000E 01	0.1000E 01	0.0	0.6220E 00
0.6239E 00	0.1981E 00	0.1192E-06	0.0	0.9987E 00	0.1000E 01	0.1000E 01	0.0	0.5826E 00
0.7439E 00	0.2362E 00	0.1192E-06	0.0	0.9998E 00	0.1000E 01	0.1000E 01	0.0	0.5393E 00
0.8800E 00	0.2794E 00	0.1192E-06	0.0	0.9994E 00	0.1000E 01	0.1000E 01	0.0	0.4974E 00
0.1000E 01	0.3175E 00	0.1192E-06	0.0	0.1000E 01	0.1000E 01	0.1000E 01	0.0	0.4655E 00

Nomenclature for Level I Computer Program

FORTRAN symbol	Mathematical symbol	Unit	Description
AK	k_R	cm/sec	chemical reaction rate constant for char combustion
AKE	K^*		specific elutriation rate constant
AKEI	$\int_0^y K^*/\lambda \, dy$		
AKEMAX			maximum value of elutriation rate constant
AKF	k_f	cm/sec	mass transfer coefficient for char combustion
ALAM	$\lambda = k_c/k_R$	-	reactivity of char
ALAMA	ψ_a	-	$= \int_0^1 \phi \, y^2 \, dy = \overline{d_c^2}/d_{cm}^2$
ALAMI	$\int_0^y 1/\lambda \, dy$	-	
ALAMV	ψ_v	-	$= \int_0^1 \phi \, y^3 \, dy = \overline{d_c^3}/d_{cm}^3$
ALAMAF	ψ_{af}	-	$= \int_0^1 \phi_f \, y^2 \, dy$
ALAMVF	ψ_{vf}	-	$= \int_0^1 \phi_f \, y^3 \, dy$
ALFO, ALF1, ALF2			dummy parameters
ANDP		-	number of sub-intervals in the interval of DPO
AT	A_t	cm^2	cross sectional area
BB		-	dimensionless parameters
BBC, BC	B_{cw}	-	dimensionless parameter
BC1	B_{cf}	-	adjusting factor for elutriation rate constant

FORTRAN symbol	Mathematical symbol	Unit	Description
BETA		-	calcium to sulfur ratio in the total
CABS	$[C_a]/[S]$	-	solids input
CC	C_c	-	dimensionless parameter
COXAV	$\overline{C_{O2}}$	$gmol/cm^3$	average oxygen concentration
COX0	$C_{O2,0}$	$gmol/cm^3$	oxygen concentration at z=0
D	$\mathcal{D}_{O2}$	cm^2/sec	diffusivity of oxygen
DB	D_B	cm	average bubble diameter
DCM	d_{cm}	cm	maximum diameter of coal particles
DETC	$\Delta\eta_c$	-	step size for combustion efficiency iteration
DDP	Δd_c	cm	interval size of d_c axis
DPAV		cm	average than particle size in a size interval
DPCR		cm	critical diameter for elutriation (char diameter whose terminal velocity equals gas velocity)
DPF		cm	diameter of inlet char
DPFO		cm	extra memory for DPF
DPL	d_ℓ	cm	mean diameter of limestone particles
DT	D_t	cm	column diameter
DTH		sec	step size for θ iteration
DY	Δy	-	interval size of y
E		-	relative error for B_{cw} iteration
E1, E2, EE1, EE2, ETC1, ETC2		-	relative error of B_{cw} from the previous iteration step
ETC	η_c	-	coal combustion efficiency

FORTRAN symbol	Mathematical symbol	Unit	Description
EB	ε_B	-	volume fraction of bubbles
EBC1		-	difference between the values of B_{cf} assumed and calculated
EBMAX		-	tolerance limit for EBC1
EC			$(A_t/W_b) < K^* y^3>$
EE		sec	difference betweem the values of Θ assumed and calculated
EETCM		-	tolerance limit for η_c iteration
ELOBS		-	fraction of carbon elutriated
EMF	ε_{mf}	-	void fraction of bed at $u = u_{mf}$
ETC	η_c	-	combustion efficiency
ETCOLD		-	value of ETC from the previous iteration
ETHMAX	Θ_{max}	sec	maximum value of Θ
EXAIR	EAR	-	excess air ratio
FMO	F_m	gmol/sec	molar mass flow rate of outlet gas
FMTH	F_{mth}	gmol/sec	the critical molar mass flow rate of air
FR	F_r	-	Froude Number
FRACT		-	weight fraction of particles in the corresponding size interval
FRACTO		-	extra memory for FRACT
FREEFV	U_t	cm/sec	terminal velocity (or freefall velocity)
G	g	cm/sec^2	gravity acceleration
HCARBN		g	hold-up of carbon in the bed
HCHAR		g	hold-up of char in the bed

FORTRAN symbol	Mathematical symbol	Unit	Description
HLMF	L_{mf}	cm	bed height at $u = u_{mf}$
HRC		-	mass fraction of carbon in the bed
IELUTR		-	index for choosing elutriation correlation
IMODEL		-	index for choosing gas phase model
INDBOI, INDETC, INDTH		-	index for B_{cw}, η_c, and θ iterations
INDX			index for defining grids of d_c
MAIR		g/gmol	average molecular weight of air
MC	M_c	g/gmol	atomic weight of C
MCA	M_{Ca}	g/gmol	atomic weight of C_a
MH2	M_{H2}	g/gmol	molecular weight of H_2
MH2O	M_{H2O}	g/gmol	molecular weight of H_2O
MN2	M_{N2}	g/gmol	molecular weight of N_2
MO2	M_{O2}	g/gmol	molecular weight of O_2
MS	M_S	g/gmol	atomic weight of ξ
NAM1,NAM2			name of coal (A-Type variables)
NDP			number of sub-interval in the interval of DPO (This value can be changed artificially). NDP $\geq$ 1
N			number of size distribution inputs (see READ (5,1001) statement)
P	p	atm	pressure
PASH		-	fraction of ash elutriated
PHI	Φ	-	size distribution density function for char particles, number fraction basis

FORTRAN symbol	Mathematical symbol	Unit	Description
PHIFW	ϕ_f^*	-	size distribution density function for char fed to the bed, weight fraction basis
PHIF	ϕ_f	-	size distribution density function for char bed to the bed, number fraction basis
PHITTL		-	size distribution density function for char, weight fraction basis
RE	R_{ep}	-	Particle Reynolds Number for DPCR
RET	R_{ep}	-	Particle Reynolds Number for terminal velocity
RHOASH	ρ_A	g/cm^3	density of coal ash
RHOC	ρ_c	g/cm^3	density of coal
RHOG	ρ_g	g/cm^3	density of gas
RHOLCA		$g(Ca)/cm^3$ (limestone)	density of Ca in limestone
RHOLS	$\rho_{\ell f}$	g/cm^3	density of limestone
RHOP	ρ_{ch}	g/cm^3	density of char
SC3	S_c	-	Schmidt Number
SHP	Sh_p	-	Sherwood Number
THI, THE, THET, THE, THETA	Θ	sec	mean residence time of limestone
THETM	Θ_{max}	sec	maximum value of Θ
TK	$\bar{T}$	°K	average bed temperature
UB	U_B	cm/sec	bubble rising velocity
VISC	μ	g/cm·sec	viscosity of gas
UO	u_o	cm/sec	superficial gas velocity
UMF	u_{mf}	cm/sec	minimum fluidizing velocity

FORTRAN symbol	Mathematical symbol	Unit	Description
US			
UT	U_t	cm/sec	terminal velocity of char particle
UTF	U_t	cm/sec	terminal velocity of char particle
UCF		cm^3/sec	volumetric flow rate of coal
VISC	μ		viscosity
VLS		cm^3/sec	volumetric feed rate of limestone
VMF	V_{mf}	cm^3	bed volume at $u = u_{mf}$
WBED	W_b	g	total bed weight
WCOAL	$w_{coal,f}$	g/sec	mass feed rate of coal
WLS	$w_{\ell f}$	g/sec	mass feed rate of limestone
XA	X_{Af}	-	mass fraction of ash in coal (dry basis)
XC	X_C	-	mass fraction of carbon in char (dry basis)
XCF	X_{Cf}	-	mass fraction of carbon in coal (dry basis)
XCV	X_{CV}	-	mass fraction of volatile carbon in coal (dry basis)
XINF		-	mole fraction of oxygen in the gas outlet when combustion is completed
XLCA	$X_{\ell Ca}$	-	mass fraction of Ca in limestone
XLS			
XN	X_N		mass fraction of nitrogen in coal (dry basis)
XO	X_O		mass fraction of oxygen in coal (dry basis)
XGO	y_{O2}		mole fraction of oxygen in the outlet stream

FORTRAN symbol	Mathematical symbol	Unit	Description
XGOO	$y_{O2.0}$	-	mole fraction of oxygen in the feed
XH	X_H		mass fraction of hydrogen in coal (dry basis)
XLCA	$X_{Ca,\ell}$		mass fraction of Ca in limestone
XNEW			corrected value of unknown from subrontine CRRECT
XS	X_S		mass fraction of sulfur in coal (dry basis)
XO	X_O		mass fraction of oxygen in coal (dry basis)
XW	X_{H2O}		mass fraction of moisture in coal (dry basis)
XX			dummy parameter
Y (active)	y	-	dimensionless char size
Y(pop)	Y	-	dimensionless function
YA, YB, YC, YA1, YB1, YC1			dummy variables for integration
YY	Y	-	dimensionless function
ZF	Z_f	-	dimensionless function

SECTION VIII

Manual of Level II Computer Program

8.1 Description of the Main Program

After introducing constants and assumed parameters, subroutine DESIGN is called at ISN 24 to feed the data of design parameters into the program. From subroutine DESIGN we have the first output listing.

The size distribution of adsorbent particles is then fed from ISN 25 to ISN 27. The different mean diameters of adsorbent particles are calculated in the section from ISN 28 to ISN 35. The mean size of bed particles is assumed to be equal to that of adsorbent particles as seen at ISN 36. The composition of adsorbent is fed at ISN 37.

Composition and heating value of coal are read at ISN 38. The size distribution of coal particles is fed from ISN 43 to ISN 45. Then the surface volume average diameter of coal particles, DCF, is calculated. The mean diameter of char particles in the bed, DCAV, is approximated by the statement at ISN 54.

DCAV = (3.0/5.0) DCF (8-1)

This relationship is derived based on the following consideration; The average size of char particles is needed to calculate the specific surface area of char particles per unit volume of emulsion, $a_c = \rho_{cN} \langle d_c^2 \rangle$. By the use of carbon mass fraction, x , a_c can be written as

$$a_c = \frac{6\rho_\ell (1-\epsilon_{mf})x}{d_{c,sv}\, \rho_{cf}\, X_{cf}} \tag{8-2}$$

where $d_{c,sv}$ is the surface-volume mean diameter of coal or char particles and is expressed as

$$d_{c,sv} = d_{cm}\psi_v/\psi_a \tag{8-3}$$

where $\psi_a = \int_0^1 y^2 \phi \, dy$ and $\psi_v = \int_0^1 y^3 \phi \, dy$ are the second and third moments of size distribution. If the effect of elutriation can be neglected, ψ_a and ψ_v can be written as (see Horio and Wen (1975a)):

$$\psi_a/\psi_{af} = \begin{cases} a_c\,(1-2/B_{cw}) + 2/B_{cw}^2 & \text{(SCR) (8-4d)} \\ 1-\exp(-B'^2_{cw}/2)\int_0^1 \exp\,(B'_{cw}\, y^2/2)\,dy & \text{(FDC) (8-4b)} \end{cases}$$

$$\psi_v/\psi_{vf} = \begin{cases} a_c\,(1-\frac{3}{B_{cw}} + \frac{6}{B^2_{cw}}) - \frac{6}{B^3_{cw}} & \text{(SRC) (8-5a)} \\ a_c[1 - \frac{3}{B'_{cw}} + \frac{3}{B'_{cw}} \exp(-\frac{B'_{cw}}{2})\int_0^1 \exp(\frac{B'_{cw}}{2}\, y^2)\,dy] & \text{(FDC) (8-5b)} \end{cases}$$

where

$$a_c = \begin{cases} 1/(1-e^{-B_{cw}}) & \text{(SRC)} \\ 1/(1-e^{-B'_{cw}/2}) & \text{(FDC)} \end{cases}$$

$$B'_{cw} \equiv \frac{\rho_c\, X_c\, d_{cm}^2}{4 M_C\, \Theta\, D_{O2}\, \bar{C}_{O2}} \qquad \text{for FDC}$$

and (SRC) and (FDC) represents Surface Reaction Control and Film Diffusion Control respectively.

In most of the cases the value of B_{cw} is small enough to approximate

$$\psi_a = \begin{cases} (1/3)\,\psi_{af} & \text{(SRC) (8-6a)} \\ (2/3)\,\psi_{af} & \text{(FDC) (8-6b)} \end{cases}$$

$$\psi_v = \begin{cases} (1/4)\,\psi_{vf} & \text{(SRC) (8-7a)} \\ (2/5)\,\psi_{vf} & \text{(FDC) (8-7b)} \end{cases}$$

Then,

$$d_{c,sv} = \begin{cases} (3/4)\ d_{e,sv,f} & \text{(SRC)} \quad (8\text{-}8a) \\ (3/5)\ d_{c,sv,f} & \text{(FDC)} \quad (8\text{-}8b) \end{cases}$$

In coal combustors the rate is mainly controlled by gas film diffusion. Therefore, we have Equation (8-1).

At ISN 55 operating conditions, such as bed height, average bed pressure, average bed temperature expected and average cooling water temperature are fed. At the same time the value of overall heat transfer coefficient, UHEAV, is fed. If the proper heat transfer correlation is available, UHEAV should be calculated elsewhere from the operating conditions. Among the input variables in this read statement either WAD or CABS and either UF or EXAIR must be zero. If there is no coal feed (WCOAL = 0), UF has to be specified instead of EXAIR.

The parameter ξ_{CO}, ξ_{H2} and ξ_{H2S} introduced by Equation (5-12) must be specified here.

At ISN 60 the actual heat of combustion, QCOAL, accounting for partial combustion is calculated from the heat of complete combustion, QCOALC and ξ_{CO} (GZCO).

The read statement at ISN 60 is for the parameter IGNITE. IGNITE is 0 for the case of no combustion and is 1 for combustion. This parameter is to control the computation. If IGNITE equals zero, the computation skips the combustion calculation - ISN 37 - 408.

The solids feed temperature, TSF, is specified by the statement of ISN 62 as 298 °K. This statement can be changed depending on the operating condition.

From ISN 63 through ISN 87 the statements are used for the overall gas phase material balance. The statements of ISN 78-87 define the value of AG(I,J) which are the coefficients of Eqs. (3-41), (3-44) and (3-49). Statements of ISN 88-93 are for calculating the density of char and adsorbent particles and the calcium to sulfur ratio, C_a/S, or mass feed rate of adsorbents, WAD. WCAD at ISN 94 is the mass flow rate of calcined adsorbents. Right after this calculation we have the second group of output listing, giving the compositions of adsorbents and coal, size distributions and average particle sizes.

The assumed temperature TAV is substituted into T(I) at ISN 108.

Then, subroutine HYDRO is called for calculating bed expansion, bubble characteristics, gas interchange coefficient, etc.

In this program the compartments are numbered as shown in Figure 9. The bottom compartment is numbered 2 and the inlet gas is numbered 1.

ISN 145 specifies the fractional loss of carbon due to elutriation, ELLOSS. The amount of solids elutriated is defined at ISN 148. There could be three steady state solutions for a combustion problem. Two of them, upper and lower, are stable solutions but the middle solution is unstable. The temperature iteration is needed because of the temperature dependent coefficients of heat balance equations.

Before the combustion calculations are performed, initial temperature and combustion efficiencies are assumed at ISN 149 and 152. High temperature and high efficiency should be assumed to get the stable solution. The DO loop 600 starting from ISN 164 is a large iteration loop for temperature calculation. The gas flow rates in both emulsion and bubble phases are calculated in the DO loop 150. The parameter M1 in the statement of ISN 174 is defined previously in subroutine HYDRO and denotes the top

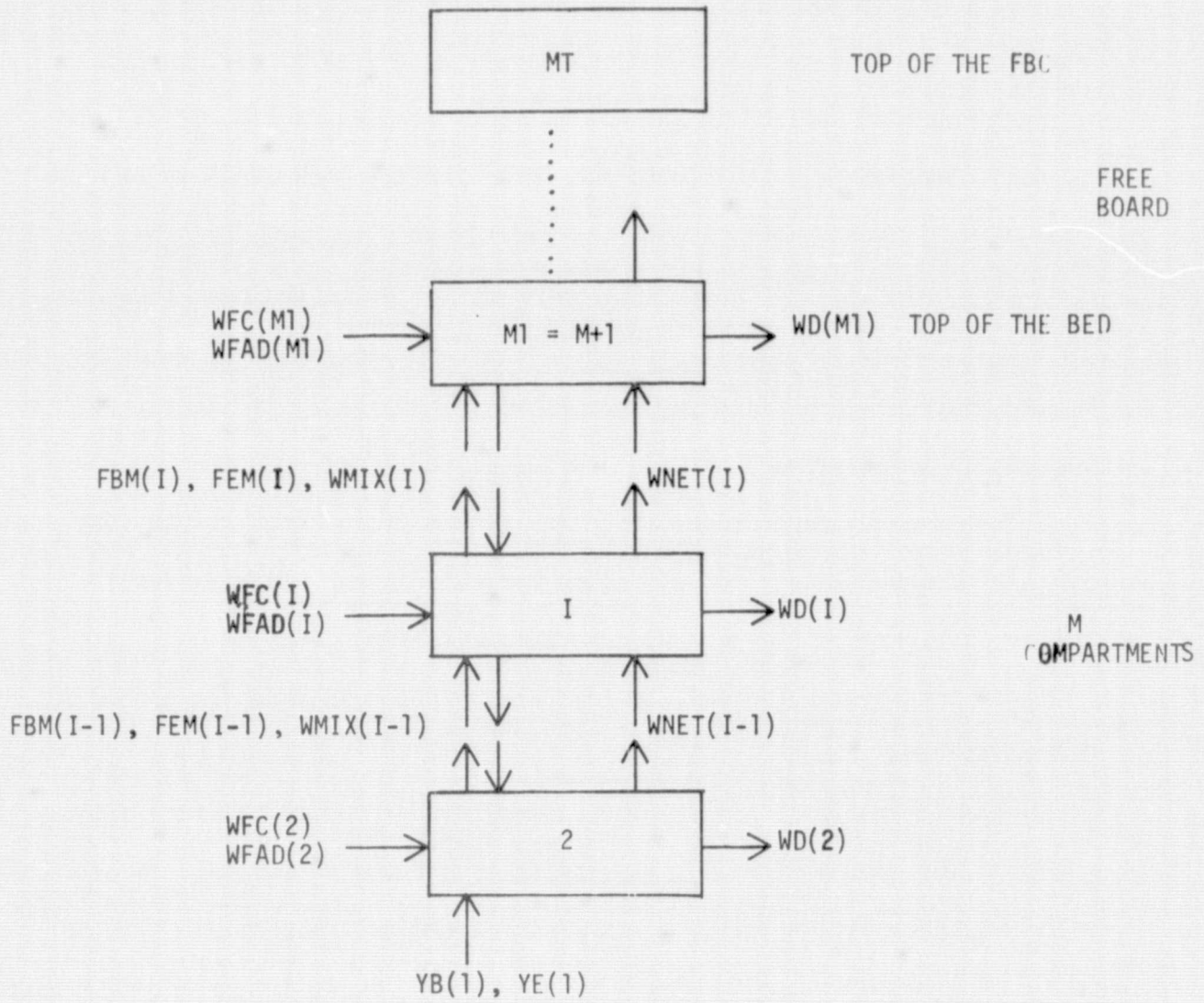


FIGURE 9. ILLUSTRATION OF THE COMPARTMENTS AND NUMBERING IN LEVEL II PROGRAM

compartment number. However, due to the change in the calculated temperature the expansion of bed can be different from the previously obtained value and so is the parameter M1. Therefore, M1 newly obtained from HYDRO is compared with the old value, M1OLD, at ISN 172. If there is no change in M1, the calculation in the section of ISN 193-192 is skipped except in the first iteration.

The DO loops 55, 56, and 57 are provided for the arrangement of solids feed to each compartment. The statement at ISN 189 is for the calculation of char flow rate corresponding to the coal feed in each compartment. The statement at ISN 190 is for the additive feed rate. In these statements MFEED, ZF (J), FFC (J) and FFAD (J) are supplied from subroutine DESIGN.

The DO loops 60, 61 and 62 give the distribution of solid discharge rate from compartments. MDIS, ZDIS(J), and FD(J) are also defined in subroutine DESIGN.

Calculation of gas phase material balance is performed in the section, ISN 202-248. Combustion efficiency based on oxygen consumption, ETCG is calculated. Net flow rate WNET(I) and the back mixing flow rate WMIX(I) are, then, calculated in the section of ISN 272 and 276. The coefficients of the solid phase carbon balance Eq. (5-1) are calculated by the statements between ISN 285 to 308. Then, subroutine SIMQ is called. The results from the subroutine are substituted into the array X(I) at ISN 306. It must be recalled that the compartments are numbered starting from 2.

The combustion efficiency, ETCC, based on carbon consumption is calculated at ISN 315. ETCG and ETCC should agree with each other. Should these differ largely, initial guess value for combustion efficiency is altered and the calculations are repeated. CRRECT subroutine is used to achieve this agreement between ETCG and ETCC.

The temperature calculation is then performed based on Equation (3-96). The coefficients are defined first and the subroutine SIMQ is called at ISN 373.

The average norm between the new temperature profile and the previous profile is calculated finally at ISN 382 and checked for the tolerance limit at ISN 384.

Results are printed out at ISN 406. The sulfur capture calculations are performed in the rest of the main program. Effective C_a to S molar ratio including the sulfur supply from inlet gas, CABSE, is defined at ISN 420. If IGNITE is zero, the sulfur in the coal is not released. Therefore, effect of IGNITE is considered at ISN 417.

The sulfur release rate in each compartment is computed at ISN 421-427. By the statements at ISN 430 and 431 the starting values of sulfur concentrations in both bubble and emulsion phases are set for the calculation. The sulfur retention efficiency, ETS, is set as unity for the initiation of the iteration. The statements from ISN 432 to ISN 435 are necessary for applying Regula Falsi method by using subroutine CRRECT.

By the statement at ISN 439, the average conversion of adsorbent ES is calculated from the overall balance. The rate constant is calculated at ISN 440 calling the function subprogram AKAD.

Then the same calculation scheme as that of combustion calculation is applied, i.e. subroutine GPHASE is called to calculate YB(I+1) and YE(I+1) from YB(I) and YE(I). The sulfur retention efficiency can be obtained from YB(M1) and YE(M1) as stated at ISN 453. The error between the assumed and calculated sulfur efficiency is fed to subroutine CRRECT at ISN 455. After the convergence of η_S the results of sulfur retention and the outlet gas concentration XG(1)~XG(7) are printed out.

In the final section the pressure drop calculation is performed.

