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FLUIDIZED BED COMBUSTOR MODELING

M. Horio
P. Rengarajan
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C.Y. Wen

January, 1977

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

West Virginia University

College of Engineering
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
**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 consist 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 $\text{SO}_2$ 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 $\text{SO}_2$ 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.

**Key Words (Suggested by Author(s))**

Fluidized Bed Combustion

**Distribution Statement**

Unclassified - unlimited

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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

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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.
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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 those 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.

A great deal of work has been done in Great Britain 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.

2. Description of gas and solids contacting process.

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

\[
\frac{D_{Bm} \cdot D_B}{D_{Bm} - D_{Bo}} = \exp (-0.5 \frac{Z}{D_t})
\]

(2-1)

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; **P₀**: perforated plate; **Pₑ**: porous plate or screen

<table>
<thead>
<tr>
<th>Investigators</th>
<th>Dc, cm</th>
<th>Solid particles</th>
<th>dp, cm</th>
<th>umf, cm/s</th>
<th>u₀/umf</th>
<th>No. of holes in the distributor, N₀</th>
</tr>
</thead>
<tbody>
<tr>
<td>Werther(1973)</td>
<td>20</td>
<td>Quartz sand</td>
<td>0.0083</td>
<td>1.8</td>
<td>5</td>
<td>P₀</td>
</tr>
<tr>
<td></td>
<td>100</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Chiba(1973)</td>
<td>20</td>
<td>Crushed silica</td>
<td>0.0089</td>
<td>0.57</td>
<td>10-39</td>
<td>Pₑ, 241</td>
</tr>
<tr>
<td>Geldart(1971)</td>
<td>30.8</td>
<td>Sand</td>
<td>0.0128</td>
<td>1.2</td>
<td>2.6-7.7</td>
<td>Pₑ, 100</td>
</tr>
<tr>
<td>Rowe(1972)</td>
<td>30 X 20*</td>
<td>Alumina</td>
<td>0.021</td>
<td>2.54</td>
<td>1.25-2.5</td>
<td></td>
</tr>
<tr>
<td></td>
<td>30 X 30*</td>
<td>Carbon</td>
<td>0.0296</td>
<td>8.0</td>
<td>1.3-1.7</td>
<td></td>
</tr>
<tr>
<td></td>
<td>30 X 20*</td>
<td>Quartz</td>
<td>0.0135</td>
<td>2.75</td>
<td>2.2-6.6</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>Ballotini</td>
<td>0.0325</td>
<td>8.0</td>
<td>1.6-2.4</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>Glass powder</td>
<td>0.0268</td>
<td>5.5</td>
<td>1.7-2.7</td>
<td></td>
</tr>
<tr>
<td>Whitehead(1967)</td>
<td>61 X 61*</td>
<td>Silica sand</td>
<td>0.015</td>
<td>2.5</td>
<td>2.8-6.6</td>
<td>T, 16</td>
</tr>
<tr>
<td></td>
<td>61 X 61*</td>
<td>M.S. cat.</td>
<td>0.015</td>
<td>2.0</td>
<td>1.5-25</td>
<td>Pₑ, 79</td>
</tr>
<tr>
<td></td>
<td>122 X 122*</td>
<td>Glass beads</td>
<td>0.0242</td>
<td>7.56</td>
<td>1.5-2.5</td>
<td></td>
</tr>
<tr>
<td></td>
<td>122 X 122*</td>
<td>Glass beads</td>
<td>0.0175</td>
<td>4.7</td>
<td>1.5-2.7</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>U.O.P. cat.</td>
<td>0.0060</td>
<td>0.418</td>
<td>2-10</td>
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<tr>
<td></td>
<td></td>
<td>Coal</td>
<td>0.0450</td>
<td>19.4</td>
<td>1.5-1.75</td>
<td></td>
</tr>
<tr>
<td>Toei(1965)</td>
<td>10 X 10*</td>
<td>Glass beads</td>
<td>0.0137</td>
<td>2.25</td>
<td>1.5-4.0</td>
<td>P₀, 1850</td>
</tr>
<tr>
<td>Kobayashi</td>
<td>10.0</td>
<td>Crushed silica</td>
<td>0.0210</td>
<td>2.85</td>
<td>2-9.7</td>
<td>Pₑ, 37</td>
</tr>
<tr>
<td>Mawa(1971)</td>
<td>15.0</td>
<td>Sand</td>
<td>0.016</td>
<td>2.4</td>
<td>3.1-5.2</td>
<td>Pₑ, 37</td>
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<tr>
<td>Tomita(1971)</td>
<td>31.4</td>
<td>Sand</td>
<td>0.0202</td>
<td>4.0</td>
<td>4.25</td>
<td>Pₑ, 575</td>
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<tr>
<td></td>
<td>37.8</td>
<td></td>
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<td></td>
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<td></td>
</tr>
<tr>
<td></td>
<td>59.9</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Baumgarten(1960)</td>
<td>7.6</td>
<td>Glass beads</td>
<td>0.0074</td>
<td>0.727</td>
<td>2-84</td>
<td>P₀</td>
</tr>
<tr>
<td>Park(1969)</td>
<td>10.0</td>
<td>Conductive coke</td>
<td>0.0086</td>
<td>0.63</td>
<td>4-10</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>0.0156</td>
<td>1.83</td>
<td>1.5-6</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>0.0344</td>
<td>6.8</td>
<td>1.5-3</td>
<td></td>
</tr>
<tr>
<td>Button(1968)</td>
<td>50</td>
<td>Sand</td>
<td>0.0071</td>
<td>1.0**</td>
<td>2-15</td>
<td>Pₑ, 78</td>
</tr>
<tr>
<td>Fryer(1974)</td>
<td>22.9</td>
<td>Sand</td>
<td>0.0071</td>
<td>1.70</td>
<td>1.47</td>
<td>B, 61</td>
</tr>
</tbody>
</table>

* 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

<table>
<thead>
<tr>
<th>Author(s)</th>
<th>Equation</th>
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<tr>
<td>Yasui et al. (1958)</td>
<td>( D_B = 1.6 \rho_d d_p \left( \frac{u_o}{u_{mf}} - 1 \right)^{0.63} \cdot Z )</td>
</tr>
<tr>
<td>Kato and Wen (1969)</td>
<td>( D_B = 1.4 \rho_d d_p \left( \frac{u_o}{u_{mf}} \right) Z + D' B_0 )</td>
</tr>
<tr>
<td>Park et al. (1969)</td>
<td>( D_B = 33.3 d_p 1.5 \left( \frac{u_o}{u_{mf}} - 1 \right)^{0.77} Z )</td>
</tr>
<tr>
<td>Whitehead et al. (1967)</td>
<td>( D_B = 9.76 \left( \frac{u_o}{u_{mf}} \right) 0.33(0.032Z)^{0.54} )</td>
</tr>
<tr>
<td>Rowe et al. (1972)</td>
<td>( D_B = -A + BZ + C \left( \frac{u_o}{u_{mf}} \right) ) ( + DZ(\frac{u_o}{u_{mf}}) + E \left( \frac{u_o}{u_{mf}} \right)^2 )</td>
</tr>
<tr>
<td>Geldart (1971)</td>
<td>( D_B = D' B_0 + 0.027 (u_o - u_{mf})^{0.94} Z )</td>
</tr>
<tr>
<td>Chiba et al. (1973)</td>
<td>( D_B = D''_B {Z^{7/6} - 1} (Z - Z_B) / (D''_B + 1)^{2/7} ) for ( Z &lt; Z_k )*</td>
</tr>
<tr>
<td>Mori and Wen (1975)</td>
<td>( \frac{D_{max} - D_B}{D_{max} - D_{Bo}} = e^{-0.3Z/D_t} )</td>
</tr>
<tr>
<td>Rowe (1976)</td>
<td>( D_B = (u_o - u_{mf})^{0.5} (Z + Z_o)^{3/4} / g^{1/4} ** )</td>
</tr>
</tbody>
</table>

* Numerical method is used to calculate \( D_B \) for \( Z > Z_k \).  
  \( D_{Bo} = (6G/\pi)^{0.4}/g^{0.2} \) 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 volumetric gas flow rate through a nozzle (cm³/sec)

** \( Z_o \) is a constant characterizing a distributor.

Original page is of poor quality.
\[ D_{Bm} = 0.652 \left[ A_t \left( u_o - u_{mf} \right) \right]^{0.4} \] (2-2)

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

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,

\[ \frac{dD_B}{dz} = \frac{0.3}{D_t} (D_{Bm} - D_B) \] (2-4)

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

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

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

* = Wall correction factor from Uno and Kinter (1956) was used in these works.
+ = The relation $u_B = u_B - (u_o - u_{mf})$ was applied to obtain $u_B$. 

ORIGINAL PAGE OF POOR QUALITY
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:

\[ u_B = u_0 - u_m f + K_B \sqrt{gD_B} \]  

(2-6)

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)).

\[ \text{upward flow rate of particles} = (u_o - u_m) A_t f_w (1 - \varepsilon_m) \text{ cm}^3/\text{sec} \]

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 \( \{1 - \varepsilon_B (1 + f_w)\}\{f_w (u_o - u_m)\} \). The mean cycle time for circulation \( \Theta_c \) is given as the sum of the residence times of upward and downward movements.

\[ \Theta_c = L_f [1/\overline{u_B} + \{1 - \varepsilon_B (1 + f_w)\}/(f_w (u_o - u_m))] \tag{2-7} \]

where \( \overline{u_B} \) denotes the average rising velocity of the bubble.
The average bubble fraction $\bar{e}_B = (L_f - L_{mf})/L_f$ is approximated by

$$\bar{e}_B = (u_o - u_{mf})/u_B$$

(2-8)

$u_B$ 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:

$$\theta_c = L_{mf}/(u_o - u_{mf}) f_w$$

(2-9)

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 backflow 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)).

$$E_Z \hat{=} \frac{(u_o - u_{mf}) f_w \Delta Z}{1 - e_B}$$

(2-10)

where $\Delta Z$ 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,

$$\frac{dW_e}{dt} = A_t K^* \cdot \frac{W_c}{W_b} \phi^* \, dy \quad [\text{g/sec}]$$ \hspace{1cm} (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

<table>
<thead>
<tr>
<th>Source</th>
<th>Formula</th>
<th>Conditions</th>
</tr>
</thead>
</table>
| A. Zenz and Weil (1958) †     | \[
\frac{K^*}{\rho u_o} = \begin{cases} \\
5.27 \times 10^{-5} \left(\frac{u_o^2}{gd_p \rho_s}\right)^{1.87} & \frac{u_o^2}{gd \rho_s^2} \leq 581.8 \\
4.97 \times 10^{-3} \left(\frac{u_o^2}{gd_p \rho_s}\right)^{1.15} & \frac{u_o^2}{gd \rho_s^2} \geq 581.8
\end{cases}
\] |                                                                                                                     |
| B. Yagi and Aoji (1955) ††    | \[
\frac{K^* d_p}{\mu} = Fr \left[0.0015 Re_t^{0.6} + 0.01 Re_t^{1.2}\right]
\] |                                                                                                                     |
| 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 $\equiv \left(\frac{u_o - u_t}{gd_p}\right)^2$, Re $\equiv d_p u_t \rho_g / \mu$
Figure 1. Elutriation rate constant determined by fitting experimental values of carbon combustion efficiency ($\beta$ 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:

$$F_i = F_{i0} + F_{i10} \exp (-a_i Z) \quad (2-12)$$

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):

\[ K_{BE} = \frac{1}{D_B} \]  
(C.G.S. Unit) (2-13)

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

\[ h_j = \frac{d_p}{0.0007 + 0.556 \frac{d_p}{d_p} \left( \frac{A_L}{n_d} (u_o - u_{mf}) \right)^{0.35}} \]  
(C.G.S. Unit) (2-14)

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).

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

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

\[
\text{total surface area} = \frac{\text{surface area}}{\text{volume of bed}} \times \frac{\text{total volume}}{\text{total volume of char per unit volume of bed}}
\]

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 popu-
lation 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 - SO₂ 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.

\[
\begin{align*}
CH_4 &= 0.201 - 0.469 \, X_{vm} + 0.241 \, X_{vm}^2 \\
H_2O &= 0.157 - 0.868 \, X_{vm} + 1.338 \, X_{vm}^2 \\
CO_2 &= 0.135 - 0.900 \, X_{vm} + 1.906 \, X_{vm}^2 \\
CO &= 0.423 - 2.653 \, X_{vm} + 4.845 \, X_{vm}^2 \\
H_2O &= 0.409 - 2.389 \, X_{vm} + 4.554 \, X_{vm}^2 \\
\text{Tar + Other} &= -0.325 + 7.279 \, X_{vm} - 12.880 \, X_{vm}^2
\end{align*}
\]

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

<table>
<thead>
<tr>
<th>LEVEL</th>
<th>DEFINITION</th>
<th>PERFORMANCE</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td><strong>DEFINITION</strong></td>
<td><strong>PERFORMANCE</strong></td>
</tr>
<tr>
<td></td>
<td>Total</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Gas phase</td>
<td>Temperature</td>
</tr>
<tr>
<td></td>
<td>Bulk solid mixing</td>
<td>Volume fraction of char</td>
</tr>
<tr>
<td></td>
<td>Axial variation of char size</td>
<td>Surface area of char per unit vol. of char</td>
</tr>
<tr>
<td></td>
<td>distribution</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Level I</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Not specified*</td>
<td>Uniform</td>
</tr>
<tr>
<td></td>
<td>Complete mixing</td>
<td>Uniform</td>
</tr>
<tr>
<td></td>
<td>Not considered</td>
<td>Uniform</td>
</tr>
<tr>
<td></td>
<td>Level II</td>
<td></td>
</tr>
<tr>
<td></td>
<td>BAM**</td>
<td>Axially distributed</td>
</tr>
<tr>
<td></td>
<td>Single phase backflow</td>
<td>Axially distributed</td>
</tr>
<tr>
<td></td>
<td>cell model</td>
<td>Uniform</td>
</tr>
<tr>
<td></td>
<td>Not considered</td>
<td>Axially distributed</td>
</tr>
<tr>
<td></td>
<td>Level III</td>
<td></td>
</tr>
<tr>
<td></td>
<td>BAM**</td>
<td>Axially distributed</td>
</tr>
<tr>
<td></td>
<td>Two phase backflow</td>
<td>Axially distributed</td>
</tr>
<tr>
<td></td>
<td>cell model</td>
<td>Axially distributed</td>
</tr>
<tr>
<td></td>
<td>Two phase backflow</td>
<td>Axially distributed</td>
</tr>
<tr>
<td></td>
<td>cell model</td>
<td>Axially distributed</td>
</tr>
</tbody>
</table>

* 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 but complicated treatment is possible introducing additional parameters.

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

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

where \( k_c \) is the overall rate constant and is given by

\[ k_c = \frac{1}{(1/k_{cf} + 1/k_{cR})} \quad (2-18) \]

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

\[ k_{cR} = \left( \frac{T}{1000} \right) \exp (17.9 - \frac{35,700}{RT}) \quad (2-19) \]

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 - \text{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 - \text{SO}_2 reaction.
The reaction rate per limestone particle can be expressed as

(Borgwardt (1970))

\[ r_L = \frac{n}{e} \frac{d^3}{dp} k_{VL} (T, f_L) \frac{C_{SO_2}^m}{m} \]  

\[ m = 1.088 \neq 1 \]

where \( k_{VL} (T, f_L) \) 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 \( k_{VL} \). Therefore, in the present FBC model development a function sub-routine is prepared for the average value of \( k_{VL} \) 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.
<table>
<thead>
<tr>
<th>No.</th>
<th>Reaction</th>
<th>Per unit vol. of emulsion</th>
<th>Per one particle</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>CaO + SO$_2$ + 0.5 O$_2$ = CaSO$_4$</td>
<td>$r_1^*$</td>
<td>$r_1$</td>
</tr>
<tr>
<td>2</td>
<td>CaO + H$_2$S = CaS + H$_2$O</td>
<td>$r_2^*$</td>
<td>$r_2$</td>
</tr>
<tr>
<td>3</td>
<td>C + O$_2$ = CO$_2$</td>
<td>$r_3^*$</td>
<td>$r_3$</td>
</tr>
<tr>
<td>4</td>
<td>C + 0.5 O$_2$ = CO</td>
<td>$r_4^*$</td>
<td>$r_4$</td>
</tr>
<tr>
<td>5</td>
<td>C + H$_2$O = CO + H$_2$</td>
<td>$r_5^*$</td>
<td>$r_5$</td>
</tr>
<tr>
<td>6</td>
<td>S(char) + O$_2$ = SO$_2$</td>
<td>$r_6^*$</td>
<td>$r_6$</td>
</tr>
<tr>
<td>7</td>
<td>S(char) + H$_2$ = H$_2$S</td>
<td>$r_7^*$</td>
<td>$r_7$</td>
</tr>
<tr>
<td>8</td>
<td>N$<em>2$ (char) + $\alpha</em>{\text{nox}}$ $x^*$ O$_2$</td>
<td>$r_8^*$</td>
<td>$r_8$</td>
</tr>
</tbody>
</table>

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

$$M_g = \text{col} \begin{pmatrix} M_{g1} \\ M_{g1} \end{pmatrix} = \text{col} \begin{pmatrix} M_{O_2}, & M_{CO_2}, & M_{SO_2}, & M_{H_2O}, & M_{CO}, & M_{H_2S}, & M_{H_2}, & M_{NO_x}, & M_{N_2} \end{pmatrix}$$

$$M_s = \text{col} \begin{pmatrix} M_{s1} \\ M_{s1} \end{pmatrix} = \text{col} \begin{pmatrix} M_{CaO}, & M_{CaSO_4}, & M_{CaS}, & M_{C}, & M_{S}, & M_{N_2} \end{pmatrix}$$

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

$$A M_g + B M_s = 0$$

(3-3)
where A and B are

\[
\begin{array}{cccccccccc}
   & O_2 & CO_2 & SO_2 & H_2O & CO & H_2S & H_2 & NO_x & N_2 \\
\hline
i=1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
(2) & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
(3) & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
(4) & -0.5 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
(5) & 0 & 0 & 0 & 0 & -1 & 1 & 0 & 0 & 0 \\
(6) & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
(7) & 0 & 0 & 0 & 0 & 0 & 0 & 1 & -1 & 0 \\
(8) & -\alpha_{n,ox} & 0 & 0 & 0 & 0 & 0 & 0 & 2\alpha_{nox} & 1-\alpha_{nox} \\
\end{array}
\]

\[
A \equiv \{a_{ij}\} \quad (3-4)
\]

\[
\begin{array}{ccccccc}
   & CaO & CaSO_4 & CaS & C & S & N_2 \\
\hline
i=1 & -1 & 1 & 0 & 0 & 0 & 0 \\
(2) & -1 & 0 & 1 & 0 & 0 & 0 \\
(3) & 0 & 0 & 0 & 0 & 1 & 0 \\
(4) & 0 & 0 & 0 & 0 & 0 & -1 \\
(5) & 0 & 0 & 0 & 0 & 0 & -1 \\
(6) & 0 & 0 & 0 & 0 & 0 & 0 \\
(7) & 0 & 0 & 0 & 0 & 0 & -1 \\
(8) & 0 & 0 & 0 & 0 & 0 & 0 \\
\end{array}
\]

\[
B \equiv \{b_{ij}\} \quad (3-5)
\]

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

\[
C = \{C_1, C_2, C_3, C_4, C_5, C_6, C_7, C_8, C_9\} \quad (3-6)
\]

\[
= \{C_{O_2}, C_{CO_2}, C_{SO_2}, C_{H_2O}, C_{CO}, C_{H_2S}, C_{H_2}, C_{NO_x}, C_{N_2}\}
\]
3-2. Reaction Rates

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

\[
\dot{r}_i^* = \frac{\text{gmol}}{\text{sec.cm}^3 (\text{emulsion})}
\]

Here emulsion refers to the dispersed solids. The voidage is assumed to be \( \varepsilon \).

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

\[
\dot{r}_{ij}^* \text{ or } \dot{r}_{ij} \text{ (emulsion)}
\]

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

\[
R_i^* = R_i = \sum_{i=1}^{n} r_i^* \text{ or } \sum_{i=1}^{n} r_i
\]

The rate of reactions 1 and 2 can be expressed as

\[
\dot{r}_i^* = \rho_{N_L} \dot{r}_i \text{ (emulsion)}
\]

where the \( \rho_{N_L} \) denotes the number of limestone (or dolomite) particles per unit volume of emulsion and the reaction rate for single particle, \( \dot{r}_i^* \), is supposed to be written by the first order rate equation regarding the reactant concentration \( C_3 \) (SO\(_2\)) or \( C_6 \) (H\(_2\)S) as follows:
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:

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

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

\[
  r_3^\prime = \pi \frac{d_c^2 k_3 (T, d_c)}{6} C_1 \tag{3-14}
\]

\[
  r_4^\prime = \pi \frac{d_c^2 k_4 (T, d_c)}{6} C_4 \tag{3-15}
\]

\[
  r_5^\prime = \pi \frac{d_c^2 k_5 (T, d_c)}{6} C_4 \tag{3-16}
\]

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

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

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

\[
  \alpha_6 = \alpha_7 = \frac{X_{SF}^N}{M_S} / \left( \frac{X_{CF}^N}{M_C} \right) \tag{3-18}
\]

\[
  \alpha_8 = \left( \frac{X_{NF}^N}{M_N} \right) / \left( \frac{X_{CF}^N}{M_C} \right) \tag{3-19}
\]
3.3. Overall Carbon Balance

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

Let \( \phi \) denote the overall size distribution density function for char particles. The function \( \phi \) is defined so that

\[
\phi (y) \, dy = \text{number fraction of char particles whose dimensionless diameter lies in the region between } y \text{ and } y + dy. \quad (3-20)
\]

\[
\int_0^1 \phi (y) \, dy = 1 \quad (3-21)
\]

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

\[
y = \frac{d_c}{d_{cm}} \quad (3-22)
\]

An average over the range \( y = 0-1 \) for an arbitrary variable \( A \) is defined by

\[
\langle A \rangle \equiv \int_0^1 \phi (y) \, A (y) \, dy \quad (3-23)
\]

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

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

\[
\psi_v \equiv \langle y^3 \rangle = \frac{<d_c^3>}{d_{cm}^3}
\]

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

\[
(\text{average reactivity of char}) = \pi d_{cm}^2 \langle y^2 k_i (T, y) \rangle \quad (i = 3-5) \quad (3-24)
\]
elutriation rate of char: $n_{ce}$
size distribution of char: $\phi_e$

oxygen concentration
$C_{O2} = C_{O2,1}$

char size distribution, $\phi$
total number of char particles, $N_c$
bed temperature, $T$

$C_{O2} = C_{O2,0}$

cooling tubes

coal feed rate, $n_{cf}$
size distribution of coal, $\phi_f$
limestone feed rate, $n_L$

air

$\phi_w = \phi$
withdrawal rate of char, $n_{cw}$
withdrawal rate of limestone, $n_{Lw} = n_{Lf}$

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, \( \eta_c \), is defined as

\[
\eta_c = \frac{M_c N_c \pi d_{cm}^2}{w_{cf} X_{Cf}} \sum_{i=3}^{5} \frac{k_i y^2}{C_j}
\]  

(3-25)

where \( j = \begin{cases} 
1 & \text{for } i = 3 \text{ or } 4 \\
4 & \text{for } i = 5
\end{cases} \)

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

\[
w_{cf} X_{Cf} \left( \frac{\pi}{6} d_{cm}^3 \rho_{ch} X_C \eta_{cw} \psi_w - \frac{\pi}{6} d_{cm}^3 \rho_{ch} X_C \eta_{ce} \psi_e \right) \\
\text{(feed) (withdrawal) (elutriation)}
\]

\[
= M_c N_c \pi d_{cm}^2 \sum_{i=3}^{5} \frac{k_i y^2}{C_j}
\]  

(3-26)

(react)

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:

\[ w_{cf} = \frac{n}{6} d_{cm}^{3} \psi_{vf} n_{cf} \rho_{cf} \]  

(3-27)

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

\[ n_{c} = 1 - \frac{(n_{cw} \psi_{vw} + n_{ce} \psi_{ve}) X_{c} \rho_{cf}}{n_{cf} \psi_{vf} \rho_{cf} X_{cf}} \]  

(3-28)

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

\[ n_{ce} \psi_{ve} = \frac{\Lambda_{t} N_{c}}{W_{b}} < k^{s} \gamma^{3} > \]  

(3-29)

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

\[ \frac{n_{cw}}{n_{cf}} = \frac{(1 - n_{c}) \psi_{vf}}{\psi_{vw} + \Theta \Lambda_{t} < k^{s} \gamma^{3} >} \frac{X_{cf} \rho_{cf}}{X_{c} \rho_{ch}} \]  