To calculate the distributor pressure drop the average temperature is assumed to be

(average temperature at distributor) = (T(1)+T(2))/2

By using the gas velocity at the distributor orifice, UOR, the pressure drop is calculated by

$$\Delta P_{dis} = (U_{OR}/0.6)^2 \rho_g/2g$$

The pressure drop in the fluidized bed section is assumed to be equal to the weight of bed material per unit cross sectional area and the calculation is done at ISN 481.

The pressure drop of fixed bed section, if it exists, is calculated by using Ergun's Equation. The index IFBC at ISN 484 is zero if there is no fixed bed section at the top of the bed. IFBC is defined in subroutine HYDRO.

Finally the bubble hydrodynamic results are printed out at ISN 494.

In this program, an empirical correlation to calculate the NO_x concentration in the outlet gas is incorporated (Ruth (1976)).

$$AN = 2.9 \times 10^{-8} (EXAIR)^{0.449}$$

where

AN = gmol NO_2 emission/cals. fuel burned.

EXAIR = excess air, in fraction.

8-2. Input to the Program

The input data for Level II program is read as shown in the following table. All INTEGER variables are right justified.

TABLE 7

	Columns	Variable	Example	Type
Card 1	1-4	A1	NCB	Alphanumeric
	5-8	A2	DATA	Characters
	9-12	A3	1.2	
	13-16	A4	1.3	
Card 2	1-10	MTB	4	INTEGER
Card 3	1-10	ZB (1)	0.0	REAL
	11-20	ATB (1)	4181.0	REAL
	21-30	ZB (2)	50.0	REAL
	31-40	ATB (2)	4181.0	REAL
	41-50	ZB (3)	100.0	REAL
	51-60	ATB (3)	13415.5	REAL
	61-70	ZB (4)	200.0	REAL
	71-80	ATB (4)	13415.5	REAL
Card 4	1-10	MTHE	3	INTEGER
Card 5	1-10	ZHE (2)	20.0	REAL
	11-20	AHE (1)	0.0	REAL
	21-30	DTUBE (1)	0.0	REAL
	31-40	PV (1)	0.0	REAL
	41-50	PH (1)	0.0	REAL
	51-60	IARR (1)	0	INTEGER
Card 6	1-10	ZHE (3)	60.0	REAL
	11-20	AHE (2)	0.145	REAL
	21-30	DTUBE (2)	5.4	REAL
	31-40	PV (2)	9.9	REAL
	41-50	PH (2)	11.43	REAL
	51-60	IARR (2)	4	INTEGER
Card 7	1-10	ZHE (4)	200.0	REAL
	11-20	AHE (3)	0.0	REAL
	21-30	DTUBE (3)	0.0	REAL
	31-40	PV (3)	0.0	REAL
	41-50	PH (3)	0.0	REAL
	51-60	IARR (3)	0	INTEGER

	Columns	Variable	Example	Type
Card 8	1-10	MFEED	1	INTEGER
Card 9	1-10	ZF(1)	12.7	REAL
	11-20	FFC (1)	1.0	REAL
	21-30	FFAD (1)	1.0	REAL
Card 10	1-10	MDIS	1	REAL
Card 11	1-10	ZDIS (1)	0.0	REAL
	11-20	FD (1)	1.0	REAL
Card 12	1-10	AND	288.0	REAL
	11-20	DNZL	0.3734	REAL
	21-30	DTHICK	2.54	REAL
Card 13	1-10	DEAV	5.0	REAL
	11-20	FW	0.15	REAL
Card 14	1-10	NDPAD	8	INTEGER
Card 15	1-10	DPADF (1)	0.0045	REAL
	11-20	DPADF (2)	0.0066	REAL
	21-30	DPADF (3)	0.0125	REAL
	31-40	DPADF (4)	0.0250	REAL
	41-50	DPADF (5)	0.0500	REAL
	51-60	DPADF (6)	0.1003	REAL
	61-70	DPADF (7)	0.1680	REAL
	71-80	DPADF (8)	0.3175	REAL
Card 16	1-10	FRACTA (1)	0.1720	REAL
	11-20	FRACTA (2)	0.0500	REAL
	21-30	FRACTA (3)	0.1220	REAL
	31-40	FRACTA (4)	0.2250	REAL
	41-50	FRACTA (5)	0.2200	REAL
	51-60	FRACTA (6)	0.1510	REAL
	61-70	FRACTA (7)	0.0590	REAL
	71-80	FRACTA (8)	0.0010	REAL
Card 17	1-4	NAMEL1	LIME	Alphanumeric
	5-8	NAMEL2	ST18	Characters
Card 18	1-10	XCACO3	0.820	REAL
	11-20	XMGCO3	0.020	REAL
Card 19	1-4	NAMEC1	PTGH	Alphanumeric
	5-8	NAMEC2	COAL	Characters

	Columns	Variable	Example	Type
Card 20	1-10	XCF	0.504	REAL
	11-20	XCV	0.222	REAL
	21-30	XH	0.046	REAL
	31-40	XS	0.027	REAL
	41-50	XO	0.043	REAL
	51-60	XN	0.014	REAL
	61-70	XW	0.013	REAL
	71-80	QCOAL	7900.0	REAL
Card 21	1-10	NDPC	8	INTEGER
Card 22	1-10	DPCF (1)	0.0045	REAL
	11-20	DPCF (2)	0.0066	REAL
	21-30	DPCF (3)	0.0125	REAL
	31-40	DPCF (4)	0.0250	REAL
	41-50	DPCF (5)	0.0500	REAL
	51-60	DPCF (6)	0.1003	REAL
	61-70	DPCF (7)	0.1680	REAL
	71-80	DPCF (8)	0.3175	REAL
Card 23	1-10	FRACTC (1)	0.0750	REAL
	11-20	FRACTC (2)	0.0310	REAL
	21-30	FRACTC (3)	0.0880	REAL
	31-40	FRACTC (4)	0.1290	REAL
	41-50	FRACTC (5)	0.2120	REAL
	51-60	FRACTC (6)	0.3440	REAL
	61-70	FRACTC (7)	0.1190	REAL
	71-80	FRACTC (8)	0.0020	REAL
Card 24	1-10	HLMF	0.0	REAL
	11-20	VMF	0.0	REAL
	21-30	HLF	67.056	REAL
	31-40	PAV	4.0	REAL
	41-50	TAV	1083.0	REAL
	51-60	TWAV	530.0	REAL
	61-70	UHEAV	0.005832	REAL
Card 25	1-10	WCOAL	14.679	REAL
	11-20	WAD	0.0	REAL
	21-30	CABS	2.2	REAL
	31-40	UF	0.0	REAL
	41-50	TF	298.0	REAL
	51-60	PF	4.1	REAL
	61-70	EXAIR	17.4	REAL
	71-80	XGF(1)	0.21	REAL
Card 26	1-10	XGF(2)	0.0	REAL
	11-20	XGF(3)	0.0	REAL
	21-30	XGF(4)	0.0	REAL
	31-40	XGF(5)	0.0	REAL
	41-50	XGF(6)	0.0	REAL
	51-60	XGF(7)	0.0	REAL
	61-70	GZCO	0.0	REAL
	71-80	GZH2S	0.0	REAL

	Columns	Variable	Example	Type
Card 27	1-10	GZH2	0.0	REAL
Card 28	1-10	IGNITE	1	INTEGER

8-3. Output of the Program

The output of a typical run of Level II program is following.

NCB DATA 1.2 1.3

HT.ABOVE DISTRIBUTOR,CM	CROSS SECTIONAL AREA OF BED,SQ.CM.
0.0000	4180.602
50.0000	4180.602
100.0000	13415.500
150.0000	13415.500

HEIGHT,CM	SP.HEAT TRANS.AREA,SQ.CM/CL.CM	DIA.OF TUBES,CM	VER.PITCH,CM	HOR.PITCH,CM	TUBES ARRNGT
20.00	0.0000	0.000	0.000	0.000	0
60.00	0.1450	5.400	9.900	11.430	4
300.00	0.0000	0.000	0.000	0.000	0

SOLIDS FEED LEVEL	FRACTION COAL FED	FRACTION LIMESTONE FED
12.70	1.0000	1.0000

SOLIDS DISCHARGE LEVEL	FRACTION DISCHARGED
66.00	1.0000

NO.OF DISTRIBUTOR HOLES = 288.0

NOZZLE DIAMETER = 0.3734 CM

DISTRIBUTOR THICKNESS = 2.5400 CM

AVERAGE CELL SIZE = DZAV = 5.000 CM

FW = 0.150

ORIGINAL PAGE IS
OF POOR QUALITY

NO.	HEIGHT	CELL VOLUME	CELL EFF.VOL.	TUBE VOL.FR.	SP.HE.AREA	TUBE DIA.	VER.PITCH	HOR.PITCH	TUBE ARRNGT
2	5.00	2.0903E 04	2.0903E 04	-0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0
3	10.00	2.0903E 04	2.0903E 04	-0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0
4	15.00	2.0903E 04	2.0903E 04	-0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0
5	20.00	2.0903E 04	2.0903E 04	-0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0
6	25.00	2.0903E 04	1.6811E 04	1.958E-01	1.450E-01	5.400E 00	9.900E 00	1.143E 01	4
7	30.00	2.0903E 04	1.6811E 04	1.958E-01	1.450E-01	5.400E 00	9.900E 00	1.143E 01	4
8	35.00	2.0903E 04	1.6811E 04	1.958E-01	1.450E-01	5.400E 00	9.900E 00	1.143E 01	4
9	40.00	2.0903E 04	1.6811E 04	1.958E-01	1.450E-01	5.400E 00	9.900E 00	1.143E 01	4
10	45.00	2.0903E 04	1.6811E 04	1.958E-01	1.450E-01	5.400E 00	9.900E 00	1.143E 01	4
11	50.00	2.0903E 04	1.6811E 04	1.958E-01	1.450E-01	5.400E 00	9.900E 00	1.143E 01	4
12	55.00	2.2623E 04	1.8194E 04	1.958E-01	1.450E-01	5.400E 00	9.900E 00	1.143E 01	4
13	60.00	2.6193E 04	2.1066E 04	1.957E-01	1.450E-01	5.400E 00	9.900E 00	1.143E 01	4
14	65.00	3.0025E 04	3.0025E 04	-0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0
15	70.00	3.4119E 04	3.4119E 04	-0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0
16	75.00	3.8474E 04	3.8474E 04	-0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0
17	80.00	4.3092E 04	4.3092E 04	-0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0
18	85.00	4.7971E 04	4.7971E 04	-0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0
19	90.00	5.3112E 04	5.3112E 04	-0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0
20	95.00	5.8515E 04	5.8515E 04	-0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0
21	100.00	6.4180E 04	6.4180E 04	-0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0
22	105.00	6.7077E 04	6.7077E 04	-0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0
23	110.00	6.7077E 04	6.7077E 04	-0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0
24	115.00	6.7077E 04	6.7077E 04	-0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0
25	120.00	6.7077E 04	6.7077E 04	-0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0
26	125.00	6.7077E 04	6.7077E 04	-0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0
27	130.00	6.7077E 04	6.7077E 04	-0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0
28	135.00	6.7077E 04	6.7077E 04	-0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0
29	140.00	6.7077E 04	6.7077E 04	-0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0
30	145.00	6.7077E 04	6.7077E 04	-0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0
31	150.00	6.7077E 04	6.7077E 04	-0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0

COMPT.NO.	HEIGHT	BED DIA.	BED C/S AREA
1	0.00	7.296E 01	4.181E 03
2	5.00	7.296E 01	4.181E 03
3	10.00	7.296E 01	4.181E 03
4	15.00	7.296E 01	4.181E 03
5	20.00	7.296E 01	4.181E 03
6	25.00	7.296E 01	4.181E 03

7	30.00	7.296E 01	4.181E 03
8	35.00	7.296E 01	4.181E 03
9	40.00	7.296E 01	4.181E 03
10	45.00	7.296E 01	4.181E 03
11	50.00	7.296E 01	4.181E 03
12	55.00	7.873E 01	4.868E 03
13	60.00	8.451E 01	5.609E 03
14	65.00	9.028E 01	6.401E 03
15	70.00	9.605E 01	7.246E 03
16	75.00	1.018E 02	8.143E 03
17	80.00	1.076E 02	9.093E 03
18	85.00	1.134E 02	1.010E 04
19	90.00	1.191E 02	1.115E 04
20	95.00	1.249E 02	1.226E 04
21	100.00	1.307E 02	1.342E 04
22	105.00	1.307E 02	1.342E 04
23	110.00	1.307E 02	1.342E 04
24	115.00	1.307E 02	1.342E 04
25	120.00	1.307E 02	1.342E 04
26	125.00	1.307E 02	1.342E 04
27	130.00	1.307E 02	1.342E 04
28	135.00	1.307E 02	1.342E 04
29	140.00	1.307E 02	1.342E 04
30	145.00	1.307E 02	1.342E 04
31	150.00	1.307E 02	1.342E 04

LIMEST18 XCACO3 = 0.820 XMGCO3 = 0.020

DPADF , CM	WT.FRACTION
0.0045	0.1720
0.0066	0.0500
0.0125	0.1220
0.0250	0.2250
0.0500	0.2200
0.1003	0.1510
0.1680	0.0590
0.3175	0.0010

SURFACE VOLUME MEAN DIA. = DPADH = 0.0084 CM WEIGHT MEAN DIA. = DPADR = 0.0338 CM

PTGHCOAL XCF = 0.504 XCV = 0.222 XH = 0.046 XS = 0.027 XO = 0.043 XN = 0.014 XA = 0.144 XW = 0.013
QCOAL = 7900.00 CALS/GM QCCALC = 7900.00 CALS/GM

DPCF , CM	WT.FRACTION
0.0045	0.0750
0.0066	0.0310
0.0125	0.0880
0.0250	0.1290
0.0500	0.2120
0.1003	0.3440
0.1680	0.1190
0.3175	0.0020

SURFACE VOL MEAN DIA OF COAL FEED = DCF = 0.0151 CM DCAV = 0.0113

```
&OPCF
HLMF=   0.0000000E 00,VMF=   0.0000000E 00,HLF=   0.6705600E 02,PAV=   0.4000000E 01,TAV=   0.1083000E 04,TWAV=   0.5300000E 03,
UHEAV=   0.5832002E-02,WCOAL=   0.1467900E 02,WAD=   0.3282995E 01,WCAD=   0.2064861E 01,CABS=   0.2200000E 01,UF=   0.8261148E 01,
TF=   0.2980000E 03,PF=   0.4100000E 01,EXAIR=   0.1739988E 00,XGF=   0.2100000E 00,   0.0000000E 00,   0.0000000E 00,
   0.0000000E 00,   0.0000000E 00,   0.0000000E 00,   0.0000000E 00,   0.0000000E 00,   0.7900000E 00,GZCO=   0.0000000E 00,GZH2S=   0.0000000E 00,
GZH2=   0.0000000E 00,IGNITE=          1,MGAS=   0.2883998E 02,FMTH=   0.4932879E 01,FMF=   0.5791199E 01,FMO=   0.5987882E 01,
RHOCAD=   0.1509496E 01,RHOCH=   0.1275399E 01,&END
```

RESULTS ,ALL TEMPERATURES IN CENTIGRADE

ETC,XAV,TAV,ITRIAL,= 0.9282E 00 0.1547E-01 0.7759E 03 2

I	YB	YE	X	Z	T	ZAVG	TPB	TPE	WNET	RR
1	1.7649E-01	1.7649E-01	2.2911E-01	0.0000E-01	2.5000E 01	0.0000E-01	2.5000E 01	2.5000E 01	0.0000E-01	0.0000E-01
2	1.4254E-01	6.2926E-04	1.5489E-02	5.0000E 00	8.1018E 02	2.5000E 00	8.1994E 02	8.1349E 02	-2.4873E 00	1.3585E 00
3	1.2045E-01	3.4815E-04	1.5498E-02	1.0000E 01	8.1177E 02	7.5000E 00	8.1962E 02	8.1426E 02	-4.0672E 00	8.6195E-01

4	1.0528E-01	2.4077E-04	1.5512E-02	1.5000E 01	8.0772E 02	1.2500E 01	8.1398E 02	8.0969E 02	5.5171E 00	5.9139E-01
5	9.4397E-02	1.8879E-04	1.5497E-02	2.0000E 01	8.0047E 02	1.7500E 01	8.0554E 02	8.0213E 02	8.7384E 00	4.2278E-01
6	8.6908E-02	2.0366E-04	1.5485E-02	2.5000E 01	7.9027E 02	2.2500E 01	7.9457E 02	7.9190E 02	8.2085E 00	3.5593E-01
7	8.0132E-02	2.3937E-04	1.5475E-02	3.0000E 01	7.8088E 02	2.7500E 01	7.8456E 02	7.8244E 02	7.7231E 00	3.2534E-01
8	7.4165E-02	2.5170E-04	1.5466E-02	3.5000E 01	7.7246E 02	3.2500E 01	7.7566E 02	7.7391E 02	7.2958E 00	2.8565E-01
9	6.8851E-02	2.6140E-04	1.5459E-02	4.0000E 01	7.6520E 02	3.7500E 01	7.6793E 02	7.6650E 02	6.9153E 00	2.5373E-01
10	6.4066E-02	2.6696E-04	1.5453E-02	4.5000E 01	7.5929E 02	4.2500E 01	7.6158E 02	7.6037E 02	6.5727E 00	2.2786E-01
11	5.9717E-02	2.6707E-04	1.5448E-02	5.0000E 01	7.5488E 02	4.7500E 01	7.5672E 02	7.5569E 02	6.2613E 00	2.0656E-01
12	5.5623E-02	2.4199E-04	1.5444E-02	5.5000E 01	7.5210E 02	5.2500E 01	7.5348E 02	7.5257E 02	5.9656E 00	1.8104E-01
13	5.1632E-02	1.9679E-04	1.5442E-02	6.0000E 01	7.5129E 02	5.7500E 01	7.5212E 02	7.5130E 02	5.6774E 00	1.5223E-01
14	4.7458E-02	1.2982E-04	1.5440E-02	6.5000E 01	7.5298E 02	6.2500E 01	7.5315E 02	7.5238E 02	5.3711E 00	1.1368E-01
15	4.5989E-02	9.1061E-05	1.5440E-02	6.7056E 01	7.5357E 02	6.6028E 01	7.5352E 02	7.5277E 02	4.0499E 00	8.3421E-02

(ETS,FS,CABS,CABSE)=
0.8287E 00 0.3767E 00 0.2200E 01 0.2200E 01

HT.	ZAVG	YB	YE	SRELB	SRELE
5.0000E 00	2.5000E 00	1.7521E-04	1.5273E-04	1.2371E-03	1.9960E-03
1.0000E 01	7.5000E 00	2.8519E-04	9.6245E-05	8.8743E-04	1.1662E-03
1.5000E 01	1.2500E 01	3.5280E-04	6.7316E-05	6.2775E-04	7.8293E-04
2.0000E 01	1.7500E 01	3.9330E-04	4.9834E-05	4.4650E-04	5.6564E-04
2.5000E 01	2.2500E 01	4.1103E-04	4.7158E-05	2.7792E-04	4.1097E-04
3.0000E 01	2.7500E 01	4.1817E-04	4.8617E-05	2.2689E-04	4.0402E-04
3.5000E 01	3.2500E 01	4.1789E-04	4.5376E-05	1.8268E-04	3.7271E-04
4.0000E 01	3.7500E 01	4.1250E-04	4.2360E-05	1.4985E-04	3.4477E-04
4.5000E 01	4.2500E 01	4.0373E-04	3.9581E-05	1.2577E-04	3.1955E-04
5.0000E 01	4.7500E 01	3.9287E-04	3.7036E-05	1.0812E-04	2.9658E-04
5.5000E 01	5.2500E 01	3.8102E-04	3.2307E-05	1.0077E-04	2.8369E-04
6.0000E 01	5.7500E 01	3.6864E-04	2.6217E-05	1.0015E-04	2.7445E-04
6.5000E 01	6.2500E 01	3.5668E-04	1.8126E-05	1.1579E-04	2.8237E-04
6.7056E 01	6.6028E 01	3.5284E-04	1.2594E-05	4.2837E-05	9.4976E-05

OUTLET GAS CONCENTRATION

O2	CO2	SO2	H2O	CO	H2S	H2	NOX
0.4560E-01	0.1635E 00	0.3500E-03	0.5742E-01	0.0000E 00	0.0000E 00	0.0000E 00	0.1839E-04

PRESSURE DROP ACROSS THE DISTRIBUTOR = 1.1519E 01

COMP.NO	PRESSURE DROP IN THE BED
2	2.2891E 00
3	2.3895E 00
4	2.4784E 00
5	2.5522E 00
6	2.7447E 00
7	2.6809E 00
8	2.6883E 00
9	2.6951E 00
10	2.7010E 00
11	2.7060E 00
12	2.7601E 00
13	2.8600E 00
14	2.8334E 00
15	1.2331E 00

PRESSURE DROP IN THE FIXED BED SECTION = 0.0000E-01

&OPCF1
ICR= 0,IFBC= 0,HCR= 0.0000000E 00,HLF= 0.6705600E 02,HLMF= 0.4842171E 02,VMF= 0.1791724E 06,BEDVOL=
0.3013810E 06,EFFVOL= 0.2672749E 06,SOLVOL= 0.1791724E 06,TETUBE= 0.1131662E 00,HAREA= 0.2526380E 05,QTRANS=
0.7488019E 05,CVCL= 0.2484568E 00,QAREA= 0.2963932E 01,HELT= 0.2945155E 01,CELU= 0.7362888E 00,CLCSS= 0.7550509E 00,
WDIS= 0.1215159E 01,&END

I	HEIGHT	ZAVG	AV.BUBBLE DIA	BUBBLE VEL.	BUBBLE FRAC.	CLOUD FRAC.	SUP.VELOCITY	MIN.FLU.VEL.
2	5.000	2.500	4.6841E 00	7.9420E 01	3.9342E-01	3.9493E-01	3.1921E 01	1.5135E-01
3	10.000	7.500	6.0753E 00	8.6646E 01	3.6680E-01	3.6808E-01	3.1944E 01	1.5094E-01
4	15.000	12.500	7.4372E 00	9.2428E 01	3.4324E-01	3.4437E-01	3.1809E 01	1.5163E-01
5	20.000	17.500	8.7680E 00	9.7457E 01	3.2370E-01	3.2471E-01	3.1588E 01	1.5217E-01
6	25.000	22.500	9.4458E 00	1.0350E 02	2.7268E-01	2.7348E-01	3.8902E 01	1.5315E-01
7	30.000	27.500	9.4862E 00	1.0713E 02	2.8959E-01	2.9042E-01	3.8556E 01	1.5423E-01
8	35.000	32.500	9.5258E 00	1.0695E 02	2.8762E-01	2.8845E-01	3.8245E 01	1.5490E-01

```
  9   40.000    37.500     9.5645E 00      1.0679E 02      2.8583E-01      2.8666E-01      3.7974E 01      1.5579E-01
 10   45.000    42.500     9.6025E 00      1.0668E 02      2.8426E-01      2.8509E-01      3.7750E 01      1.5641E-01
 11   50.000    47.500     9.6397E 00      1.0662E 02      2.8294E-01      2.8377E-01      3.7579E 01      1.5683E-01
 12   55.000    52.500     9.6748E 00      1.0395E 02      2.6860E-01      2.6942E-01      3.2172E 01      1.5710E-01
 13   60.000    57.500     9.7068E 00      9.9224E 01      2.4214E-01      2.4291E-01      2.7891E 01      1.5731E-01
 14   65.000    62.500     1.0229E 01      9.4817E 01      2.4917E-01      2.5000E-01      1.9675E 01      1.5759E-01
 15   67.056    66.028     1.0937E 01      9.2637E 01      2.0535E-01      2.0605E-01      1.8687E 01      1.5715E-01

CORE USAGE       OBJECT CODE=    59536 BYTES,ARRAY AREA=    24484 BYTES,TOTAL AREA AVAILABLE=   131072  BYTES

DIAGNOSTICS        NUMBER OF ERRORS=        0, NUMBER OF WARNINGS=        1, NUMBER OF EXTENSIONS=        0

COMPILE TIME=     7.04 SEC,EXECUTION TIME=     10.18 SEC,     23.08.56     FRIDAY         1 JUL 77    WATFIV - JAN 1976 V1L5

        $IBSYS                                                                  1407.
```

ORIGINAL PAGE
OF POOR QUALITY

Nomenclature of Level II Program

FORTRAN Symbol	Mathematical Symbol	Unit	Description
AAA	-	-	matrix coefficients
AG	-	mole fraction	outlet gas composition (O_2, CO_2, SO_2, H_2O, CO, H_2S, H_2, N_2)
AHE	a_{HE}	cm^2/cm^3	specific heat transfer area
AHEAV	$a_{HE,i}$	cm^2/cm^3	specific heat transfer area in each compartment
AKB	k_c	cm/sec	overall surface reaction rate constant for coal combustion in the bubble phase
AKBE	$K_{BE,i}$	1/sec	gas exchange coefficient in the ith compartment
AKE	k_c	cm/sec	overall surface reaction rate constant for coal combustion in the emulsion phase
AKO	$\hat{k}_{v\ell}$	1/sec	volumetric reaction rate constant for SO_2 reaction
ALFA	-	-	temperature matrix coefficient
AND	N_d	-	number of distributor holes
ANOX	NO_x	mole fraction	NO_x concentration in the effluent gas
AT	$A_{t,i}$	cm^2	cross sectional area of the bed at each location
ATB	-	cm^2	cross sectional area of the FBC at specified locations
BBB	-	-	matrix coefficient
BEDVOL	V	cm^3	total bed volume
BETA	-	-	temperature matrix coefficient
CABS	$[C_a]/[S]$	mole ratio	mole ratio of calcium to sulfur in feed solids
CABSE	$[C_a]_f/[S]_f$	mole ratio	effective ratio of calcium to sulfur in the feed (gas and solids)
CADF	C_{sf}	Cal/g°C	heat capacity of additives fed

FORTRAN Symbol	Mathematical Symbol	Unit	Description
CCF	C_{cf}	Cal/g°C	heat capacity of coal fed
CELU	W_e	g/sec	elutriation rate of unburnt char
CGM	C_{gm}	Cal/gmol°K	molar heat capacity of gas
CGMF	C_{gmf}	Cal/gmol°K	molar heat capacity of gas at feed temperature
CLOSS	-	g/sec	total carbon loss
CS	C_s	Cal/g°K	heat capacity of solids
DB	D_B	cm	bubble diameter
DBAV	$D_{B,av}$	cm	average bubble size of each compartment
DENOM	-	gmol/sec	total sulfur fed into the bed
DCAV	d_c	cm	average particle size
DELT	-	-	temperature matrix coefficient
DNZL	-	cm	diameter of distributor holes
DPADH	-	cm	surface volume mean diameter of additives (used in hydrodynamic calculations)
DPADR	d_p	cm	weight mean diameter of additives (used for reaction calculations)
DPB	d_ℓ	cm	particle diameter of additives
DPDIS	-	cm H_2O	pressure drop across the distributor
DPFIX	-	cm H_2O	pressure drop in the fixed bed section
DPFLU	-	cm H_2O	pressure drop in the fluidized section
DT	$D_{t,i}$	cm	diameter of the bed at each location
DTHICK	-	cm	distributor plate thickness
DVBB	ΔV_i	cm^3	volume of compartment
DVBBEF	-	cm^3	effective volume of compartment eccluding tubes

FORTRAN Symbol	Mathematical Symbol	Unit	Description
DZAV	-	cm	average compartment size
EFFVOL	-	cm^3	effective volume of bed eccluding tubes
ELLOSS	-	wt. fraction	elutriation loss
EMF	ε_{mf}	-	void fraction at minimum fluidization
ETC	η	-	carbon combustion efficiency
ETCA	-	-	assumed carbon combustion efficiency
ETCC	-	-	combustion efficiency based on carbon consumption
ETCG	-	-	combustion efficiency based on oxygen consumption
ETCP	-	-	efficiency of pyrolysis
ETS	-	-	efficiency of sulfur capture
ETUBE	$\varepsilon_{tube,i}$	-	tube volume fraction in each compartment
EXAIR	EAR	-	excess air
FBM	F_{BM}	gmol/sec	molar flow rate of gas in bubble phase
FD	-	-	fraction of total solids discharged at each location
FEM	F_{EM}	gmol/sec	molar flow rate of gas in emulsion
FFAD	-	-	fraction of total additives fed at each location
FFC	-	-	fraction of total coal fed at each location
FMF	F_{mf}	gmol/sec	molar flow rate of inlet gas
FMO	F_m	gmol/sec	total molar flow rate of gas in the bed
FMTH	F_{mth}	gmol/sec	theoretical feed rate of inlet gas

FORTRAN Symbol	Mathematical Symbol	Unit	Description
FS	f_ℓ	-	fractional conversion of additives
FW	f_w	-	volume fraction of wake to bubble
G	g	980.1 cm/sec^2	acceleration due to gravity
GZCO	ξ_{CO}	-	ratio of CO formation rate to carbon combustion rate
GZH2	ξ_{H_2}	-	ratio of H_2 formation rate from coal to sum of H_2 and H_2O formation rate from coal
GZH2S	ξ_{H_2S}	-	ratio of H_2S formation rate to sulfur feed rate
H(I),H(I+1)	h_i h_{i+1}	cm	height of the bottom and top of each compartment above distributor
HAREA	-	cm^2	total heat transfer area
HCR	-	cm	critical bed height
HLF	L_f	cm	height of the fluidized (expanded) bed
HLMF	L_{mf}	cm	height of minimum fluidization
ICR	-	-	indicator for critical bed height
IFBC	-	-	indicator for the fixed bed section
IGNITE	-	-	index for combustion calculation (= 1, combustion, = 0, no combustion)
MAIR	M_{air}	g/mole	molecular weight of air

FORTRAN Symbol	Mathematical Symbol	Unit	Description
MC	M_c	g/g atm	atomic weight of carbon
MCACO3	M_{CaCO_3}	g/g atm	molecular weight of $CaCO_3$
MCAO	M_{CaO}	g/g atm	molecular weight of CaO
MCASO4	M_{CaSO_4}	g/g atm	molecular weight of $CaSO_4$
MCO	M_{CO}	g/g atm	molecular weight of CO
MCO2	M_{CO_2}	g/g atm	molecular weight of CO_2
MDIS	-	-	number of solids discharge locations
MFEED			number of solids feed locations
MGAS	M_g	g/g mole	molecular weight of feed gas
MH2	M_{H_2}	g/g mole	molecular weight of hydrogen
MH2O	M_{H_2O}	g/g mole	molecular weight of water
MH2S	M_{H_2S}	g/g mole	molecular weight of H_2S
MMGCO3	M_{MgCO_3}	g/g mole	molecular weight of $MgCO_3$
MMGO	M_{MgO}	g/g mole	molecular weight of MgO
MN2	M_{N_2}	g/g mole	molecular weight of nitrogen
MO2	M_{O_2}	g/g mole	molecular weight of oxygen
MS	M_s	g/g atm	atomic weight of sulfur
MSO2	M_{SO_2}	g/g mole	molecular weight of SO_2
MT	-	-	total number of divisions of the FBC + 1
MTB	-	-	number of specified locations

FORTRAN Symbol	Mathematical Symbol	Unit	Description
NAMEC1 NAMEC2	-	-	name of coal
NAMEL1 NAMEL2	-	-	name of limestone
NDPAD DPADF FRACTA	-	cm wt. fraction	size distribution of limestone particles - number of size intervals (NDPAD), upper bound of each size interval (DPADF), weight fraction (FRACTA)
NDPC DPCF FRACTC		cm wt. fraction	size distribution of coal particles - number of size intervals (NDPC), upper bound of each size interval (DPCF), weight fraction (FRACTC)
PAV	P	atm	average pressure of the FBC
PF	-	atm	inlet gas pressure at the distributor
PH	P_h	cm	horizontal pitch of the cooling coils
PI	π	3.141593	mathematical constant
PV	P_v	cm	vertical pitch of the cooling coils
QAREA	-	$Cal/cm^2 sec$	heat transfer rate per cm^2 heat transfer area
QCLCN	q_ℓ	Cal	total heat of calcination of limestone
QCOAL	q_c	Cal/g	heating value of coal for incomplete combustion
QCOALC	-	Cal/g	heating value of coal for complete combustion
QIN	-	Cal/sec	sensible heat carried in by feed solids and gas
QTRANS	-	Cal/sec	total heat transferred to the coolant
QVOL	-	$Cal/sec\ cm^3$	heat transfer rate per cm^3 of bed
RG	R	cc·atm/gmol·K	gas constant
RHOAD	$\rho_{\ell f}$	g/cm^3	density of limestone

FORTRAN Symbol	Mathematical Symbol	Unit	Description
RHOASH	ρ_A	g/cm^3	density of ash
RHOC	ρ_{cf}	g/cm^3	density of coal
RHOCAD	ρ_ℓ	g/cm^3	density of calcined additives
RHOCH	ρ_{ch}	g/cm^3	density of char
RHOFG	-	g/cm^3	density of feed gas
RHOGAS	ρ_g	g/cm^3	density of gas in the bed
RR		g/sec	rate of combustion in each compartment per unit carbon concentration
RR (I)	-	Cal/sec	heat generation rate minus heat consumption rate in each compartment
RRB	-	g/sec	rate of combustion of carbon in the bubble phase in each compartment
RRE	-	g/sec	rate of combustion of carbon in the emulsion phase in each compartment
S (I)	-	-	index for net flow (-1, for downward flow, +1, for upward flow)
SRELB	-	gmol/sec	sulfur release rate in the bubble phase
SRELE	-	gmol/sec	sulfur release rate in the emulsion phase
T	T	°K	bed temperature
TAV	-	°K	average bed temperature
TCAR	-	g/sec	total carbon available for combustion
TCRATE	-	g/sec	total carbon combustion rate
TETUBE	-	-	total volume fraction of tubes
TF	T_g	°K	inlet gas temperature
THET	Θ	sec	residence time in the top compartment

FORTRAN Symbol	Mathematical Symbol	Unit	Description
TNORM	-	°K	temperature for convergency criterion
TOLD	-	°K	bed temperature in the previous iteration
TPB	-	°K	temperature of particles in the bubble phase
TPE	-	°K	temperature of particles in the emulsion phase
TSF	T_{sf}	°K	temperature of feed solids
TW	T_w	°K	temperature of coolant
TWAV	-	°K	average coolant temperature
UB	u_b	cm/sec	bubble velocity
UF	u_f	cm/sec	superficial gas velocity at the distributor at the inlet temperature and pressure
UHE	u	$Cal/cm^2 sec°K$	overall heat transfer coefficient
UHEAV	-	$Cal/cm^2 sec°K$	average overall heat transfer coefficient
UMF	u_{mf}	cm/sec	minimum fluidization velocity
UO	u_o	cm/sec	superficial gas velocity
VISC	μ	g/cm sec	viscosity of gas in the bed
VMF		cm^3	volume of bed at minimum fluidization
WAD	$w_{\ell f}$	g/sec	total limestone feed rate
WCAD	-	g/sec	total calcined additives feed rate
WCOAL	w_{cf}	g/sec	total coal feed rate
WELT	-	g/sec	total solids elutriated
WFAD	-	g/sec	feed rate of calcined additives at each location
WFC	-	g/sec	feed rate of char at each location
WMIX	w_{mix}	g/sec	upward and downward flow rate of solids due to backflow

FORTRAN Symbol	Mathematical Symbol	Unit	Description
WNET	w_{net}	g/sec	net flow rate of solids
X	x	wt. fraction	carbon concentration in the bed
XAV SAVIC	-	wt.fraction	average carbon concentration in the bed (IC denotes initial condition)
XC	x_f	wt. fraction	total carbon content in the coal
XCACO3	$x_{\ell Ca}$	wt. fraction	$CaCO_3$ content in the limestone
XCAO	-	wt. fraction	CaO content in the additives
XCF	-	wt. fraction	weight fraction of fixed carbon in the coal (d b)
XCV	-	wt. fraction	weight fraction of volatiles in the coal (d b)
XCF (I)	y_i	mole fraction	feed gas composition (O_2, CO_2, SO_2, H_2O, CO, H_2S, H_2, N_2)
XH	-	wt. fraction	weight fraction of hydrogen in the coal (d b)
XMGCO3	-	wt. fraction	$MgCO_3$ content in limestone
XN	-	wt. fraction	weight fraction of nitrogen in coal (d b)
XO	-	wt. fraction	weight fraction of oxygen in coal (d b)
XS	-	wt. fraction	weight fraction of sulfur in coal(d b)
YAV	-	mole fraction	average oxygen concentration in the bed
YB	y_B	mole fraction	bubble phase concentration of oxygen in combustion calculations or sulfur dioxide in SO_2 calculations
YBO	-	mole fraction	bubble phase concentration of oxygen
YE	y_E	mole fraction	emulsion phase concentration of oxygen in combustion calculations or sulfur dioxide in SO_2 calculations
YEO	-	mole fraction	emulsion phase concentration of oxygen

FORTRAN Symbol	Mathematical Symbol	Unit	Description
Z	Z	cm	height above the distributor
ZAVG	-	cm	average height of the compartment
ZB	-	cm	specified location
ZDIS ZF	-	cm	locations of discharge and feed
ZHE	-	cm	locations of bottom and top of the cooling coils

Section IX

MANUAL OF COMPUTER SUB-PROGRAMS

In this section the sub-programs used in the computer programs (Level I and II) are explained in detail. Following Table 9 shows the list of subroutines in alphabetical order. Except the subroutine SIMQ which is the duplication of one of the subroutines in SSP supplied by IBM, explanation is given for each sub-program.

TABLE 8

LIST OF ORIGINAL COMPUTER SUB-PROGRAMS

No.	Title	Used in	Functions
1	ACTIV	Level I	Calculation of the reactivity of char λ_c, for given data of y, d_{cm}, ρ_g, μ, $\mathcal{D}_{O2}$, k_{co}, u_o.
2	AKAD	Level II	Calculation of the rate constant of sulfur capturing reaction, $k_{v\ell}$ for given data of f_ℓ, d_ℓ and T.
3	AKK	Level II	Calculation of the combustion rate constant k_c and the temperature of char particles T_c for given t, p, d_c and y_{O2}
4	AREA	Level II	Calculation of A_t for a given height above distribution, z
5	CRRECT	Level I & II	Calculation of the value of an unknown parameter assumed for the next trial of Regula Falsi iteration
6	DESIGN	Level II	Input subroutine for the design parameters of the bed. Redistribution of the parameters for each elemental volume
7	FREEFV	Level I	Calculation of the free fall velocity (terminal velocity) of particle of given property (d_p,) in the gas of given property (ρ_g,μ_g)

(Table 9 Continued)

No.	Title	Used in	Functions
8	GPHASE	Level II	GPHASE given the value of gaseous species concentrations in bubble and emulsion phases of the ith compartment, y_{Bi} and y_{Ei}, from a given hydrodynamic and kinetic informations and the values of $y_{B,i-1}$ and $y_{E,i-1}$. It is assumed there that the reaction is first order about the relevant species.
9	HEIGHT	Level II	Calculation of the effective height of the bed excluding the volume occupied by tubes.
10	HFATI	Level II	Calculation of the bed height above the distributor at any given corss-sectional area of the bed.
11	HYDRO	Level II	Calculation of the bubble hydrodynamics-minimum fluidizing velocity, superficial velocity, bubble size, bubble fraction, cloud fraction, bubble velocity and location of the fixed bed section above the fluidized bed section, computation of height at minimum fluidization or height of fluidized bed.
12	POP	Level I	Calculation of the size distribution density function of char in the bed.
13	VOLUME	Level II	Calculation of the effective volume of the bed for the given height of the fluidized bed.

9-1. Function ACTIV

Reactivity of char, λ_c, is calculated in this sub-program based on the equation:

$$\lambda_c = 1/(k_{cR}/k_{cf} + 1)$$

k_{cR} must be fed as an input but k_{cf} is calculated in the subprogram by assuming Sh = 2. The value of Sherwood number can be changed as a function of Reynolds number easily, since Reynolds number is also computed in this sub-program although it is not used. Then the mass transfer coefficient is given as

$$k_f = Sh \cdot \mathcal{D}_{O2}/d_c$$

where $d_c = d_{cm} \cdot y$

The inputs and outputs of this sub-program are,

Inputs to the sub-program: Y, DCM, RHOG, VISC, D, AK, UO

Output from the sub-program: ACTIV

Nomenclature Code	Model variable	Description	Unit
AK	k_{cR}	chemical reaction rate constant	cm/sec
AKF	k_{cf}	mass transfer coefficient	cm/sec
ACTIV	λ_c	reactivity of char	-
D	$\mathcal{D}_{O2}$	diffusivity of oxygen	cm^2/sec
DCM	d_{cm}	maximum diameter of char particles	cm
RHOG	ρ_g	gas density	g/cm^3
UO	u_o	gas superficial velocity	cm/sec
VISC	μ	gas vescosity	g/cm·sec
Y	y	dimensionless particle diameter of char	-

9-2. Function AKAD

Mean overall rate constant for sulfur capturing reaction, $\hat{k}_{v\ell}$, is computed by this function sub-program. The sub-program shown in this report is for temporary use because of the lack of general kinetic data. This function is designed based on the data by Borgwardt (1972) for Type 4 limestone. The condition of Borgwardt is summarized as follows:

1) reaction: limestone - SO_2
2) temperature: 1253 °K
3) particle size: 0.0096~0.13 cm

Mean overall reaction rate constant is calculated by the equation,

$$\hat{k}_{v\ell} = k'_{v\ell} \; S_g \; \hat{\lambda}_\ell \; (\hat{f}_\ell, d_\ell)$$

where $k'_{v\ell}$ is defined as

$$k'_{v\ell} = 3.72 \times 10^{-3} \exp (- 17.5 \times 10^3/RT)$$

This value of activation energy was obtained by Wen and Ishida (1973). By using Borgwardt (1972)'s data the specific surface S_g is correlated with temperature (calcination temperature) as

$S_g = - 193.75\ T + 275{,}000 \quad cm^2/g \quad T > 1100\ K$. For $T < 1100\ K$, $S_g = S_g$ at 1100 K

From Borgwardt's experiment the relationships between λ_ℓ and f_ℓ are obtained. The data are reformed using Equations (3-65) and (3-66) and the function $\hat{\lambda}_\ell\ (\hat{f}_\ell)$ is calculated for each particle diameter. The results are stored in the sub-program. Linear interpolation on the semi-logarithmic space is applied to obtain the value of $\hat{\lambda}_\ell$ for the arbitrary input of $\hat{f}_\ell$ and d_ℓ. The equations for the interpolation are:

$$\hat{\lambda}_{\ell a} \equiv \left(\frac{\hat{\lambda}_{\ell a2}}{\hat{\lambda}_{\ell a1}}\right)^{\frac{\hat{f} - \hat{f}_1}{\hat{f}_2 - \hat{f}_1}} \hat{\lambda}_{\ell a1}$$

$$\hat{\lambda}_{\ell b} \equiv \left(\frac{\hat{\lambda}_{\ell b2}}{\hat{\lambda}_{\ell b1}}\right)^{\frac{\hat{f} - \hat{f}_1}{\hat{f}_2 - \hat{f}_1}} \hat{\lambda}_{\ell b1}$$

$$\hat{\lambda}_{\ell} = \frac{\hat{\lambda}_{\ell a}}{\hat{\lambda}_{\ell b}}^{\frac{\ell n(d_{\ell}/d_{\ell b})}{\ell n(d_{\ell a}/d_{\ell b})}} \hat{\lambda}_{\ell b}$$

To improve the validity of this function sub-program, kinetic data covering wide temperature and particle size ranges are needed. The direct combination of a kinetic model for one particle will not be effective due to the computation time limitation. It is, therefore, recommended to provide the value of $\hat{k}_{v\ell}$ over the wide conditions such as

$T = 950\sim1350$ °K

$d_{\ell} = 0.01\sim0.5$ cm

and apply the interpolation not only for f_{ℓ} and d_{ℓ} but also T.

The inputs and outputs of this sub-program are,

Inputs: FS, DP, T

Outputs: AKAD

Nomenclature Code	Model variable	Description
AKAD	$\hat{k}_{v\ell}$	mean overall reaction rate constant
ALIME	$\hat{\lambda}_{\ell}$	mean reactivity of adsorbent
DP	d_{ℓ}	particle diameter of adsorbent
DP1, DP2, DP3	$d_{\ell a}, d_{\ell b}$	particle diameters of stored data
FB(I)	$\hat{f}_{\ell i}$	mean conversion data grid
FS	$\hat{f}_{\ell}$	mean conversion
RR(I), RB(I), RC(I)		mean reactivity data corresponding to the particle sizes of DP1, DP2, and DP3 respectively.
R1	$\hat{\lambda}_{\ell a}$	
R2	$\hat{\lambda}_{\ell b}$	
XXX	$\frac{\ell n\ (d_{\ell}/d_{\ell b})}{\ell n\ (d_{\ell a}/d_{\ell b})}$	

9-3. Subroutine AKK

Combustion rate constant, k_c, and the temperature of char particle are calculated by this subroutine. At first, the char particle temperature is assumed to be equal to the bed temperature. Applying Equation (3-101) the following equation is used for the criterion equation for testing the assumed value of char particle temperature:

$$\text{Error} = T_c - T - \frac{7900\ k_c p\ y_{O2}/RT'}{\frac{2\lambda'}{d_c} + \frac{T_c^4 - T^4}{T_c - T}}$$

$$T' \equiv (T_c + T)/2$$

where

$\sigma = 1.36 \times 10^{-12}$

$\varepsilon' = 0.5$

$\lambda' = 0.5659 \times 10^{-4} + 1.07 \times 10^{-7} T'$

are used.

For calculating k_c the following data are used:

$k_{cR} = (T_c/1000) \exp (17.9 - 35.7/(0.001986\ T_c))$

$Sh = 2$

$\mathcal{D} = 4.26\ (T'/1800)^{1.75}\ /P$

Subroutine CRRECT is applied for correcting the assumed value of T_c.