(3-30)

where \( \Theta \) denotes the mean residence time of limestone at the steady state,

\[ \Theta = \frac{N_{c}}{n_{cw}} = \frac{N_{c} / n_{cw}}{n_{cw}} \]  

(3-31)

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

\[ \Theta = \frac{(1 - \varepsilon_{mf}) V_{mf}}{w_{lf} / \rho_{lf} + (\pi/6) d_{cm}^{3} \psi_{vw} n_{cw} + (n_{cw} \psi_{lw} X_{Af} / \rho_{A})(1 - \varepsilon_{Ae})} \]  

(3-32)

where the parameter \( \varepsilon_{Ae} \) denotes the ratio of the ash elutriation rate to the total ash formation rate. The numerical value of \( \varepsilon_{Ae} \) must be evaluated based on ash elutriation rate constant. In this study, however, \( \varepsilon_{Ae} \) 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) = \( \frac{w_{cf} X_S f \eta_c}{M_S} + \frac{\gamma_{SO_2, f}}{y_{H_2S, f}} \)

2. (total sulfur capture rate by adsorbent) = \( \frac{w_{LE} X_L Ca \bar{\eta}_L}{M_C a} \)

where \( \bar{\eta}_L \) is the average conversion of adsorbent (limestone or dolomite) in the bed and is defined as

\[
\bar{\eta}_L = \int_0^1 \phi_L (\eta_L) \eta_L \, d\eta_L
\]

\( \phi_L (\eta_L) \) is the density function of the distribution of adsorbent conversion and has the feature

\[
\int_0^1 \phi_L (\eta_L) \, d\eta_L = 1
\]

In addition,

3. (total sulfur capture rate) = \( N_L \frac{\pi}{6} \left( \hat{k}_{v1} C_3 + \hat{k}_{v2} C_6 \right) \)

where

\[
\hat{k}_{v1} = \frac{1}{L_f} \int_0^{L_f} \left[ C_3 \int_0^1 \hat{\eta}_L \phi_L \, d\eta_L \right] \, dZ
\]

\[
\hat{k}_{v2} = \frac{1}{L_f} \int_0^{L_f} \left[ C_6 \int_0^1 \hat{\eta}_L \phi_L \, d\eta_L \right] \, dZ
\]

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:

\[
\frac{n_S}{[S]} = \frac{[C_a]}{[S]} \quad (3-35)
\]

\[
\hat{f}_k = \frac{N_k M_{Ca} \left( \hat{k}_{v1} C_3 + \hat{k}_{v2} C_6 \right)}{n_k \rho \rho_f X_{k, Ca}} \quad (3-36)
\]

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

\[
\hat{f}_k = N_k M_{Ca} \left( \hat{k}_{v1} (T, d_k) C_3 + \hat{k}_{v2} (T, d_k) C_6 \right) / \left\{ n_k \rho \rho_f X_{k, Ca} \right\} \quad (3-37)
\]

3-5. Overall Mass Balance for Gas Phase Species

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

\[
F_{m, th} = \left( \frac{w_{cf} X_{cf}/M_C Y_{O2,f}}{A_2} \right) / A_2 \quad (3-38)
\]

where

\[
A_2 \equiv \left( X_{cf}/M_C \right) / \left( \left( X_{cf}/M_C \right) + 0.5 \left( X_{HF}/M_H2 \right) + \left( X_{SF}/M_S \right) - \left( X_{O2}/M_O2 \right) \right) \quad (3-39)
\]

The excess air ratio, EAR, is defined by

\[
EAR = \frac{F_{mf}}{F_{m, th}} - 1 \quad (3-40)
\]

Neglecting the \(CH_4\) formation, the mole fraction of oxygen at the top of the bed is obtained as follows:
\[
Y_{O2} = [(1 + \text{EAR}) Y_{O2,f} - \frac{M_C Y_{O2,f} A_2}{X_{cf}} - (2 - \xi_{CO}) \frac{X_{cf}}{2M_C n_c}]
\]
\[
+ (1 - \xi_{H2}) \frac{X_{hf}}{2M_{H2}} + (1 - \xi_{H2S}) \frac{X_{Sf}}{M_S} - \frac{X_{Of}}{M_{O2}} \]
\]
\[
/ [1 + \text{EAR} + \frac{A_1 A_2 M_C Y_{O2,f} + w_{Sf}}{X_{cf}} \frac{X_{Ca}}{M_{Ca}} + \frac{X_{Mg}}{M_{Mg}}] \] (3-41)

where

\[
\xi_{CO} \equiv \frac{\text{CO formation rate}}{\text{carbon consumption rate}}
\]
\[
\xi_{H2} \equiv \frac{\text{amount of H}_2 \text{ formed}}{\text{amount of H}_2 \text{ and H}_2O \text{ formed}} \] (3-42)
\[
\xi_{H2S} \equiv \frac{\text{sulfur release rate in the form of H}_2\text{S}}{\text{total sulfur feed rate}}
\]

\[
A_1 \equiv (X_{cf} n_c \xi_{CO}/2M_C) + (X_{of}/M_{O2}) + (1 + \xi_{H2}) (X_{hf}/2M_{H2})
\]
\[
+ (X_{hf}/M_{H2O}) \] (3-43)

The outlet concentration of CO\textsubscript{2}, CO, H\textsubscript{2}, H\textsubscript{2}O, SO\textsubscript{2}, H\textsubscript{2}S and NO\textsubscript{x} can then be given as follows:

\[
Y_{CO2} = \frac{1}{F_m} \left[ \frac{w_{cf} X_{cf}}{M_C} \left(1 - \xi_{CO}\right) n_c + w_{hf} \frac{X_{Ca}}{M_{Ca}} + \frac{X_{Mg}}{M_{Mg}} + F_{mf} Y_{CO2,f} \right] \] (3-44)
\[
Y_{CO} = \frac{1}{F_m} \left[ \frac{w_{cf} X_{cf}}{M_C} \xi_{CO} n_c + F_{mf} Y_{CO,f} \right] \] (3-45)
\[
Y_{H2} = \frac{1}{F_m} \left[ \frac{w_{cf} X_{hf}}{M_{H2}} + \frac{w_{cf} X_{hf}}{M_{H2O}} + F_{mf} Y_{hf} + F_{mf} Y_{H2f} + F_{mf} Y_{H2S,f} \right] \] (3-46)
\[
- \left( F_{mf} (Y_{H2S,f} + Y_{SO2,f}) + \frac{w_{cf} X_{Sf}}{M_S} \right) \xi_{H2S} \xi_{H2} \]
\[
Y_{H2S} = \frac{1}{F_m} \left[ \frac{w_{cf} X_{hf}}{M_{H2}} + \frac{w_{cf} X_{hf}}{M_{H2O}} + F_{mf} Y_{hf} + F_{mf} Y_{H2f} + F_{mf} Y_{H2S,f} \right] \] (3-47)

\[
- \left( F_{mf} (Y_{H2S,f} + Y_{SO2,f}) + \frac{w_{cf} X_{Sf}}{M_S} \right) \xi_{H2S} \left(1 - \xi_{H2} \right) \]

\[
\text{ORIGINAL PAGE IS OF POOR QUALITY} \]
FIGURE 4  SCHEMATIC ILLUSTRATION OF THE GAS PHASE MODEL
\[ y_{\text{SO}_2} = \frac{1 - n_S}{F_m} \left[ \frac{w_{\text{cf}} X_{\text{Sf}}}{M_S} + F_{\text{mf}} (y_{\text{SO}_2,f} + y_{\text{H}_2\text{S},f}) \right] \]

\[ y_{\text{H}_2\text{S}} = \frac{1}{F_m} \left[ \frac{w_{\text{cf}} X_{\text{Sf}}}{M_S} + F_{\text{mf}} (y_{\text{H}_2\text{S},f} + y_{\text{SO}_2,f}) \right] \epsilon_{\text{H}_2\text{S}} \]

The total molar flow rate, \( F_m \), is written as:

\[ F_m = (1 + \text{EAR}) F_{\text{m,th}} + A_1 w_{\text{cf}} + w_{\text{ef}} \left( \frac{X_{\lambda \text{Ca}}}{M_{\text{Ca}}} + \frac{X_{\lambda \text{Mg}}}{M_{\text{Mg}}} \right) \]

### 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,

\[ \text{(reaction rate in bubble-cloud wake)} = (\varepsilon_{ci} - \varepsilon_{Bi}) AV_{i,ef} g_{B,i} \]

\[ \text{(reaction rate in emulsion phase)} = (1 - \varepsilon_{ci}) AV_{i,ef} g_{E,i} \]

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

\[ R_{Bi} = \frac{\alpha_{B,i}}{\alpha_{B,i} - 1} \]

\[ \alpha_{Bi} = \varepsilon_{\text{mf}} u_{B,i} / u_{\text{mf}} \]
The bubble fraction, $e_{Bi}$, is given by

$$e_{Bi} = \frac{(u_o - u_{mf})/u_B}{i} \quad (3-54)$$

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

$$y_{B,i} = \{y_{Bj,i}\} \quad (j = 1-9) \quad (3-55)$$

$$y_{E,i} = \{y_{Ej,i}\} \quad (j = 1-9)$$

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:

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

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

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

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

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

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

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

$$F_{mBE,i} y_{BE,i} = F_{mBE,i} y_{B,i} \quad \text{if } F_{mBE,i} > 0 \quad (3-58)$$

$$F_{mBE,i} y_{BE,i} = F_{mBE,i} y_{E,i} \quad \text{if } F_{mBE,i} < 0$$

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

$$K_{mBE,i} = K_{BE,i}/(R T_i/p) \quad (3-59)$$
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, $\phi_k$, introduced in section 3-4, therefore, satisfies the population balance equation (see Appendix II).

$$N_k \frac{d(\phi_k (df_k/d\theta)^*)}{df_k} = n_{kf} \phi_k - n_{lw} \phi_k \quad (3-60)$$

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

$$n_{lf} = n_{lw} \quad (3-61)$$

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

$$\frac{d(\phi_k \lambda_k)}{df_k} = B_k (\phi_{lf} - \phi_k) \quad (3-62)$$

where relative reactivity of the adsorbent $\lambda_k$ is defined by

$$\lambda_k = \frac{k_{v1}(T,d_k,F_k)}{k_{v1}(T,d_k,0)} \quad (SO_2 \, reaction) \quad (3-63)$$

or

$$\lambda_k = \frac{k_{v2}(T,d_k,F_k)}{k_{v2}(T,d_k,0)} \quad (H_2S \, reaction)$$

and the parameter $B_k$ is defined as follows:

$$B_k = \begin{cases} \frac{n_{kf} \rho \phi_{lf} \lambda_k \rho \phi_{lf} \lambda_k \rho \phi_{lf} \lambda_k}{N_k M_{Ca} k_{v1}(T,d_k,0) C_3} \quad (SO_2 \, reaction) \\ \frac{n_{kf} \rho \phi_{lf} \lambda_k \rho \phi_{lf} \lambda_k \rho \phi_{lf} \lambda_k}{N_k M_{Ca} k_{v2}(T,d_k,0) C_6} \quad (H_2S \, reaction) \end{cases} \quad (3-64)$$
The solution of Equation (3-62) for the case of fresh limestone feed, namely \( \phi_{\beta} = \delta(f_{\beta}) \), is given as follows (see Appendix III):

\[
\phi_{\beta} (f_{\beta}, \bar{T}, d_{\beta}) = \frac{\frac{B_{\beta}}{\lambda_{\beta}} \exp \left[ - \int_{0}^{f_{\beta}} \frac{B_{\beta}}{\lambda_{\beta}} \, df_{\beta} \right]}{1 - \exp \left[ - \int_{0}^{1} \frac{B_{\beta}}{\lambda_{\beta}} \, df_{\beta} \right]}
\] (3-65)

Therefore,

\[
\hat{k}_{\nu i}(\bar{T}, d_{\beta}) = \int_{0}^{1} k_{\nu i} (\bar{T}, d_{\beta}, f_{\beta}) \phi_{\beta} \, df_{\beta}
\]

\[
= k_{\nu i} (\bar{T}, d_{\beta}, 0) \int_{0}^{1} \lambda_{\beta} \phi_{\beta} \, df_{\beta}
\]

\[
= k_{\nu i} (\bar{T}, d_{\beta}, 0) \hat{\lambda}_{\beta}
\] (3-66)

Using the parameter \( B_{\beta} \) defined by Equation (3-64), the relation (3-37) can be written in a simple form

\[
\hat{f}_{\beta} = \frac{\hat{\lambda}_{\beta}}{B_{\beta}}
\] (3-67)

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 \( \hat{f}_{\beta}, \bar{T} \) and \( d_{\beta} \) by the following technique:

1. Specify \( \bar{T} \) and \( d_{\beta} \)
2. Specify \( B_{\beta} \)
3. Obtain \( \phi_{\beta} (f_{\beta}) \) from (3-65) and calculate \( \hat{\lambda}_{\beta} \)
4. Obtain \( \hat{f}_{\beta} \) from (3-67)
5. Specify another \( B_{\beta} \) and repeat 2-4
6. Specify another \( \bar{T} \) and \( d_{\beta} \) and repeat 2-5
7. \( \hat{\lambda}_{\beta} = \hat{\lambda}_{\beta} (\hat{f}_{\beta}, \bar{T}, d_{\beta}) \) (3-68)
In order to consider the size distribution of the adsorbent, the distribution density function $\phi_{\xi S}(d_\xi)$ is introduced as

$$\left( \begin{array}{c}
\text{number fraction of absorbent} \\
\text{particles which have the} \\
\text{diameter between } d_\xi \text{ and } d_\xi + \Delta d_\xi \\
\end{array} \right)
\frac{d(d_\xi)}{d_\xi} = \phi_{\xi S}(d_\xi) \ d(d_\xi)$$

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

$$< \hat{\lambda}_\xi > = \int_{0}^{d_{\max}} \hat{\lambda}_\xi (\hat{f}_\xi, \overline{T}, d_\xi) \ \phi_{\xi S}(d_\xi) \ d(d_\xi) \quad (3-69)$$

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, $\theta_c$, 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.
POINTS NOT INCLUDED IN LEAST SQUARES CALCULATION

\[ t_c \] BURN-OUT TIME (s)

\[ (d_i^2) \] (INITIAL AVERAGE CHAR PARTICLE DIAMETER)\(^2\)(mm\(^2\))

- \( d_a = 0.39 \text{ mm} \);
- \( m = 3.6 \text{g CARBON} \);
- \( U_0 = 46 \text{ mm/s} \);
- \( \rho_c = 720 \text{ kg CARBON/m}^3 \)

(a) \( U = 214 \text{ mm/s} \); (b) \( U = 300 \text{ mm/s} \); (c) \( U = 383 \text{ mm/s} \)

-Burn-out time as a function of the initial average char particle diameter (Avdesian and Davidson (1973)).
\[ n_{d,i} = \begin{cases} > 0 & \text{if } v_{E,i} < 0 \\ 0 & \text{if } v_{E,i} \geq 0 \end{cases} \quad i = 2, I_t \]

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

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:

\[ N_{B,i} \phi_{B,i}(0) \frac{dy}{dy_{B,i,y}} = \begin{cases} n_{BE,i} - n_{EB,i} - n_{B,i-1} + n_{B,i} & \text{if } \text{i = 1, I}_c \\ n_{B,i} + n_{u,i} + n_{d,i+1} + n_{w,i} & \text{if } \text{i = 1, I}_t \end{cases} \]

\[ N_{E,i} \phi_{E,i}(0) \frac{dy}{dy_{E,i,y}} = \begin{cases} n_{EB,i} - n_{BE,i} - n_{E,i-1} - n_{E,i} & \text{if } \text{i = 1, I}_c \\ -n_{d,i+1} + n_{u,i} + n_{d,i} + n_{w,i} & \text{if } \text{i = 1, I}_t \end{cases} \]

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

\[ \int_0^1 \phi_{B,i} \, dy = \int_0^1 \phi_{E,i} \, dy = 1 \]

The assumption of complete mixing in each compartment is expressed by

\[ N_{B,i} / \Delta V_{sB,i} = n_{B,i} / \Delta V_{sB,i} = n_{BE,i} / \Delta V_{EB,i} \]

\[ N_{E,i} / \Delta V_{sE,i} = n_{d,i} / \Delta V_{sE,i} = n_{u,i} / \Delta V_{sE,i} \]

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:

\[
\Delta V_{sB,i} = \Delta V_{i,ef} e_{B,i} f' W \\
\Delta V_{sE,i} = \Delta V_{i,ef} (1 - e_{B,i} (1 + f' W))(1 - e_{mf}) \\
v_{B,i} = (u_o - u_{mf}) A_t, i f' W (1 - e_{mf}) \\
v_{EB,i} = K_{sBE,i} \Delta V_{i,ef} (1 - e_{B,i}) \\
v_{BE,i} = v_{EB,i} + v_{B,i} - v_{B,i+1} + \varepsilon_{B,i} f' W \Delta V_{i,ef} x_{Cf}^{MC} (1/\rho_{cf} - X_{Af}/\rho_A) \\
v_{u,i} = \begin{cases} v_{E,i} & \text{(if } v_{E,i} > 0) \\ 0 & \text{(if } v_{E,i} \leq 0) \end{cases} \quad i = 2, l_t \quad (3-84) \\
v_{d,i} = \begin{cases} v_{E,i} & \text{(if } v_{E,i} < 0) \\ 0 & \text{(if } v_{E,i} \geq 0) \end{cases} \quad i = 2, l_t \quad (3-85)
\]

From a volume balance for the \( i \)th level

\[
v_{E,i} = v_{net,i} - v_{B,i} \quad (3-86)
\]

The overall volume balance for the \( i \)th compartment gives

\[
v_{net,i+1} = v_{net,i} + v_{B,i} - v_{B,i+1} + v_f,i - v_w,i - \Delta V_{i,M_C}^{MC} x_{Cf}^{MC} \left\{ \left( \varepsilon_{Wi} - \varepsilon_{W,i} \varepsilon_{B,i} \right) r_{cB,i}^* + (1 - \varepsilon_{W,i} - e_{B,i}) r_{CE,i}^* \right\} \\
X(1/\rho_{cf} - X_{Af}/\rho_A) \quad (3-87)
\]

In Equations (3-83) and (3-87) \( \rho_A \) denotes the density of ash particles formed after combustion, and \( r_{cB,i}^* \) and \( r_{CE,i}^* \) are defined as

\[
\begin{align*}
    r_{cB,i}^* &= r_{3B,i}^* + r_{4B,i}^* + r_{5B,i}^* \\
    r_{CE,i}^* &= r_{3E,i}^* + r_{4E,i}^* + r_{5E,i}^*
\end{align*}
\quad (3-88)
\]
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.

$$v_{u,1} = v_{d,1} = v_{B,1} = 0 \quad (3-89)$$

$$v_{u,I_t} + 1 = v_e \quad (3-90)$$

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

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:

$$(dy/d\theta)^*_{B,i} = -\frac{2 M_c}{\rho_{ch} \bar{X}_c \bar{d}_{cm}} (k_3 \bar{C}_1 + k_4 \bar{C}_1 + k_5 \bar{C}_4)_{B,i} \quad (3-91)$$

$$(dy/d\theta)^*_{E,i} = -\frac{2 M_c}{\rho_{ch} \bar{X}_c \bar{d}_{cm}} (k_3 \bar{C}_1 + k_4 \bar{C}_1 + k_5 \bar{C}_4)_{E,i} \quad (3-92)$$

These equations are adequate to determine the axial distribution of size distribution function $\phi_B$ and $\phi_E$ 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 satisfies 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)

\[ w_{B,i-1} x_{B,i-1} + w_{EB,i} x_{E,i} + \Delta \rho_{i} \varepsilon_{B,i} \frac{f^*_{w} r_{CB,i}}{r_{CB,i}} M_{C} \]  

(3-93)

(cloud-emulsion phase)

\[ w_{d,i+1} x_{E,i+1} + w_{u,i-1} x_{E,i-1} + w_{BE,i} x_{B,i} + \frac{w_{f,i} x_{f,i}}{r_{CB,i}} \]

\[ = \left( w_{d,i} + w_{u,i} + w_{EB,i} + w_{w,i} \right) x_{E,i} + \Delta \rho_{i} \left( \varepsilon_{c,i} - \varepsilon_{B,i} \frac{f^*_{w}}{r_{CB,i}} \right) M_{C} \]  

(3-94)

where

\[ w_{B,i} = \rho_{B,i} \]

\[ w_{E,i} = \rho_{E,i} \]

\[ w_{BE,i} = \rho_{BE,i} \]

\[ w_{EB,i} = \rho_{EB,i} \]

\[ w_{u,i} = \rho_{u,i} \]

\[ w_{d,i} = \rho_{d,i} \]

and correspondingly

\[ w_{u,1} = w_{d,1} = w_{B,1} = 0 \]

\[ w_{u,I_{t}} + 1 = \rho_{u,I_{t}} + 1 \]

\[ w_{B,I_{t}} + 1 = w_{d,I_{t}} + 1 = 0 \]  

(3-95)
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)

For $i = I_t$ (top compartment)

\[
N_{B,i} \frac{d}{dy} [\Phi_{B,i}(dy/d\Theta)]_{BW,i} = n_{EB,i} \Phi_{E,i} + n_{B,i-l} \Phi_{B,i-l} - (n_{BE,i} + n_{B,i}) \Phi_{B,i}
\]

For $i = 1$ (bottom compartment)

\[
N_{B,i} \frac{d}{dy} [\Phi_{B,i}(dy/d\Theta)]_{BW,i} = n_{EB,i} \Phi_{E,i} - (n_{BE,i} + n_{B,i}) \Phi_{B,i}
\]

\[
N_{E,i} \frac{d}{dy} [\Phi_{E,i}(dy/d\Theta)]_{CE,i} = n_{BE,i} \Phi_{E,i} - n_{EB,i} \Phi_{E,i} + n_{f,i} \Phi_{f,i}
\]

\[
+ n_{u,i} \Phi_{E,i-l} - n_{E,i} \Phi_{E,i} - (n_{d,i} + n_{w,i}) \Phi_{E,i}
\]

\[
+i = 2, I_t - 1 \quad (3-70)
\]

\[
(i = 2, I_t - 1) \quad (3-71)
\]
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:

\[ c_s \left( (S_i - 1) \ T_{\text{net},i} + w_{\text{mix},i} \right) T_{i+1} \]

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

\[-[c_s \left( S_i \ T_{\text{net},i} + (S_i - 1) \ T_{\text{net},i-1} + w_{\text{mix},i} \right.
\]

\[ + w_{\text{mix},i-1} + w_{\text{wi}} + c_{gm,i} F_{gm} ] T_i \]

(heat flow out from ith cell)

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

(heat flow in from i-1th cell)

\[ + r^* M_i \Delta V_i \left( q_c / X_{ef} \right) - w_{ef} q_i \Delta V_i,ef \left( 1 - e_{\text{Bi}} / V_{mf,ef} \right) \]

(heat generated by combustion of limestone)

\[ + w_{fi} c_{sfi} \left( T_{i} - T_{wi} \right) \]

(heat consumed by calcination of limestone)

\[ + w_{fi} c_{sfi} T_{fi} = U_i c_{H2O} \Delta V_i \left( T_i - T_{wi} \right) \]

(sensible heat recovered by cooling tubes)

where

\[ S_i = \begin{cases} 0 & \text{if } w_{\text{net},i} \leq 0 \\ 1 & \text{if } w_{\text{net},i} > 0 \end{cases} \]
The reaction rate $r_{ci}^*$ in Equation (3-96) is defined by

$$r_{ci}^* = (e_{c,i} - e_{B,i}) r_{cB,i}^* + (1 - e_{c,i} - e_{tube,i}) r_{cE,i}^* \quad (3-98)$$

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

$$w_{\text{net},i} - w_{\text{net},i-1} = w_{f,i} (1 - X_{vf,i}) - w_{w,i} - r_{c,i} M_{AV} \quad (3-99)$$

$$w_{\text{mix}}' = (u_o - u_{mf}) A_f p_s (1 - \varepsilon_{mf}) \quad (3-100)$$

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:

$$\frac{2\lambda'}{d_c} (T_c - T) + \varepsilon' \sigma (T_c^4 - T^4) = r_c (T_c) M_{AV} c_c / X_{Cf} \pi d_p^2 \quad (3-101)$$

where $\varepsilon'$ is the emissivity of particles, $\lambda'$ is the thermal conductivity of the gas surrounding char particles and $\sigma$ 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:

\[ N_c \frac{d\phi^*}{dy} + n_{cw} \phi = n_{cf} \phi_f - n_{ce} \phi_e \]  (4-1)

where

\[ R^* \equiv (dy/d\theta)^* = -2 M c_r^* / (\pi d_c^2 \rho_{cm} \rho_{ch} X_c) \]  (4-2)
\[ r_c^* \equiv \Sigma r_{ci} \Delta V_i / \Sigma \Delta V_i \hat{\phi} (N_c/V_mC_c) \pi d_c^2 k_{c0} \lambda_c (y) \bar{C}_{O2} \]  (4-3)