The inputs and outputs of this sub-program are,

Inputs: T, P, DC, YO2, RG

Outputs: AKR, TP

Nomenclature Code	Model variable	Description	Unit
AKF	k_{cf}	mass transfer coeeficient	
AKR	k_{cR}	chemical reaction constant	
AKS	k_c	overall combustion rate constant	
COND	λ'	thermal conductivity of gas	
D	$\mathcal{D}$	diffusivity of oxygen	cm^2/sec
EM	ε'	emissivity	
ETS	Error		
ETSMAX	max(Error)	tolerance limit for iteration	°K
SHP	Sh	Sherwood number	-
SIGM	σ		
T	T	bed temperature	°K
TAV	T'	average temperature for gas film	°K
TP	T_c	char particle temperature	°K

9-4. Subroutine AREA

By using this subroutine the cross sectional area of the bed can be calculated at any given height. Into subroutine DESIGN a set of ~~the~~ data z_j and A_j, j = 1~MTB is fed and stored in the common address before subroutine AREA is called.

For a given height z, z_{j-1} and z_j are searched so that

$$z_{j-1} \leq z < z_j$$

Then, the cross sectional area A correspondint to z is obtained by the following equation:

$$A = \pi r^2$$

$$r = \left[1 + \frac{z - z_{j-1}}{z_j - z_{j-1}} \cdot \left\{\left(\frac{A_j}{A_{j-1}}\right)^{1/2} - 1\right\}\right] r_{j-1}$$

$$r_{j-1} = (A_{j-1}/\pi)^{1/2}$$

where it is assumed that the diameter in between z_{j-1} and z_j is proportional to the height. The diameter D_t is also calculated.

The inputs and outputs of this sub-program are,

Inputs: ZI

Other parameters supplied from common(GEN/:ZB(J), ATB(J), J = 1, MTB

Nomenclatures Code	Model variable	Description	Unit
ATB(J)	A_j	bed cross section at $z=z_j$	cm^2
ATI	A_t	bed cross section at z=z	cm^2
DTI	D_t	equivalent diameter of bed at z=z	cm
RI	n	radius at z=z	cm
ZB(J)	z_j	height from the distributor where the data for cross-sectional area is given	cm
ZI	z	height from the distributor	cm

9-5. Subroutine CRRECT

Subroutine CRRECT provides the assumed value for the unknown variable to be used in the next iteration of Regula Falsi method and also judges if the iteration has converged.

The regula Falsi iteration has two different periods,

Period 1: the root is not captured in the interval (INDX = 0)

Period 2: the root is captured in the interval (INDX = 1) as illustrated in Figure 10.

The parameter INDX is an indicator of the periods and INDX = 2 indicates that the iteration has converged. During period 1 the search for the root is repeated by proceeding in one direction specified by the sign of increment for X, DX. Once the root is captured in the interval, Newton-Raphson scheme is applied.

To apply this subroutine the following statements must be prepared in the program from where CRRECT is called.

1) Initial assumption for the unknown parameter, X

2) Value for differential increment, ΔX

3) Tolerance limit for ERROR: E

4) Initial value for INDX the error, INDX = 0

5) DO loop for iteration

6) A statement to get off from the DO loop when INDX = 2.

Therefore the program looks like

```
X = ......
DX = ....... (positive for the search by increaseing X and negative
              for the search by decreasing X).

EMAX = ..... (must be always positive)
INDX = 0
```

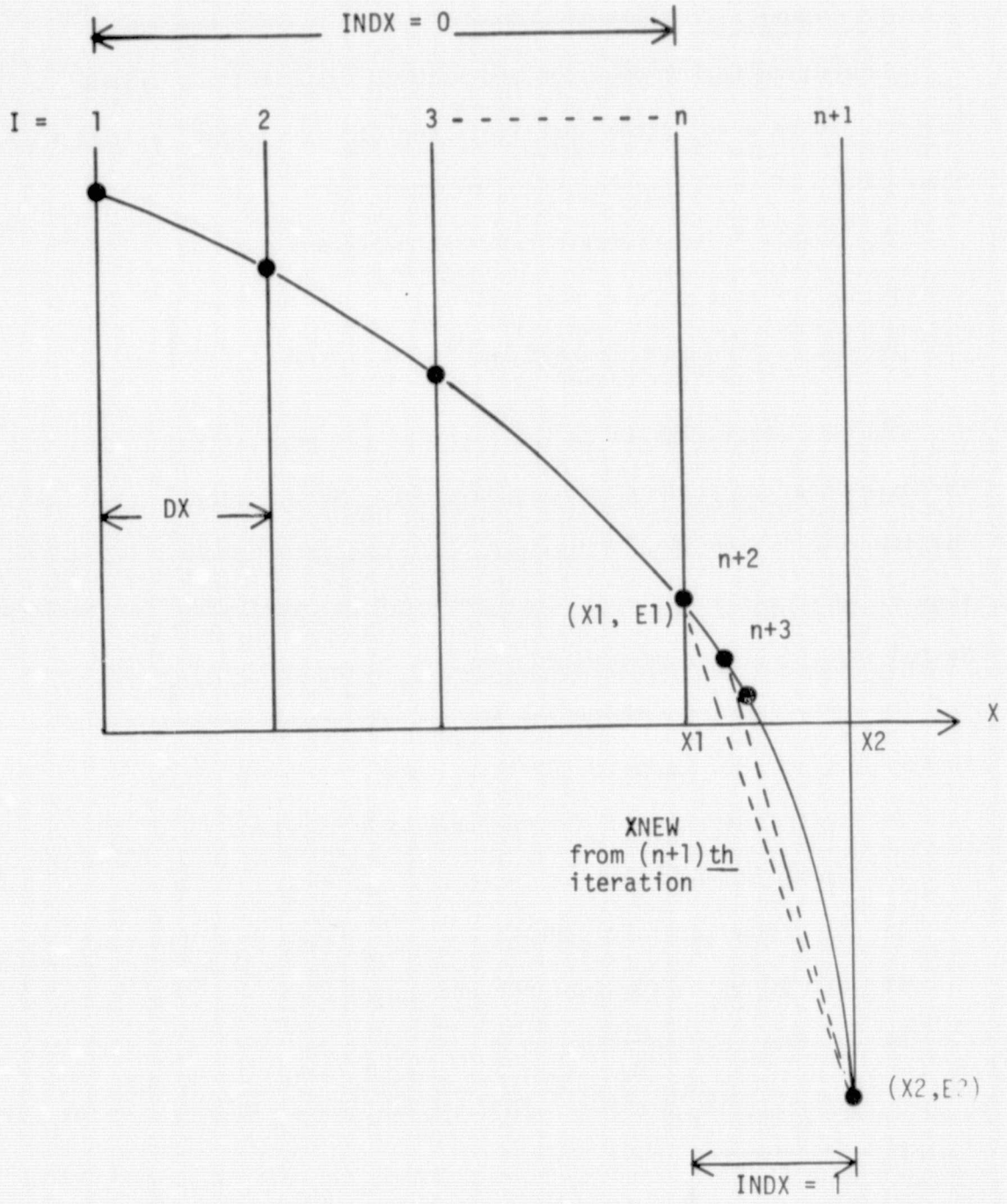


FIGURE 10. ILLUSTRATION FOR REGULA FALSI METHOD

```
      DO  000  I = 1, ΔΔ  (ΔΔ is for the maximum acceptable number of trials)
      E = function F (X)
      CALL  CRRECT (I, INDX, DX, X1, X2, X, E1, E2, E, EMAX)
      IF (INDX. EQ. 2) GO  TO   XXX
000   CONTINUE
XXX   CONTINUE
```

The initial value of X and the sign of DX are very important factor to get a successful result from the iteration. If there are multiple roots, special consideration for choosing these values is needed.

In the ordinary case it is recommended to start from the maximum or minimum possible value of the unknown X.

The inputs to the subroutine are, the number of trial (i.e. DO loop variable), I, INDX, increment DX, assumed value of X, error E and the tolerance limit EMAX. The results of previous iterations, i.e. X1 and X2 and the corresponding values E1 and E2 are additional inputs to the subroutine. However, these values are always renewed by the subroutine. The outputs from the subroutine are INDX, X1, X2, E1, E2 and the value X for next assumption.

Subroutine CRRECT can be applied to the multi-dimensional search problem. In this case, the unknowns are X_1 ..... X_m and, therefore, DX_1 .... DX_m, E_1 ..... E_m and $EMAX_1$ ..... $EMAX_m$ are needed. The main program must have the following structure:

```
      X1 = ....
      DX1 = .....
      EMAX1 = .....
      INDX1 = 0
      DO      m       I1 = 1, ΔΔ
```

```
      X2 = ....
      DX2 = ....
      EMAX2 = .....
      INDX2 = 0
      DO     m-1     I2 = 1, ΔΔ


      Xm = .....
      DXm = .....
      EMAXm = .....
      INDXm = 0
      DO     1       Im = 1, ΔΔ


      EM = Fm (X1 .... Xm)

     CALL CRRECT (Im, INDXm, DXm, Xm1, Xm2, Xm, Em1, Em2, Em, EMAXm)

  1  If (INDXm. EQ. 2) GO TO A1

  A1 CONTINUE

      E2 = F2 (X1 ..... Xm)

     CALL CRRECT (I2, INDX2, DX2, X21, X22, X2, E21, E22, E2, EMAX2)
(m-1) IF  (INDX2. EQ.2) GO TO A(m-1)
A(m-1) CONTINUE


      E1 = F1 (X1 ..... Xm)
      CALL CRRECT (I1, INDX1, DX1, X11, X12, X1, E11, E12, E1, EMAX1)
 m    IF (INDX1. EQ.1) GO TO Am
 Am   CONTINUE
```

9-6. Subroutine Design

All the design parameters are fed into the main program by calling this subroutine. The axial variation of the bed cross-section with respect to the bed height (A_t vs. z), the locations of the heat transfer tubes, the specifications of the tubes (specific heat transfer area, tube diameter, vertical pitch, horizontal pitch, tubes arrangement), solids feed locations and the fractions of feed through each nozzle, solids discharge locations and the fractions of materials discharged through each discharger nozzle and diameter of the distributor tubes and thickness of the distributor plate are the bed design parameters fed into the program.

Specific heat transfer area of the coil in a section of the bed refers to the outside surface area of the coils available for heat transfer per unit volume of the bed in that section. The tubes arrangement is coded into four divisions, and in the program it is denoted as IARR (I). If IARR (I) is(1) it refers to the vertical triangular arrangement;(2) the vertical rectangular arrangement; (3) horizontal in line arrangement, and (4) horizontal staggered arrangement.

If the specific heat transfer area is not given, but the tube diameter is given, the former can be calculated from the expression

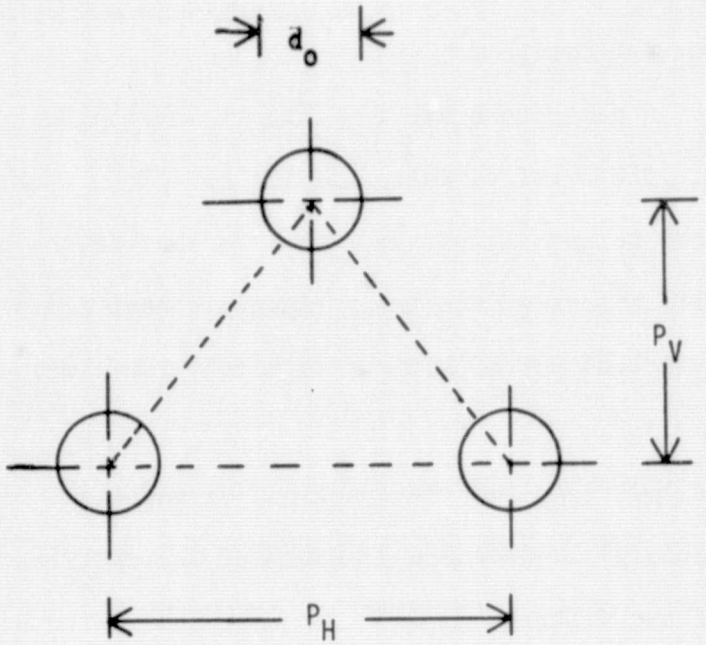
$$a_{HE} = \pi d_o/(P_H \cdot P_V)$$

where a_{HE} is the specific heat transfer area [cm^2/cm^3 (bed)].

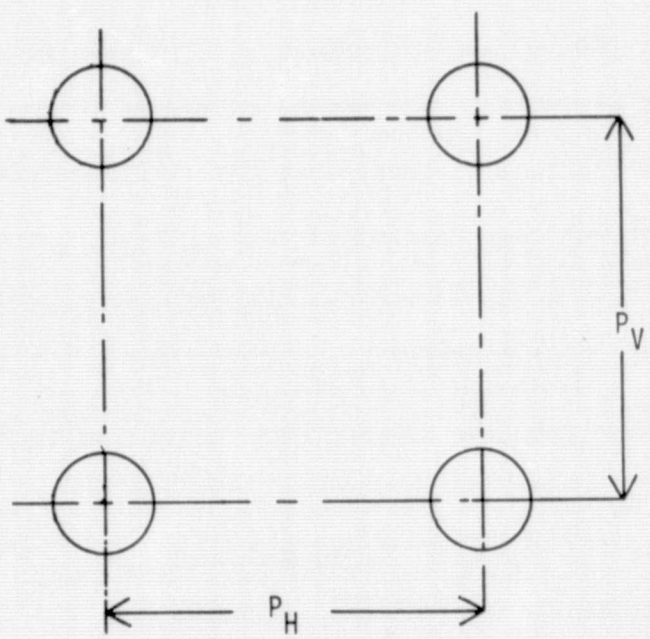
d_o is the outside diameter of cooling coils

P_H is the horizontal pitch

P_V is the vertical pitch



(a) triangular arrangement



(b) rectangular arrangement

FIGURE 11 ILLUSTRATION FOR THE ARRANGEMENT OF HORIZONTAL COOLING TUBES

For the triangular arrangement as shown in the Figure 19,

$$a_{HE} = \frac{\text{Total heat transfer area}}{\text{Total volume}}$$

$$\frac{(\frac{1}{2})\ (\ \pi\ d_o\ L)}{(\frac{1}{2})\ P_H\ P_V\ L} = \frac{\pi\ d_o}{P_H P_V}$$

For the rectangular arrangement,

$$a_{HE} = \frac{\pi\ d_o}{P_H\ P_V L} = \frac{\pi\ d_o}{P_H P_V}$$

The height of an elemental volume of bed corresponding to each compartment is chosen. The height should be so chosen that the total number of compartments is always less than the maximum dimensions allowed by the program. After having chosen the elemental volume, the specifications of the heat transfer tubes are computed for each compartment. Also, the diameter and area for each location are calculated. The differential volume of each compartment, and the effective volume excluding the volume occupied by the heat transfer tubes are computed.

Volume occupied by tubes per unit volume of bed is given as follows:

(for rectangular arrangement): $$\frac{\frac{\pi}{4} d_o^2 \cdot L}{P_H \cdot P_V \cdot L} = \frac{d_o}{4}\ a_{he}$$

(for the triangular arrangement): $$\frac{\frac{1}{2}\ (\ \frac{\pi}{4}\ d_o^2\ )\ L}{\frac{1}{2}\ P_H\ P_V} = \frac{d_o}{4}\ a_{he}$$

Tube volume fraction is, then, equal to

ε_{tube} = 1 - effective vol./total volume

For each compartment, the height, volume, effective volume, tube fraction specific heat transfer area, tube outer diameter, vertical pitch, horizontal pitch and tube arrangement are printed out in additions to the diameter and cross-sectional area of the bed for each location.

So, essentially, subroutine DESIGN takes care of the design parameters and distributes them to each compartment.

Nomenclature

Code	Model Variables	Description	Unit
A1, A2, A3, A4	-	ALPHANUMERIC CHARACTERS	-
ABED	$A_{t,i}$	Area of the FBC at each location	cm^2
AHE	a_{HE}	Specific heat transfer area	cm^2/cm^3
AHEAV	$a_{HE,i}$	Specific heat transfer area in each compartment	cm^2/cm^3
AND	n_d	Number of distributor holes	-
ATB	$A_{t,i}$	Cross-sectional area of the FBC	cm^2
DBED	$D_{t,i}$	Diameter of the FBC at each location	cm
DEAV	ΔZ	Average cell or compartment height	cm
DNZL	-	Diameter of distributor holes	cm
DTHICK	-	Distributor plate thickness	cm
DTUBE	d_o	Heat transfer tubes outside diameter	cm
DTUBEI	$d_{o,i}$	Tube outside diameter in each compartment	cm

Nomenclature (Cont'd)

Code	Model Variables	Description	Unit
DVB	-	Volume of each compartment	cm^3
DVBEFF	-	Effective volume of each compartment	cm^3
ETUBE	ϵ_{tube}	Tube volume fraction	-
FD	-	Fraction of total solids discharged at each location	-
FFC	-	Fraction of total coal fed at each location	-
FFAD	-	Fraction of total additive fed at each location	-
IARR	-	Tubes arrangement code	-
IARRNG	-	Tubes arrangement code for each compartment	-
MDIS	-	No. of solids discharge locations	-
MFEED	-	No. of solids feed locations	-
MTB	-	No. of specified locations	-
MTHE	-	No. of coil locations	-
PH	P_H	Horizontal pitch of the coils	cm
PHI	$P_{H,i}$	Horizontal pitch in each compartment	cm
PI	π	Pi	3.1415926
PV	P_V	Vertical pitch of the coils	cm
PVI	$P_{v,i}$	Vertical pitch in each compartment	cm
ZB, ZHE, ZF, ZDIS	Z_i	Height above the distributor	cm
ZDIS	Z_{dis}	Location of solids discharge	cm
ZHE	-	Locations of the bottom and top of the heat transfer coils	cm
Z(I), Z(I+1)	Z_i, Z_{i+1}	Locations of the bottom and top of the ith compartment above the distributor	cm

9-7. Function FREEFV

This function gives the terminal velocity of single particle based on the equation

$$(\rho_p - \rho_g)\, g d_p^2 / 18\,\mu \qquad Re_p \leq 0.4$$

$$4\{(\rho_p - \rho_g)g\}^2 / (225\,\rho_g\,\mu)^{1/3}\, d_p \qquad 0.4 < Re_p \leq 500$$

$$\{3.1\,(\rho_p - \rho_g)g\, d_p/\rho_g\}^{1/2} \qquad 500 < Re_p < 200{,}000$$

where the particle is assumed to be spherical. The inputs to this function sub-program are d_p, ρ_p, ρ_g and μ.

Nomenclature Code	Model variable	Description	Unit
DP	d_p	particle diameter	cm
FREEFV	u_t	terminal velocity	cm/sec
G	g	gravity acceleration	cm/sec^2
RET	Re_t	Reynolds number for u_t	-
RHOG	ρ_g	gas denisty	g/cm^3
RHOP	ρ_p	particle density	g/cm^3
UT	u_t	terminal velocity	cm/sec
VISC	μ	viscosity	g/cm·sec

9-8. Subroutine GPHASE

This subroutine is designed for solving Equations (5-2) and (5-3) or (5-4) and (5-5) simultaneously. The value of parameters in the equations and the concentrations of gas coming into the ith compartment, YBO and YEO must be fed to the subroutine. The outputs are the concentrations of gas coming out from the ith compartment, YB1 and YE1.

Equations (5-2)~(5-5) are modified into the general form and are solved and analytically to obtain YB1 and YE1. The solutions are

$$Y_{B,i} = \frac{F_{Bm,i-1}\, Y_{B,i-1} + \alpha_1 F_{Em,i-1}\, Y_{E,i-1} + GENB}{F_{Bm,i} + \alpha_1 F_{Em,i} + a_{c,i}\, \Delta V_i\, (k_{cB,i}/T_B' + \alpha_1 k_{cE,i}/T_E')p/R}$$

$$Y_{E,i} = (F_{Bm,i-1}\, Y_{E,i-1} + GENE)/D_1 + \alpha_1 Y_{B,i}$$

where

$$\alpha_1 \equiv K_{BE,i}\, (p/RT_i)\, \Delta V_i\, \varepsilon_{bi}/D_1$$

$$D_1 \equiv F_{Em,i} + \{(1 - \varepsilon_{c,i} - \varepsilon_{tube,i})\, a_{c,i}\, k_{cE,i}/T_E' + K_{BE,i}\, \varepsilon_{b,i}/T_i\}\, (p/R)\Delta V_i$$

$$T_B' \equiv (T_i + T_{cB,i})/2$$

$$T_E' \equiv (T_i + T_{cE,i})/2$$

where GENB and GENE are the generation rate of concerning species in the bubble phase and that in the emulsion phase. In the case of combustion GENB and GENE are set as zero in the main program. While for SO_2/H_2S calculation GENB and GENE represents the SO_2/H_2S formation rate which is assumed to be proportional to combustion rate.

The inputs and outputs of this subroutine are:

Inputs: AKB, AKE, AM, PAV, RG, ETUBE, EPB, EPC, AKBE, DVBB, FBMO, FEMO, FBMO, FEMO, FBM, FEM, T, TB, TE, YBO, YEO, GENB, GENE

Outputs: YB1, YE1

Nomenclature Code	Model Variable	Description	Unit
AM	a_c	specific surface area of char particle in the bed	cm^2/sec^3
AKB	k_{cB}	combustion rate constant in the bubble phase	
AKBE	K_{BE}	gas interchange coefficient	1/sec
AKE	k_{cE}	combustion rate constant in the emulsion phase	
ALF	α_1		
DC	d_c	particle diameter of char	cm
DVBB	ΔV_i	volume of ith compartment	cm^3
D1	D_1		
EPB	ε_B	volume fraction of bubbles	-
EPC	ε_c	volume fraction of bubbles and clouds	-
ETUBE	ε_{tube}	volume fraction of heat exchange tubes	-
FBM, FBMO	$F_{mB,i}$ $F_{mB,i-1}$	molar flow rates of gas in bubble phase	gmole/sec
FEM, FEMO	$F_{mE,i}$ $F_{mE,i-1}$	molar flow rates of gas in emulsion phase	gmole/sec
GENB, GENE	-	formation rate of the concerning species by other reactions	gmole/sec
P	p	pressure	atm
RG	R	gas constant	$cm^3 \cdot atm/gmole\ ^\circ K$
TB	T_{cB}	temperature of char particle in bubble cloud phase	$^\circ K$
TE	T_{cE}	temperature of char particle in emulsion phase	$^\circ K$
YBO, YB1	$Y_{B,i-1}$, Y_{Bi}	mole fraction in bubble phase	-
YEO, YE1	$Y_{E,i-1}$, Y_{Ei}	mole fraction in emulsion phase	-

9-9. Subroutine HFATI

This subroutine calculates the height corresponding to the given cross sectional area of the bed. The idea is basically the same as that of subroutine AREA. The height, z, corresponding to the area, A_t, is calculated by the formula,

$$z = z_{j-1} + \frac{(A_t/A_{j-1})^{1/2} - 1}{(A_j/A_{j-1})^{1/2} - 1} (z_j - z_{j-1})$$

The input to the subroutine is A_i. The output will be the diameter and height above the distributor corresponding to the given cross-sectional area.