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

\[ k_{c0} \lambda_c (y) = k_3 k_x \]  (4-4)

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

\[ \int_0^1 \phi(y) dy = 1 \]

is obtained as follows:

\[ \phi \frac{Y(y)}{\lambda_c (y)} \left[ C_c - B_c Y_f (y) \right] \]  (4-5)

where

\[ Y(y) \equiv \exp \left[ B_{cw} \int_0^y \frac{1 + (8A_c/W_b) K^*}{\lambda_c} dy \right] \]  (4-6)
\[
\begin{align*}
Z_f(y) &= \int_0^y \left( \frac{\phi_f}{\lambda} \right) dy \tag{4-7} \\
C_c &= 1 + B_c f \int_0^1 \left[ Y(y) Z_f(y) / \lambda \right] dy / \int_0^1 \left[ Y(y) / \lambda \right] dy \tag{4-8} \\
B_{cw} &= \frac{d_c \rho c h c}{2 M_c \Theta k_{c0} C_{O2}} \tag{4-9} \\
\frac{B_{cf}}{B_{cw}} &= \frac{n_{cf}}{n_{cw}} \tag{4-10} \\
\end{align*}
\]

According to the definition of \( B_{cw} \), we obtain the following relation from Equations (3-26), (3-27) and (3-31):
\[
B_{cw} = \frac{3 < \lambda_c y^2 > (1 - \eta_c)}{(\psi_v + \frac{A_t}{W_b} < \kappa^* y^3 >) \eta_c} \tag{4-11} \\
\]

The gas phase model shown in Section 3-6 gives a solution for the exit oxygen concentration in the form
\[
C_{O2,1} = f_1 \left( N_c < \lambda_c y^2 > \pi d_{cm}^2, k_{c0}, L_f, u_o, u_{mf}, C_{O2,0}, \ldots \right) \tag{4-12} \\
\]

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 \( C_{O2,0} \) 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
\[
F_m (y_{O2,0} - y_{O2,1}) = N_c < \lambda_c y^2 > \pi d_{cm}^2 \frac{k_{c0} C_{O2}}{C_{O2}} \tag{4-13} \\
\]
From Equations (3-25), (3-26) and (3-27) the outlet oxygen concentration can be related to the combustion efficiency as follows:

\[ Y_{02,1} = Y_{02,0} - \frac{w_{cf} X_{Cf}}{M_C} \eta_c \]  

(4-14)

Using Equations (4-12), (4-13) and (4-14), we can obtain the following relationship between \( \eta_c \) and \( k_{c0} \) where the term \( N_c < \lambda_c y^2 > \) and \( C_{02,1} \) are already eliminated.

\[ f_2(k_{c0}, C_{02}, \eta_c, L_f, u_o, u_{mf}, C_{02,0}, ...) = 0 \]  

(4-15)

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

\[ \bar{k}_{c0} Y_{02} = \bar{k}_{c0} \left[ Y_{02,f} \frac{F_{mf}}{F_m} - w_{cf} X_{Cf} \eta_c / M_C \right] \]  

(4-15)\(^{-}\)

In the case of plug flow we obtain

\[ \bar{k}_{c0} Y_{02} = \bar{k}_{c0} \left[ \frac{w_{cf} X_{Cf} \eta_c}{M_C F_m} \right] / \ln \left[ 1 - \frac{w_{cf} X_{Cf} \eta_c}{M_C F_{mf} Y_{02,f}} \right] \]  

(4-15)\(^{-}\)

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 \( \bar{k}_{c0} Y_{02} \) analytically and numerical solution by iteration technique becomes necessary.

By an overall heat balance, the bed temperature \( \bar{T} \) is obtained as

\[ \bar{T} = \left[ \begin{array}{c} c_{gm} F_m T_{gt} + c_{cf} w_{cf} T_{cf} + c_{lf} w_{lf} T_{lf} \\ \end{array} \right] + q_c w_{cf} (1 - \eta_c) - q_k w_{kf} + U A_{HE} \frac{T}{w} \]  

(4-16)
START

ASSUME BED TEMPERATURE, T.

ASSUME COMBUSTION EFFICIENCY, \( n_c \).

CALCULATE \( k_{cO_2} \) FROM EQUATION (4-15).

ASSUME MEAN RESIDENCE TIME, \( \theta \):

CALCULATE \( B_{cW} \) FROM EQUATION (4-9).

ASSUME CHAR HOLD-UP, \( n_c \).

CALCULATE \( n_{cw} \) FROM EQUATION (3-30).

CALCULATE \( n_c \) FROM EQUATION (3-31).

NO
TEST FOR \( n_c \) CONVERGENCE.

YES
CALCULATE \( \theta \) FROM EQUATION (3-32).

NO
TEST FOR \( \theta \) CONVERGENCE.

YES
CALCULATE \( B_{cw} \) FROM EQUATION (4-11).

NO
TEST FOR \( B_{cw} \) CONVERGENCE.

YES
CALCULATE T BY ENERGY BALANCE (4-16).

NO
TEST FOR T CONVERGENCE.

YES
STOP

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 - $I_t$) 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 5-9 may still hold even the above assumptions are made. Because of the assumption (1), equations for $\phi$ 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, $x_i$:

$$
\begin{align*}
\{(S_i - 1)w_{\text{net},i} + w_{\text{mix},i}\} x_{i+1} \\
-(S_i w_{\text{net},i} + (S_i - 1)w_{\text{net},i-1} + w_{\text{mix},i} + w_{\text{mix},i-1} + w_{\text{fi}})x_i \\
+(S_{i-1} w_{\text{net},i-1} + w_{\text{mix},i-1}) x_{i-1} \\
= T^*_c \Delta V_i,ef M_C - w_{\text{fi}}x_{fi} 
\end{align*}
$$

\text{ORIGINAL PAGE IS OF POOR QUALITY}
The net flow rate, $w_{\text{net},i}$, 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 $Y_B$ or $E_i$ denote the mole fraction of oxygen, equations (3-56) and (3-57) become,

\[
F_{Bm,i} Y_{B,i} - F_{Bm,i-1} Y_{B,i-1} + (1 - 0.5 \frac{e_{CO}}{e_{CO}}) r_{CB,i}^* v_{CB,i} e_{W,i} \]

\[= K_{BE,i} (P/RT_i) \Delta V_i e_{B,i} (Y_{E,i} - Y_{B,i}) \quad (5-2)\]

\[
F_{Em,i} Y_{E,i} - F_{Em,i-1} Y_{E,i-1} + (1 - 0.5 \frac{e_{CO}}{e_{CO}}) r_{CE,i}^* \Delta V_i \]

\[\times (1 - e_{W,i} - e_{B,i} - e_{\text{tube},i}) \quad (5-3)\]

\[= K_{BE,i} (P/RT_i) \Delta V_i e_{B,i} (Y_{E,i} - Y_{B,i}) \]

Let $Y_B$ or $E_i$ designates either mole fraction of sulfur dioxide or hydrogen sulfide, depending on the case, we get

\[
F_{Bm,i} Y_{B,i} - F_{Bm,i-1} Y_{B,i-1} + \Delta V_i e_{W,i} r_{Xf} \frac{X_{f}}{X_{c,f}} r_{CB,i}^* \]

\[= K_{BE,i} (P/RT_i) \Delta V_i e_{B,i} (Y_{E,i} - Y_{B,i}) \quad (5-4)\]
\[ F_{E,m,i} Y_{E,i} - F_{E,m,i-1} Y_{E,i-1} + \Delta V_i (1 - H_{E,i} - H_{B,i} - H_{tube,i}) \]

\[ \times (r_{E,i}^{*} - r_{E,i}^{*}) = K_{E,B,i} (P/RT_i) \Delta V_i E_{B,i} (Y_{B,i} - Y_{E,i}) \]

where the term \( (X_{SF}/X_{CF}) \) denotes the generation rate of SO\(_2\) or H\(_2\)S.

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)

\[ Y_{E,0} = Y_{B,0} = Y_{O2,0} \frac{F_m}{F_m} \]
2) For Equations (5-4) and (5-5)
\[ Y_{E,0} = Y_{B,0} = Y_{SO_2,f} \frac{F_{mf}}{F_m} \]

of \[ Y_{H_2S,f} \frac{F_{mf}}{F_m} \]

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

\[ w_{net,1} = 0 \]

\[ w_{net,I_t+1} = w_e \]

\[ w_{mix,1} = 0 \]

\[ w_{mix,I_t} = 0 \]

4) For Equation (3-96)

\[ T_0 = T_{gf} \]

\[ c_{gm0} = c_{gmf} \]

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.
FIGURE 7 (CONTINUED)

* NO  \[ T_{\text{norm}} \leq 0.01 \ast T_{\text{AV}} \]

YES

PRINT

\( SO_2 \text{ CAPTURE} \)

\( n_s = 1 \) (INITIAL VALUE)

\( f = n_s/\text{CABSE} \)

\( n_s = 1 - \frac{\text{MODEL} \text{SO}_2 \text{IN OUTLET GAS}}{\text{TOTAL MOLES S FED}} \)

\( \gamma_{B1}, \gamma_{E1} \) FROM Eqs. 5-4, 5-5

SUBROUTINE \text{CRECT}

NO

\( |n_s - n_s, \text{ASSUMED}| \leq \text{TOLERANCE} \)

YES

PRINT

STOP
Section VI

LISTS OF LEVEL I AND II COMPUTER PROGRAMS

6-1. LEVEL I PROGRAM
A MODEL FOR COMBUSTION AND FLUTRITATION BEHAVIORS OF A FLUIDIZED BED COMBUSTOR

M. HORIN 1976

MOLYCAL WEIGHT

<table>
<thead>
<tr>
<th>Species</th>
<th>Weight</th>
</tr>
</thead>
<tbody>
<tr>
<td>KAl</td>
<td>0.271</td>
</tr>
<tr>
<td>MCP</td>
<td>0.271</td>
</tr>
<tr>
<td>KH2O</td>
<td>0.271</td>
</tr>
<tr>
<td>KH2C</td>
<td>0.271</td>
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DIMENSION

<table>
<thead>
<tr>
<th>Variable</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>DPF</td>
<td>35</td>
</tr>
<tr>
<td>FRACT</td>
<td>35</td>
</tr>
</tbody>
</table>

PARAMETERS

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>NDF</td>
<td>1.0</td>
</tr>
<tr>
<td>NASH</td>
<td>1.0</td>
</tr>
<tr>
<td>ETC</td>
<td>1.0</td>
</tr>
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</table>

CONTANTS

<table>
<thead>
<tr>
<th>Constant</th>
<th>Value</th>
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</thead>
<tbody>
<tr>
<td>IF</td>
<td>1</td>
</tr>
<tr>
<td>IF2</td>
<td>2</td>
</tr>
<tr>
<td>IF3</td>
<td>3</td>
</tr>
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</table>

LIMESTONE

<table>
<thead>
<tr>
<th>Component</th>
<th>Weight</th>
</tr>
</thead>
<tbody>
<tr>
<td>KHLS</td>
<td>0.5</td>
</tr>
<tr>
<td>KHLC</td>
<td>0.2</td>
</tr>
</tbody>
</table>

OUTPUT

<table>
<thead>
<tr>
<th>Name</th>
<th>Properties</th>
</tr>
</thead>
<tbody>
<tr>
<td>NAME1, NAME2</td>
<td>XCF, XCV, XH, XS, XC, XN, XW, XN</td>
</tr>
</tbody>
</table>

ORIGINAL PAGE IS OF POOR QUALITY
CONTINUE

CALCULATION OF NUMBER FRACTION FROM WEIGHT FRACTION

DO 7 1=1,N
FRACT(1)=FRACT(1)*DPF(N)/(DPF*SUM)
7 CONTINUE

INPUT 2 OPERATING CONDITIONS

IF(T<0.0) GO TO 3

PDPF=DPF(1)

THEORETICAL AIR FLOW RATE FMT FL (MCLF/SEC)

A=2./((XH/MH*2.0+XS/MS+XC/XC0)*MC/XC+1.)
A1=XH/MH*0.5+XC/MC+XH2/XH+MC+XG0/XC-1.
A2=1+EXA2*EXA1*FMTFA xa*FMTFA1*WCCAL

IF(UN<0.0) UN=0.01

CALCULATION OF HYDRODYNAMIC PARAMETERS

UMF=(VISC/1.2)*FMTFA/(SQT(33.7)*(0.2*1.0*DPF*DPF*SUM)))
UM=0.71*SQT(G*DB)
USE=3.3*SQT(GACT)
IF(IN1=GT=US) UN=US
IF(IN1=GT=US) UN=UMF

G=10.0*UMF/UB

DPFR=DPF*G/1.0*VISCAV*(RHCP/RHOG)*G
PE=DPF*1.0*AVBPOR/RHOG/VMSC
IF(RE=LE*5.76) GC TO 12
PE=DPF/1.0*RCR
DPFR=5*2.5*AM/RHOG/VMSC/(RHCP/RHOG)*G**2)**0.33333*UM
PE=EP*1.0*RCR
IF(RE=LE*5.0) GC TO 12
DPFR =G*2.5*AM/RHOG/((RHCP/RHOG)*1.1)*G
12 CONTINUE

NUT OUT 2

WRITE (F,20044)FLUT, BETA, INXDEL, BHP, EB

CALCULATION OF THE SIZE DISTRIBUTION

INDX=)
INPVX=
A=N
ON 11 1=1,N
DPF(I)=DPF0(I)
15 CONTINUE

16 NCONT=)
A=1
INPVX=)
IF(INPVX<0.0) AND=DPF(I)*2*DPFC) INPVX=0.0
IF(INPVX>1.0) GC TO 14
IF(INPVX<1.0) GC TO 16
IF(INPVX<0.0) GC TO 14
INPVX=1.0
2=DPF(1+1)
CALCULATION OF THE REACTIVITIES OF CHAR PARTICLE ALAM(I) AND ELUTRIATION RATE CONSTANT, AKE(I)

```
0000 0040 DPO(I)=G(DP(I))
0000 0041 IF(AKE(I)>0.15) AKE(I)=AE(I)=AD(I)
0000 0042 IF(AKE(I)<0.15) AKE(I)=AE(I)=AD(I)/1.5
0000 0043 IF(AKE(I)<0.1) AKE(I)=AE(I)=AD(I)/3
0000 0044 IF(AKE(I)<0.01) AKE(I)=AE(I)=AD(I)/30
0000 0045 GO TO 25
0000 0046 CONTINUE
0000 0047 25 AKE(I)=AE(I)=AD(I)
0000 0048 GO TO 26
0000 0049 121 CONTINUE
0000 0050 AKE(I)=AD(I)*RHOG*UO*(1+1/2)*UTF*
0000 0051 (1+1/2)*UTF*
0000 0052 DPO(I)*G(DP(I))
0000 0053 IF(AKE(I)>0.15) AKE(I)=AE(I)=AD(I)
0000 0054 IF(AKE(I)<0.15) AKE(I)=AE(I)=AD(I)/1.5
0000 0055 IF(AKE(I)<0.1) AKE(I)=AE(I)=AD(I)/3
0000 0056 IF(AKE(I)<0.01) AKE(I)=AE(I)=AD(I)/30
0000 0057 GO TO 25
0000 0058 CONTINUE
0000 0059 25 AKE(I)=AE(I)=AD(I)
0000 0060 GO TO 26
0000 0061 122 CONTINUE
0000 0062 RET=DPO(I)*UTF*RHOG/VISC
0000 0063 FR=(UC-UTF)*2/(GDP(I))
0000 0064 KG=RET*AD(I)
0000 0065 AKE(I)=AD(I)*0.015*G/KG+G*KG*FR*VISC/DPI(I)
0000 0066 GO TO 123
0000 0067 123 CONTINUE
0000 0068 AKE(I)=AD(I)*0.52E-5*(UC-UTF)*2*RHOG/SQRT(G/DPI(I))*DPI(I)*UTF*RHOG/VISC**0.725*(RHOG-RHOG)*RHOG**1.15
```

ORIGINAL PAGE IS OF POOR QUALITY
CONTINUE

AEK(I)=AVE**2 *A

DO 22 J=1,L

JMT(J)=A

IF(AEK(J) .GT. A)

JMT(J) = JMT(J)**2 *L

AEK(J) = A

22 CONTINUE

CONTINUE

AK(I) = A

ALAM(I) = 0

DO 30 I = 1,L

AEK(I) = AEK(I-1)/ALAM(I-1)*AEK(I)/ALAM(I)*0.5*DY(I)*AEK(I-1)

ALAM(I) = 1./ALAM(I-1)*1./ALAM(I)*0.5*DY(I)*ALAM(I-1)

30 CONTINUE

PHITTL = SUM

SUM = 0

31 CONTINUE

A=0

B=0

DO 32 I = 2,L

PHIF(I) = PHIF(I)/PHITTL

BR = V(I) ** 2 * PHIF(I)

AA = V(I) ** 2 * BB

SUM = SUM + AA * DY(I-1) * 0.5 * SUM

SUM = SUM + B * BB * DY(I-1) * 0.5 * SUM

AA = 0

BB = 0

32 CONTINUE

ALAMVF = SUM

ALAMVF = UNION

WRITE (6,3006) SUM, ALAMVF

3006 FORMAT (*) SUM = E12.4, ALAMVF = E12.4)

OUT PUT 3 AND A

0200

VCF=WCOAL/RHOC

WLS=CABS*WCOAL*XS*MC/MS

0202

WLS=WLS/RHOLCA

VMF=HLMF*AT

0204

THETM=VMF*(*1.-EMF)/WLS

0205

THI=WCD*X*G/(-PA)/HYMASH*WLS

0206

ETHM=THETM*0.0001

0207

BDEO=THETM*WLS

0208

WRITE (6,2001) WCOAL, WLS, CABS, EXAIR, FMQ, UQ, P, TK, DT, HLMF, AK, DPCR,

1VCF, VLS, THETM, ALAMVF, ANDP, PASH, RHOCASH, ETCMAX

ALF=ALF0

A2=ALF2

DTH=THETM*0.25

DTHC=0

DTHC=0

ETC=1.*EXAIR

IF (ETC.LT.1) ETC=1.

DTHC=0.2*499999

DTHC=0.05

DTHC=0.1

EC=0.0

ITERATION OF ETC (COMBUSTION EFFICIENCY) STATES FROM HERE

0220

VCW=0

0221

BC1=0

ITERATION LOOP FOR ETC, UP TO "500 CONTINUE"

0222

DO 500 IETC=1,30

IF (IETC.LE.0) GO TO 501

INDTH=0

0224

THET=THETM/(*1.+THI*ETC)

500 CONTINUE

ITERATION LOOP FOR THET, UP TO "100 CONTINUE"

0226

DO 200 ITHET=1,30

IF (ITHET.EQ.0) ITHET=0.0001

IF (ITHET.LT.0.01) GO TO 201

XINF=EXAIR/(EXAIR+ALF2)

COX0=(EXAIR+ALF2)*P/(((1.*EXAIR)/XG00+ALF1)*RG*TK)
GO TO (41,42) IMODEL
41 CONTINUE
COXAV=1. - XINF) 1. - ETC) * XINF) * COXO
GO TO 45
42 CONTINUE
COXAV=(1.*XINF) * ETC / ALOG((1.*XINF) * ETC)
CONTINUE
CM
PLUG
GO TO 45
CONTINUE
CM
COXAV= (1. - XINF) * ETC / ALOG((1. - XINF) * ETC)
PLUG
COXAV=COXAV*COXO
CONTINUE
CM
BC=DCM*RHOC*XCIG2VOL*MC*AK*THET*COXAV
IF(ETC.EQ.1. ) GO TO 210
INDBC1=0.
BC1=0.
DBCl=100.
ITERATION FOR BC1 , UP TO "50 CONTINUE"
DO 50 IBCl=1,20
BC1=BC1
EBMAX=ABS(BC1)*0.00005
CALL POP(BC1,BC1,THET,L)
A=(ALAMV+THET*EC)/((1.-ETC)*ALAMVF)
EBCl=BC1*A-BC1
CORRECTION OF BC 1
CALL CRRECT(BC1,INDBC1,DBC1,BC11,BC1,BC12,BC1,BC11,BC12,BC1,EBC1,EBC12,EBC1,EBMAX)
IF(INDBC1.EQ.2)GO TO 51
INDBC1=INDBC1+1.
AND, ABS(BC1-BC10).LT.EBMAX) GO TO 51
CONTINUE
50 CONTINUE
CM
VCF= (1.-ETC)*VCW*(ALAMV+THET*EC)
THETA=THETM/(1. + VCF*VLS+THET*ETC)
WBED=(VCW*RHOP*VLS*TH1*VLS*ETC*RHOASH)*THET
EE=THET-THETA
CORRECTION OF THET
CALL CRRECT(THET,INDTH,ITHET1,ITHET2,THE,EE1,EE2,EE,ETHMAX)
XX=ABS(THET-ETH)
IF (XX.LE.ETHMAX) GO TO 210
THET=THE
IF (INDTH.EQ.2) GO TO 210
CONTINUE
200 CONTINUE
201 CONTINUE
WRITE(6,3000)
CONTINUE
210 CONTINUE
WBBC=0.
IF (ETC.EQ.1) GO TO 212
BCR=(1.-ETC)*3.*ALAMA/((ALAMV+THET*EC)*ETC)
212 E=BC-BBC1/(BC+BBC1)*2.
CORRECTION OF ETC
CALL CRRECT(ETC,INDETC,DET1,ETC,ETC1,ETC2,ETC,E1,E2,E,EETCM)
HR=AB/((ETC-ETCOLO)
IF (XX.EQ.6.0.-16.0) GO TO 510
IF (INDETC.EQ.2) GO TO 510
ELoss=1. -ETC-VCW*VCF
XG0=(1.-ETC)*A2*EXAIR)*XG0/(AL*EXAIR)
HCHAR=THET*VCW*RHOP
HCARBN=THET*VCF*RHOC*VCF
HRC=HCARBN*WBED
CONTINUE
500 CONTINUE
501 CONTINUE
WRITE(6,3001)
CONTINUE
510 CONTINUE
AL1=AT/(WBED*EC)
YA1=0.
YB1=0.
YCl=0.
PHIF1(1)=0.
PHIW1(1)=0.
PHIE1(1)=0.
DO 500 I=2,L
YA2=YA1
YA2=YA1
CONTINUE 520
DO 530 I=201
PXFW=PHFW+1/PHFW(L)
PHFW=PHFW+1/PHFW(L)
CONTINUE 530
ECLOSE=L/ETC-VCW/VCF
XGO=(1-ETC)*2+EXAIR)*XGOO/(A1+EXAIR)
HCHAR=THET*VCW*RHOC*XCF
HCARB=THET*VCW*RHOC*XCF
HC=HCARB/WBED
OUT PUT 5 (RESULTS)
WRITE(6,2000) NAM1,NAM2,XCF,XCV,XH,XS,XG,XN,XW,(DPF(I),FRACP(I),I=1,11,N)
WRITE(6,2001) IELUTR,BETA,MODEL,EB,EB
WRITE(6,2002) XCOAL,WLS,CABS,EXAIR,FMO,UO,P,TK,DT,HLMF,AK,OPCR,
VCF,VLS,THETM,ALAMVF,ANDP,PASH,RHOSH,EETC,ETHMAX
WRITE(6,2003) Y(1),DPF(I),PHIF(I),PHI(I),PHIFW(I),PHIWW(I),PHIEW(I),I=1,11,L
WRITE(6,3005) Y(1),DPF(I),PHIF(I),PHI(I),PHIFW(I),PHIWW(I),PHIEW(I),I=1,11,L
CONTINUE 700
CONTINUE 800
GO TO 10
1000 FORMAT(2A4.7F8.0,14)
1001 FORMAT(2A4.7F8.0,14)
2000 FORMAT(1H1,1X,10F12.4)
2001 FORMAT(1H1,1X,10F12.4)
2002 FORMAT(1H1,1X,10F12.4)
2003 FORMAT(1H1,1X,10F12.4)
2004 FORMAT(1H1,1X,10F12.4)
2005 FORMAT(1H1,1X,10F12.4)
3000 FORMAT(1H1,1X,10F12.4)
3001 FORMAT(1H1,1X,10F12.4)
3002 FORMAT(1H1,1X,10F12.4)
3003 FORMAT(1H1,1X,10F12.4)
3004 FORMAT(1H1,1X,10F12.4)
3005 FORMAT(1H1,1X,10F12.4)
3006 FORMAT(1H1,1X,10F12.4)
3007 FORMAT(1H1,1X,10F12.4)
3008 FORMAT(1H1,1X,10F12.4)
3009 FORMAT(1H1,1X,10F12.4)
3010 FORMAT(1H1,1X,10F12.4)
3011 FORMAT(1H1,1X,10F12.4)
3012 FORMAT(1H1,1X,10F12.4)
3013 FORMAT(1H1,1X,10F12.4)
3014 FORMAT(1H1,1X,10F12.4)
3015 FORMAT(1H1,1X,10F12.4)
3016 FORMAT(1H1,1X,10F12.4)
3017 FORMAT(1H1,1X,10F12.4)
3018 FORMAT(1H1,1X,10F12.4)
3019 FORMAT(1H1,1X,10F12.4)
3020 FORMAT(1H1,1X,10F12.4)
3021 FORMAT(1H1,1X,10F12.4)
3022 FORMAT(1H1,1X,10F12.4)
3023 FORMAT(1H1,1X,10F12.4)
3024 FORMAT(1H1,1X,10F12.4)
3025 FORMAT(1H1,1X,10F12.4)
3026 FORMAT(1H1,1X,10F12.4)
3027 FORMAT(1H1,1X,10F12.4)
3028 FORMAT(1H1,1X,10F12.4)
3029 FORMAT(1H1,1X,10F12.4)
3030 FORMAT(1H1,1X,10F12.4)
3031 FORMAT(1H1,1X,10F12.4)
3032 FORMAT(1H1,1X,10F12.4)
3033 FORMAT(1H1,1X,10F12.4)
3034 FORMAT(1H1,1X,10F12.4)
3035 FORMAT(1H1,1X,10F12.4)
3036 FORMAT(1H1,1X,10F12.4)
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
C
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.LT.E)INDX=1
IF(INDX.EQ.1)GO TO 150
10 X1=X2
E1=E2
XNEW=XNEW+DX
RETURN
150 CONTINUE
XNEW=(X1-X2)*E2/(E2-E1)+X2
RETURN
END
SUBROUTINE POP(BC, BC1, THET, L)

THIS SUBROUTINE

CALCULATES THE SIZE DISTRIBUTION DENSITY FUNCTION
PHI(I) AND SECOND AND THIRD MOMENTS AND AVERAGE VALUE OF
ELUTRIATION CONSTANT * PARTICLE VOLUME
FOR GIVEN BC, BC1 AND THET.

COMMON Y(201), DY(200), PHIF(201), PHI(201), AKE(201), AKEI(201), YY(201)
1, ZF(201), CC, ALAMV, ALAMA, EC, WBED, AT
Z, ALAM(201), ALAMI(201)
ZFC::= 0.
SUM1=0.
SUM2=0.
X1= 0.
DO 100 I=1, L
A=(ALAMI(I)*THET*AKEI(I)*AT/WBED)*BC
IF(A.LT.0.1E-30)A=0.0
YY(I)=EXP(A)
X2=X1
IF(I.EQ.1)GO TO 100
ZF(I)=1./YY(I)+1./YY(I-1))**0.5*PHIF(I)*DY(I)+ZF(I-1)
X1=YY(I)/ZF(I)/ALAM(I)
SUM1=(YY(I)/ALAM(I)+YY(I-1)/ALAM(I-1))**0.5*DY(I)+SUM1
SUM2=(X1+X2)**0.5*DY(I)+SUM2
CONTINUE
100 SUM2=0.
SUM3=0.
A11=0.
A12=0.
A31=0.
A32=0.
DO 200 I=1, L
PHI(I)=(-BC1*ZF(I)+CC)*YY(I)/ALAM(I)
A11=PHI(I)**2
A21=A11**2
A12=A11*YY(I)
A31=A21*AKEI(I)
SUM1=(A11**2)*0.5*DY(I)+SUM1
SUM2=(A21+A32)*0.5*DY(I)+SUM2
SUM3=(A31+A32)*0.5*DY(I)+SUM3
CONTINUE
200 SUM2=SUM1
SUM3=SUM2
ALAMV=SUM3
ALAMA=SUM1
RETURN
END
FUNCTION ACTIV (Y,DCM,RHOG,VISC,D,AK,UD)

REACTIVITY OF CHAR AS A FUNCTION OF PARTICLE SIZE, GAS VELOCITY AND TEMPERATURE

DP=Y*DCM
IF(DP.LE.0.00001)DP=0.00001
SC3=(VISC/(PHOG*D))**0.3333
REP=UO*RHOG*DP/VISC
A1=0.1
SHP=REP**1.2*A1*SC3
SHP=2.
AKF=SHP*D/DP
ACTIV=1./(AK/AKF+1.)
RETURN
END
FUNCTION FREEFV(DP,RHOP,RHOG,VISC)
CALCULATION OF TERMINAL VELOCITY LT
FREE FALL VELOCITY

G=980.1
UT=(RHOP-RHOG)*G*DP*DP/(18.*VISC)
RET=UT*RHOG*DP/VISC
IF(RET.LE.5.76)GO TO 40

UT=(((RHOP-RHOG)*G)**2*4.)/(225.*RHOG*VISC)**0.33333*DP
RET=UT*RHOG*DP/VISC
IF(RET.LE.54.0)GO TO 40

UT=SQRT((RHOP-RHOG)*3.1*G*DP/RHOG)
FREEFV=UT
RETURN
END
6-2. LEVEL II PROGRAM
SIZE DISTRIBUTION OF LIMESTONE OR DOLOMITE PARTICLES

NDPAD : TOTAL NUMBER OF SIZE INTERVALS
DPADF : UPPER ROUND OF EACH SIZE INTERVAL
FRACFA : WEIGHT FRACTION

RFAC(5.1000) NDPAD
READ(5.1001)(DPADF(I),I=1,NDPAD)
READ(5.1001)(FRACFA(I),I=1,NDPAD)

SUM = FRACFA(I)*2.0 / DPADF(I)
DPADR = FRACFA(I)*SUM / DPADF(I)

DO 10 I = 2,NDPAD

DPBAR = (DPADF(I) + DPADF(I-1)) * 0.5
SUM = FRACFA(I) / DPBAR + SUM
DPADR = FRACFA(I) * DPBAR + DPADR
10 CONTINUE

DPADH = 1.0 / SUM

DPADH : SURFACE VOLUME MEAN DIAMETER FOR HYDRODYNAMIC CALCULATION
DPADR : WEIGHT MEAN DIAMETER FOR REACTION RATE CALCULATION

DPB = DPADH

DPB : AVERAGE PARTICLE SIZE OF BED PARTICLES

COMPOSITION OF ADDITIVES

READ(5.1010)NAMEL1,NAMEL2,XCACO3,XMGO3

COMPOSITION AND NET HEATING VALUE OF COAL

READ(5.1010)NAMEC1,NAMEC2,XCF,XCV,XH,XS,XN,XW,OCOAL
XCF+XCV

XCF : FIXED CARBON
XCV : VOLATILE CARBON
XH : HYDROGEN
XS : SULPHUR
XN : NITROGEN
XW : MOISTURE

QCAL : CAL/GRAM

OPERATING CONDITIONS (BED CONDIT)
IF (TF .EQ. 0.0) TF = 298.0

XGF (1) : FEED GAS COMPOSITION (MOLE FRACTION)

<table>
<thead>
<tr>
<th>XGF</th>
<th>CO2</th>
<th>CO</th>
<th>H2O</th>
<th>H2S</th>
<th>H2</th>
<th>N2</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.2</td>
<td>0.2</td>
<td>0.2</td>
<td>0.2</td>
<td>0.2</td>
<td>0.2</td>
<td>0.2</td>
</tr>
</tbody>
</table>

GZCO, GZH2S, GZH2 --- USED ONLY FOR FUEL RICH CASE
GZCO : (C0 FORMATION RATE)/ (CARBON COMBUSTION RATE)
GZH2S : (H2S FORMATION RATE)/ (SULPHUR FEED RATE)
GZH2 : (H2 FORMATION RATE FROM COAL)/(H2+H20 FROM COAL)

QCOALC : HEAT OF COMPLETE COMBUSTION CAL/G (COAL)
QCOAL : HEAT OF INCOMPLETE COMBUSTION CAL/G (COAL)

QCOAL = QCOALC - 67636.*GZCO*XG / MC

RFAD = IF (WCOAL .LE. 0.0) 1000.0 IF (WCOAL .GT. 0.0) 0.0

A2 = (1.0 - GZCO)*WCOAL*(1.0 - XW)/MC

FMTH = MC*(1.0 - XW)/MC + FMF / (1.0 - XW)

FMF = FMF*FMTH

AG(1,2) = (AG(1,1) - GZCO*XG*0.5/MC + AG(1,3)*MC/MGOF)*FMF/(1.0 - XW)

AG(1,3) = (AG(1,2) - AG(1,4)*MC/MGOF)*WCOAL/FMO

AG(1,4) = (AG(1,3) - WCOAL*(1.0 - XW)*MGOF*FMF/(1.0 - XW)) / (MC/MGOF)

AG(1,5) = (AG(1,4) - WCOAL*XG*0.5/MC + AG(1,6)*MC/MGOF)*FMF/(1.0 - XW)

AG(1,6) = (AG(1,5) - GZCO*XG*0.5/MC + AG(1,7)*MC/MGOF)*FMF/(1.0 - XW)

AG(1,7) = AG(1,6) + AG(1,4)

RHOCH : DENSITY OF CHAR
RHOCAO : DENSITY OF CALCINED ADDITIVE

RHOC = (1.0 - XH - XO)*RHOC

IF (IGNITE.EQ.0.0) RHOCAO = RHOC

RHOCAO = (XCAO3*MCACO3 + XMGCO3*MMGD/MMGCC3)*WCAO0.0

ICAB5 = WAD*XCAO3/MCACO3 + 1.0 - XH)*XMS + (XG (3) + XG (6) + MF)

IF (IGNITE.EQ.0.0) RHOCAO = RHOAD

IF (CABS.EQ.0.0) AND (WAD.EQ.0.0)

[WRITE (*,2000) NAME1, NAME2, XCAO3, XMGCO3, (DPADF(I), FPACTA(I), 1 = 1, NOPAD)
DO 25 I = 1, 46
ZAVG(1) = 0.0
X(1) = 0.0
DATA RR(1), RRB(1), RRE(1) = 300.0
T(1) = TAV
CONTINUE

WRITE (6, 2010) DPADH, DPADR
WRITE (6, 2020) NAMEC, NAMEC2, XCF, XCV, XP, XS, XD, XN, XA, XW, OCOAL, OCOALC
WRITE (6, 2030) OPCF, FRACTC(I), I = 1, NDPC
WRITE (6, 2040) OCF, OCAV
WRITE (6, 2050) OPCF
T(1) = TAV
Y(1) = YAV
Y(1) = YAV

DO 25 I = 2, 46
ZAVG(I) = ZAVG(I) + H(I) + M(I-1)
CONTINUE

IF (HLF .LE. FO .AND. VMF .GE. 0.0) VMF = VOLUME(FLMF)
CALL HYDRO
DO 611 I = 2, MT
ZAVG(I) = ZAVG(I) + (H(I) + M(I-1)) * 0.5
CONTINUE

IF (IGNITE .EQ. 0) GO TO 630
ETC = 0.0
YAV = XGF(1)
XCF = XDGAL * XC/(WAD + WAD) * (1 - XM)
FMF = FMO - FEM(I) * AT(I) * PAV
FBM = FMO - FEM(I)
IF (UOW .LE. UMF(I)) FEM(I) = 0.0
115 CONTINUE

IF (IGNITE .EQ. 0) GO TO 630
CONTINUE

C QCLCN = HEAT CONSUMED BY CALCINATION. THIS HEAT CONSUMPTION IS
DISTRIBUTED UNIFORMLY TO EACH COMPT. HAVING TEMP > 900 KELVIN.
C QIN = SENSIBLE HEAT CARRIED IN BY THE FEED SOLIDS AND GAS.
C QIN = (CADF * WAD + CCF * XCF) * TSF - 273) + CGMF * FMF * (TF - 273)
C QCLCN = (42500.0 * XFCO3 / WCAD + WCAD) * (1 - XM) + 23810.0 * XMCO3 / WMCO3) * WAD
C CGMF = 6.8 + 0.5 * (TAV - 273)
C CS = 0.215
C ELLOSS = 0.07
C IF (IFBC .GT. 0) ELLOSS = 0.0
C CELU = WCAD * XC * ELLOSS * (1 - XM)
C WELT = CELU / 0.25
C TAV = 12000
C A4 = WCAD * XC * (1 - XM) * (1 - ELLOSS) / (FMF * MC)
C AMODF = 10.0 * RHOCAD * (1.0 - EMF) / (RHOCAD * DCF)
C PREPARATORY STATEMENTS FOR THE WHOLE ITERATION.
C ETCA = 0.9975
C YAV = FMF * XGF(1) / FMF + A4 * ETCA * (1.0 - 0.5 * GZC3)
C DO 130 I = 2, 46

98 WRITE (6, 2010) DPADH, DPADR
99 WRITE (6, 2020) NAMEC, NAMEC2, XCF, XCV, XP, XS, XD, XN, XA, XW, OCOAL, OCOALC
100 WRITE (6, 2030) OPCF, FRACTC(I), I = 1, NDPC
101 WRITE (6, 2040) OCF, OCAV
102 WRITE (6, 2050) OPCF
103 WRITE (6, 2060) OPCF
104 T(1) = TAV
105 Y(1) = YAV
106 CONTINUE
BOUNDARY CONDITION OF OXYGEN CONCENTRATION

YBO(I) = AG(I,1) + AG(1,2) * ETC
YEO(I) = YBO(I)
YB(I) = YBO(I)
YE(I) = YEN(I)

M1OLD = M1

FROM HERE TO THE STATEMENT NO. 600 : TEMPERATURE ITERATION LOOP

CALL HYDRO

DO 600 ITRIAL = 1, 30

IF (I.EQ.1) FEM(I) = UMF(I) * AT(I) * (1.0 - ETC(I)) * PAV(RG * T(I))

IF (I.EQ.1) FEM(I) = UMF(I) * AT(I) * (1.0 - ETC(I)) * PAV(RG * T(I))

IF(UO(I)).LT.UMF(I) FEM(I) = FMO

FBO(I) = FMO - FEM(I)

IF (ITRIAL .LT. NCF) AND (M1.EQ.M1OLD) GO TO 170

IF(I.EQ.I) FEM(I) = UMF(I) * AT(I) * (1.0 - ETC(I)) * PAV(RG * T(I))

DO 56 I = 2, M1

WF(I) = WFC(I) + WCOAL * (XA(I) + XC(I) * (1.0 - ETC(I)) * (1.0 - XW))

WFAD(I) = WFAD(I) + WCA(I) * FFAD(I)

WF(I) = WF(I) + WFC(I)

WF(I) = WFC(I) + WCOAL * (XA(I) + XC(I) * (1.0 - ETC(I)) * (1.0 - XW))

WFAD(I) = WFAD(I) + WCA(I) * FFAD(I)

DO 133 I = 2, M1

TOLD(I) = T(I)

FROM THE STATEMENT NO. 200 TO 300 : ITERATION OF MATERIAL HALANCE BASED ON THE GIVEN TEMPERATURE PROFILE. GAUSS SEIDEL METHOD

INDEX = 0

DO 200 NT = 1, 30

DET = -0.05

EETCM = 0.01

DO 201 NT = 1, 30

WNET1 = WCA(I) * (1.0 - ETC(I)) * (1.0 - XW)

XAV(C(I)) = WCA(I) * (1.0 - ETC(I)) * (1.0 - XW)

TAVB = (T(I) + TPB(I)) / 2.

TAVB = (T(I) + TPB(I)) / 2.

AM = AMODF * X(I)

X(I) = XAVIC

GENB AND GENE : GENERATION RATE OF OXYGEN

GENB = 0.

GENB = 0.

TCRATE = 0.0

DO 235 I = 2, M1

CALL AKK(AKB, T(I), PAV, DCAV, TPD(I), YB(I), RG)

TAVB = (T(I) + TPB(I)) / 2.

TAVB = (T(I) + TPB(I)) / 2.

TAVE(I) = 1.0

AM = AMODF * X(I)

CALL GPHASF (AKB, AKF, AM, PAV, FG, ETUBE(I), EBR(I), EPC(I),

AKB1(I), DVAR(I), FBM1(I), FEM1(I), FEM1(I), TAVB, TAVE, YB(I),

2(I), YE(I), YB(I), YE(I), GENB, GENE)

1 = DVAR(I) * MC

RR(I) = A(K * RRE(I)) * YB(I) * AKB/I TAVB

RRE(I) = A(K * RRE(I)) * (1.0 - EPC(I) - EPC(I) * YE(I)) * AMOTE / TAVE

RR(I) = A(K * RRE(I)) / X(I)

ORIGINAL PAGE IS OF POOR QUALITY
TCRATE = TCRATF + RRB(I) + RPF(I)

WRITE (6,202) I,RRB(I),RPF(I),RR(I),YE(I),YE(I)

WRITE (6,203) I,RRB(I),RRE(I),RR(I),YE(I)

WRITE (6,204) I,WF(I),WFAD(I),AKB(I),AKE(I)

CONTINUE

ETC = MF*XGF(I)+WCOAL*(1.-XW)*XC/MOP-FEM(M1)*YB(M1)-FEM(M1)*YF(M1)

ETC = ETCG/FMTH*XGF(1)-FLL0S

RPF(I) = RR(I) * TCAR / TCRATE

RRE(I) = RRE(I) * TCAR / TCRATE

BB = AKE(I) * DVBH(I) * EP9(I) * PAV / (PG * T(I))

YB(I) = 0.0

YF(I) = (-YB(I)*R8+BRJ,)/(BB+F_M(I))

IF(J1.GT.MDIS)GO TO 61

WD(M1)=WD(M1)+WDIS*FD(J)

CONTINUE

WMIX(I) = AT(I)*(1.0-ETUBE(I))*ETC(I)+WCAD*YF(I)+WCOAL*(1.-XW)*XC*WFD(I)

WORDER(I) = WD(I)+WDIS*FD(J)

CONTINUE

WMIX : UP- AND DOWN-WARD SOLID MIXING FLOW WHICH IS SUPERPOSED ON FLOW OF SOLIDS. G/SEC

WNET(I) : NET FLOW RATE OF SOLID FROM THE TOP OF I-TH COMPARTMENT. POSITIVE VALUE MEANS THE UPWARD FLOW.

DO 255 I=2,NI

WNET(I)=WNET(I-1)+WF(I)+WFAD(I)-WDIS*FD(J)

IF(J1.GT.0) S(I)=1.

WMIX(I)=AT(I)*(1.0-ETUBE(I))*ETC(I)+WCAD*YF(I)+WCOAL*(1.-XW)*XC*WFD(I)

WORDER(I) = WD(I)+WDIS*FD(J)

CONTINUE

WMIX : UP- AND DOWN-WARD SOLID MIXING FLOW WHICH IS SUPERPOSED ON FLOW OF SOLIDS. G/SEC

WNET(I) : NET FLOW RATE OF SOLID FROM THE TOP OF I-TH COMPARTMENT. POSITIVE VALUE MEANS THE UPWARD FLOW.

DO 255 I=2,NI

WNET(I)=WNET(I-1)+WF(I)+WFAD(I)-WDIS*FD(J)

IF(J1.GT.0) S(I)=1.

WMIX(I)=AT(I)*(1.0-ETUBE(I))*UD(I)-UMF(I)*EMF(I)+RHOCAD*FW
IF(WMIX(I).LT.0.9)WMIX(I)=0.45
CONTINUE
WMIX(M1)=0.

CARBON CONCENTRATION CALCULATION.

MM=M*M
DO 411 I=1,MM
AAA(I)=0.
DO 412 I=1,M
BBB(I)=0.
AAA(1)=-RR(2)-WMIX(2)-WNET(2)*S(2)-WD(2)
AAA(M1)=WMIX(2)+(S(2)-1.)*WNF_T(2)
AAA(MM)=-RR(M1)-WMIX(M)-S(M1)*WNET(M1)-(S(M)-1.)*WNET(M)-WD(M1)
AAA(MM-M)=S(M)*WNET(M)+WMIX(M)

11=I+1
IF (WFC(I1).NE.0.0 OR. WFA_D(I1)*NE.*0.0)
BBB(I)=-WFC'(11)*A1/(WFC(11)+WFA_D(I1))
CONTINUE

20=M-1
DO 270 1=20,M0
II=(1-11*M+I
L1=I+1
AAA(I1)=-RR(I1)-WMIX(I1)-WMIX(T)-S(I1)*WNET(I1)-(S(T)-1.)*WNET(T)-WD(I1)
AAA(II-M)=S(I)*WNET(I)+WMIX(I)
AAA(TI+M)=(S(I1)-1.)*WNET(I1)+WMIX(I1)

CALL SIMQ(AAA, BBB, M, KS)
SUM=0.
SUM2=0.
DO 280 1=1, M
X(I+1) = BBB(I)
SUM2=SUM2+X(I+1)
XAV=SUM2/FLOAT(M)
SUM=0.
DO 285 I=2, M1
SUM=RR(I)*X(I)+SUM
CONTINUE

CLOS = SUM - CFLU
ETCC = 1.0 - SUM / ( WCOAL * XC * (1.-XW) *(1.-ELLOSS) )
DO 220 I = 2, M1
WRITE (6,206) I,WO(I),WNET(I),X(I),ETCC, XAV
C*WRITE (6,3400) I,WO(I),WNET(I),X(I),ETCC, XAV
C*DO 211 ETC = 1. - CLOS / ( WCOAL * XC * (1.-XW) )
C*DO 220 ETC = 1.0 - CLOS / ( WCOAL * XC * (1.-XW) )
C*DO 220 ETC = 1.0 - CLOS / ( WCOAL * XC * (1.-XW) )
C* CALL CORRECT (NT,INDEX,OFTC,ETC1,ETC2,ETCA,EL,EF,ETCM)

IF (INDEX. EQ. 2) GO TO 211
CONTINUE

201 WRITE (6,3400)
FORMAT (I*0.10X. & ETCA HAS NOT CONVERGED. S.NO. = 3400')
CONTINUE

E= ETCC - ETCA
EE = ETCC - ETCA
CALL CORRECT (NT,INDEX,OFTC,ETC1,ETC2,ETCA,EL,EF,ETCM)
IF (INDEX. EQ. 2) GO TO 211
CONTINUE

3400 FORMAT (I*0.10X. & ETCA HAS NOT CONVERGED. S.NO. = 3400')
3201 CONTINUE
3202 CONTINUE
3203 SUM=0.
3204 SUM=0.
3205 SUM=RR(I)*X(I)+SUM
3206 SUM=RR(I)*X(I)+SUM
3207 CONTINUE
3208 CONTINUE

C THE DEFINITION OF RR(I) IS CHANGED FOR TEMPERATURE CALCULATIONS.
C RR(I)=HEAT GENERATION RATE/HEAT CONSUMPTION RATE IN THE ITH COMPARTMENT.

10C=0
DO 291 1=2, M1
IF (T(I1).LT.900.) 291,291,292
I0C=10C+1
CONTINUE

DOCAL = 0.0
IF (10C .GT. 0) DOCAL = OCLCN/FLOAT(10C)
DO 295 1=2, M1
AOCAL=1.
IF (T(I).LE.900.) AOCAL=0.

CLOS = SUM - CFLU
ETCC = 1.0 - SUM / ( WCOAL * XC * (1.-XW,))

STOP
END
RR(I) = RR(I) * X(I) / SUM * QCAL * WCAL * ETC - DQCAL * AQCAL

CONTINUE

CALCULATION OF TEMPERATURE

A1 = CADF * WAD / WCAD
A2 = CCF / (XAD * (1.0 - ETC) * XC)
A3 = CGM / FMO

ALFA(I) = (S(I) + WMIX(I) + WMIX(I) + WD(I)) * CS + A3 + UHE(I) * AHEAV(I) * DVBB(I)

DELTA(I) = RR(I) * A1 * WFAD(I) + A2 * WFC(I) * (TSF - 273.1) + UHE(I) * AHEAV(I) * DVBB(I)

CONTINUE

DO 310 I = N

I1 = I - 1

ALFA(I) = (S(I) + WMIX(I) + WMIX(I) + WD(I)) * CS + A3 + UHE(I) * AHEAV(I) * DVBB(I)

BETA(I) = O.

GAMA(I) = (S(I) + WMIX(I) + WMIX(I) + WS(I)) * CS + A3

DELTA(M) = RR(M) * A1 * WFAD(M) + A2 * WFC(M) * (TSF - 273.1) + UHE(M) * AHEAV(M) * DVBB(M)

CONTINUE

DO 501 I = 1, MM

AAA(I) = 0.