This subroutine is called from subroutine HYDRO to determine the level of $u_o = u_{mf}$. This situation does not occur at the cylindrical section, but occurs at the tapered section. Therefore, we never have the situation of $A_t = A_j = A_{j-1}$, and the trouble of dividing by zero is automatically avoided. The explanation of computer codes is the same as that given in the subroutine DESIGN.

9-10. Function Height

This function sub-program calculates the height of the bed for the given effective volume of the bed. Effective volume is the total volume of the bed minus the volume occupied by the tubes. The input to the subroutine is the effective volume, and the output is the bed height. The explanation of computer codes is the same as that in the subroutine HYDRO.

9-11. Subroutine HYDRO

This subroutine essentially calculates the bubble hydrodynamics of the bed. Following is the list of equations used in this sub-program.

$$u_{mf} = \left(\frac{\mu d_p}{\rho_g}\right) \{[33.7^2 + 0.0408\, d_p^3 g\, (\rho_p - \rho_g)\rho_g/\mu^2]^{1/2} - 33.7\}$$

(Wen-Yu Equation)

$$D_{Bi} = D_{Bmax,i} - (D_{Bmax,i} - D_{B,i-1})e^{-0.3\Delta z_i/D_{t,i}}$$

$$D_{B,1} = 0.347\, [A_{t,1}(u_{o,i} - u_{mf,i})/n_d]^{0.4}$$

(Miwa's Equation)

$$D_{Bmax,i} = 0.652\, [A_{t,i}\, (u_{o,i} - u_{mf,i})]^{0.4}$$

(Mori-Wen Equation)

$$u_{B\infty,i} = 0.711 \quad gD_{B,i}$$

$$u_{BS,i} = 0.355 \quad gD_{t,i}$$

$$u_{B,i} = u_{B\infty,i} + u_{o,i} - u_{mf}$$

$$\varepsilon_{B,i} = (u_{o,i} - u_{mf})/u_{B,i}$$

$$\varepsilon_{c,i} = \varepsilon_{B,i} + \alpha_B/(\alpha_{B-1})$$

$$\alpha_B \equiv \varepsilon_{mf}\, u_{B,i}/u_{mf}$$

In this subroutine, the following method is used to determine the bed height. The bubble hydrodynamics is calculated for each elemental volume (chosen already in the SUBROUTINE DESIGN). The height of the bed is the summation of the heights of each elemental volume accounted. When the total height reaches the given expanded bed height the iteration is stopped. In case the expanded bed height is not given, but the height at the minimum fluidization is given, then the volume of bed corresponding to the minimum fluidization height is calculated, and used as the criterion for determining the expanded bed height.

The program is also designed to take into consideration the formation of a fixed bed section over the fluidized bed section.

First, the volume of bed at minimum fluidization is evaluated in the case when bed height is not given. Subroutine HYDRO is called inside the temperature iteration loop till the convergency is obtained. Depending upon the temperature of the bed, the hydrodynamic parameters and the bed height are determined. If more number of compartments are needed than for the earlier iteration, then for the excess number of compartments the temperature, carbon concentration, bubble and emulsion phase oxygen concentrations are taken as those corresponding to the last compartment in the earlier iteration.

Knowing the temperature, the density and viscosity of the gas, minimum fluidizing velocity and superficial velocity are calculated for each compartment using the equations given earlier. The bubble diameter above the distributor is calculated knowing the u_{mf}, u_o and number of distributor holes on the gird. u_o is compared with u_{mf}. Since the corss-sectional area of the bed increases as the height increases, the superficial velocity decreases. If at any instance, u_o is less than or equal to u_{mf}, it means the presence of a fixed bed section. Then different calculations are to be performed for the fixed bed section. Four different cases are analyzed:

1. Expanded bed height given, no fixed bed section:

For each compartment, the bubble hydrodynamics is calculated. u_{mf}, u_o and D_b are calculated at the bottom and top of each compartment. The average value of these variables are used to compute the bubble size, bubble fraction, and cloud fraction for each compartment. The iteration is performed till the height of the last compartment reaches the expanded bed height.

2. Expanded bed height given, fixed bed section present:

The bubble hydrodynamics is calculated for each compartment. As the height increases, u_o is decreasing, and when it is smaller than u_{mf}, cirtical height has been reached. The critical height corresponds to the height of the bed above the distributor at which the fixed bed section starts. At this location u_o is equal to u_{mf}. Above this height, there is no fluidization, and the bubble fraction is zero. The presence of critical height and fixed bed are tagged by the symbols ICR and IFBC. If they are greater than zero, critical height and fixed bed section are present.

For each compartment the volume of solids and the effective height of the solids are calculated. Sum of these heights would be the height of the bed at minimum fluidization.

3. Height at minimum fluidization given, no fixed bed section:

Instead of basing the convergency criterion directly on the minimum fluidization height, the volume of the bed at minimum fluidization is used. This would help avoid any inaccuracy involved in the calculation of the effective solids height in each compartment. Also, it would be easy to determine the total bed height when the effective volume of solids in the bed equals the volume at the minimum fluidization. The sums of each compartment volume, effective volume of solids (excluding the bubbles and tubes) and the effective height of solids are computed. The iteration continues till the effective solids volume equals to volume at minimum fluidization. If it exceeds V_{mf}, the excess solid volume corrected for the expansion and tube fraction is subtracted from the effective

(excluding tube volume) volume of the bed to give the correct volume of the bed. From this effective volume of the bed, the expanded bed height is calculated.

4. Height at minimum fluidization given, fixed bed section present:

As before, computations are performed till u_o becomes smaller than u_{mf}. In the fixed bed section, the bubble fraction is zero. Fixed bed is equivalent to the condition of minimum fluidization. Total volume of the bed is the sum of the effective volume of the fluidized bed section and the difference in the minimum fluidization volume and the volume of solids in the fluidized section. Total height of the bed is computed from the total volume of the bed.

Nomenclature
(SUBROUTINE HFAI, HYDRO, AND VOLUME)

Code	Model Variables	Description	Unit
AHEAV	a_{he}	Specific heat transfer area for each compartment	cm^2/cm^3
AND	n_d	No. of distributor holes	-
AT	$A_{t,i}$	Cross-sectional area of the bed at each location	cm^2
DB	D_B	Bubble diameter	cm
DBAV	$D_{B,av}$	Average bubble size of each compartment	cm
DBED	$D_{t,i}$	Diameter of the FBC	cm
DBMAX	D_{Bm}	Maximum bubble size	cm
DPB	d_p	Average particle diameter in the bed	cm
DTUBE, DTUBEI	d_o	Diameter of heat transfer coils	cm
DVB, DVBB	ΔV_i	Volume of each compartment	cm^3
DVBBEF, DVBEFF	-	Effective volume of each compartment (excluding tubes)	cm^3
EMF	ε_{mf}	Void fraction at minimum fluidization	-
EPB	ε_b	Bubble fraction	-
EPC	ε_c	Cloud fraction	-
ETUBE	$\varepsilon_{tube,i}$	Tube volume fraction in each compartment	-
FMF	F_{mf}	Molar flow rate of inlet gas	gmol/sec
FMO	F_m	Total molar flow rate of gas	-
G	g	Acceleration due to gravity	cm/sec^2
HCR	-	Critical bed height ($u_o = u_{mf}$)	cm
H(I), H(I+1)	h_i, h_{i+1}	Height of the bottom and top of each compartment above the distributor	cm
HLF	L_f	Height of the fluidized bed (expanded)	cm
HLMF	L_{mf}	Height of minimum fluidization	cm
ICR	-	Indicator for critical bed height	-

ORIGINAL PAGE IS
OF POOR QUALITY

Nomenclature (Cont.)

Code	Model Variables	Description	Unit
IFBC	-	Indicator for the fixed bed section	
ITUBE, IARRNG	-	Tube arrangement code for each compartment	
M	-	Total number of compartments in the expanded bed	-
M1	-	Total number of locations compartment	
MGAS	M_g	Molecular weight of gas	g/gmol
PAV	P_{av}	Average pressure of the FBC	atm
PHI	PH_i	Horizontal pitch of the coils for each compartment	cm
RG	R	Gas constant	$atm \cdot cm^3/gmol \cdot K$
RHOCAD	ρ_ℓ	Density of calcined additives	g/cm^3
RHOGAS	ρ_g	Density of fluidizing gas	g/cm^3
SOLVOL	-	Volume of bed, total	cm^3
SUM	-	Height of solids alone (no bubble), total	cm^3
SUMEFF	-	Volume of solids alone, total	cm^3
SUMV		effective volume of the bed	cm^3
T	T	Temperature of the bed	°K
UB	u_b	Bubble velocity	cm/sec
UBR	u_{br}	Bubble rising velocity	cm/sec
UBS	u_{bs}	Slug velocity	cm/sec
UF	u_f	Superficial gas velocity at the inlet pressure	cm/sec
UO	u_o	Superficial gas velocity	cm/sec
UMF	u_{mf}	Minimum fluidization velocity	cm/sec
VMF	-	Volume of bed at minimum fluidization	cm^3
X	x	Carbon concentration	wt. fraction
YB	-	Bubble phase oxygen concentration	mole fraction
YE	-	Emulsion phase oxygen concentration	mole fraction

9-12. Subroutine POP

The calculations of the size distribution density function $\phi(y_i)$, second and third moments of ϕ and the average value of elutriation constant are performed in this subroutine by the use of Equations (4-5)~(4-8).

The major inputs to the subroutine are BC, BC1, THET and L. The major outputs from the subroutine are PHI (I), (I=1, L), ALAMA, ALAMV and EC. Numerical integrations are performed by trapezoidal method.

Nomenclature Code	Model Variable	Description	Unit
AKE (I)	$K^*(y_i)$	elutriation rate constant	$g \cdot cm^2/sec$
AKEI(I)		$\int_0^{y_i} (K^*/\lambda_c)\, dy$ defined in the main program	$g \cdot cm^2/sec$
ALAMA		$\int_0^1 \phi\, y^2\, dy$	-
ALAM(I)	$\lambda_c(y_i)$	reactivity of coal for $y = y_i$	-
ALAMI(I)		$\int_0^{y_i} (1/\lambda_c(y))dy$ calculated in the main program	-
ALAMV	ψ_v	$\int_0^1 \phi\, y^3\, dy$	-
A, A11, A12, A21, A22, A31, A32		dummy variables	cm^2
AT		bed cross section	
BC	B_{cw}	defined by Eq. (4-9)	-
BC1	B_{cf}	defined by Eq. (4-10)	-
CC	C_c	defined by Eq. (4-8)	-
DY(i)		increment of y; $y_i - y_{i-1}$	-
EC		$(A_t/W_b) < K^* y^3 >$	-
L		total number of grids on y-coordinate	-

(Cont.)

Nomenclature Code	Model Variable	Description	Unit
PHIF(I)	$\phi(y_i)$	size distribution density function	-
SUM1, SUM2, SUM3		dummy variables for integration	-
THET	Θ	mean residence time of limestone	sec
WBED	W_b	total bed weight	g
X1, X2		dummy variables	
Y(I)	y_i	dimensionless char size	-
YY(I)	$Y(y_i)$	defined by Eq. (4-6)	-
ZF(I)	$Z_f(y_i)$	defined by Eq. (4-7)	-

9-13. Function Volume

This function sub-program calculates the effective volume of the bed for the given height above the distributor.

The input to the subroutine is the height and the output is the effective volume. Any division by a small number (zero) causing exponential underflow or overflow is taken care of by the IF statement preceding the DO loop.

If (ZZ - FLOAT(N-1)* DZAV · GT · 0.01 * DZAV) N = N+1. This statement avoids the computation for infinitesmal difference in height (ZZ - FLOAT(N) * DZAV) that would arise because of the hexadecimal storage of numbers. The explanation of computer codes is the same as that given in the subroutine HYDRO.

SECTION X

COMPUTED RESULTS

The performance of the model (Level I and II) is examined for a set of operating conditions based on the data reported by the National Coal Board, England. Combustion efficiency, axial bed temperature profile, carbon concentration in the bed, oxygen and SO_2 concentrations in the bubble phase and emulsion phases, bubble diameter and sulfur dioxide cpature efficiency are the key variables computed in the models to evaluate the FBC performance. The effect of bed geometry, bed temperature, excess air, molar ratio of calcium to sulfur in the feed and the presence of internals on these variables is examined. These results are presented in Figures 12 and 18. The results depict the trends that can be expected in the range of operating conditions selected for simulation. The accuracy of the results cannot be quantitatively assessed at this point due to lack of experimental data on the performance parameters. However, from a mechanistic point of view the models can simulate experimental performance of a FBC quite closely taking into consideration the various physical and chemical phenomena occurring in the bed.

Figure 12 presents the various profiles obtained using the Level II model for a uniform (non-tapered) bed. The calculated combustion efficiency is about 93 percent while the remaining 7 percent accounts for carbon loss largely due to elutriation. The carbon loss in the solids withdrawn is negligible (0.2 percent of carbon fed) since the carbon concentration in the bed and the amount of solids withdrawn are small.

Table 9 shows the comparison of the calculated results with experimental data. The agreement between predicted results and the experimental data are satisfactory.

Y_B - mole fraction oxygen in bubble phase

Y_E - mole fraction oxygen in emulsion phase

ELUTRIATION =7%

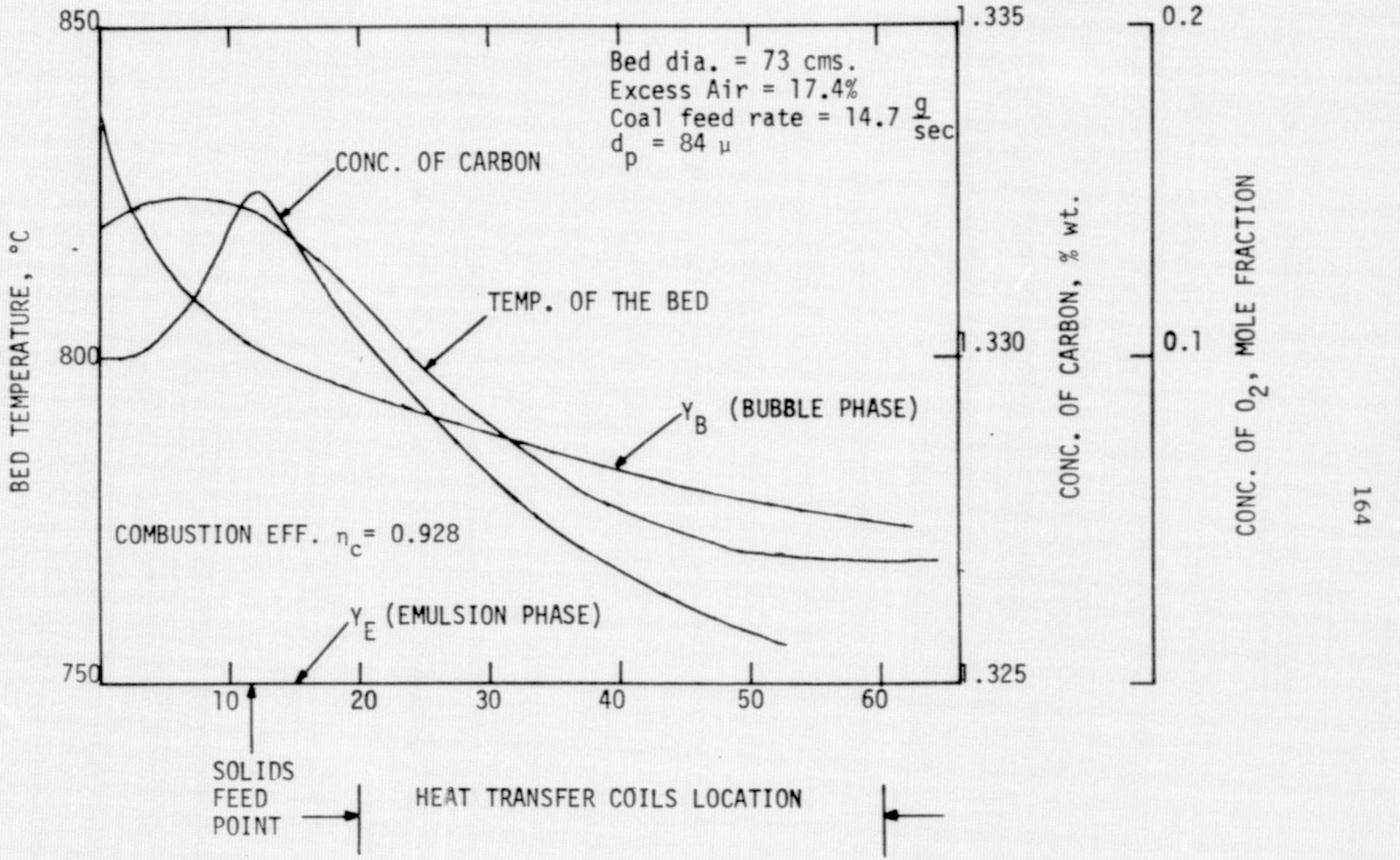


FIGURE 12. TEMPERATURE PROFILE, CARBON CONCENTRATION IN THE BED AND O_2 CONCENTRATION PROFILES ALONG THE BED HEIGHT FOR THE UNIFORM BED (LEVEL II MODEL).

TABLE 9 COMPARISON OF CALCULATED RESULTS WITH EXPERIMENTAL DATA FROM NATIONAL COAL BOARD.

Variable	NCB DATA	COMPUTED RESULTS
Combustion Efficiency	92.8%	92.84%
Average Bed Temp.	1470°F (799°C)	1457°F (791.5°C)
Outlet gas concentration		
Oxygen	4.3% v	4.6% v
Carbon dioxide	13.9% v	16.36% v
Sulfur dioxide	400 ppm	374 ppm
Sulfur capture efficiency	83%	81.69%

Figure 13 shows the profiles of temperature for the tapered bed. The combustion efficiency is 99+ percent. The high combustion efficiency estimated is largely due to negligible elutriation loss from the bed because of the presence of a fixed bed section above the fluidized bed section. The large temperature gradient observed in Figure 13, is because of poor solids mixing. In order to provide a fixed bed portion in the tapered bed u_o/u_{mf} is selected to be around 2.0 in the fluidized bed section which is considerably less than the ratio in the non-tapered bed.

Figure 14 shows the SO_2 concentration profile for the uniform bed. The SO_2 concentration in the emulsion phase is lower than in the bubble phase due to absorption of SO_2 by the calcined limestone in the emulsion phase. Bubble phase SO_2 concentration increases because of higher combustion rate (higher SO_2 release rate) in the bubble phase. Concentration of carbon in the cloud-wake phase of the bubble is higher than that in the emulsion phase, becuase the fines char particles are preferentially carried by the bubbles. The SO_2 capture efficiency is around 82 percent which compares favorably with 83% reported by the National Coal Board.

Figure 15 shows an increase in the sulfur capture efficiency with increase in [Ca/S] ratio in the feed. In order to obtain an environmentally acceptable level of SO_2 in the flue gas, the molar ratio of calcium to sulfur should be at least twice the stoichiometric amount. Test data reported by NCB for similar operating conditions are shown in the Figure 15.

The effect of bed temperatures on the sulfur capture efficiency (η_s) is shown in Figure 16. The decrease is η_s at higher temperatures is due to decrease in the reactivity of the calcined limestone particles. The reactivity is strongly dependent on the pore structure. At high temperatures, the

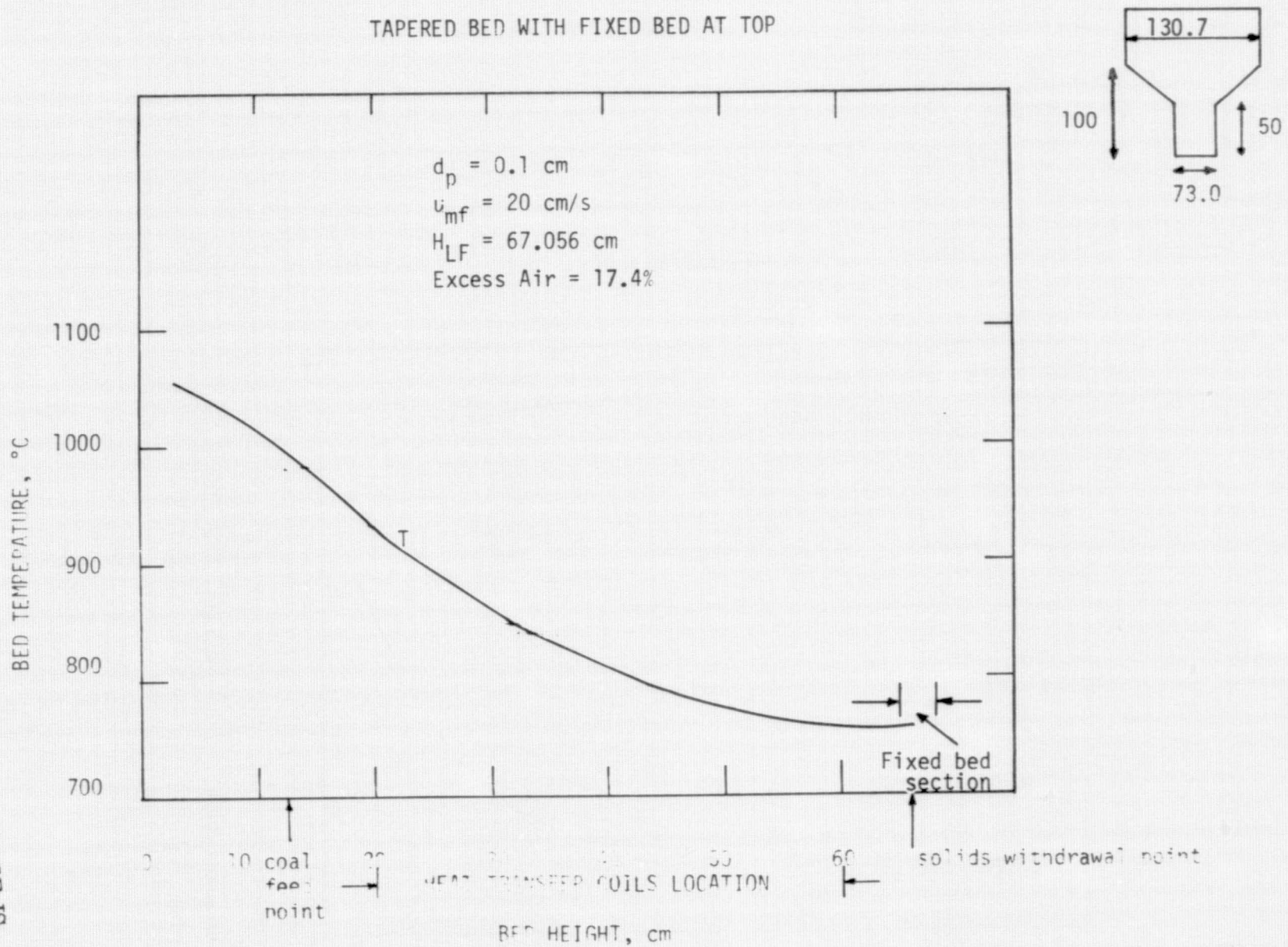


FIGURE 13. TEMPERATURE PROFILE IN THE TAPERED BED (LEVEL II MODEL).