DO 502 I = 1, MM

BBB(I) = DELTA(I + 1)

AAA(I) = ALFA(I)

AAA(M) = -BETA(I)

AAA(M - 1) = -GAMA(I)

I1 = I - 1 + M

AAA(I) = ALFA(I + 1)

AAA(I - 1) = -GAMA(I + 1)

AAA(I + 1) = -BETA(I + 1)

CONTINUE

CALL SIMO(AAA, BBB, MM)

TAV = 0.

DO 504 I = 2, MM

T(I) = BBB(I - 1) + 273.1

WRITE (6, 207) I, T(I)

CONTINUE

WRITE (16, 208) TAV

C207 FORMAT ('6F15.5

DO 504 I = 2, MM

WRITE (16, 3001) TAV

CONTINUE

FORMAT ('5F15.5

WRITE (16, 3003)

DO 610 I = 2, MM

CONTINUE

HAREA = HAREA + A1

QTRANS = UHE(I) * A1 + (T(I) - TW(I)) + QTRANS

RR(I) = RR(I) / DVBBEF(I)

ZAVG(I) = (H(I - 1) + H(I)) / 2.0

CONTINUE

QVOL = QTRANS / BEDVOL

IF (HAREA < NE. 0.0) QAREA = QTRANS / HAREA
TPB(I)=T(1)  
TPE(I)=TPE(I)-273.  
TAV=TAV-273.  
WRITE(6,2001)ETC,XAV,TAV,ITRIAL,(I,YB(I),YE(I),X(I),H(I),T(I))  
TA=TAV+273.  
DO 710 I=2,M1  
SREL(I)=0.  
SREL(I)=0.  
SREL(I)=0.  
SREL(I)=0.  
SRELE(I)=0.  
SRELB(I)=0.  
A2=0.  
A2=0.  
A2=0.  
A2=0.  
DO 800 ITRY=1,30  
FS=ETS/CABSE  
AK0=AKAD(FS,DPA,TA)*A2  
A3=1.  
A3=1.  
A3=1.  
A3=1.  
DO 740 I=2,M1  
11=1-1  
AK=AK0  
AK=AK0  
AK=AK0  
AK=AK0  
CALL GPHASE(AK,AK,AM,PAV,KG,ETUBE(I),EPB(I),EPC(I),  
1AKBE(I),DVBE(I),FBM(I),FEM(I),TPB(I),TPE(I),WNET(I),RR(I),I=1,M1)  
ETSC=1.-((FBM(I)*YE(M1)*FEM(M1)*YF(M1))/DENOM
C

CONTINUE
453  CALL CRRECT(TRY,INDX,ETS,EETSN1,ETS,F1,E2,EE,ETSN)
454  IF(INDX.EQ.2) GO TO 810
455  CONTINUE
456  CONTINUE
457  WRITE(6,3500)  ETS HAS NOT CONVERGED. S.NO. = 3500/
458  3500 FORMAT('0*,10X,T')
459  810 CONTINUE

C MAIN OUTPUT 4

C ***********************
C ALL THE PRESSURE DROP GIVEN IN CM OF WATER
C ***********************
C PRESSURE DROP CALCULATION ACROSS THE DISTRIBUTOR

470  WRITE(6,2051)
471  M1 = M1
472  IF (IFBC .EQ. 0) N1 = M1 - 1
473  DPFLU = (1.0-EMF)*(1.0-EPB(I))*(H(I)-H(I-1)) * RHOCAD
474  WRITE(6,2052) I, DPFLU
475  CONTINUE
476  IF (IFBC .EQ. 0) GO TO 930

C PRESSURE DROP CALCULATIONS IN THE FLUIDIZED RED SECTION

477  WRITE(6,2057) 1.000 FORMAT(110)
478  1001 FORMAT(8F10.0)
479  1010 FORMAT(2A4,10X,' XCACO3 = ',F6.3,'XMGCO3 = ',F6.3,'WT.FRAC
480  1011 FORMAT(8F10.0)
481  2000 FORMAT(4/10X,'RESULTS , ALL TEMPERATURES IN C AN

556  XNEW=XNEW+DX  
557  RETURN  
558  100 CONTINUE  
559  IF(E1.EQ.E1.LT.0.) GO TO 110  
560  E1=E  
561  X1=XNEW  
562  GO TO 150  
563  110 E2=E  
564  X2=XNEW  
565  150 CONTINUE  
566  XNEW=(X1-X2)*E2/(E2-E1)*X2  
567  RETURN  
568  END  

569  SUBROUTINE SIMO(A,B,N,KS)  
570  DIMENSION A(2116).B(46)  
571  C FORWARD SOLUTION  
572  TOL=0.0  
573  KS=0  
574  JJ=N  
575  JY=J+1  
576  BIGA=0  
577  IT=J-J  
578  DO 65 J=1,N  
579  DO 30 I=J,N  
580  SEARCH FOR MAXIMUM COEFFICIENT IN COLUMN  
581  IJ=IT+I  
582  IF(ABS(BIGA)-ABS(A(IJ))=20.30.30  
583  20 BIGA=A(IJ)  
584  IMAX=I  
585  30 CONTINUE  
586  TEST FOR PIVOT LESS THAN TOLERANCE ( SINGULAR MATRIX )  
587  IF(ABS(BIGA) TOL)=35.35.40  
588  35 KS=1  
589  WRITE(6,100) KS  
590  100 FORMAT('NO SOLUTION*',KS=':1(2X)')  
591  STOP  
592  INTERCHANGE ROWS IF NECESSARY  
593  40 X=J+N*(J-2)  
594  I=IMAX-J  
595  DO 50 K=J,N  
596  SAVE=A(I1)  
597  A(I1)=B(IMAX)  
598  B(IMAX)=SAVE  
599  DIVIDE EQUATION BY LEADING COEFFICIENT  
600  A(I1)=A(I1)/BIGA  
601  SAVE=B(IMAX)  
602  B(IMAX)=B(J)  
603  B(J)=SAVE/BIGA  
604  ELIMINATE NEXT VARIABLE  
605  IF( J-N) 55.70.55  
606  55 IX=N*(J-1)  
607  DO 65 IX=JY,N  
608  IXJ=IXS+IX  
609  IXJ=IXJ+I  
610  A(IXJ)=A(IXJ)-(A(IXJ)*A(JJX))  
611  60 B(IX)=B(IX)-3(J)*A(IXJ)
SUBROUTINE CPHASE(AKR,AKE,AM,PAV,FG,ETURE,EPB,EPD,AKBE,DVHR,FBMO,
& *CONTINUE,FEM,T,TE,YBO,YBG,YBI,YE1,G,GENE)
DI= ((1.0+ETURE-EPD)*AM*AKE/TF+AKBE*EPB/T)*PAV/PG*DVBB+FEM
ALF=AKBE*FPR*DVBB*PAV/(DL*RG*T)_
D2 = FBM+ALF*FFMO+(EPD-EPB)*AKBE/TB+
IF (D2 .GE. 0.0) YBI = 0.0
IF (D2 .LT. 0.0) YBI=(FBMO*YBO+GENB+ALF*FFMO*YEO)/D2
YBI=YE0*YEO/D1+ALF*YR1
RFTURN
END

FUNCTION AKAD(FS,DP,T)
COMMON ZHE(N),AHE(N),PV(N),PH(N),ZF(N),FFC(N),
& ORIGINAL PAGE IS
& OF POOR QUALITY
1) \text{FFAD}(46), \text{ZDIS}(46), \text{FD}(46), \text{AHEAV}(101), \text{ETUBE}(101), \text{DB}(46), \text{MFFED}, \text{MDIS} 976.
2) \text{PHI}(101), \text{PV}(101), \text{DVE}(101), \text{CT}(101), \text{PHI}(101), \text{ZDIS}(101), \text{ABED}(101), \text{ATB}(101), \text{DTUBE}(101), \text{DB}(46).
3) \text{DIMENSION DTUBE}(46), \text{IARR}(46), \text{MDIS}(97/6).
4) \text{COMMON /DEHYD/ OSED} 011, \text{ABED}(101), \text{DTUHF}(101).
5) \text{COMB}/ GEN/ \text{AND/ DNLZ/ DTHICK/ FW}
6) \text{COMMON/DEMAIN/AND/ONZL/DTIS/ DTHICK/ FW}
7) \text{DIMENSION DTUSE}(46), \text{IARR}(46)
8) \text{C AXIAL VARIATION OF BED CROSS SECTION}
9) \text{C 965.}
10) \text{READ (5,1000) A1, A2, A3, A4}
11) \text{READ (5,1001) MTB, (ZB(J), ATB(J), ATR(J), J = 1, MTB)}
12) \text{IARRNG} 1 2 3 4
13) \text{C} \text{--- VERTICAL TRIANGULAR ARRANGEMENT}
14) \text{C} \text{--- VERTICAL RECTANGULAR ARRANGEMENT}
15) \text{C} \text{--- HORIZONTAL INLINV ARRANGEMENT}
16) \text{C} \text{--- HORIZONTAL STAGGERED ARRANGEMENT}
17) \text{HEAT EXCHANGE TUBES}
18) \text{READ (5,1007) MTHE, (ZHE(J+1), AHE(J), DTUBE(J), PV(J), PH(J))}
19) \text{IARR(J), J = 1, MTHE}
20) \text{LOCATION OF FEED AND DISCHARGE}
21) \text{READ (5,1001) *FEED, (ZF(J), FFC(J), FFAD(J), J = 1, MFFED)}
22) \text{READ (5,1001) MDIS, (ZDIS(J), FD(J), J = 1, MDIS)}
23) \text{DISTRIBUTOR}
24) \text{READ (5,1003) AND, DNLZ, DTHICK}
25) \text{DO 100 J = 1, MTHE}
26) \text{IF (AHE(J) .GT. 0.0) GO TO 110}
27) \text{IF (DTUBE(J) .ED. 0.0) GO TO 110}
28) \text{AHE(J) = PI . DE. DTUBE(J) / (PH(J)*PV(J))}
29) \text{CONTINUE}
30) \text{CONDITION FOR COMPUTING AVERAGE CELL SIZE}
31) \text{READ (5,1003) DZAV, FW}
32) \text{N = IFIX (ZB(MTB)/DZAV)}
33) \text{IF (ZB(MTB) - FLOAT(N) * DZAV - GT. 0.1 * DZAV) N = N + 1}
34) \text{IF (N .LT. (101)*1) GO TO 215}
35) \text{WRITE (6,2000) N}
36) \text{FORMAT (*9,20X, *ARRAY SIZE FOR Z TOO SMALL, N > (101), TRACE DZAV 210.)}
37) \text{1 IN SUBROUTINE DESIGN, MAKE SURE N < Z ARRAY SIZE, N = '9T5) 1022.}
38) \text{STOP}
39) \text{CONTINUE}
40) \text{WRITE (6,2005) A1, A2, A3, A4}
41) \text{WRITE (6,2001)}
42) \text{WRITE (6,2002) (ZB(J), ATB(J), J = 1, MTB)}
43) \text{WRITE (6,2003) (ZHE(J+1), AHE(J), DTUBE(J), PV(J), PH(J), IFR(J), J = 1, MTHE)}
44) \text{WRITE (6,2005)}
45) \text{WRITE (6,2006) (ZF(J), FFC(J), FFAD(J), J = 1, MFFED)}
46) \text{WRITE (6,2007)}
47) \text{WRITE (6,2008) (ZDIS(J), FD(J), J = 1, MDIS)}
48) \text{WRITE (6,2009) AND, DNLZ, DTHICK, DZAV, FW}
49) \text{SPECIFIC HEAT EXCHANGE AREA CALCULATION FOR EACH COMPARTMENT}
50) \text{Z(1) = ZB(1)}
51) \text{ABED(1) = ATB(1)}
52) \text{DBED(1) = SQRT(4.0 * ABED(1) / PI)}
53) \text{DVEB(1) = 0.0}
54) \text{DVEEFF(1) = 0.0}
55) \text{ZHE(1) = 0.0}
56) \text{IARRNG(1) = 0}
57) \text{DO 10 I = 1, N}
58) \text{Z(I+1) = Z(I) + DZAV}
59) \text{IF (I .EQ. 196) Z(I+1) = ZB(MTB)}
60) \text{Z(I+1) = Z(I) + DZAV}
61) \text{Z(I+1) = Z(I) + DZAV}
62) \text{IF (ZHE(J) .LE. Z(I), AND. ZHE(J+1) .GE. Z(I+1)) GO TO 30}
63) \text{IF (ZHE(J) .LE. Z(I) + D, AND. ZHE(J+1) .LT. Z(I+1)) GO TO 30}
DENOM = Z(I+1) - Z(I)  
F1 = (Z(I+1) - ZHE(J) / DENOM  
F2 = (Z(I) - ZHE(J) / DENOM  
AHEAV(I+1) = F1 * AHEJ + F2 * AHE(J-1)  
DTUBE(I+1) = F1 * DTUBE(J) + F2 * DTUBE(J-1)  
PV(I+1) = F1 * PV(J) + F2 * PV(J-1)  
PH(I+1) = F1 * PHJ + F2 * PH(J-1)  
GOTO 40  
AHEAV(I+1) = AHEJ  
DTUBE(I+1) = DTUBE(J)  
PV(I+1) = PV(J)  
PH(I+1) = PH(J)  
IARRNG(I+1) = IARR(J)  
GOTO 50  
CONTINUE  
CELL VOL CALCULATION  
CALL AREA ( Z(I+1), ABED(I+1), ABED(I+1) )  
DVB(I+1) = 0.5 * (ABED(I+1)+ABEO(I)) * (Z(I+1)-Z(I))  
EFFECTIVE CELL VOLUME EXCLUDING THE VOLUME OCCUPIED BY THE HEAT EXCHANGE TUBES  
DVBEFF(I+1) = DVB(I+1) * (1.0 - 0.25 * AHEAV(I+1) * DTUBE(I+1))  
TUHF: VOLUME FRACTION  
ETUBE(I+1) = 1.0 - DVBEFF(I+1) / DVB(I+1)  
CONTINUE  
WRITE (6,2010) M = N+1  
MT = M1  
DO 60 I = 2, M1  
WRITE (6,2012) I,Z(I),DVB(I),DVBEFF(I),PH(I),IARRNG(I)  
60 CONTINUE  
WRITE (6,2013) I,Z(I),DVB(I),DVBEFF(I)  
CONTINUE  
WRITE (6,2014) M = N+1  
DO 70 I = 1, M1  
WRITE (6,2015) I,Z(I),DVB(I),DVBEFF(I),PH(I),IARRNG(I)  
70 CONTINUE  

SUBROUTINE HYDRO

REAL MGAS

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

COMMON /DEHYD/ DBFD(101), ABED(101), DTUBF(101),

LPHI(101), PVI(101), FD(46), AHEAV(101), ETUSE(101), DB(46), MFEED.

COMMON/DEMAIN/ ANDsDNZL, DTHTCK, FW

COMMON /HYMAIN/ UC1(46), UMF(46), H(46), AT(46), OT(46), E(46), FPB(46), UFG(46), DVFB(46), DVBOEF(46), DBAV(46), DB(46), HCMF, VMF, FMF, FMF, UF, PF, TF, RG, MGAS, DPFIX, DPFLU, DDPD, RHOCAD

3EMF, YB(46), PAV, HCR, ABED(46), DETVOL, EFFVOL, SOLVOL, TETUBE, ICR, IFAC

COMMON /GEN/ Z(101), DLV, FF(101), ZB(46), ATB(46), PI, DZAV, MTB, MTF, M1

C CALCULATION OF BUBBLE HYDRODYNAMICS

I=0

SUM=0.0

SUMEFF=0.0

$EDVOL = 0.0

SUMV = 0.0

ICR = 0

MCR = 0.0

DTUBE(1) = 0.0

I = I + 1

IF (I * LE. M1) GO TO 5

T(I) = T(M1)

X(I) = X(M1)

YR(I) = YR(M1)

YE(I) = YE(M1)

C CALCULATION OF MINIMUM FLUIDIZING VELOCITY

CONTINUE

IF (IFRC .GT. 0) GO TO 11

H(I) = Z(I)

DT(I) = DBED(I)

AT(I) = ABFD(I)

DVBB(I) = DV(I)

DVBEFF(I) = DVRFF(I)

CONTINUE

TEMP = T(I)

IF (I .GT. 1) GO TO 16

UMF(I) = MIN. FLUIDIZING VEL. AT THE H(I) LEVEL ABOVE THE

DISTRIBUTOR

AL = 33.7**2 + 0.040B / (DPF/VISC)

1 ** 2 * DPH * G * (RHOCAD - PHOGAS) * RHOGAS

UMF(I) = VISC/(DPH*RHOGAS) * (SORT(A1) - 33.7)

IF (I .GT. 1) GO TO 7

UO(I) = FMF * MGAS / RHOGAS / AT(I)

GO TO 15

DB(I) = 0.347 * (AT(I) * (UO(I) - UMF(I)) / AND ) **0.4

GO TO 15

C --- SUPERFICIAL GAS VEL. AT H(I) LEVEL ABOVE DISTRIBUTOR

UO(I) = FMQ * RG * T(I) / (PAV*AT(I) * (1.0 - FTUE(I))

IF (IFBC .GT. 0) GO TO 125

IF (ABS(UO(I)) - UMF(I)) .LE. 0.01 * UMF(I) GO TO 18

IF (UO(I) .GT. 1.0, UMF(I)) GO TO 10

GO TO 17

ICR --- INDICATOR FOR THE CRITICAL HEIGHT WHERE UO = UMF

ICR = 1

C BUBBLE SIZE CALCULATIONS

DBMAX = 0.652 * (AT(I) * (1.0 - FTUE(I)) * ABS(UO(I) - UMF(I))) **0.4

IF (DBMAX .GT. PH(1)) GO TO 14

IF IFARRNG(I) * GT. 2 AND PH(1) .GE. 0.5 * DB(I-1) DBMAX = PH(1)

DBMAX = (DBMAX - DB(I-1)) * EXP(-0.3 * (H(I) - H(I-1))/DT(I))

DBAV(I) = 0.5 * (DB(1) + DB(I-1))

AKBE(1) = 11.0 / DBAV(1)
CALCULATIONS FOR UBR —— BUBBLE RISING VEL, AT MIN. FLUIDIZATION,
UBS —— BUBBLE VEL. AT SLUGGING CONDITIONS,
UB —— ABS. BUBBLE RISING VELOCITY,
EPC —— BUBBLE FRACTION,
EFC —— CLOUD FRACTION

UBR = 0.711 * SORT ( G * DAVB(I) )
UBS = 0.355 * SORT ( G * (DT(I)+DT(-1))/2.0 )
IF (UBR > GT, UBS) UBR = UBS
UDAV = 0.5 * ( UN(I) + UN(I-1) )
UMFAV = 0.5 * ( UMIF(I) + UMIF(I-1) )
UB(I) = UDAV - UMFAV + UBR
EPC(I) = ( UDAV - UMFAV ) / UB(I) * ( 1.0 - ETUBE(I) )
ALFB = EMF * UB(I) / UMFV
EFC(I) = EPC(I) * ALFB / ( ALFB - 1.0 )
IF (EPC(I) > GT, 0.7) EPC(I) = 0.7
IF (EPC(I) < (0.99 - ETUBE(I)) EPC(I) = 0.99 - ETUBE(I)
BEDVOL = BEDVOL + DVB(I)
SUMV = SUMV + DVB(I)
SOLVOL = DVB(I) - DVB(I) * EPC(I)
SOLM = SUMV - SOLVOL
SUM = SUM + SOLVOL / ( 0.5 * (AT(I) + AT(-I)) )
IF (ICR > GT, 0) GO TO 35
IF (HLF < NE) GO TO 20

TEST FOR CONVERGENCE
IF (ABS(SUMEFF-VMF) > LT, 0.01*VMF) GO TO 125
IF (SUMEFF > LT, VMF) GO TO 15
VOL = SUMV / (SUMEFF*VMF) * (1.0 - ETUBE(I)) / (1.0 - EPC(I) - STUNE(I))
H(I) = HEIGHT(VOL)
CALL AREA ( H(I), AT(I), AT(I) )
SUMV = SUMV - DVB(I)
SUM = SUM - SOLVOL / ( 0.5 * (AT(I) + AT(-I)) )
DVB(I) = 0.5 * ( AT(I) + AT(-I) ) * ( H(I) - H(I-1) )
DVB(I) = DVB(I) * ( 1.0 - 0.25 * AHEAV(I) * DTUBE(I) )
GO TO 16
CONTINUE

TEST FOR CONVERGENCE
IF (ABS(H(I)-HLF) > LE, 1.0E-3*HLF) GO TO 125
IF (H(I) > LT, HLF) GO TO 15
H(I) = HLF
BEDVOL = BEDVOL - DVB(I)
SUMV = SUMV - DVB(I)
SUMEFF = SUMEFF - SOLVOL
SUM = SUM - SOLVOL / ( 0.5 * (AT(I) + AT(I)) )
DVB(I) = 0.5 * ( AT(I) + AT(-I) ) * ( H(I) - H(I-1) )
DVB(I) = DVB(I) * ( 1.0 - 0.25 * AHEAV(I) * DTUBE(I) )
GO TO 16
CONTINUE

IF (ABS(H(I)-HLF) > LE, 1.0E-3*HLF) GO TO 125
IF (H(I) > LT, HLF) GO TO 15
H(I) = HLF
BEDVOL = BEDVOL - DVB(I)
SUMV = SUMV - DVB(I)
SUMEFF = SUMEFF - SOLVOL
SUM = SUM - SOLVOL / ( 0.5 * (AT(I) + AT(I)) )
DVB(I) = 0.5 * ( AT(I) + AT(-I) ) * ( H(I) - H(I-1) )
DVB(I) = DVB(I) * ( 1.0 - 0.25 * AHEAV(I) * DTUBE(I) )
GO TO 16
CONTINUE

10 UMFV = UMIF(I)
64 AT(I) = FMD * RG * T(I) / ( PAV * UN(I) * (1.0 - FTUBE(I)) )
65 CALL HFAT ( AT(I), DT(I), H(I) )
66 ICR = 1
67 DVBR(I) = 0.5 * ( AT(I) + AT(-I) ) * ( H(I) - H(I-1) )
68 DVBH(I) = DVBH(I) * ( 1.0 - 0.25 * AHEAV(I) * DTUBE(I) )
69 GO TO 17
70 
35 125
71 HCR = H(I)
72 IF (ABS(H(I)-HLF) > LE, 1.0E-3*HLF) GO TO 125
73 IF (ABS(VMF-SUMEFF) > LE, 0.01*VMF) GO TO 125
74 I = I + 1
75 DAVB(I) = 0.0
76 UM(I) = 0.0
77 AKBE(I) = 1000.0
78 EPB(I) = 0.0
79 FPC(I) = 0.0
80 IF (VMF < EQ, 0.0) GO TO 45

FIXED RED CONDITIONS

881 VOL = SUMV + ( VMF - SUMEFF )
892 H(I) = HEIGHT(VOL)

ORIGINAL PAGE IS OF POOR QUALITY
CONTINUE

IF (VMF *EQ* 0.0) H(I) = HLF

CALL AREA ( H(I), DT(I), AT(I) )

DVBB(I) = 0.5 * (AT(I) + AT(I-1)) * (H(I) - H(I-1))

DVBBEI(I) = DVBB(I) * (0.1 + 0.25 * AHEAV(I) * DTUBEI(I))

BEDVOL = BEDVOL + DVBBEI(I)

SUMV = SUMV + DVBBEI(I)

SUMEFF = SUMEFF + DVBBEI(I)

SUM = SUM + DVBBEI(I) / (0.5 * (AT(I) + AT(I-1)))

IFRC = 1

GO TO 13

M1 = I

TETUBE = 1.0 - SUMV/SEDVOL

EFFVOL = SUMV

SOLVOL = SUMEFF

M = M1 - 1

WRITE(6,204)

WRITE(6,206) 1, M1

WRITE(6,207) 4, H(I), DBAV(I), UBI(I), FPB(I), EPC(I), UG(I), UMF(I)

SUBROUTINE A ( ZI, DTI, ATI )

COMMON /GEN/ Z(101), DVFFFEFF(101), ZB(46), ATR(46), PI, DZA5, MTR, MT, M1, M1

C

CALCULATION OF THE CROSS SECTIONAL AREA GIVEN THE HEIGHT ABOVE

THE DISTRIBUTION

IF ( ZI > Z(J) ) GO TO 10

RMJ = SORT ( ATR(J) / PI )

A = ( ZI - ZB(J-1) ) / ( ZB(J) - ZB(J-1) )

B = SORT ( ATR(J) / ATR(J-1) ) - 1.0

RI = ( 1.0 + A * B ) * RMJ

DTI = 2.0 * PI

ATI = PI * RI ** 2

GO TO 20

CONTINUE

RETURN

END

SUBROUTINE HFA ( ATI, DTI, ZI )

COMMON /GEN/ Z(101), DVFFFEFF(101), ZB(46), ATR(46), PI, DZA5, MTR, MT, M1, M1

C

CALCULATION OF THE HEIGHT GIVEN THE CROSS SECTIONAL AREA

RI = SORT ( ATI / PI )

DTI = 2.0 * PI

IF ( ATI > ATB(J) ) GC TO 10

A = SORT ( ATI / ATB(J-1) ) - 1.0

B = SORT ( ATB(J) / ATB(J-1) ) - 1.0

C = ZB(J) - ZB(J-1)

ZI = ZB(J-1) + A * C / R

GO TO 20

CONTINUE

RETURN

END

FUNCTION HEIGHT ( ZZV )

COMMON /GEN/ Z(101), DVFFFEFF(101), ZB(46), ATR(46), PI, DZA5, MTR, MT, M1, M1

C

CALCULATION OF THE HEIGHT GIVEN THE EFFECTIVE VOLUME OF THE BED

EXCLUDING THE VOLUME OCCUPIED BY THE TUNES

H = 0.0
SUM = 0.0

DO 100 I = 2, MT

SUM = SUM + DVBEFF(I)

H = H + DZAV

IF ( SUM + LT. VV ) GO TO 100

H = ( VV - SUM ) * DZAV / DVBEFF(I) + H

GO TO 110

CONTINUE

HEIGHT = H

RETURN

END

FUNCTION VOLUME (ZZ)

COMMON /GEN/ Z(101), DVBEFF(101), ZB(46), ATB(46), PI, DZAV, MT3, MT, M1

CALCULATION OF THE EFFECTIVE VOLUWF OF THE BED GIVEN THE HEIGHT

N = IFIX (ZZ/DZAV)+1

IF ( ZZ - FLOAT(N-1) * DZAV + GT. 0.01 * DZAV ) N = N + 1

SUM = 0.0

DO 100 I = 2, N

SUM = SUM + DVBEFF(I)

IF ( I + LT. N ) GO TO 100

A = 1.0 - ( ZZ - Z(N) ) / DZAV

SUM = SUM - DVBEFF(I) * A

CONTINUE

VOLUME = SUM

RETURN

END
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,

\[
\begin{align*}
\text{IELUTR} = 1 & \quad \text{Correlation A} \\
\text{IELUTR} = 2 & \quad \text{Correlation B} \\
\text{IMODEL} = 1 & \quad \text{Homogeneous complete mixing} \\
\text{IMODEL} = 2 & \quad \text{Homogeneous plug flow}
\end{align*}
\]

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,

\[
\frac{u}{u_0} (\text{DPCR}) = \frac{u}{u_0}
\]
From ISN 84 to ISN 91 a new grid is introduced at the point \( d_c = DPCR \) and FR\(ACT(I) \) vs DP\(F(I) \) relation is modified. Then from ISN 92 to 139 the value of size distribution density function for the coal particle PH\(I(\omega) \) corresponding to each interval of DP\((\omega) - DP(\omega + 1) \) is found from the FR\(ACT(k) \) 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
\[
\int_0^{\gamma_i} \left( \frac{1}{\lambda_c} \right) dy \quad \text{and} \quad \int_0^{\gamma_i} \left( \frac{K^*}{\lambda_c} \right) dy
\]
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 \( n_c (\text{= ETC}) \), \( \Theta (\text{= THET}) \) and \( B_{cf} (\text{= BC1}) \) 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 \( \Theta \) and \( B_{cf} \) are used.

ETC iteration is started from
\[
ETC = \begin{cases} 
1 & \text{if EXAIR} \geq 0 \\
1 + \text{EXAIR} & \text{if EXAIR} < 0
\end{cases}
\]
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. Subroutine 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 \( \Theta \), 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 289-311 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.

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<th>Column</th>
<th>Variable</th>
<th>Example</th>
<th>Type</th>
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<td></td>
<td>4-8</td>
<td>NAM2</td>
<td>S</td>
</tr>
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<td>SCF</td>
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<td>65-72</td>
<td>DPL</td>
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<td>73-80</td>
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7-3. Output of the Program

The output of a typical run of Level I program is following.
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<tr>
<th></th>
<th>0.0460</th>
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<td>0.2000</td>
<td>0.02E-02</td>
<td>0.02E-02</td>
<td>0.01E-01</td>
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<tr>
<td>P1</td>
<td>0.6600</td>
<td>0.10E+00</td>
<td>0.11E-02</td>
<td>0.10E-02</td>
<td>0.10E-02</td>
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<tr>
<td>P2</td>
<td>0.12E+01</td>
<td>0.20E+00</td>
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<td>0.11E-02</td>
<td>0.11E-02</td>
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<td>P5</td>
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<td>0.20E+00</td>
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<td>P6</td>
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<td>0.20E+00</td>
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<td>0.20E+00</td>
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GAS PHASE MODEL: NO. 1  

EFFECT OF CLUTERAT1ON ON COMBUSTION EFFICIENCY  

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<thead>
<tr>
<th>Y</th>
<th>PHIF</th>
<th>PHI</th>
<th>PHI W</th>
<th>PHIEW</th>
<th>AKE</th>
<th>ALAM</th>
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ORIGINAL PAGE IS OF POOR QUALITY
# Nomenclature for Level I Computer Program

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<th>FORTRAN symbol</th>
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<th>Unit</th>
<th>Description</th>
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<tbody>
<tr>
<td>AK</td>
<td>(k_R)</td>
<td>cm/sec</td>
<td>chemical reaction rate constant for char combustion</td>
</tr>
<tr>
<td>AKE</td>
<td>(K^*)</td>
<td></td>
<td>specific elutriation rate constant</td>
</tr>
<tr>
<td>AKEI</td>
<td>(\int_0^y K^* / \lambda \ dy)</td>
<td></td>
<td>maximum value of elutriation rate constant</td>
</tr>
<tr>
<td>AKEMAX</td>
<td></td>
<td></td>
<td>maximum value of elutriation rate constant</td>
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<tr>
<td>AKF</td>
<td>(k_f)</td>
<td>cm/sec</td>
<td>mass transfer coefficient for char combustion</td>
</tr>
<tr>
<td>ALAM</td>
<td>(\lambda = k_c/k_R)</td>
<td>-</td>
<td>reactivity of char</td>
</tr>
<tr>
<td>ALAMA</td>
<td>(\psi_a)</td>
<td></td>
<td>(= \int_0^1 \phi \ y^2 \ dy = \frac{d^2}{d_c^2/d_c^m})</td>
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<tr>
<td>ALAMI</td>
<td>(\int_0^y 1/\lambda \ dy)</td>
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<tr>
<td>ALAMV</td>
<td>(\psi_v)</td>
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<td>(= \int_0^1 \phi \ y^3 \ dy = \frac{d^3}{d_c^2/d_c^m})</td>
</tr>
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<td>ALAMAF</td>
<td>(\psi_{af})</td>
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<td>(= \int_0^1 \phi_f \ y^2 \ dy)</td>
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<tr>
<td>ALAMVF</td>
<td>(\psi_{vf})</td>
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<td>(= \int_0^1 \phi_f \ y^3 \ dy)</td>
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<tr>
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<td>dummy parameters</td>
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<tr>
<td>ANDP</td>
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<td>number of sub-intervals in the interval of DPO</td>
</tr>
<tr>
<td>AT</td>
<td>(A_t)</td>
<td>cm(^2)</td>
<td>cross sectional area</td>
</tr>
<tr>
<td>BB</td>
<td></td>
<td>dummy parameters</td>
<td></td>
</tr>
<tr>
<td>BBC, BC</td>
<td>(B_{cw})</td>
<td></td>
<td>dimensionless parameter</td>
</tr>
<tr>
<td>BC1</td>
<td>(B_{cf})</td>
<td></td>
<td>dimensionless parameter</td>
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</table>

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*ORIGINAL PAGE IS OF POOR QUALITY*
<table>
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<th>Unit</th>
<th>Description</th>
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<td>BETA</td>
<td>[Ca]/[S]</td>
<td>-</td>
<td>calcium to sulfur ratio in the total solids input</td>
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<tr>
<td>CABS</td>
<td>C_{c}</td>
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<td>dimensionless parameter</td>
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<td>COXAV</td>
<td>C_{O2}</td>
<td>gmol/cm³</td>
<td>average oxygen concentration</td>
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<tr>
<td>COX0</td>
<td>C_{O2,0}</td>
<td>gmol/cm³</td>
<td>oxygen concentration at z=0</td>
</tr>
<tr>
<td>D</td>
<td>D_{O2}</td>
<td>cm²/sec</td>
<td>diffusivity of oxygen</td>
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<tr>
<td>DB</td>
<td>D_{B}</td>
<td>cm</td>
<td>average bubble diameter</td>
</tr>
<tr>
<td>DCM</td>
<td>d_{cm}</td>
<td>cm</td>
<td>maximum diameter of coal particles</td>
</tr>
<tr>
<td>DETC</td>
<td>\Delta n_c</td>
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<td>step size for combustion efficiency iteration</td>
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<td>DDP</td>
<td>\Delta d_{C}</td>
<td>cm</td>
<td>interval size of d_{C} axis</td>
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<td>DPAV</td>
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<td>average than particle size in a size interval</td>
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<tr>
<td>DPCR</td>
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<td>-</td>
<td>critical diameter for elutriation</td>
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<tr>
<td>DPF</td>
<td>cm</td>
<td>-</td>
<td>diameter of inlet char</td>
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<td>dm</td>
<td>-</td>
<td>extra memory for DPF</td>
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<td>DPL</td>
<td>d_{Z}</td>
<td>cm</td>
<td>mean diameter of limestone particles</td>
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<tr>
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<td>D_{T}</td>
<td>cm</td>
<td>column diameter</td>
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<tr>
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<td>sec</td>
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<td>step size for \theta iteration</td>
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<tr>
<td>DY</td>
<td>\Delta y</td>
<td>-</td>
<td>interval size of y</td>
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<tr>
<td>E</td>
<td>-</td>
<td>-</td>
<td>relative error for B_{cw} iteration</td>
</tr>
<tr>
<td>E1, E2, EE1, EE2, ETC1, ETC2</td>
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<td>-</td>
<td>relative error of B_{cw} from the previous iteration step</td>
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<tr>
<td>ETC</td>
<td>\eta_{C}</td>
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<td>coal combustion efficiency</td>
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<td>FORTRAN symbol</td>
<td>Mathematical symbol</td>
<td>Unit</td>
<td>Description</td>
</tr>
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<tr>
<td>EB</td>
<td>$\varepsilon_B$</td>
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<td>volume fraction of bubbles</td>
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<td>difference between the values of $B_{cf}$ assumed and calculated</td>
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<td>void fraction of bed at $u = u_{mf}$</td>
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<tr>
<td>ETC</td>
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<td>combustion efficiency</td>
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<td>EAR</td>
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<td>molar mass flow rate of outlet gas</td>
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<td>Froude Number</td>
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<td>$U_t$</td>
<td>cm/sec</td>
<td>terminal velocity (or freefall velocity)</td>
</tr>
<tr>
<td>G</td>
<td>g</td>
<td>cm/sec$^2$</td>
<td>gravity acceleration</td>
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<td>g</td>
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<tr>
<td>HCHAR</td>
<td>g</td>
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<td>atomic weight of Ca</td>
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<td>g/gmol</td>
<td>molecular weight of H_2</td>
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<td>g/gmol</td>
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<td>g/gmol</td>
<td>molecular weight of N_2</td>
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<td>M_{O2}</td>
<td>g/gmol</td>
<td>molecular weight of O_2</td>
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<td>M_S</td>
<td>g/gmol</td>
<td>atomic weight of ( \xi )</td>
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<td>name of coal (A-Type variables)</td>
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<td>number of size distribution inputs (see READ (5,1001) statement)</td>
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<td>atm</td>
<td>pressure</td>
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<td>fraction of ash elutriated</td>
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<td>\Phi</td>
<td>-</td>
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<td>FORTRAN symbol</td>
<td>Mathematical symbol</td>
<td>Unit</td>
<td>Description</td>
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<td>Particle Reynolds Number for DPCR</td>
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<td>RET</td>
<td>$R_{ep}$</td>
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<td>Particle Reynolds Number for terminal velocity</td>
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<td>density of coal ash</td>
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<tr>
<td>RHOC</td>
<td>$\rho_c$</td>
<td>g/cm³</td>
<td>density of coal</td>
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<td>RHOG</td>
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<td>g/cm³</td>
<td>density of gas</td>
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<td>$\rho_{ch}$</td>
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<td>$Sh_p$</td>
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<td>Sherwood Number</td>
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<td>$\theta$</td>
<td>sec</td>
<td>mean residence time of limestone</td>
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<tr>
<td>TETHM</td>
<td>$\theta_{max}$</td>
<td>sec</td>
<td>maximum value of $\theta$</td>
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<td>TK</td>
<td>$\bar{T}$</td>
<td>°K</td>
<td>average bed temperature</td>
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<td>$U_B$</td>
<td>cm/sec</td>
<td>bubble rising velocity</td>
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<td>$\mu$</td>
<td>g/cm·sec</td>
<td>viscosity of gas</td>
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<td>$u_o$</td>
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<td>superficial gas velocity</td>
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<td>$u_{mf}$</td>
<td>cm/sec</td>
<td>minimum fluidizing velocity</td>
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<td>Mathematical symbol</td>
<td>Unit</td>
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<td>$u_t$</td>
<td>cm/sec</td>
<td>terminal velocity of char particle</td>
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<td>cm/sec</td>
<td>terminal velocity of char particle</td>
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<td>cm$^3$/sec</td>
<td>volumetric flow rate of coal</td>
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<tr>
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<tr>
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<tr>
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<td>Unit</td>
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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.

\[
DCAV = \left(\frac{3.0}{5.0}\right) DCF \tag{8-1}
\]

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, \( a_c = \frac{\rho_c}{\rho_{cf}} \cdot d_{c}^{2} \).

By the use of carbon mass fraction, \( x \), \( a_c \) can be written as

\[
a_c = \frac{6\rho \left(1 - \epsilon_{mf}\right)x}{d_{c,sv} \rho_{cf} X_{cf}} \tag{8-2}
\]

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

\[
d_{c,sv} = \frac{d_{cm} \psi_{v}}{\psi_{a}} \tag{8-3}
\]
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, \( \psi_a \) and \( \psi_v \) can be written as (see Horio and Wen (1975a)):

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

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

where

\[
a_c = \begin{cases} 
    1/(1 - e^{-B_{cw}}) & \text{(SRC)} \\
    1/(1 - e^{-B_{cw}^2 / 2}) & \text{(FDC)}
\end{cases}
\]

\[
B_{cw}^c = \frac{\rho_c X_c d_{cm}^2}{4M_C \Theta D_{CO2} C_{CO2}} \quad \text{for FDC}
\]

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

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

\[
\psi_v = \begin{cases} 
    (1/4) \psi_{vf} & \text{(SRC)} \\
    (2/5) \psi_{vf} & \text{(FDC)}
\end{cases}
\] (8-7a)
Then,
\[
\begin{align*}
\frac{3}{4} d_{e,sv,f} &= \frac{3}{5} d_{c,sv,f} \\
\text{(SRC) (8-8a)}\\
\frac{3}{5} d_{c,sv,f} &= \text{(FDC) (8-8b)}
\end{align*}
\]

In coal combustors the rate is mainly controlled by gas 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 \( \xi_{CO}, \xi_{H_2}, \text{ and } \xi_{H_2S} \) introduced by Equation (8-12) 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 \( \xi_{CO} (GZCO) \).

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, Ca/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 Ml 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 \( M_1 \). Therefore, \( M_1 \) newly obtained from HYDRO is compared with the old value, \( M_{10LD} \), at ISN 172. If there is no change in \( M_1 \), 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 Ca 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 445 are necessary for applying Regula Falsi method by using subroutine CRRECT.

By the statement at ISN 439, the average conversion of adsorbent FS 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 the results of sulfur retention and the outlet gas concentration XG(1) ... 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

\[(\text{average temperature at distributor}) = \frac{(T(1)+T(2))}{2}\]

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

\[\Delta p_{\text{dis}} = \left(\frac{U_{\text{OR}}}{0.6}\right)^2 \rho_g / 2g\]

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\textsubscript{x} concentration in the outlet gas is incorporated (Ruth (1976)).

\[ AN = 2.9 \times 10^{-8} (\text{EXAIR})^{0.449} \]

where

AN = \text{gmol NO}\textsubscript{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.

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<th>Variable</th>
<th>Example</th>
<th>Type</th>
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8-3. Output of the Program

The output of a typical run of Level II program is following.
### Heat Transfer Area Data

<table>
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<tr>
<th>HEIGHT, CM</th>
<th>SP. HEAT TRANS. AREA, SQ.CM/GL.CM</th>
<th>DIA. OF TUBES, CM</th>
<th>VER. PITCH, CM</th>
<th>HOR. PITCH, CM</th>
<th>TUBES ARRNGT</th>
</tr>
</thead>
<tbody>
<tr>
<td>20.00</td>
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<td>0.0000</td>
<td>0.0000</td>
<td>0.0000</td>
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### SOLIDS Feed Level

- **SOLIDS FEED LEVEL:** 12.70
- **FRACTION COAL FED:** 1.0000
- **FRACTION LIMESTONE FED:** 1.0000

### SOLIDS Discharge Level

- **SOLIDS DISCHARGE LEVEL:** 66.00
- **FRACTION DISCHARGED:** 1.0000

### Heights

<table>
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<tr>
<th>NO.</th>
<th>HEIGHT</th>
<th>CELL VOLUME</th>
<th>CELL EFF.VCL.</th>
<th>TUBE VOL.FR.SP.HE.AREA</th>
<th>TUBE DIA.</th>
<th>VER. PITCH</th>
<th>HOR. PITCH</th>
<th>TUBES ARRNGT</th>
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</thead>
<tbody>
<tr>
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<td>2.090E-04</td>
<td>-0.000E-01</td>
<td>0.000E-01</td>
<td>0.000E-01</td>
<td>0.000E-01</td>
<td>0.000E-01</td>
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<td>0.000E-01</td>
<td>0.000E-01</td>
<td>0.000E-01</td>
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<td>0.000E-01</td>
<td>0.000E-01</td>
<td>0.000E-01</td>
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</table>

### Additional Parameters

- **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
<table>
<thead>
<tr>
<th>LIMEST18</th>
<th>XCaCO3 = 0.820</th>
<th>XMgCO3 = 0.020</th>
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<table>
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<th></th>
<th></th>
<th>WT. FRACTION</th>
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<td>0.1720</td>
<td></td>
</tr>
<tr>
<td>0.0066</td>
<td>0.0500</td>
<td></td>
</tr>
<tr>
<td>0.0125</td>
<td>0.1220</td>
<td></td>
</tr>
<tr>
<td>0.0125</td>
<td>0.0125</td>
<td></td>
</tr>
<tr>
<td>0.0500</td>
<td>0.0250</td>
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<tr>
<td>0.1175</td>
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- **SURFACE VOLUME**
- **MEAN DIA.** = DPADH = 0.0084 CM
- **WEIGHT MEAN DIA.** = DPADR = 0.0338 CM

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<th>XCF = 0.504</th>
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<td>QCAL = 7900.00 CALS/GM</td>
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<table>
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<th>QCCALC = 7900.00 CALS/GM</th>
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<td>0.1175</td>
<td>0.0010</td>
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- **SURFACE VOL MEAN DIA OF COAL FEED** = DCF = 0.0151 CM
- **DCAV** = 0.0113 CM

**RESULTS:** ALL TEMPERATURES IN CENTIGRADE

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<th>C.1547E-01</th>
<th>C.7759E 03</th>
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Outlet Gas Concentration

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Pressure Drop Across the Distributor = 1.1519E 01

Pressure Drop in the Bed

Pressure Drop in the Fixed Bed Section = 0.0000E-01

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<th>BUBBLE VEL.</th>
<th>BUBBLE FRACT.</th>
<th>CLOUD FRACT.</th>
<th>SUP.VELOCITY</th>
<th>MIN.FLU.VELO.</th>
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9 40.000 37.500 5.5645E 00 1.6639E 02 2.8583E-01 2.8646E-01 3.7924E 01 1.579E-01
10 45.000 42.500 9.6025E 00 1.0668E 02 2.8422E-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 2.8060E-01 2.8417E-01 3.7502E 01 1.5710E-01
13 60.000 57.500 9.7068E 00 1.0395E 02 2.8216E-01 2.8391E-01 3.7750E 01 1.5715E-01
14 65.000 62.500 1.0229E 01 1.0417E 01 2.4917E-01 2.5000E-01 1.9675E 01 1.5731E-01
15 67.056 66.028 1.0937E 01 1.0937E 01 2.0535E-01 2.0605E-01 1.8687E 01 1.5759E-01