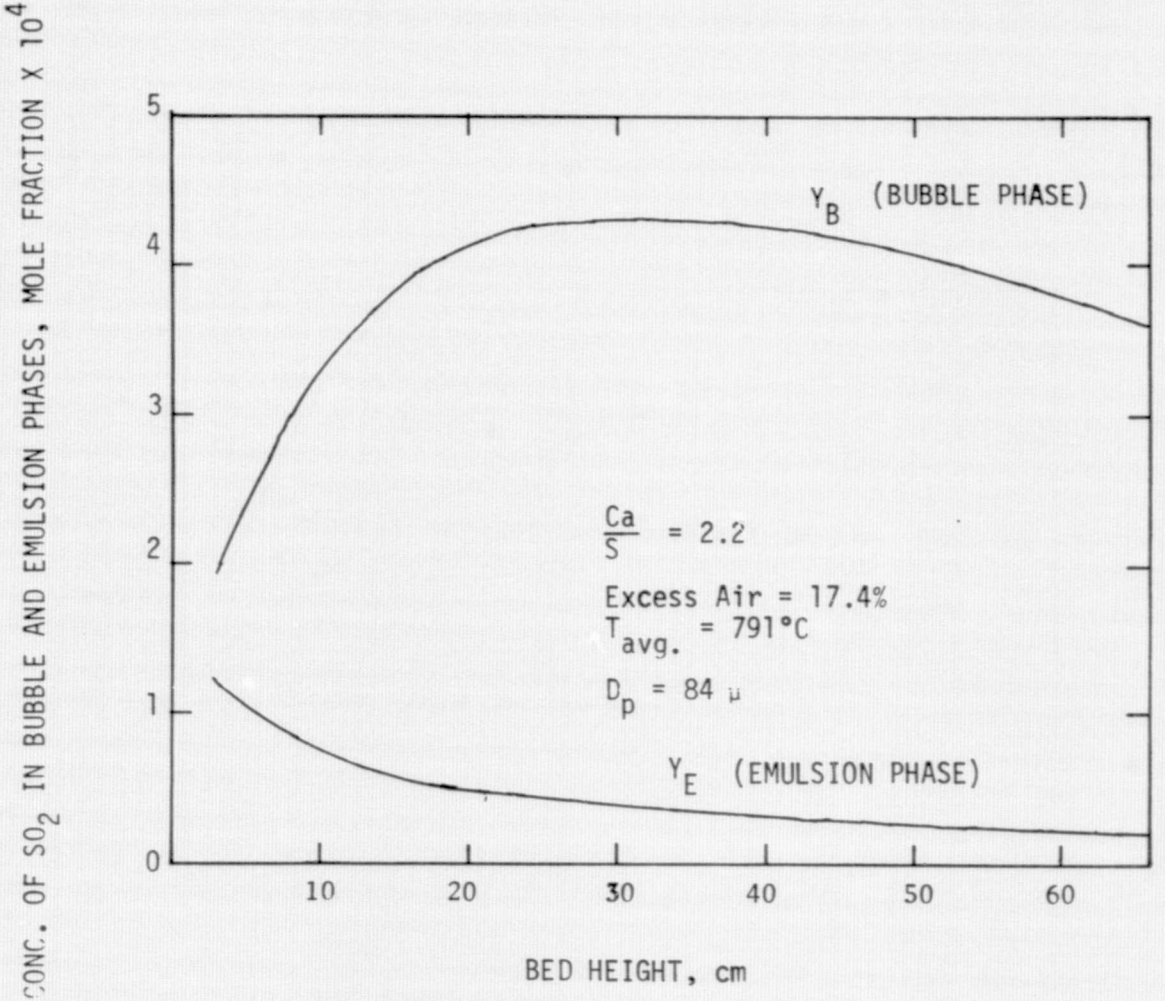


FIGURE 14. CONCENTRATION PROFILE OF SO_2 IN THE UNIFORM BED.

LEVEL II

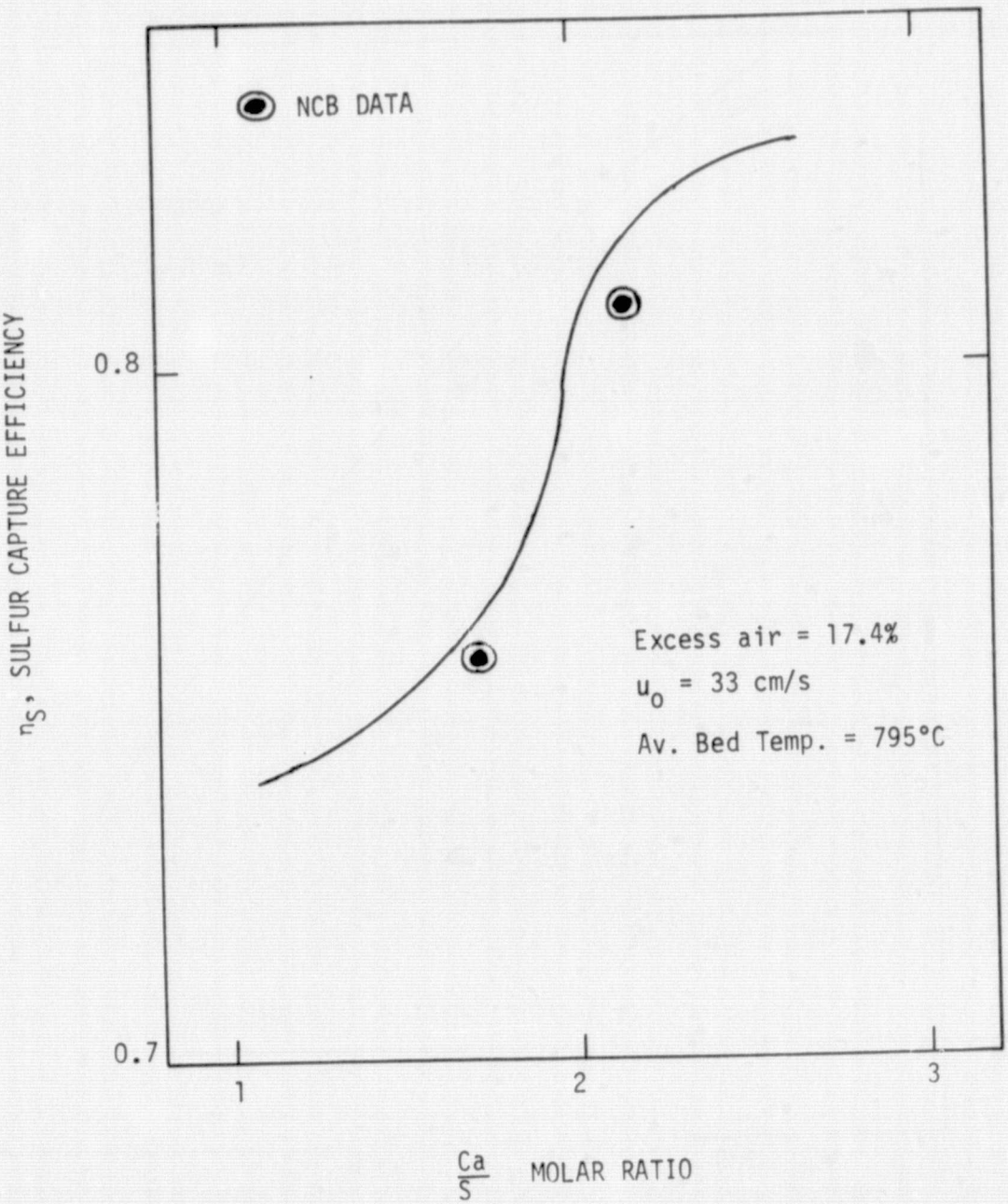


FIGURE 15. EFFECT OF CALCIUM TO SULFUR RATIO IN FEED ON SULFUR CAPTURE EFFICIENCY.

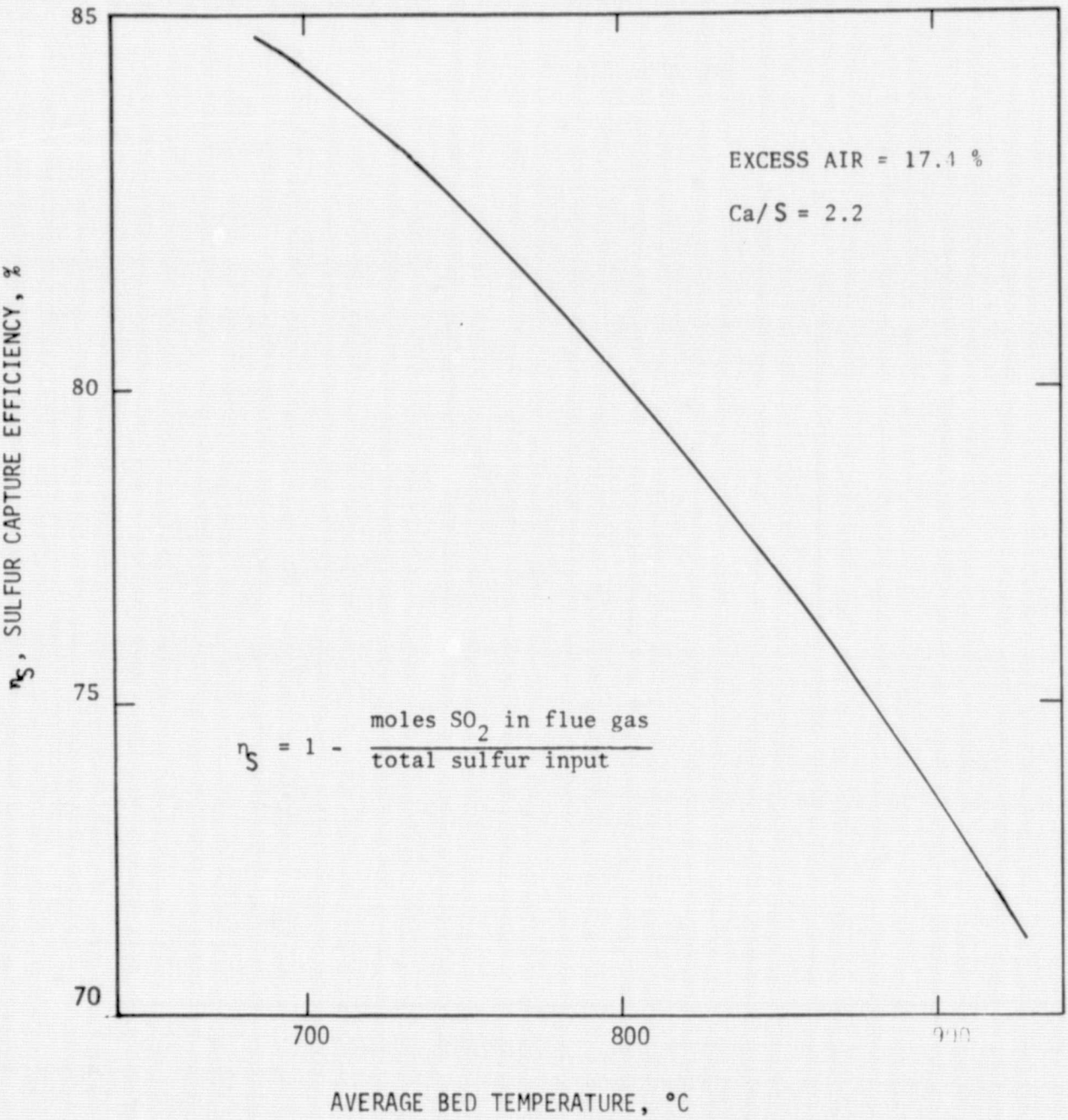


FIGURE 16. EFFECT OF BED TEMPERATURE ON SULFUR CAPTURE EFFICIENCY.

porosity decreases due to formation of very dense sulfate layer resulting in lower reactivity of the limestone particles. Although the trend observed in Figure 16 indicates that lower temperatures are suited for higher sulfur capture efficiency, from the standpoint of combustion efficiency it is not economical to operate at low temperatures. Furthermore, the calcination of limestone particles cannot occur at temperatures below 650°C.

In a bubbling fluidized bed model, the bubble diameter is one of the important parameters which affects the performance of the bed. It is well known that the bubble size increases as the gas flow rate is increased and also increases along the bed height above the distributor. Bubble diameter is also affected by bed geometry and presence of coils in the bed. Figure 17 is a plot of bubble diameter versus bed height for a uniform bed with and without coils. The coils hinder bubble growth and cause the large bubbles to break resulting in smaller bubble diameters. This effect is observed in beds with horizontal coils. In beds where vertical coils are present the effect may not be quite the same.

The Level I model is used to calculate the combustion efficiency (η_c) as a function of excess air. The model calculates the elutriation loss from experimental correlations. Figure 18 shows the combustion efficiency and carbon concentration in the bed as a function of excess air. The initial increase in η_c is due to a higher oxygen concentration in the bed. However, at higher values of excess air, the elutriation loss will become greater and offset the increase in η_c due to higher oxygen concentration. The combustion efficiency at extremely large excess air ratio will be expected to drop.

LEVEL II

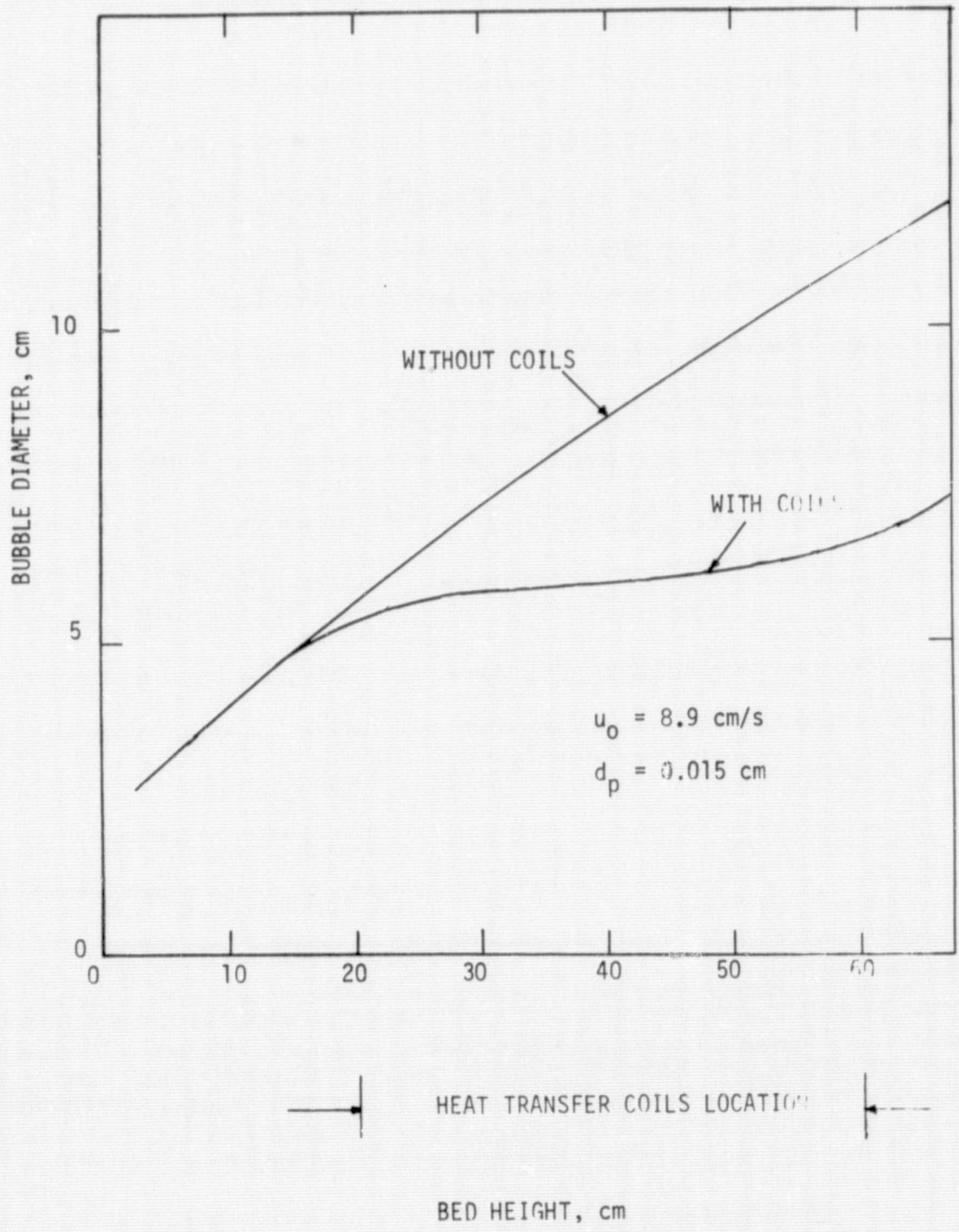


FIGURE 17. BUBBLE DIAMETER ALONG THE BED HEIGHT FOR THE UNIFORM BED.

LEVEL I

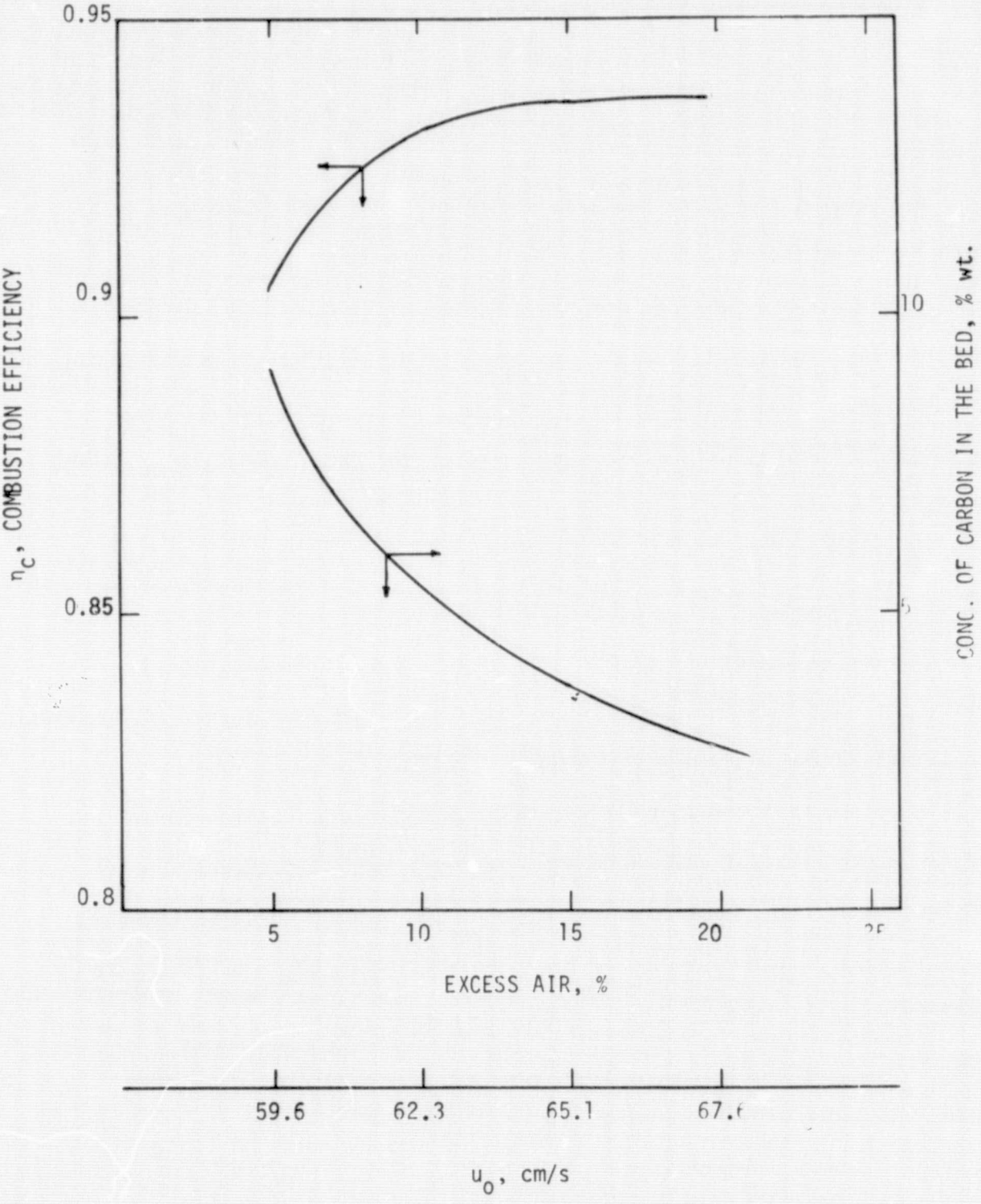


FIGURE 18. EFFECT OF EXCESS AIR ON COMBUSTION EFFICIENCY IN THE UNIFORM BED.

SECTION XI

CONCLUSIONS AND RECOMMENDATIONS

The general fluidized bed coal combustor (FBC) model developed in this study is a valuable tool in predicting the performance of the combustor under various operating conditions and bed geometry. The simulation results indicate that the model predicts the combustion efficiency, bed temperature profile, oxygen and sulfur dioxide concentration profiles and sulfur retention efficiency within the range of observed data from pilot scale FBC units.

Due to the complexities of the various physical and chemical processes occurring in the bed, the general FBC model is divided into various levels with increasing degree of complexity in each level. This approach is convenient both from the standpoint of conceptualization and ease of computation. Two levels of the FBC model are described in this study.

In the Level I model, the char particle size distribution, shrinkage, and the elutriation of char particles are considered in deriving the basic FBC equations. The population balance approach is used to calculate the particle size distribution in the bed. Solids in the bed are assumed to be completely mixed. The gas phase model is formulated so that either plug flow or complete mixing in the gas phase can be used. Temperature variations, bubble hydrodynamics and SO_2-limestone reactions are not considered in Level I model. Elutriation of char particles is calculated using available correlations in the literature for the elutriation rate constant.

In Level II model, the single phase backflow compartment model is used to describe the solids mixing in the bed. For the gas phase, a modified

version of the Bubble Assemblage Model is employed. Axial variations of temperature, carbon concentration in the bed, combustion efficiency, oxygen concentration in the bubble phase and emulsion phase are calculated in the model. Also included in the model is the SO_2-limestone reactions which are used to calculate the sulfur retention efficiency and the SO_2 concentration in the flue gas.

Level I model is derived for a uniform (non-tapered) bed whereas Level II model is applicable for both tapered and non-tapered bed geometry. When used in combination with Level I model, Level II model can cover a wide range of FBC operating conditions.

The FBC models developed in this study have been demonstrated that they are capable of predicting the performance of experimental FBC units within a reasonable level of accuracy. However, the models are by no means complete and efforts to seek further improvements are being undertaken. In the absence of experimental data on the various parameters, the model has not been refined sufficiently. The accuracy and sensitivity of the various parameters have not been tested in depth. The user is therefore cautioned against interpreting the results beyond the range of applicability specified in the model equations.