1407.
## Nomenclature of Level II Program

<table>
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<th>Mathematical Symbol</th>
<th>Unit</th>
<th>Description</th>
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<td>-</td>
<td>-</td>
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<tr>
<td>AG</td>
<td>-</td>
<td>mole fraction</td>
<td>outlet gas composition ( (O_2, CO_2, SO_2, H_2O, CO, H_2S, H_2, N_2) )</td>
</tr>
<tr>
<td>AHE</td>
<td>( a_{HE} )</td>
<td>( \text{cm}^2/\text{cm}^3 )</td>
<td>specific heat transfer area</td>
</tr>
<tr>
<td>AHEAV</td>
<td>( a_{HE,i} )</td>
<td>( \text{cm}^2/\text{cm}^3 )</td>
<td>specific heat transfer area in each compartment</td>
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<tr>
<td>AKB</td>
<td>( k_c )</td>
<td>( \text{cm/sec} )</td>
<td>overall surface reaction rate constant for coal combustion in the bubble phase</td>
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<tr>
<td>AKBE</td>
<td>( K_{BE,i} )</td>
<td>1/sec</td>
<td>gas exchange coefficient in the ( i )th compartment</td>
</tr>
<tr>
<td>AKE</td>
<td>( k_c )</td>
<td>( \text{cm/sec} )</td>
<td>overall surface reaction rate constant for coal combustion in the emulsion phase</td>
</tr>
<tr>
<td>AKO</td>
<td>( \hat{k}_{VL} )</td>
<td>1/sec</td>
<td>volumetric reaction rate constant for ( \text{SO}_2 ) reaction</td>
</tr>
<tr>
<td>ALFA</td>
<td>-</td>
<td>-</td>
<td>temperature matrix coefficient</td>
</tr>
<tr>
<td>AND</td>
<td>( N_d )</td>
<td>-</td>
<td>number of distributor holes</td>
</tr>
<tr>
<td>ANOX</td>
<td>( \text{NO}_x )</td>
<td>mole fraction</td>
<td>( \text{NO}_x ) concentration in the effluent gas</td>
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<tr>
<td>AT</td>
<td>( A_{t,i} )</td>
<td>( \text{cm}^2 )</td>
<td>cross sectional area of the bed at each location</td>
</tr>
<tr>
<td>ATB</td>
<td>-</td>
<td>( \text{cm}^2 )</td>
<td>cross sectional area of the FBC at specified locations</td>
</tr>
<tr>
<td>BBB</td>
<td>-</td>
<td>-</td>
<td>matrix coefficient</td>
</tr>
<tr>
<td>BEDVOL</td>
<td>( V )</td>
<td>( \text{cm}^3 )</td>
<td>total bed volume</td>
</tr>
<tr>
<td>BETA</td>
<td>-</td>
<td>-</td>
<td>temperature matrix coefficient</td>
</tr>
<tr>
<td>CABS</td>
<td>( [C_a]/[S] )</td>
<td>mole ratio</td>
<td>mole ratio of calcium to sulfur in feed solids</td>
</tr>
<tr>
<td>CABSE</td>
<td>( [C_a]_f/[S]_f )</td>
<td>mole ratio</td>
<td>effective ratio of calcium to sulfur in the feed (gas and solids)</td>
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<tr>
<td>CADF</td>
<td>( C_{sf} )</td>
<td>Cal/g°C</td>
<td>heat capacity of additives fed</td>
</tr>
<tr>
<td>FORTRAN Symbol</td>
<td>Mathematical Symbol</td>
<td>Unit</td>
<td>Description</td>
</tr>
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<tr>
<td>CCF</td>
<td>$C_{cf}$</td>
<td>Cal/g°C</td>
<td>heat capacity of coal fed</td>
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<tr>
<td>CELU</td>
<td>$W_e$</td>
<td>g/sec</td>
<td>elutriation rate of unburnt char</td>
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<tr>
<td>CGM</td>
<td>$C_{gm}$</td>
<td>Cal/gmol°C</td>
<td>molar heat capacity of gas</td>
</tr>
<tr>
<td>CGMF</td>
<td>$C_{gmf}$</td>
<td>Cal/gmol°C</td>
<td>molar heat capacity of gas at feed temperature</td>
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<tr>
<td>CLOSS</td>
<td>-</td>
<td>g/sec</td>
<td>total carbon loss</td>
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<tr>
<td>CS</td>
<td>$C_s$</td>
<td>Cal/g°C</td>
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<td>DB</td>
<td>$D_B$</td>
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<tr>
<td>DBAV</td>
<td>$D_{B,av}$</td>
<td>cm</td>
<td>average bubble size of each compartment</td>
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<tr>
<td>DENOM</td>
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<td>gmol/sec</td>
<td>total sulfur fed into the bed</td>
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<tr>
<td>DCAV</td>
<td>$d_c$</td>
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<tr>
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<td>$d_p$</td>
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<td>weight mean diameter of additives (used for reaction calculations)</td>
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<td>$d_k$</td>
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<td>EMF</td>
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<td>ETCG</td>
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<td>combustion efficiency based on oxygen consumption</td>
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<td>$\epsilon_{tube,i}$</td>
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<td>EAR</td>
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<td>molar flow rate of gas in bubble phase</td>
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<td>fraction of total solids discharged at each location</td>
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<td>fraction of total additives fed at each location</td>
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<td>$F_{mf}$</td>
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<td>molar flow rate of inlet gas</td>
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<td>theoretical feed rate of inlet gas</td>
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<td>Unit</td>
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<td>g</td>
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<td>$E_{CO}$</td>
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<tr>
<td>GZH2</td>
<td>$E_{H_2}$</td>
<td>-</td>
<td>ratio of $H_2$ formation rate from coal to sum of $H_2$ and $H_2O$ formation rate from coal</td>
</tr>
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<td>-</td>
<td>ratio of $H_2S$ formation rate to sulfur feed rate</td>
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<td>H(I),H(I+1)</td>
<td>$h_i$, $h_{i+1}$</td>
<td>cm</td>
<td>height of the bottom and top of each compartment above distributor</td>
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</tr>
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<td>height of the fluidized (expanded) bed</td>
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<td>-</td>
<td>index for combustion calculation $(=1, \text{ combustion, } =0, \text{ no combustion})$</td>
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<td>g/mole</td>
<td>molecular weight of air</td>
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<tr>
<td>FORTRAN Symbol</td>
<td>Mathematical Symbol</td>
<td>Unit</td>
<td>Description</td>
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<tr>
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<td>$M_c$</td>
<td>g/g atm</td>
<td>atomic weight of carbon</td>
</tr>
<tr>
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<td>$M_{CaCO_3}$</td>
<td>g/g atm</td>
<td>molecular weight of CaCO$_3$</td>
</tr>
<tr>
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<td>$M_{CaO}$</td>
<td>g/g atm</td>
<td>molecular weight of CaO</td>
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<td>$M_{CaSO_4}$</td>
<td>g/g atm</td>
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<td>$M_{CO}$</td>
<td>g/g atm</td>
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<td>g/g atm</td>
<td>molecular weight of CO$_2$</td>
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<td>number of solids discharge locations</td>
</tr>
<tr>
<td>MFEED</td>
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<td>number of solids feed locations</td>
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<td>molecular weight of feed gas</td>
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<td>g/g mole</td>
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</tr>
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<td>g/g mole</td>
<td>molecular weight of water</td>
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<td>g/g mole</td>
<td>molecular weight of H$_2$S</td>
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<td>$M_{MgO}$</td>
<td>g/g mole</td>
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<td>-</td>
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<tr>
<td>FORTRAN Symbol</td>
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<td>Unit</td>
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<td>NAMEC2</td>
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<td>NAMELI</td>
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<td>NDPAD</td>
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<td>size distribution of limestone particles - number of size intervals (NDPAD), upper bound of each size interval (DPADF), weight fraction (FRACTA)</td>
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<tr>
<td>DPADF</td>
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<td>atm</td>
<td>average pressure of the FBC</td>
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<td>PF</td>
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<td>atm</td>
<td>inlet gas pressure at the distributor</td>
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<td>PH</td>
<td>P_h</td>
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<td>P_v</td>
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<td>vertical pitch of the cooling coils</td>
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<td>Cal/cm^2/sec</td>
<td>heat transfer rate per cm^2 heat transfer area</td>
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<td>q_L</td>
<td>Cal</td>
<td>total heat of calcination of limestone</td>
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<td>q_C</td>
<td>Cal/g</td>
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<td>Cal/g</td>
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<td>Cal/sec</td>
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<td>heat transfer rate per cm^3 of bed</td>
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<td>gas constant</td>
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<td>FORTRAN Symbol</td>
<td>Mathematical Symbol</td>
<td>Unit</td>
<td>Description</td>
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<td>------------------------------------------</td>
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<tr>
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<td>g/cm³</td>
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<tr>
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<td>$\rho_{cf}$</td>
<td>g/cm³</td>
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<td>$\rho_{\ell}$</td>
<td>g/cm³</td>
<td>density of calcined additives</td>
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<td>$\rho_{ch}$</td>
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<td>RR</td>
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<td>rate of combustion in each compartment per unit carbon concentration</td>
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<td>Cal/sec</td>
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<td>g/sec</td>
<td>rate of combustion of carbon in the bubble phase in each compartment</td>
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<td>g/sec</td>
<td>rate of combustion of carbon in the emulsion phase in each compartment</td>
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<td>-</td>
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<td>sulfur release rate in the bubble phase</td>
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<td>gmol/sec</td>
<td>sulfur release rate in the emulsion phase</td>
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<td>T</td>
<td>°K</td>
<td>bed temperature</td>
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<td>°K</td>
<td>average bed temperature</td>
</tr>
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<td>TCAR</td>
<td>-</td>
<td>g/sec</td>
<td>total carbon available for combustion</td>
</tr>
<tr>
<td>TCRATE</td>
<td>-</td>
<td>g/sec</td>
<td>total carbon combustion rate</td>
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</tr>
<tr>
<td>TF</td>
<td>$T_g$</td>
<td>°K</td>
<td>inlet gas temperature</td>
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<td>residence time in the top compartment</td>
</tr>
<tr>
<td>FORTRAN Symbol</td>
<td>Mathematical Symbol</td>
<td>Unit</td>
<td>Description</td>
</tr>
<tr>
<td>----------------</td>
<td>---------------------</td>
<td>------------</td>
<td>------------------------------------------------------------------</td>
</tr>
<tr>
<td>TNORM</td>
<td>-</td>
<td>°K</td>
<td>temperature for convergency criterion</td>
</tr>
<tr>
<td>TOLD</td>
<td>-</td>
<td>°K</td>
<td>bed temperature in the previous iteration</td>
</tr>
<tr>
<td>TPB</td>
<td>-</td>
<td>°K</td>
<td>temperature of particles in the bubble phase</td>
</tr>
<tr>
<td>TPE</td>
<td>-</td>
<td>°K</td>
<td>temperature of particles in the emulsion phase</td>
</tr>
<tr>
<td>TSF</td>
<td>T_{sf}</td>
<td>°K</td>
<td>temperature of feed solids</td>
</tr>
<tr>
<td>TW</td>
<td>T_{w}</td>
<td>°K</td>
<td>temperature of coolant</td>
</tr>
<tr>
<td>TWAV</td>
<td>-</td>
<td>°K</td>
<td>average coolant temperature</td>
</tr>
<tr>
<td>UB</td>
<td>u_{b}</td>
<td>cm/sec</td>
<td>bubble velocity</td>
</tr>
<tr>
<td>UF</td>
<td>u_{f}</td>
<td>cm/sec</td>
<td>superficial gas velocity at the distributor at the inlet temperature and pressure</td>
</tr>
<tr>
<td>UHE</td>
<td>u</td>
<td>Cal/cm²sec°K</td>
<td>overall heat transfer coefficient</td>
</tr>
<tr>
<td>UHEAV</td>
<td>-</td>
<td>Cal/cm²sec°K</td>
<td>average overall heat transfer coefficient</td>
</tr>
<tr>
<td>UMF</td>
<td>u_{mf}</td>
<td>cm/sec</td>
<td>minimum fluidization velocity</td>
</tr>
<tr>
<td>UO</td>
<td>u_{o}</td>
<td>cm/sec</td>
<td>superficial gas velocity</td>
</tr>
<tr>
<td>VISC</td>
<td>u</td>
<td>g/cm sec</td>
<td>viscosity of gas in the bed</td>
</tr>
<tr>
<td>VMF</td>
<td>-</td>
<td>cm³</td>
<td>volume of bed at minimum fluidization</td>
</tr>
<tr>
<td>WAD</td>
<td>W_{lf}</td>
<td>g/sec</td>
<td>total limestone feed rate</td>
</tr>
<tr>
<td>WCAD</td>
<td>-</td>
<td>g/sec</td>
<td>total calcined additives feed rate</td>
</tr>
<tr>
<td>WCOAL</td>
<td>W_{cf}</td>
<td>g/sec</td>
<td>total coal feed rate</td>
</tr>
<tr>
<td>WELT</td>
<td>-</td>
<td>g/sec</td>
<td>total solids elutriated</td>
</tr>
<tr>
<td>WFAD</td>
<td>-</td>
<td>g/sec</td>
<td>feed rate of calcined additives at each location</td>
</tr>
<tr>
<td>WFC</td>
<td>-</td>
<td>g/sec</td>
<td>feed rate of char at each location</td>
</tr>
<tr>
<td>W MIX</td>
<td>w_{mix}</td>
<td>g/sec</td>
<td>upward and downward flow rate of solids due to backflow</td>
</tr>
<tr>
<td>FORTRAN Symbol</td>
<td>Mathematical Symbol</td>
<td>Unit</td>
<td>Description</td>
</tr>
<tr>
<td>----------------</td>
<td>---------------------</td>
<td>--------</td>
<td>-------------</td>
</tr>
<tr>
<td>WNET</td>
<td>$w_{net}$</td>
<td>g/sec</td>
<td>net flow rate of solids</td>
</tr>
<tr>
<td>X</td>
<td>x</td>
<td>wt. fraction</td>
<td>carbon concentration in the bed</td>
</tr>
<tr>
<td>XAV SAVIC</td>
<td>-</td>
<td>wt.fraction</td>
<td>average carbon concentration in the bed (IC denotes initial condition)</td>
</tr>
<tr>
<td>XC</td>
<td>$x_f$</td>
<td>wt. fraction</td>
<td>total carbon content in the coal</td>
</tr>
<tr>
<td>XCACO3</td>
<td>$x_{\text{Ca}}$</td>
<td>wt. fraction</td>
<td>CaCO$_3$ content in the limestone</td>
</tr>
<tr>
<td>XCAO</td>
<td>-</td>
<td>wt. fraction</td>
<td>CaO content in the additives</td>
</tr>
<tr>
<td>XCF</td>
<td>-</td>
<td>wt. fraction</td>
<td>weight fraction of fixed carbon in the coal (d b)</td>
</tr>
<tr>
<td>XCV</td>
<td>-</td>
<td>wt. fraction</td>
<td>weight fraction of volatiles in the coal (d b)</td>
</tr>
<tr>
<td>XCF (I)</td>
<td>$y_i$</td>
<td>mole fraction</td>
<td>feed gas composition ($O_2$, $CO_2$, $SO_2$, $H_2O$, $CO$, $H_2S$, $H_2$, $N_2$)</td>
</tr>
<tr>
<td>XH</td>
<td>-</td>
<td>wt. fraction</td>
<td>weight fraction of hydrogen in the coal (d b)</td>
</tr>
<tr>
<td>XMGC03</td>
<td>-</td>
<td>wt. fraction</td>
<td>MgCO$_3$ content in limestone</td>
</tr>
<tr>
<td>XN</td>
<td>-</td>
<td>wt. fraction</td>
<td>weight fraction of nitrogen in coal (d b)</td>
</tr>
<tr>
<td>XO</td>
<td>-</td>
<td>wt. fraction</td>
<td>weight fraction of oxygen in coal (d b)</td>
</tr>
<tr>
<td>XS</td>
<td>-</td>
<td>wt. fraction</td>
<td>weight fraction of sulfur in coal (d b)</td>
</tr>
<tr>
<td>YAV</td>
<td>-</td>
<td>mole fraction</td>
<td>average oxygen concentration in the bed</td>
</tr>
<tr>
<td>YB</td>
<td>$y_B$</td>
<td>mole fraction</td>
<td>bubble phase concentration of oxygen in combustion calculations or sulfur dioxide in SO$_2$ calculations</td>
</tr>
<tr>
<td>YBO</td>
<td>-</td>
<td>mole fraction</td>
<td>bubble phase concentration of oxygen</td>
</tr>
<tr>
<td>YE</td>
<td>$y_E$</td>
<td>mole fraction</td>
<td>emulsion phase concentration of oxygen in combustion calculations or sulfur dioxide in SO$_2$ calculations</td>
</tr>
<tr>
<td>YEO</td>
<td>-</td>
<td>mole fraction</td>
<td>emulsion phase concentration of oxygen</td>
</tr>
<tr>
<td>FORTRAN Symbol</td>
<td>Mathematical Symbol</td>
<td>Unit</td>
<td>Description</td>
</tr>
<tr>
<td>----------------</td>
<td>--------------------</td>
<td>------</td>
<td>--------------------------------------------</td>
</tr>
<tr>
<td>Z</td>
<td>Z</td>
<td>cm</td>
<td>height above the distributor</td>
</tr>
<tr>
<td>ZAVG</td>
<td>-</td>
<td>cm</td>
<td>average height of the compartment</td>
</tr>
<tr>
<td>ZB</td>
<td>-</td>
<td>cm</td>
<td>specified location</td>
</tr>
<tr>
<td>ZDIS</td>
<td>-</td>
<td>cm</td>
<td>locations of discharge and feed</td>
</tr>
<tr>
<td>ZF</td>
<td>-</td>
<td>cm</td>
<td>locations of bottom and top of the cooling coils</td>
</tr>
<tr>
<td>ZHE</td>
<td>-</td>
<td>cm</td>
<td></td>
</tr>
</tbody>
</table>
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

<table>
<thead>
<tr>
<th>No.</th>
<th>Title</th>
<th>Used in</th>
<th>Functions</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>ACTIV</td>
<td>Level I</td>
<td>Calculation of the reactivity of char ( \lambda_c ), for given data of ( y, d_{cm}, \rho_g, \mu, D_{O2}, k_{co}, u_0 ).</td>
</tr>
<tr>
<td>2</td>
<td>AKAD</td>
<td>Level II</td>
<td>Calculation of the rate constant of sulfur capturing reaction, ( k_{vl} ), for given data of ( f_x, d_x ), and ( T ).</td>
</tr>
<tr>
<td>3</td>
<td>AKK</td>
<td>Level II</td>
<td>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} ).</td>
</tr>
<tr>
<td>4</td>
<td>AREA</td>
<td>Level II</td>
<td>Calculation of ( A_t ) for a given height above distribution, ( z ).</td>
</tr>
<tr>
<td>5</td>
<td>CRRECT</td>
<td>Level I &amp; II</td>
<td>Calculation of the value of an unknown parameter assumed for the next trial of Regula Falsi iteration</td>
</tr>
<tr>
<td>6</td>
<td>DESIGN</td>
<td>Level II</td>
<td>Input subroutine for the design parameters of the bed. Redistribution of the parameters for each elemental volume</td>
</tr>
<tr>
<td>7</td>
<td>FREEFV</td>
<td>Level I</td>
<td>Calculation of the free fall velocity (terminal velocity) of particle of given property ( (d'_p) ) in the gas of given property ( (\rho_g, \mu_g) ).</td>
</tr>
</tbody>
</table>
(Table 9 Continued)

<table>
<thead>
<tr>
<th>No.</th>
<th>Title</th>
<th>Used in</th>
<th>Functions</th>
</tr>
</thead>
<tbody>
<tr>
<td>8</td>
<td>GPHASE</td>
<td>Level II</td>
<td>GPHASE given the value of gaseous species concentrations in bubble and emulsion phases of the ith compartment, $y_{g_i}$ and $y_{E_i}$, from a given hydrodynamic and kinetic informations and the values of $y_{g_{i-1}}$ and $y_{E_{i-1}}$. It is assumed there that the reaction is first order about the relevant species.</td>
</tr>
<tr>
<td>9</td>
<td>HEIGHT</td>
<td>Level II</td>
<td>Calculation of the effective height of the bed excluding the volume occupied by tubes.</td>
</tr>
<tr>
<td>10</td>
<td>HFATI</td>
<td>Level II</td>
<td>Calculation of the bed height above the distributor at any given cross-sectional area of the bed.</td>
</tr>
<tr>
<td>11</td>
<td>HYDRO</td>
<td>Level II</td>
<td>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.</td>
</tr>
<tr>
<td>12</td>
<td>POP</td>
<td>Level I</td>
<td>Calculation of the size distribution density function of char in the bed.</td>
</tr>
<tr>
<td>13</td>
<td>VOLUME</td>
<td>Level II</td>
<td>Calculation of the effective volume of the bed for the given height of the fluidized bed.</td>
</tr>
</tbody>
</table>
9-1. Function ACTIV

Reactivity of char, \( \lambda_c \), is calculated in this sub-program based on the equation:

\[
\lambda_c = \frac{1}{(k_{cR}/k_{cf} + 1)}
\]

\( k_{cR} \) 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

\[
k_f = Sh \cdot \frac{D_{O2}}{d_c}
\]

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: \( ACTIV \)

<table>
<thead>
<tr>
<th>Nomenclature Code</th>
<th>Model variable</th>
<th>Description</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>AK</td>
<td>( k_{cR} )</td>
<td>chemical reaction rate constant cm/sec</td>
<td></td>
</tr>
<tr>
<td>AKF</td>
<td>( k_{cf} )</td>
<td>mass transfer coefficient cm/sec</td>
<td></td>
</tr>
<tr>
<td>ACTIV</td>
<td>( \lambda_c )</td>
<td>reactivity of char</td>
<td></td>
</tr>
<tr>
<td>D</td>
<td>( D_{O2} )</td>
<td>diffusivity of oxygen cm²/sec</td>
<td></td>
</tr>
<tr>
<td>DCM</td>
<td>( d_{cm} )</td>
<td>maximum diameter of char particles cm</td>
<td></td>
</tr>
<tr>
<td>RHOG</td>
<td>( \rho_g )</td>
<td>gas density g/cm³</td>
<td></td>
</tr>
<tr>
<td>UO</td>
<td>( u_o )</td>
<td>gas superficial velocity cm/sec</td>
<td></td>
</tr>
<tr>
<td>VISC</td>
<td>( \mu )</td>
<td>gas viscosity g/cm·sec</td>
<td></td>
</tr>
<tr>
<td>Y</td>
<td>( y )</td>
<td>dimensionless particle diameter of char</td>
<td></td>
</tr>
</tbody>
</table>
9-2. Function AKAD

Mean overall rate constant for sulfur capturing reaction, \( k_{\text{vL}} \), 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 - SO₂
2) temperature: 1253 K
3) particle size: 0.0096-0.13 cm

Mean overall reaction rate constant is calculated by the equation,

\[ \hat{k}_{vL} = k' \cdot S \cdot \lambda_l \cdot (f_l, d_l) \]

where \( k' \) is defined as

\[ k' = 3.72 \times 10^{-3} \exp (-17.5 \times 10^3/RT) \]

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

\[ S_g = -193.75 T + 275,000 \quad \text{cm}^2/\text{g} \quad T > 1100 \text{ K} \]
\[ S_{g} = S_{g, 1100 \text{ K}} \]

For \( T < 1100 \text{ K} \), \( S_{g} = S_{g, 1100 \text{ K}} \)

From Borgwardt's experiment the relationships between \( \lambda_l \) and \( f_l \) are obtained. The data are reformed using Equations (3-56) and (3-66) and the function \( \hat{\lambda}_l \) (\( \hat{f}_l \)) 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 \( \hat{\lambda}_l \) for the arbitrary input of \( \hat{f}_l \) and \( d_l \). The equations for the interpolation are:
\[ \dot{\lambda}_{\alpha} = \left( \frac{\lambda_{\alpha 2}}{\lambda_{\alpha 1}} \right)^{\frac{f_2 - f_1}{f_2 - f_1}} \dot{\lambda}_{\alpha 1} \]

\[ \dot{\lambda}_{\beta} = \left( \frac{\lambda_{\beta 2}}{\lambda_{\beta 1}} \right)^{\frac{f_2 - f_1}{f_2 - f_1}} \dot{\lambda}_{\beta 1} \]

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 \( \dot{k}_{v\lambda} \) over the wide conditions such as

\[ T = 950-1350 \degree K \]
\[ d_{\lambda} = 0.01-0.5 \text{ cm} \]

and apply the interpolation not only for \( f_{\lambda} \) and \( d_{\lambda} \) but also \( T \).
The inputs and outputs of this sub-program are,

Inputs: FS, DP, T  
Outputs: AKAD

<table>
<thead>
<tr>
<th>Nomenclature Code</th>
<th>Model variable</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>AKAD</td>
<td>( \hat{k}_v )</td>
<td>mean overall reaction rate constant</td>
</tr>
<tr>
<td>ALIME</td>
<td>( \hat{\lambda}_k )</td>
<td>mean reactivity of adsorbent</td>
</tr>
<tr>
<td>DP</td>
<td>( d_k )</td>
<td>particle diameter of adsorbent</td>
</tr>
<tr>
<td>DP1, DP2, DP3</td>
<td>( d_{ka}, d_{kb} )</td>
<td>particle diameters of stored data</td>
</tr>
<tr>
<td>FB(I)</td>
<td>( \hat{f}_{ki} )</td>
<td>mean conversion data grid</td>
</tr>
<tr>
<td>FS</td>
<td>( \hat{f}_k )</td>
<td>mean conversion</td>
</tr>
<tr>
<td>RR(I), RB(I), RC(I)</td>
<td></td>
<td>mean reactivity data corresponding to the particle sizes of DP1, DP2, and DP3 respectively.</td>
</tr>
</tbody>
</table>

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:

\[
\text{Error} = T_c - T - \frac{7900 k_c p \gamma_{O2}/RT_c}{\frac{2A}{d_c} + \frac{T_c^4 - T^4}{T_c - T} e^{-0.5}}
\]

\( T' = \frac{(T_c + T)}{2} \)
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:

\[ k_{cR} = \left( \frac{T_c}{1000} \right) \exp \left( 17.9 - \frac{35.7}{(0.001986 T_c)} \right) \]

\( \text{Sh} = 2 \)

\[ D = 4.26 \left( \frac{T'}{1800} \right)^{1.75} \frac{1}{P} \]

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

<table>
<thead>
<tr>
<th>Nomenclature Code</th>
<th>Model variable</th>
<th>Description</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>AKF</td>
<td>( k_{cf} )</td>
<td>mass transfer coefficient</td>
<td></td>
</tr>
<tr>
<td>AKR</td>
<td>( k_{cR} )</td>
<td>chemical reaction constant</td>
<td></td>
</tr>
<tr>
<td>AKS</td>
<td>( k_c )</td>
<td>overall combustion rate constant</td>
<td></td>
</tr>
<tr>
<td>COND</td>
<td>( \lambda' )</td>
<td>thermal conductivity of gas</td>
<td></td>
</tr>
<tr>
<td>D</td>
<td>( D )</td>
<td>diffusivity of oxygen</td>
<td>cm²/sec</td>
</tr>
<tr>
<td>EM</td>
<td>( \varepsilon' )</td>
<td>emissivity</td>
<td></td>
</tr>
<tr>
<td>ETS</td>
<td>Error</td>
<td></td>
<td></td>
</tr>
<tr>
<td>ETSMAX</td>
<td>max(Error)</td>
<td>tolerance limit for iteration</td>
<td>°K</td>
</tr>
<tr>
<td>SHP</td>
<td>Sh</td>
<td>Sherwood number</td>
<td></td>
</tr>
<tr>
<td>SIGM</td>
<td>( \sigma )</td>
<td></td>
<td></td>
</tr>
<tr>
<td>T</td>
<td>( T )</td>
<td>bed temperature</td>
<td>°K</td>
</tr>
<tr>
<td>TAV</td>
<td>( T' )</td>
<td>average temperature for gas film</td>
<td>°K</td>
</tr>
<tr>
<td>TP</td>
<td>( T_c )</td>
<td>char particle temperature</td>
<td>°K</td>
</tr>
</tbody>
</table>
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 \(A_j\), \(j = 1-\text{MTB}\) 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 \(A\) corresponding to \(z\) is obtained by the following equation:

\[
A = \pi r^2
\]