Several simplifying assumptions have been made at various stages of model development to overcome computational difficulties. These assumptions should be re-examined as more data from experimental units become available. Furthermore, the correlations available in the literature for estimating bubble hydrodynamic quantities, elutriation rate constant, etc. need considerable refinement. For example, the correlations available to estimate the bubble diameter and bubble rising velocity do not take into consideration the presence

of cooling coils in the bed. Modifications of the empirical correlations to extend the range of applicability to these operating conditions could improve the validity of the model predictions. Extreme discrepencies between prediction of the elutriation rate constant from available correlations exist. It is not unusual for these correlations to give predictions differing by several orders of magnitude. Improvements in accuracy of experimental data is needed to extend the range of applicability of the model.

Correlations of elutriation rates which take into account the effect of shrinkage of char particles, presence of fine fly ash particles, fluidizing gas velocity, temperature and other hydrodynamic variables, need to be included in the model to accurately estimate the elutriation loss from the bed. Correlations presently used in the model are not satisfactory.

The devolatilization of coal as it is fed into the bed has not been considered in the computations. The devolatilized products can cause increase in temperatures or form a reducing zone near the feed point. This effect should be considered in detail.

A major effort is needed in refining the SO_2-limestone reaction kinetics. The reactivity of the calcined limestone depends on the temperature, particle diameter and the conversion in the bed. Presently available rate expressions do not consider all these variables. These variables have to be analyzed in detail to improve the rate expressions used in the model.

LITERATURE CITED

1. Avedesian, M. M. and J. F. Davidson, Trans. Instn. Chem. Engrs. 51, 121 (1973).

2. Basov, V. A., V. I. Mankhevka, T. Kh. Melik-Akhnazaro and D. I. Orachko, Int. Chem. Eng. 9, 263 (1969).

3. Baumgarten, P. K. and R. L. Pigford, A.I.Ch.E. Journal 6, 115 (1960).

4. Bethell, F. V. and D. N. Gill, B. B. Morgan, Fuel 52, 121 (1973).

5. Borgwardt, R. H., Environmental Sci. and Tech. 4, 59, (1970).

6. Borgwardt, R. H. and R. D. Harvey, Environmental Sci. Tech. 6, 350 (1972).

7. Botton, R., Symp. on Fluid Particle and Fluidization, Part II, A.I.Ch.E. Annual Meeting, Los Angeles, Dec. 1, 1968.

8. Chiba, T., K. Terashima and H. Kobayashi, J. Chem. Engrs. Japan 6, 78 (1973).

9. Davidson, J. F., R. C. Paul, J. S. Smith, and H. A. Duxbury, Trans. Inst. Chem. Engrs. 37, 323 (1959).

10. Donsi, G., L. Massimilla, S. Cresctelli and G. Volpicelli, Powder Tech. Vol. 6, 217 (1972).

11. Field, M. A., D. W. Gill, B. B. Morgan, and P. G. W. Hawksley, "Combustion of Pulverized Coal" BCURA, (1967).

12. Fryer, C. and O. E. Potter, Fluidization Technology, McGraw Hill, Vol. 1, 171 (1975).

13. Gabor, J. D., C.E.P. Symp. 62 Ser. No. 7, 5,(1966).

14. Geldart, D., Powder Tech. Vol. 4, 41 (1970/1971).

15. Harrison, D. and L. S. Leung, Trans. Ins. Chem. Engrs. 40, 146 (1962).

16. Horio, M. and C. Y. Wen, Proc. of International Fluidization Conference Pacific Grove, Ca. (1975a), "Fluidization Technology", Vol. II, p. 289, McGraw Hill, (1976), paper presented at 80th National Meeting, Los Angeles CA, Dec. (1975b).

17. Ishida, M. and C. Y. Wen, A.I.Ch.E. Symp. Ser. 69, No. 128, 1 (1973).

18. Kato, T. and C. Y. Wen, Chem. Eng. Sci., 24, 1351 (1969).

19. Kobayashi, H., F. Arai and T. Sunagawa, Chem. Engrs. (Japan), 31, 239 (1967).

20. Kobayashi, H., Chiba, T. and K. Ihora, Proc. of 36th Annual Meeting of Society of Chem. Engrs. Japan, 36, 2 (1971).

21. Kunii, D., Y. Yoshida and I. Hiraki Proc. of International Symp. on Fluidization, Netherlands University Press, 243, 1967.

22. Large, J. F., Y. Martinie and M. A. Bergougnou, paper presented at International Powder and Bulk Solid Handling and Processing Conference Mag., 11-13, Rosemont, 1976.

23. Leva, M. and C. Y. Wen, "Fluidization" by Davidson and Harrison, p. 647, Academic Press, 1971.

24. Levenspiel, O., D. Kunii and T. Fitzgerald, Powder Tech. 2, 87, (1968/1969).

25. Miwa, K., S. Mori, T. Kato and I. Muchi, Chem. Eng., Tokyo, 35, 777 (1971).

26. Mori, S. and C. Y. Wen, A.I.Ch.E. Journal, 21, 109, (1975).

27. Mori, S. and C. Y. Wen, paper presented at International Fluidization Conference, Pacific Grove, III-5, (1975).

28. Park, W. H., W. K. Kang, C. E. Capes and G. L. Osberg, Chem. Eng. Sci., 24, 851, (1969).

29. Rowe, P. N. and B. A. Partridge, Proc. Symp. Interation between Fluids and Particles, P. A. Rotenburg (ed), Inst. Chem. Engrs., 135, June (1962), Trans, Ins. Chem. Engrs. 43, T 157 (1965).

30. Rowe, P. N. and D. J. Everett, Trans. Inst. Chem. Eng. 50, 55, (1972).

31. Rowe, P. N., "Fluidization" by Davidson and Harrison, Academic Press, p. 142, (1971), Chem. Eng. Sci., 31, 285, (1976).

32. Rowe, P. N. and R. Matsuno, Chem. Eng. Sci., 26, 923 (1971).

33. Ruth, L. A., "Fluidization Technology", ed. by D. L. Kearins, Vol. II, p. 321, McGraw Hill (1976).

34. Sutherland, K. S., Trans. Inst. Chem. Engrs., 39, 188, (1961).

35. Tanaka, I. and H. Shinohara, J. Chem. Engrs. of Japan, 5, 51, (1972).

36. Toei, R., R. Matsuno and Y. Nagai, Mem. Fac. Eng., Kyoto Univ. 28, 428, (1966).

37. Toei, R., R. Matsuno, H. Kojima, Y. Nagai and K. Nakagawa, Chem. Eng. Tokyo, 29, 851, (1965).

38. Tomita, M. and T. Adachi, Proc. 36th Annual Meeting of Soc. Chem. Engrs., Japan II, pp. 169, Tokyo (1971).

39. Uno, S. and R. C. Kintner, A.I.Ch.E. Journal 2, 420, (1956).

40. Wen, C. Y. and R. F. Hashinger, A.I.Ch.E. Journal, 6, 220, (1960).

41. Wen, C. Y. and M. Ishida, Environmental Sci. Tech. 7, 703, (1973).

42. Whitehead, A. B., A.I.Ch.E. Meeting, Detroit, "Fluidization"ed. by Davidson and Harrison, Academic Press Chap. 19, (1973).

43. Woollard, I. N. M. and O. E. Potter, A.I.Ch.E. Journal, 14, 388 (1968).

44. Yagi, S. and T. Aochi, paper presented at the Soc. of Chem. Engrs. (Japan), Fall Meeting, (1955).

45. Yasui, G., and L. N. Johanson, A.I.Ch.E. 4, 445, (1958).

46. Zenz, F. A. and N. A. Weil, A.I.Ch.E. Journal, 4, 472, (1958).

NOMENCLATURE

(except Appendix II)

A	matrix defined by Eq. (3-4)	-
A_{HE}	total heat exchange area	cm^2
A_t	cross sectional area of bed	cm^2
a_{HE}	specific heat transfer area based on outside area of tubes and volume of bed minus internals	cm^2/cm^3(bed)
B	matrix defined by Eq. (3-5)	-
B_{cf}	$B_{cw} n_{cf}/n_{cw}$	-
B_{cw}	$d_{cm}\rho_{ch} X_C/(2M_C \Theta \overline{k_{c0} C_{O2}})$	-
B_ℓ	constant defined by Eq. (3-64)	-
C_c	constant defined by Eq. (4-8)	-
C_i	concentration of gaseous species i	mol/cm^3
c_{gm}	molar heat capacity of gas	cal/gmol·°K
c_{gmf}	molar heat capacity of gas at feed temperature	cal/gmol·°K
c_s	heat capacity of solid	cal/g·°K
c_{sf}	heat capacity of solid at feed temperature	cal/g·°K
D_B	bubble size	cm
D_{Bo}	initial bubble size	cm
D_{Bm}	maximum bubble size	cm
D_t	bed diameter	
d_A	ash particle size	cm
d_c	particle diameter of coal or char	cm
d_{cm}	maximum diameter of coal particles	cm
d_ℓ	particle diameter of additives (limestone or dolomite)	cm
EAR	excess air ratio	-

E_z	axial dispersion constant of solids	cm^2/sec
F_{Bm}	molar flow rate of gas through bubble phase	gmol/sec
F_{Em}	molar flow rate of gas through emulsion phase	gmol/sec
F_m	total molar flow rate of gas	gmol/sec
F_{mf}	molar flow rate of inlet gas	gmol/sec
F_{mth}	theoretical feed rate of inlet gas	gmol/sec
F_r	Froude number	-
f_ℓ	conversion of limestone	-
f_W	volume fraction of wake to bubble proper	-
f'_W	volume fraction of wake to bubble proper effective for reaction	-
g	acceleration due to gravity	cm/sec^2
h_j	maximum height of jets above distributor	cm
I_t	total number of cells	-
K^*	specific elutriation rate constant	$g/cm^2 \cdot sec$
$K_{BE,i}$	gas exchange coefficient in ith cell	1/sec
$K_{mBE,i}$	modified gas exchange coefficient (Eq.3-59)	$1/sec \cdot cm^3$
$K_{sBE,i}$	solids exchange coefficient in ith cell	1/sec
k_c	overall surface reaction rate constant for coal combustion	cm/sec
k_{cf}	film diffusion coefficient	cm/sec
k_{cR}	chemical reaction constant	cm/sec
k_{c0}	value of k_c for the maximum particle size	cm/sec
k_i	overall surface reaction rate constant of reaction i, (i=3,4 or 5)	cm/sec
k_{vi}	overall volume reaction rate constant of reaction i, (i=1 or 2)	1/sec
L_f	fluidized bed height	cm
L_{mf}	minimum fluidization height	cm

M_i	atomic or molecular weight of species i	g/mol
N_D	number of holes in distributor	
N_A	number of ash particles held up in the bed	-
N_c	number of char particles held up in the bed	-
N_{ci}	number of char particles held up in ith cell	-
N_ℓ	number of adsorbent particles held up in the bed	-
$\vec{n}$	number mass velocity vector of char particles	$1/cm^2 \cdot sec$
n_{Aw}	number of ash particle withdrawn per unit time	1/sec
n_{ce}	number of char particles elutriated per unit time	1/sec
n_{cf}	number of coal particles fed to the bed per unit	1/sec
n_{cw}	number of coal particles withdrawn per unit time	1/sec
n_d	downward flow of particles	1/sec
n_u	upward flow of particles	1/sec
n_{eW}	number of char particles transferred from emulsion phase to wake phase per unit time	1/sec
$n_{\ell f}$	number rate of limestone particles fed to the bed	1/sec
$n_{\ell w}$	number rate of limestone particles withdrawn from the bed	1/sec
n_{WE}	number of char particles transferred from wake phase to emulsion phase in the ith cell per unit time	1/sec
p	average pressure in the bed	atm
q_c	lower heating value of coal on dry basis adjusted for CO	cal/g
q_ℓ	heat of calcination of limestone	cal/g
R	gas constant 82.05 $cm^3 \cdot atm/gmol/°K$ or 1.987	cal/gmol.°K
$R^*=(dy/d\theta)^*$;	dimensionless shrinking rate of char	1/sec
R_B	ratio of cloud sphere volume to bubble volume	-
$R = \{r_i^*\}$	reaction rate vector for reactions 1-8	$gmol/sec \cdot cm^3$ (emulsion
$R_g^* = R\ A$	total formation rate vector for gaseous species	$gmol/sec \cdot cm^3$ (emulsion)
$R_s^* = R\ B$	total formation rate vector for solid phase species	$gmol/sec \cdot cm^3$ (emulsion)
R_{e_t}	terminal Reynold's number	

r^*_{cBi}, r^*_{cEi}	reaction rates defined by Eqs. (3-88)	gmol/sec·cm^3 (emulsion)
r^*_i	rate of reaction i	gmol/sec·cm^3 (emulsion)
r^*_{iB}, r^*_{iE}	rates of reaction i in emulsion phase and in bubble phase	gmol/sec·cm^3 (emulsion)
r^*_{gij}, r^*_{sij}	formation rates of species M_{gj} or M_{sj} by reaction i	gmol/sec·cm^3 (emulsion)
$r^*_{\ell B}$, $r^*_{\ell E}$	rates of sulfur capture in bubble phase and in emulsion phase	gmol/sec·cm^3 (emulsion)
r'_i	rate of ith reaction for one particle	gmol/sec
r_c	reaction rate per char particle	gmol/sec
r_ℓ	reaction rate per limestone particle	gmol/sec
S_i	internal surface area of calcined limestone	cm^2/g
T	local bed temperature	°K
T_{gf}	temperature of feed gas	°K
T_i	temperature of i^{th} compartment	°K
T_{sf}	temperature of feed solids	°K
T_w	temperature of cooling water	°K
U	overall heat transfer coefficient of cooling tubes based on outside tube diameter	cal/cm^2·sec.°K
u_o	superficial gas velocity	cm/sec
u_B	bubble rising velocity	cm/sec
u_{mf}	minimum fluidization velocity	cm/sec
u_t	terminal velocity	cm/sec
V	volume of bed (total including tubes)	cm^3
V_{ef}	volume of bed excluding tubes	cm^3
v_B	volumetric flow rate of solids in bubble-wake phase excluding voids	cm^3/sec
v_{BE}, v_{EB}	volumetric solids exchange rates from bubble-wake phase to emulsion phase and from emulsion phase to bubble-wake phase respectively	cm^3/sec

v_d	volumetric down flow rate of solids in emulsion phase excluding voids	cm^3/sec
v_E	volumetric flow rate of solids in emulsion phase excluding voids	cm^3/sec
v_e	volumetric elutriation rate	cm^3/sec
v_f	volumetric feed rate excluding voids	cm^3/sec
v_{net}	volumetric net flow rate excluding voids	cm^3/sec
v_u	volumetric upward flow rate of solids in emulsion phase excluding voids	cm^3/sec
v_w	volumetric withdrawal rate of solids excluding voids	cm^3/sec
W_b	total weight of bed material	g
w_B	solids mass flow rate in bubble-wake phase	g/sec
w_{BE}, w_{EB}	solids mass exchange rates from bubble-wake phase to emulsion phase and from emulsion phase to bubble-wake phase	g/sec
W_c	total weight of char in the bed	g
w_{cf}	coal feed rate, dry basis	g/sec
w_d	solids down flow rate in emulsion phase	g/sec
w_e	elutriation rate of unburned char	g/sec
w_E	solids mass flow rate in emulsion phase	g/sec
w_f	feed rate of solids	g/sec
$w_{\ell f}$	limestone feed rate, uncalcined basis	g/sec
w_{mix}	upward and downward flow rate due to backflow of solids	g/sec
w_{net}	net flow rate of solids	g/sec
w_u	solids upward flow rate in emulsion phase	g/sec
w_w	withdrawal rate of solids	g/sec
w_W	mass flow rate of wake	g/sec
X_C	mass fraction of carbon in char	-
X_h	mass fraction of water in coal	-

X_{if} (i=A,C,H,N,O,S)	mass fraction of ash, carbon, hydrogen, nitrogen, oxygen, sulfur and in coal (dry basis)	-
$X_{\ell Ca}$	mass fraction of calcium in limestone	-
X_{vf}	mass fraction of volatiles, dry basis	-
X_{VM}	mass fraction of volatiles dry ash free basis	-
x	mass fraction of carbon in the bed	-
x_B	mass fraction of carbon in bubble-wake phase	-
x_E	mass fraction of carbon in emulsion phase	-
x_f	mass fraction of carbon in solids feed	-
Y(y)	function defined by Eq. (4-6)	-
Y_B, Y_E	mole fractions of oxygen in bubble and emulsion phases	-
Y'_B, Y'_E	mole fractions of SO_2 or H_2O in bubble and emulsion phase	-
$y = d_c/d_{cm}$	dimensionless diameter of char particle	-
$y_{j,f}$	mole fraction of gaseous species j in the feed stream	-
y_{Bj}, y_{Ej}	mole fractions of gaseous species j in bubble phase and in emulsion phase	-
Y_B, Y_E	mole fraction vectors of gases in bubble phase and emulsion phase	-
Z	height above distributor	cm
$Z_f(y)$	function defined by Eq. (19)	-

Greek Symbols

β	adjusting factor of elutriation rate constant	-
ε'	emissivity	-
ε_b	volume fraction of bubbles	-
ε_c	volume fraction of clouds and bubbles	-
ε_{mf}	volume fraction of bed at $u_o = u_{mf}$	-
ε_{tube}	volume fraction of internal tubes	-
ε_w	volume fraction of cloud and wake	-
η_c	combustion efficiency of coal	-
η_S	efficiency of sulfur capture	-
θ	time	sec
Θ	mean residence time of solids	sec
θ_c	mean circulation time of particles	sec
λ_c	$= k_c/k_{c0}$	-
λ_ℓ	reactivity of limestone defined by Eq.(e-63)	-
μ	viscosity of gas	gm/cm·sec
ξ_{Ae}	weight fraction ash particles elutriated from bed	-
$\xi_{CO}, \xi_{H2}, \xi_{H2S}$	parameters defined by Eq. (3-42)	-
ρ_A	density of ash	g/cm^3
ρ_{cf}	density of coal	g/cm^3
ρ_{ch}	density of char	g/cm^3
ρ_g	density of gas	g/cm^3
ρ_ℓ	density of lime or calcined dolomite	g/cm^3
$\rho_{\ell f}$	density of limestone or dolomite	g/cm^3
ρ_s	density of solids	g/cm^3

ρ_{Nc}	number of char particles per unit volume of bed	$1/cm^3$
$\rho_{N\ell}$	number of adsorbent particles per unit volume of bed	$1/cm^3$
ϕ	size distribution density function of char particles	-
ϕ_B, ϕ_E	size distribution density functions of char in bubble-wake phase and in emulsion phase	-
ϕ_e	size distribution density function of elutriated char particles	-
ϕ_f	size distribution density function of char particles fed to the bed	-
ϕ_ℓ	distribution density function of adsorbent conversion	-
$\phi_{\ell f}$	conversion distribution density function of adsorbent fed to the bed	-
ϕ_w	size distribution density function of withdrawn char particles	-
ψ_v	$= \int_0^1 \phi\, y^3\, dy$	-
ψ_{ve}	$= \int_0^1 \phi_e\, y^3 dy$	-
ψ_{vw}	$= \int_0^1 \phi_w\, y^3 dy$	-

Subscripts

B	bubble or bubble phase
b	bulk density or bed
C	carbon
c	coal, char, cloud or circulation
ch	char
d	downward flow

C-3

E	emulsion phase
ef	effective (excluding the tubes)
f	feed
g	gas
HE	heat exchange
ℓ	lime or limestone
mf	minimum fluidization
s	solid
u	upward flow
W	wake
w	withdrawal or cooling water
Z	axial
0	Z = 0
1	Z = L_f

APPENDIX I

Mean Residence Time of Absorbent Particles, Θ

The number of absorbent particles, char particles and ash particles are indicated by N_ℓ, N_c and N_A. The total volume in the bed occupied by solids is $(1 - \varepsilon_{mf})V_{mf}$ and is calculated from the following equation:

$$(1 - \varepsilon_{mf})V_{mf} = \frac{\pi}{6} N_\ell \overline{d_\ell^3} + \frac{\pi}{6} d_{cm}^3 N_c \psi_{vw} + \frac{\pi}{6} \overline{d_A^3} N_A \qquad (I\text{-}1)$$

Substituting the definition of Θ, namely

$$\Theta = N_\ell/n_{\ell f} = N_c/n_{cw} = N_A/n_{Aw} \qquad (3\text{-}31)$$

we get

$$\Theta = \frac{(1 - \varepsilon_{mf})\, V_{mf}}{\frac{\pi}{6}\left(n_{\ell f} \overline{d_\ell^3} + n_{cw} d_{cm}^3 \psi_{vw} + n_{Aw} \overline{d_A^3}\right)} \qquad (I\text{-}2)$$

By the use of the relations,

$$\frac{\pi}{6} n_{\ell f} \overline{d_\ell^3} = w_{\ell f}/\rho_{\ell f}$$

$$\frac{\pi}{6} n_{cw} d_{cm}^3 \psi_{vw} = \frac{(1 - \eta_c)\, w_{cf}}{\rho_{cf}} - \frac{\pi}{6} d_{cm}^3 n_{ce} \psi_{ve}$$

and

$$\frac{\pi}{6} n_{Aw} \overline{d_A^3} = \frac{\eta_c w_{cf} X_{Af} (1 - \xi_{Ae})}{\rho_A}$$

we have

$$\Theta = \frac{(1 - \varepsilon_{mf})V_{mf}}{\frac{w_{\ell f}}{\rho_{\ell f}} + \left(\frac{\pi}{6}\right) d_{cm}^3 \psi_{vw} n_{cw} + \frac{\eta_c w_{cf} X_{Af}}{\rho_A} (1 - \xi_{Ae})} \qquad (3\text{-}32)$$

APPENDIX II

Derivation of Population Balance Equations

Consider a m-dimensional state space of the state variable

$$x = (X_1, X_2 \ldots X_m)$$

The state variables can be particle size, density, conversion, temperature, etc. Population balance is made around a small segment of state space, dV,

$$dV = dX_1 \; dX_2 \ldots dX_m \qquad \text{(II-1)}$$

The kinetic equations relating the change of the state on one particle at a given condition are assumed to be known. The equation can be given as:

$$\left(\frac{dX_i}{d\theta} \right)^* = R_i \; (x) \qquad (i = 1\text{~}m) \qquad \text{(II-2)}$$

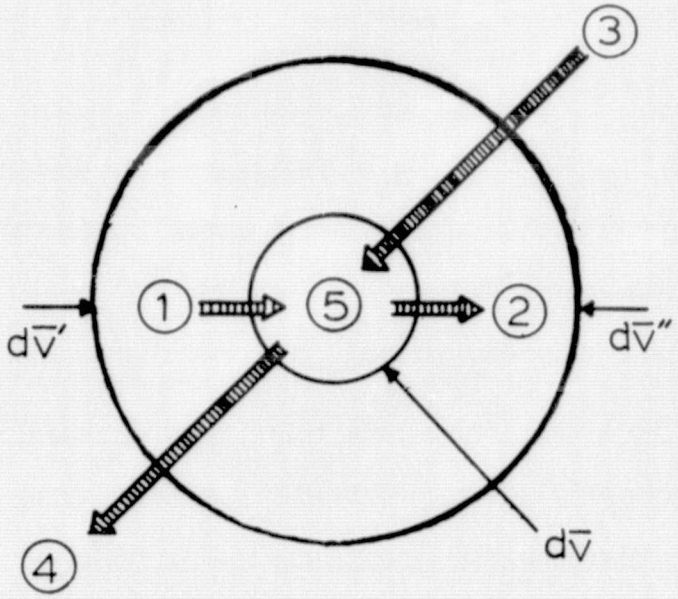
As the result of a change in the state variable described in Equation (II-2), particles in the subspace dv enter into the subspace dv continuously.

$$dV = \{dX_2 \cdot dX_3 \ldots dX_m \left(\frac{dX_1}{d\theta}\right)^* + dX_1 \cdot dX_3 \ldots dX_m \left(\frac{dX_2}{d\theta}\right)^* + \; \} \, d\theta \qquad \text{(II-3)}$$

$$= \sum_{i=1}^{m} \left[\frac{1}{dX_i} \left(\frac{dX_i}{d\theta} \right)^*_{x=x^{dv}} \right] = \sum_{i=1}^{m} \frac{R_i \; (x)}{d \quad X_i} \, dVd\theta$$

Also, the particles in the subspace dV are continuously leaving the neighbouring subspace dV''(see Figure II-1).

$$dV'' = \sum_{i=1}^{m} \frac{R_i (x + dx)}{dX_i} \, dVd\theta \qquad \text{(II-4)}$$



1, 2 = Input and output due to change in state of the particles.

3, 4 = Direct input and direct output.

5 = Accumulation.

$\bar{V}$ = State space.

FIGURE II-1 ILLUSTRATION OF THE POPULATION BALANCE.

Furthermore there are direct input and output of particles due to the feed, withdrawal, coalescence, agglomeration, breaking up, splitting or attrition.

$$\text{input} = N \phi (x) \sum_i \frac{R_i(x)}{dX_i} dVd\theta \quad \text{..... 1}$$

$$+ n_{in} \phi_{in} dVd\theta \quad \text{..... 3} \qquad \text{(II-5)}$$

$$\text{output} = N \sum_i \phi (X_j = X_j, X_i = X_i + dX_i) \qquad j = 1\sim m,\ j \neq i$$

$$\times \frac{R_i (X_i = X_i + dX_i)}{dX_i} dVd\theta \quad \text{..... 2}$$

$$+ n_{out} \phi_{out} dVd\theta \quad \text{..... 4} \qquad \text{(II-6)}$$

$$\text{accumulation} = d(N \phi (x))\, dV$$

Since the term 2 can be rewritten as follows:

$$\sum_i \phi (X_j = X_j\ X_i = X_i + dX_i) \frac{R_i(X_i = X_i + dX_i)}{dX_i} dVd\theta \qquad j = 1\sim m,\ j \neq i$$

$$= \sum_i \left(\phi (x) \frac{R_i (x)}{dX_i} + \frac{\partial \phi R_i}{\partial X_i}\right) dVd\theta \qquad \text{(II-7)}$$

We obtain the final expression of the population balance as

$$\frac{\partial N\phi}{\partial \theta} = - N \sum_i \frac{\partial \phi R_i}{\partial X_i} + n_{in} \phi_{in} - n_{out} \phi_{out} \qquad \text{(II-8)}$$

Mass balance

The relation between ϕ (density function for number fraction) and ϕ^* (density function for weight fraction) is given by

$$N \frac{\pi}{6} d_p^3 \rho_p \phi \, dV = W \phi^* \, dV \qquad \text{(II-9)}$$

because

ϕdV: fraction of the number of particles which have the state $x \sim x + dx$

$\phi^* dV$: weight fraction of particles which have the state $x \sim x + dx$

Therefore,

$$\phi = \frac{6 W}{\pi N \rho_p d_p^3} \phi^* \qquad \text{(II-10)}$$

The average mass of one particle m_p is calculated by

$$m_p \equiv \frac{W}{N} = \frac{\frac{\pi}{6} \int_x \phi(x) \rho_p d_p^3 \, dV}{\int_x \phi^*(x) \, dV} \qquad \text{(II-11)}$$

Then each term in the equation (II-8) can be written in terms of ϕ^*.

$$\frac{\partial N\phi}{\partial \theta} = \frac{6}{\pi \rho_p d_p^3} \frac{\partial W \phi^*}{\partial \theta} \qquad \text{(II-12)}$$

where the fact that $(\rho_p d_p^3)$ is not dependent on θ, but only dependent on x is used.

$$N \frac{\partial \phi R_i}{\partial X_i} = \frac{6W}{\pi} \frac{\partial [(\phi^* R_i)/(\rho_p d_p^3)]}{\partial X_i} \qquad \text{(II-13)}$$

$$= \frac{6W}{\pi} \left[\frac{1}{\rho_p d_p^3} \frac{\partial \phi^* R_i}{\partial X_i} - \frac{\phi^* R_i}{(\rho_p d_p^3)^2} \frac{\partial (\rho_p d_p^3)}{\partial X_i} \right]$$

$$\begin{pmatrix} n_{in}\ \phi_{in} \\ \text{or} \\ n_{out}\ \phi_{out} \end{pmatrix} \equiv n_X\ \phi_X = \frac{n_X\ m_{pX}}{\pi/6} \cdot \frac{\phi_X^*}{(\rho_p d_p^3)} = \frac{w_X}{\pi/6}\ \frac{\phi_X^*}{(\rho_p d_p^3)} \qquad \text{(II-14)}$$

$$\frac{\partial W\phi^*}{\partial\theta} = -W \sum_i \left[\frac{\partial\ \phi^* R_i}{\partial\ X_i} - \frac{\phi^*\ R_i}{\rho_p\ d_p^3}\ \frac{\partial(\rho_p d_p^3)}{\partial\ X_i} \right] + w_{in}\ \phi_{in}^* - w_{out}\ \phi_{out}^* \qquad \text{(II-15)}$$

A Simple Case

ρ_p = constant and $X_1 = d_p/d_{p\,m}$

$$\frac{\partial W\phi^*}{\partial\theta} = -W \sum_i \left[\frac{\partial\ \phi^*\ R_i}{\partial\ X_i} \right] + \frac{3\ W\ \phi^* R_i}{X_1} + w_{in}\phi_{in}^* - w_{out}\phi_{out}^* \qquad \text{(II-16)}$$

$3\ \frac{W\ \phi^* R_1}{X_1}$: loss of mass due to shrinkage volume balance

(ρ_p = constant $X_1 = d_p/d_{p\,m}$)

$$\frac{\partial V\phi^*}{\partial\theta} = -V \left[\sum_i \frac{\partial\ \phi^* R_i}{\partial\ X_i} - \frac{3\ \phi^* R_1}{X_1} \right] + v_{in}\ \phi_{in}^* - v_{out}\ \phi_{out}^* \qquad \text{(II-17)}$$

if ρ_p is constant the Equation (II-11) becomes

$$m_p = \frac{\pi}{6}\ \rho_p \int_\chi \phi\ d_p^3\ dV = \frac{\pi}{6}\ d_{pm}^3\ \rho_p\ \psi_v \qquad \text{(II-18)}$$

$$\psi_v \equiv \frac{V}{\frac{\pi}{6}\ d_{pm}^3\ N} \equiv \int\int\int \ldots \int_\chi \phi\ X_1^3\ dX_1\ dX_2 \ldots dX_m / \int\int\int \ldots \int dV \qquad \text{(II-19)}$$

Total Number Balance

The disappearance of particle occurs only when d_p becomes 0.

$$dX_1 = + \left(\frac{dX_1}{d\theta}\right)^*_{X_1 \to 0} d\theta = -R_1\ (x)_{X_1 \to 0}\ d\theta \qquad R_1 < 0 \qquad \text{(II-20)}$$

Then total number of particles disappeared during $d\theta$ is given by:

$$N \int_{X_2 \ldots X_m} \int \int \phi \ (X_1 = 0) \ \frac{dV dX_1}{dX_1} \ d\theta \qquad \text{(II-21)}$$

Therefore,

$$\frac{dN}{d\theta} = n_{in} - n_{out} + N \int_{X_2}^{X_m} \ldots \int \phi \ (X_1 = 0, \ x) R_1 (X_1 = 0, x) dX_2 \ldots dX_m \qquad \text{(II-21)}$$

SUMMARY

basic equation: $$\frac{\partial N\phi}{\partial \theta} = - N \sum_i \frac{\partial \phi R_i}{\partial X_i} + n_{in} \phi_{in} - n_{out} \phi_{out} \qquad \text{(II-8)}$$

or $$\frac{\partial W\phi^*}{\partial \theta} = - W \sum_i \left[\frac{\partial \phi^* R_i}{\partial X_i} - \frac{\phi^* R_i}{\rho_p \overline{d^3_p}} \frac{\partial (\rho_p d^3_p)}{\partial X_i} \right] + w_{in} \phi^*_{in} - w_{out} \phi^*_{out} \qquad \text{(II-12)}$$

where $R_i = (d X_i / d\theta)^*$

Total number balance

$$\frac{dN}{d\theta} = n_{in} - n_{out} + N \int_{X_2 \ldots X_m} \ldots \int \phi \ (x) \ R_1 \ (x) \ dX_2 \ldots . dX_m \qquad \text{(II-19)}$$

Nomenclature for Appendix II

d_p: particle diameter

d_{pm}: maximum particle diameter

dV: small volume in the state space

n: particle flow rate (number/time)

n_{in}: flow rate of direct input

n_{out}: flow rate of direct output

N: total number of particles in the system

m: dimension of state space

m_p: average mass of one particle

W: total mass of particles in the system

Θ: time

ϕ: distribution density function of x based on the number of particles

ϕ^*: distribution density function of x based on the mass of particles

ρ_p: apparent density of particle

APPENDIX III

Solution of the Population Balance Equation for Sulfur Capture Reaction

The population balance equation for sulfur capture reaction can be given by

$$\frac{dY_\ell}{df} + B_1 \frac{Y_\ell}{\lambda_\ell} = B_2 \phi_{\ell f} \qquad \text{(III-1)}$$

where

$$Y_\ell \equiv \phi_\ell \lambda_\ell$$

Integrating this equation by assuming initial value Y(0) and the integration constraint, $\int_0^1 \phi_{\ell f}\, df = 1$, we obtain

$$Y_\ell (f) = \frac{B_2 + Y(0-)}{\exp\left[\int_0^f (B_1/\lambda_\ell) df\right]} \qquad \text{(III-2)}$$

Therefore,

$$\phi_\ell(f) = \frac{B_2 + Y(0-)}{\lambda_\ell \exp\left[\int_0^f (B_1/\lambda_\ell) df\right]} \qquad \text{(III-3)}$$

The function ϕ_ℓ must satisfy the constraint

$$\int_0^1 \phi_\ell(f) df = \{B_2 + Y_\ell(0-)\} \int_0^1 \frac{df}{\lambda_\ell \exp\left(\int_0^f \frac{B_1}{\lambda_\ell} df\right)}$$

$$\equiv 1$$

Then,

$$B_2 + Y_\ell(0-) = \frac{1}{\int_0^1 \frac{df}{\lambda_\ell \exp\left(\int_0^f \frac{B_\ell}{\lambda_\ell} df\right)}} \qquad \text{(III-4)}$$

Substitute Equation (III-4) into Equation (III-3) and use the relation

$$\int_0^1 \frac{1}{\lambda_\ell} \exp\left[\int_0^f \frac{B_\ell}{\lambda_\ell} df\right] df = -\frac{1}{B_\ell}\left[\exp\left(-\int_0^1 \frac{B_\ell}{\lambda_\ell} df\right) - 1\right]$$

then we have

$$\phi_\ell(f) = \frac{(B_\ell/\lambda_\ell) \exp\left[-\int_0^f \frac{B_\ell}{\lambda_\ell} df_\ell\right]}{1 - \exp\left[-\int_0^1 \frac{B_\ell}{\lambda_\ell} df\right]} \qquad \text{(3-65)}$$

APPENDIX IV

Relation between Population Balance and Material Balance

Consider a reaction system of shrinking particles as illustrated in Figure IV-1. The system can be divided into a small complete mixing cell. The process in a single cell is described by the population balance as follows:

1) differential population balance:
$$N \frac{d\ \phi\ R^*}{dy} = r_f\ \phi_f - n_o \phi \qquad \text{(IV-1)}$$

2) boundary conditions for particle shrinking system (i.e. no particles beyond y = 1) :
$$\phi\ (1+) = 0 \qquad \text{(IV-2)}$$

3) integral constraint:
$$\int_0^1 \phi\ dy = 0 \qquad \text{(IV-3)}$$

where

$$R^* \equiv (dy/d\theta)^* = f(y, \ldots.) \qquad \text{(IV-4)}$$
$$y = d_p/d_{pm}$$

On the other hand, from the material balance

$$w_f = w_o - 4\ \pi\ d_{pm}^3\ \ N\ \rho_p < y^2\ R^* > \qquad \text{(IV-5)}$$

(input) (output)

where

$$w_o = \frac{4}{3}\ \pi\ \rho_p\ d_{pm}^3\ \ \psi_v\ n_o$$

$$\psi_v \equiv \int_0^1 \phi\ y^3 dy / \int_0^1 \phi\ dy$$

$$< y^2\ R^* > \equiv \int_0^1 \phi\ \ y^2\ R^* dy / \int_0^1 \phi\ dy$$

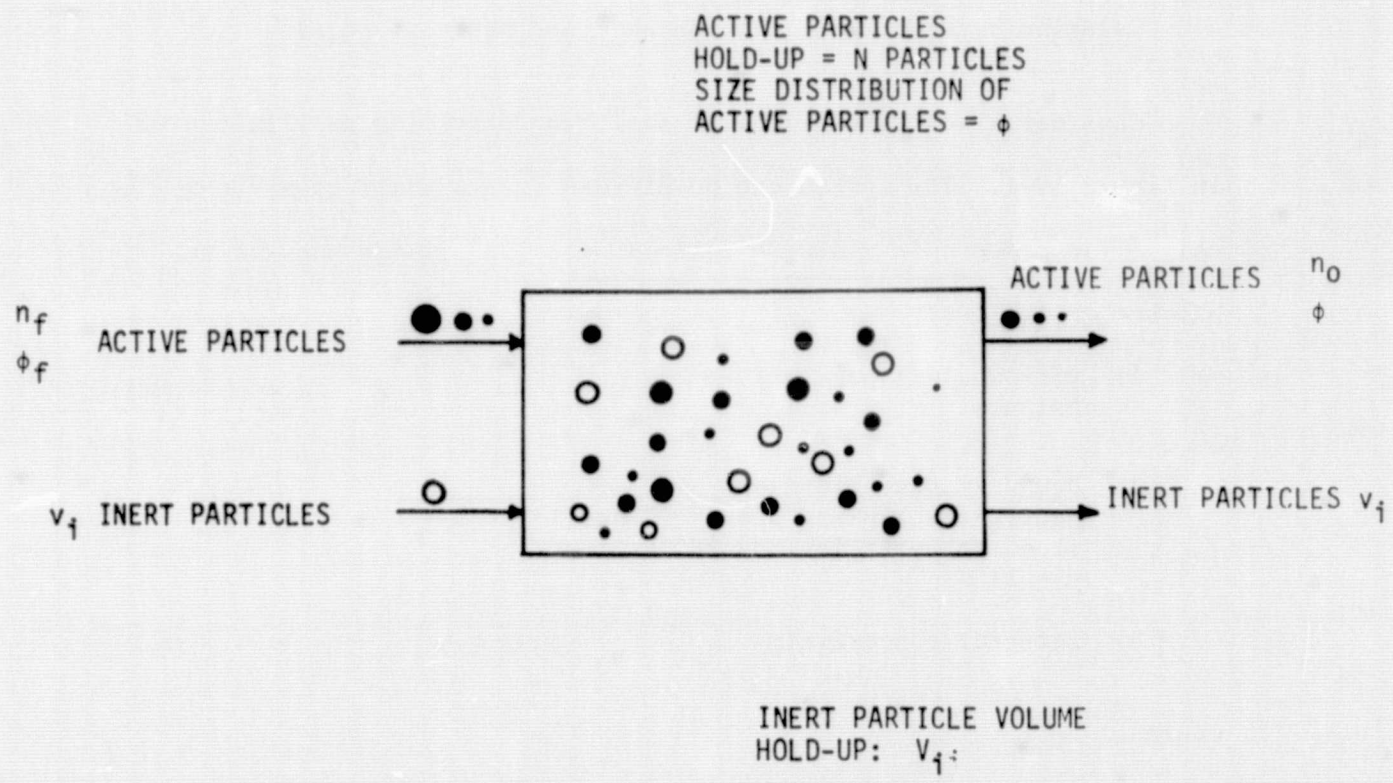


FIGURE IV-1 ILLUSTRATION FOR THE POPULATION BALANCE

Equation (IV-5) can be rearranged into the form

$$w_f = \alpha \, [\psi_v \, n_o - 3 \, N < y^2 \, R^* >] \qquad \text{(IV-5)}'$$

where

$$\alpha \equiv \frac{4}{3} \pi \rho_p \, d_{pm}^3$$

The problem is stated as follows:

Is Equation (IV-5)′ dependent on the system described by population balance?

The answer is shown below.

1) Equation (IV-5)′ is dependent on Equations (IV-1)~(IV-3)

Multiplying y^3 on both sides of Equation (IV-1) and integrate it from y = 0 to y = 1, we obtain

$$\int_0^1 [\text{ left hand side of Equation (IV-1)}] \cdot y^3 \, dy$$

$$= N \, [y^3 \, \phi \, R^* \Big|_0^{1+} - 3 \int_0^1 y^2 \, \phi \, R^* \, dy] \qquad \text{(IV-6)}$$

$$\int_0^1 [\text{ right hand side of Equation (IV-1)}] \cdot y^3 \, dy$$

$$= n_f \, \psi_{vf} - n_o \, \psi_v \int_0^1 \phi \, dy \qquad \text{(IV-7)}$$

After substituting Equations (IV-2) and (IV-3), we have the form

$$n_f \, \psi_{vf} = n \, \psi_v - 3 \, N < y^2 \, R^* >$$

By multiplying by $\frac{4}{3} \pi \, d_{pm}^3 \, \rho_p$, Equation (IV-5)′ is obtained.

2) Condition (IV-3) is derived from Equations (IV-1), (IV-2) and IV-5)′

In this case Equation (IV-6) remains in the following form:

$$\text{Equation (IV-6)} = - 3 \, N < y^2 \, R^* > \int_0^1 \phi \, dy \qquad \text{(IV-6)}'$$

Equating Equation (IV-6)' with Equation (IV-7), we obtain the value of integration of ϕ,

$$\int_0^1 \phi \, dy = \frac{n_f \psi_{vf}}{n_o \psi_v - 3 N < y^2 R^* >} = \frac{w_f}{\alpha [n_o \psi_v - 3 N < y^2 R^* >]}$$

Therefore, from Equation (IV-5)'

$$\int_0^1 \phi \, dy = 1$$

3) The overall number balance can replace Equation (IV-4)

The overall number balance equation for this system is given by

$$n_f - n_o = - N R^* (0) \phi(0) \qquad \text{(IV-8)}$$

This equation can also be derived from Equations (IV-1), (IV-2) and (IV-3).

Consider a case in which constraint (IV-3) can be ignored.

Integrating Equation (IV-1) over the interval y = 0~1 and applying Equation (IV-2), we have

$$- N \phi (0) R^* (0) = n_f - n_o \int_0^1 \phi \, dy$$

By using Equation (IV-8),

$$\int_0^1 \phi \, dy = \frac{n_f + N \phi (0) R^* (0)}{n_o} = 1$$

Conclusion

Equations (IV-1), (IV-2) and (V-3) are necessary and sufficient equations to describe the system. Material balance equation is no longer an independent equation when the system is expressed by these three equations. Therefore, there are four combinations of equations to formulate the performance equations of the system. For instance, if we use the material balance equation with the population balance equation and solve them simultaneously, it is not necessary to consider the integral constraint (IV-3). The selection of equations for constructing the numerical iteration scheme must be decided from the view point of numerical stability and rapidness of convergence.

Nomenclature for Appendix IV

d_p	diameter of active particle	cm
d_{pm}	maximum diameter of active particles	cm
n	number flow rate of active particles	1/sec
N	number hold-up of active particles	-
R^*	shrinking rate of a single particle	1/sec
v_i	volume flow rate of inert particles	cm^3/sec
V_i	volume hold-up of inert particles	cm^3
V_t	total volume of solids in the cell	cm^3
w	mass flow rate of active particles	g/sec
$y=d_p/d_{pm}$	dimensionless particle size	-
ϕ	size distribution density function	-
ρ_p	density of particles	g/cm^3

$\psi_V \equiv \int_0^1 \phi\, y^3 / \int_0^1 \phi\, dy$

Subscripts

f	feed or input
o	outlet

APPENDIX V

Elutriation Rate

Let w_e denote the total elutriation rate of coal or char [g/sec]. By using ϕ_e^*, the size distribution of elutriated particles on weight fraction basis, and ϕ_e, the size distribution of elutriated particles on number fraction basis, we have,

$$dw_e = w_e \, \phi_e^* \, dy = w_e \, \frac{y^3 \, \phi_e}{\psi_{ve}} \, dy \qquad \text{(V-1)}$$

On the other hand, the elutriation rate is given by the specific elutriation rate constant, K^*, in the form

$$\frac{dw_e}{A_t} = K^* \, \phi_b^* \, dy \qquad \text{(V-2)}$$

where ϕ_b^* is the density function of size distribution of the char particles in the bed based on the total weight of bed. ϕ^* is the size distribution density function based on the total weight of char particles in the bed and is related to ϕ_b^* by

$$W_c \, \phi^* \, dy = W_b \, \phi_b^* \, dy \qquad \text{(V-3)}$$

Substituting (V-2) and (V-3) into (V-1), we obtain

$$dw_e = w_e \, \phi_e^* \, dy = \frac{A_t \, W_c}{W_b} \, K^* \, \phi^* \, dy \qquad \text{(V-4)}$$

or by using ϕ and ϕ_e,

$$dw_e = \frac{w_e \, \phi_e}{\psi_{ve}} \, y^3 dy = \frac{A_t \, W_c}{W_b \, \psi_v} \, K^* \, \phi \, dy \qquad \text{(V-5)}$$

where

$$\psi_{ve} = \int_0^1 \phi_e \, y^3 \, dy, \quad \psi_v = \int_0^1 \phi \, y^3 \, dy$$

Now since the number of particles elutriated per unit time, n_e, and the total number of coal particles in the bed, N_c, are given by

$$n_e = w_e/(\psi_{ve} \frac{\pi}{6} d_{cm}^3 \rho_{ch})$$

$$N_c = W_c/(\psi_v \frac{\pi}{6} d_{cm}^3 \rho_{ch})$$

We obtain the final form

$$n_e \phi_e = \frac{K^* A_t}{W_b} N_c \phi \qquad \text{(V-6)}$$