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

\[ r_{j-1} = \left(\frac{A_{j-1}}{\pi}\right)^{1/2} \]

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(\(\text{GEN}/:ZB(J)\), \(\text{ATB}(J)\), \(J = 1, \text{MTB}\)

<table>
<thead>
<tr>
<th>Nomenclature Code</th>
<th>Model Variable</th>
<th>Description</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>(\text{ATB}(J))</td>
<td>(A_j)</td>
<td>bed cross section at (z=z_j)</td>
<td>(\text{cm}^2)</td>
</tr>
<tr>
<td>(\text{ATI})</td>
<td>(A_t)</td>
<td>bed cross section at (z=z)</td>
<td>(\text{cm}^2)</td>
</tr>
<tr>
<td>(\text{DTI})</td>
<td>(D_t)</td>
<td>equivalent diameter of bed at (z=z)</td>
<td>(\text{cm})</td>
</tr>
<tr>
<td>(\text{RI})</td>
<td>(n)</td>
<td>radius at (z=z)</td>
<td>(\text{cm})</td>
</tr>
<tr>
<td>(\text{ZB}(J))</td>
<td>(z_j)</td>
<td>height from the distributor where the data for cross-sectional area is given</td>
<td>(\text{cm})</td>
</tr>
<tr>
<td>(\text{ZI})</td>
<td>(z)</td>
<td>height from the distributor</td>
<td>(\text{cm})</td>
</tr>
</tbody>
</table>
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 increasing 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 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 X1, ..., Xm and, therefore, DX1, ..., DXm, E1, ..., Em and EMAX1, ..., EMAXm are needed. The main program must have the following structure:

    XI = ....
    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 I f (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)I f (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 I f (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

$$\alpha_{HE} = \pi \frac{d_o}{(P_H \cdot P_V)}$$

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

d$_o$ is the outside diameter of cooling coils

$P_H$ is the horizontal pitch

$P_V$ is the vertical pitch

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FIGURE 11 ILLUSTRATION FOR THE ARRANGEMENT OF HORIZONTAL COOLING TUBES

(a) triangular arrangement

(b) rectangular arrangement
For the triangular arrangement as shown in the Figure 19,

\[ q_{HE} = \frac{\text{Total heat transfer area}}{\text{Total volume}} \]

\[ \frac{1}{2} (\pi d_o L) \quad \frac{1}{2} p_H p_V L \quad \frac{p}{p_H V} \]

For the rectangular arrangement,

\[ q_{HE} = \frac{\pi d_o}{p_H p_V L} = \frac{\pi d_o}{p_H V} \]

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): \[ \frac{\frac{\pi d_o^2}{4} L}{p_H p_V L} = \frac{d_o}{4} a_{he} \]

(for the triangular arrangement): \[ \frac{1}{2} \left(\frac{\pi d_o^2}{4}\right) L \quad \frac{d_o}{4} a_{he} \]
Tube volume fraction is, then, equal to
\[ \epsilon_{\text{tube}} = 1 - \text{effective vol./total volume} \]

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

<table>
<thead>
<tr>
<th>Code</th>
<th>Model Variables</th>
<th>Description</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>A1, A2, A3, A4</td>
<td>-</td>
<td>ALPHANUMERIC CHARACTERS</td>
<td>-</td>
</tr>
<tr>
<td>ABED</td>
<td>( A_{t,i} )</td>
<td>Area of the FBC at each location</td>
<td>cm(^2)</td>
</tr>
<tr>
<td>AHE</td>
<td>( a_{\text{HE}} )</td>
<td>Specific heat transfer area</td>
<td>cm(^2)/cm(^3)</td>
</tr>
<tr>
<td>AHEAV</td>
<td>( a_{\text{HE},i} )</td>
<td>Specific heat transfer area in each compartment</td>
<td>cm(^2)/cm(^3)</td>
</tr>
<tr>
<td>AND</td>
<td>( n_d )</td>
<td>Number of distributor holes</td>
<td>-</td>
</tr>
<tr>
<td>ATB</td>
<td>( A_{t,i} )</td>
<td>Cross-sectional area of the FBC</td>
<td>cm(^2)</td>
</tr>
<tr>
<td>DBED</td>
<td>( D_{t,i} )</td>
<td>Diameter of the FBC at each location</td>
<td>cm</td>
</tr>
<tr>
<td>DEAV</td>
<td>( \Delta Z )</td>
<td>Average cell or compartment height</td>
<td>cm</td>
</tr>
<tr>
<td>DNZL</td>
<td>-</td>
<td>Diameter of distributor holes</td>
<td>cm</td>
</tr>
<tr>
<td>DTHICK</td>
<td>-</td>
<td>Distributor plate thickness</td>
<td>cm</td>
</tr>
<tr>
<td>DTUBE</td>
<td>( d_o )</td>
<td>Heat transfer tubes outside diameter</td>
<td>cm</td>
</tr>
<tr>
<td>DTUBEI</td>
<td>( d_{o,i} )</td>
<td>Tube outside diameter in each compartment</td>
<td>cm</td>
</tr>
</tbody>
</table>
## Nomenclature (Cont'd)

<table>
<thead>
<tr>
<th>Code</th>
<th>Model Variables</th>
<th>Description</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>DVB</td>
<td>-</td>
<td>Volume of each compartment</td>
<td>cm³</td>
</tr>
<tr>
<td>DVBEFF</td>
<td>-</td>
<td>Effective volume of each compartment</td>
<td>cm³</td>
</tr>
<tr>
<td>ETUBE</td>
<td>$e_{\text{tube}}$</td>
<td>Tube volume fraction</td>
<td>-</td>
</tr>
<tr>
<td>FD</td>
<td>-</td>
<td>Fraction of total solids discharged at each location</td>
<td>-</td>
</tr>
<tr>
<td>FFC</td>
<td>-</td>
<td>Fraction of total coal fed at each location</td>
<td>-</td>
</tr>
<tr>
<td>FFAD</td>
<td>-</td>
<td>Fraction of total additive fed at each location</td>
<td>-</td>
</tr>
<tr>
<td>IARR</td>
<td>-</td>
<td>Tubes arrangement code</td>
<td>-</td>
</tr>
<tr>
<td>IARRNG</td>
<td>-</td>
<td>Tubes arrangement code for each compartment</td>
<td>-</td>
</tr>
<tr>
<td>MDIS</td>
<td>-</td>
<td>No. of solids discharge locations</td>
<td>-</td>
</tr>
<tr>
<td>MFEED</td>
<td>-</td>
<td>No. of solids feed locations</td>
<td>-</td>
</tr>
<tr>
<td>MTB</td>
<td>-</td>
<td>No. of specified locations</td>
<td>-</td>
</tr>
<tr>
<td>MTHE</td>
<td>-</td>
<td>No. of coil locations</td>
<td>-</td>
</tr>
<tr>
<td>PH</td>
<td>$P_H$</td>
<td>Horizontal pitch of the coils</td>
<td>cm</td>
</tr>
<tr>
<td>PHI</td>
<td>$P_{H,i}$</td>
<td>Horizontal pitch in each compartment</td>
<td>cm</td>
</tr>
<tr>
<td>PI</td>
<td>$\pi$</td>
<td>Pi</td>
<td>$3.1415926$</td>
</tr>
<tr>
<td>PV</td>
<td>$P_V$</td>
<td>Vertical pitch of the coils</td>
<td>cm</td>
</tr>
<tr>
<td>PVI</td>
<td>$P_{V,i}$</td>
<td>Vertical pitch in each compartment</td>
<td>cm</td>
</tr>
<tr>
<td>ZB, ZHE, ZF, ZDIS</td>
<td>$Z_i$</td>
<td>Height above the distributor</td>
<td>cm</td>
</tr>
<tr>
<td>ZDIS</td>
<td>$Z_{\text{dis}}$</td>
<td>Location of solids discharge</td>
<td>cm</td>
</tr>
<tr>
<td>ZHE</td>
<td>-</td>
<td>Locations of the bottom and top of the heat transfer coils</td>
<td>cm</td>
</tr>
<tr>
<td>$Z(I), Z(I+1)$</td>
<td>$Z_i, Z_{i+1}$</td>
<td>Locations of the bottom and top of the ith compartment above the distributor</td>
<td>cm</td>
</tr>
</tbody>
</table>
9-7. Function FREEFV

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

\[
\begin{align*}
\text{Re}_p & \leq 0.4 \\
\frac{(\rho_p - \rho_g) g d_p^2}{18 \mu} & \quad \text{Re}_p \leq 0.4 \\
4\left(\frac{(\rho_p - \rho_g) g}{(225 \rho_g \mu)}\right)^{1/3} d_p & \quad 0.4 < \text{Re}_p \leq 500 \\
\frac{3.1 \left(\frac{\rho_p - \rho_g}{\rho_g}\right) g d_p}{\rho_g} & \quad 500 < \text{Re}_p < 200,000
\end{align*}
\]

where the particle is assumed to be spherical. The inputs to this function sub-program are \(d_p, \rho_p, \rho_g\) and \(\mu\).

<table>
<thead>
<tr>
<th>Nomenclature Code</th>
<th>Model variable</th>
<th>Description</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>DP</td>
<td>(d_p)</td>
<td>particle diameter</td>
<td>cm</td>
</tr>
<tr>
<td>FREEFV</td>
<td>(u_t)</td>
<td>terminal velocity</td>
<td>cm/sec</td>
</tr>
<tr>
<td>G</td>
<td>(g)</td>
<td>gravity acceleration</td>
<td>cm/sec²</td>
</tr>
<tr>
<td>RET</td>
<td>(\text{Re}_t)</td>
<td>Reynolds number for (u_t)</td>
<td>-</td>
</tr>
<tr>
<td>RHOG</td>
<td>(\rho_g)</td>
<td>gas density</td>
<td>g/cm³</td>
</tr>
<tr>
<td>RHOP</td>
<td>(\rho_p)</td>
<td>particle density</td>
<td>g/cm³</td>
</tr>
<tr>
<td>UT</td>
<td>(u_t)</td>
<td>terminal velocity</td>
<td>cm/sec</td>
</tr>
<tr>
<td>VISC</td>
<td>(\mu)</td>
<td>viscosity</td>
<td>g/cm·sec</td>
</tr>
</tbody>
</table>
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

\[
Y_{B,i} = \frac{F_{Bm,i-1} Y_{B,i-1} + a_1 F_{Em,i-1} Y_{E,i-1} + \text{GENB}}{F_{Bm,i} + a_1 F_{Em,i} + a_c,i \Delta V_i \left( k_{cB,i} T_B^{*} + a_1 k_{cE,i} T_E^{*} \right) / D_1}
\]

\[
Y_{E,i} = \frac{F_{Bm,i-1} Y_{E,i-1} + \text{GENE}}{D_1 + a_1 Y_{B,i}}
\]

where

\[
a_1 = k_{BE,i} \left( \frac{p}{RT_i} \right) \Delta V_i e_{bi}/D_1
\]

\[
D_1 = F_{Em,i} + \left( 1 - e_{c,i} - e_{\text{tube},i} \right) a_c,i k_{cE,i} T_E^{*}
\]

\[
+ k_{BE,i} e_{bi} T_i^{*} / \left( p/R \right) \Delta V_i
\]

\[
T_B^{*} = \left( T_i + T_{CB,i} \right) / 2
\]

\[
T_E^{*} = \left( T_i + T_{CE,i} \right) / 2
\]

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 SO2/H2S calculation GENB and GENE represents the SO2/H2S 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, FBM0, FEM0, FBMO, FEM, FBM, FEM, T, TB, TE, YBO, YEO, GENB, GENE

Outputs: YB1, YE1

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<table>
<thead>
<tr>
<th>Nomenclature Code</th>
<th>Model Variable</th>
<th>Description</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>AM</td>
<td>$a_c$</td>
<td>specific surface area of char particle in the bed</td>
<td>cm$^2$/sec $^3$</td>
</tr>
<tr>
<td>AKB</td>
<td>$k_{CB}$</td>
<td>combustion rate constant in the bubble phase</td>
<td></td>
</tr>
<tr>
<td>AKBE</td>
<td>$K_{BE}$</td>
<td>gas interchange coefficient</td>
<td>1/sec</td>
</tr>
<tr>
<td>AKE</td>
<td>$k_{CE}$</td>
<td>combustion rate constant in the emulsion phase</td>
<td></td>
</tr>
<tr>
<td>ALF</td>
<td>$a_1$</td>
<td>particle diameter of char</td>
<td>cm</td>
</tr>
<tr>
<td>DC</td>
<td>$d_c$</td>
<td>volume of $i$th compartment</td>
<td>cm$^3$</td>
</tr>
<tr>
<td>DVBB</td>
<td>$\Delta V_i$</td>
<td>volume fraction of bubbles and clouds</td>
<td></td>
</tr>
<tr>
<td>D1</td>
<td>$D_1$</td>
<td>volume fraction of bubbles</td>
<td>-</td>
</tr>
<tr>
<td>EPB</td>
<td>$\varepsilon_B$</td>
<td>volume fraction of heat exchange tubes</td>
<td>-</td>
</tr>
<tr>
<td>FBM, FBMO</td>
<td>$F_{mB,i}$, $F_{mB,i-1}$</td>
<td>molar flow rates of gas in bubble phase</td>
<td>gmole/sec</td>
</tr>
<tr>
<td>FEM, FEMO</td>
<td>$F_{mE,i}$, $F_{mE,i-1}$</td>
<td>molar flow rates of gas in emulsion phase</td>
<td>gmole/sec</td>
</tr>
<tr>
<td>GENB, GENE</td>
<td>-</td>
<td>formation rate of the concerning species by other reactions</td>
<td>gmole/sec</td>
</tr>
<tr>
<td>P</td>
<td>$p$</td>
<td>pressure</td>
<td>atm</td>
</tr>
<tr>
<td>RG</td>
<td>$R$</td>
<td>gas constant</td>
<td>cm$^3$.atm/gmole $^oK$</td>
</tr>
<tr>
<td>TB</td>
<td>$T_{CB}$</td>
<td>temperature of char particle $^oK$ in bubble cloud phase</td>
<td></td>
</tr>
<tr>
<td>TE</td>
<td>$T_{CE}$</td>
<td>temperature of char particle $^oK$ in emulsion phase</td>
<td></td>
</tr>
<tr>
<td>YBO, YB1</td>
<td>$Y_{B,i-1}$, $Y_{Bi}$</td>
<td>mole fraction in bubble phase</td>
<td>-</td>
</tr>
<tr>
<td>YEO, YE1</td>
<td>$Y_{E,i-1}$, $Y_{Ei}$</td>
<td>mole fraction in emulsion phase</td>
<td>-</td>
</tr>
</tbody>
</table>
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,

\[
z = z_{j-1} + \left( \frac{A_t}{A_j} \right)^{1/2} - 1 \quad \frac{(z_j - z_{j-1})}{(A_j/A_{j-1})^{1/2} - 1}
\]

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.
\[ u_{mf} = \left( \frac{dP}{\rho g} \right) \left[ (33.7)^2 + 0.0408 \frac{d^3}{\rho_p (\rho_p - \rho_g) \rho_g/\mu^2} \right]^{1/2} - 33.7 \]  
(Wen-Yu Equation)

\[ D_{Bi} = D_{B_{\text{max},i}} - (D_{B_{\text{max},i}} - D_{B,i-1}) e^{-0.3\Delta z_i/D_{t,i}} \]

\[ D_{B,1} = 0.347 \left[ A_{t,1} (u_{o,i} - u_{mf,i})/n_d \right]^{0.4} \]  
(Miwa's Equation)

\[ D_{B_{\text{max},i}} = 0.652 \left[ A_{t,i} (u_{o,i} - u_{mf,i}) \right]^{0.4} \]  
(Mori-Wen Equation)

\[ u_{B_{\infty},i} = 0.711 \quad g_{D,i} \]

\[ u_{BS,i} = 0.355 \quad g_{D_t,i} \]

\[ u_{B,i} = u_{B_{\infty},i} + u_{o,i} - u_{mf} \]

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

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

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

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 grid. $u_o$ is compared with $u_{mf}$. Since the cross-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, $u_0$ is decreasing, and when it is smaller than $u_{mf}$, critical 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 $u_0$ 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.
<table>
<thead>
<tr>
<th>Code</th>
<th>Model Variables</th>
<th>Description</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>AHEAV</td>
<td>a_{he}</td>
<td>Specific heat transfer area for each compartment</td>
<td>cm^2/cm^3</td>
</tr>
<tr>
<td>AND</td>
<td>n_d</td>
<td>No. of distributor holes</td>
<td>-</td>
</tr>
<tr>
<td>AT</td>
<td>A_{t,i}</td>
<td>Cross-sectional area of the bed at each location</td>
<td>cm^2</td>
</tr>
<tr>
<td>DB</td>
<td>D_B</td>
<td>Bubble diameter</td>
<td>cm</td>
</tr>
<tr>
<td>DBAV</td>
<td>D_{B,av}</td>
<td>Average bubble size of each compartment</td>
<td>cm</td>
</tr>
<tr>
<td>DBED</td>
<td>D_{t,i}</td>
<td>Diameter of the FBC</td>
<td>cm</td>
</tr>
<tr>
<td>DBMAX</td>
<td>D_{Bm}</td>
<td>Maximum bubble size</td>
<td>cm</td>
</tr>
<tr>
<td>DPB</td>
<td>d_p</td>
<td>Average particle diameter in the bed</td>
<td>cm</td>
</tr>
<tr>
<td>DTUBE, DTUBEI</td>
<td>d_o</td>
<td>Diameter of heat transfer coils</td>
<td>cm</td>
</tr>
<tr>
<td>DVB, DVBB</td>
<td>ΔV_i</td>
<td>Volume of each compartment</td>
<td>cm^3</td>
</tr>
<tr>
<td>DVBBEF, DVBEFF</td>
<td>-</td>
<td>Effective volume of each compartment (excluding tubes)</td>
<td>cm^3</td>
</tr>
<tr>
<td>EMF</td>
<td>e_{mf}</td>
<td>Void fraction at minimum fluidization</td>
<td>-</td>
</tr>
<tr>
<td>EPB</td>
<td>e_b</td>
<td>Bubble fraction</td>
<td>-</td>
</tr>
<tr>
<td>EPC</td>
<td>e_c</td>
<td>Cloud fraction</td>
<td>-</td>
</tr>
<tr>
<td>ETUBE</td>
<td>e_{tube,i}</td>
<td>Tube volume fraction in each compartment</td>
<td>-</td>
</tr>
<tr>
<td>FMF</td>
<td>F_{mf}</td>
<td>Molar flow rate of inlet gas</td>
<td>gmol/sec</td>
</tr>
<tr>
<td>FMO</td>
<td>F_m</td>
<td>Total molar flow rate of gas</td>
<td>-</td>
</tr>
<tr>
<td>G</td>
<td>g</td>
<td>Acceleration due to gravity</td>
<td>cm/sec^2</td>
</tr>
<tr>
<td>HCR</td>
<td>-</td>
<td>Critical bed height (u_o = u_{mf})</td>
<td>cm</td>
</tr>
<tr>
<td>H(I), H(I+1)</td>
<td>h_i, h_{i+1}</td>
<td>Height of the bottom and top of each compartment above the distributor</td>
<td>cm</td>
</tr>
<tr>
<td>HLF</td>
<td>L_f</td>
<td>Height of the fluidized bed (expanded)</td>
<td>cm</td>
</tr>
<tr>
<td>HLMF</td>
<td>L_{mf}</td>
<td>Height of minimum fluidization</td>
<td>cm</td>
</tr>
<tr>
<td>ICR</td>
<td>-</td>
<td>Indicator for critical bed height</td>
<td>-</td>
</tr>
<tr>
<td>Code</td>
<td>Model Variables</td>
<td>Description</td>
<td>Unit</td>
</tr>
<tr>
<td>---------</td>
<td>-----------------</td>
<td>-------------------------------------------------------</td>
<td>---------------------------</td>
</tr>
<tr>
<td>IFBC</td>
<td>-</td>
<td>Indicator for the fixed bed section</td>
<td></td>
</tr>
<tr>
<td>ITUBE,</td>
<td>-</td>
<td>Tube arrangement code for each compartment</td>
<td></td>
</tr>
<tr>
<td>IARRNG</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>M</td>
<td>-</td>
<td>Total number of compartments in the expanded bed</td>
<td></td>
</tr>
<tr>
<td>M1</td>
<td>-</td>
<td>Total number of locations compartment</td>
<td></td>
</tr>
<tr>
<td>MGAS</td>
<td>$M_g$</td>
<td>Molecular weight of gas</td>
<td>$g$/mol</td>
</tr>
<tr>
<td>PAV</td>
<td>$P_{av}$</td>
<td>Average pressure of the FBC</td>
<td>atm</td>
</tr>
<tr>
<td>PHI</td>
<td>$PH_i$</td>
<td>Horizontal pitch of the coils for each compartment</td>
<td>cm</td>
</tr>
<tr>
<td>RG</td>
<td>$R$</td>
<td>Gas constant</td>
<td>atm$\cdot$cm$^3$/g/mol$\cdot$K</td>
</tr>
<tr>
<td>RHOCAD</td>
<td>$\rho_k$</td>
<td>Density of calcined additives</td>
<td>$g$/cm$^3$</td>
</tr>
<tr>
<td>RHOGAS</td>
<td>$\rho_g$</td>
<td>Density of fluidizing gas</td>
<td>$g$/cm$^3$</td>
</tr>
<tr>
<td>SOLVOL</td>
<td>-</td>
<td>Volume of bed, total</td>
<td>cm$^3$</td>
</tr>
<tr>
<td>SUM</td>
<td>-</td>
<td>Height of solids alone (no bubble), total</td>
<td>cm$^3$</td>
</tr>
<tr>
<td>SUMEFF</td>
<td>-</td>
<td>Volume of solids alone, total effective volume of the bed</td>
<td>cm$^3$</td>
</tr>
<tr>
<td>SUMV</td>
<td>-</td>
<td></td>
<td></td>
</tr>
<tr>
<td>T</td>
<td>$T$</td>
<td>Temperature of the bed</td>
<td>°K</td>
</tr>
<tr>
<td>UB</td>
<td>$u_b$</td>
<td>Bubble velocity</td>
<td>cm/sec</td>
</tr>
<tr>
<td>UBR</td>
<td>$u_{br}$</td>
<td>Bubble rising velocity</td>
<td>cm/sec</td>
</tr>
<tr>
<td>UBS</td>
<td>$u_{bs}$</td>
<td>Slug velocity</td>
<td>cm/sec</td>
</tr>
<tr>
<td>UF</td>
<td>$u_f$</td>
<td>Superficial gas velocity at the inlet pressure</td>
<td>cm/sec</td>
</tr>
<tr>
<td>UO</td>
<td>$u_o$</td>
<td>Superficial gas velocity</td>
<td>cm/sec</td>
</tr>
<tr>
<td>UMF</td>
<td>$u_{mf}$</td>
<td>Minimum fluidization velocity</td>
<td>cm/sec</td>
</tr>
<tr>
<td>VMF</td>
<td>-</td>
<td>Volume of bed at minimum fluidization</td>
<td>cm$^3$</td>
</tr>
<tr>
<td>X</td>
<td>$x$</td>
<td>Carbon concentration</td>
<td>wt. fraction</td>
</tr>
<tr>
<td>YB</td>
<td>-</td>
<td>Bubble phase oxygen concentration</td>
<td>mole fraction</td>
</tr>
<tr>
<td>YE</td>
<td>-</td>
<td>Emulsion phase oxygen concentration</td>
<td>mole fraction</td>
</tr>
</tbody>
</table>
### 9-12. Subroutine POP

The calculations of the size distribution density function \( \phi (y_i) \), second and third moments of \( \phi \) 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, BCl, 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.

<table>
<thead>
<tr>
<th>Nomenclature Code</th>
<th>Model Variable</th>
<th>Description</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>AKE (I)</td>
<td>( K^*(y_1) )</td>
<td>elutriation rate constant</td>
<td>g·cm(^2)/sec</td>
</tr>
<tr>
<td>AKEI(I)</td>
<td>( \int_0^{y_i} (K^*/\lambda_c) ) dy</td>
<td>g·cm(^2)/sec</td>
<td>defined in the main program</td>
</tr>
<tr>
<td>ALAMA</td>
<td>( \int_0^{1} \phi y_2 ) dy</td>
<td>-</td>
<td></td>
</tr>
<tr>
<td>ALAM(I)</td>
<td>( \lambda_c(y_i) )</td>
<td>reactivity of coal for ( y = y_i )</td>
<td>-</td>
</tr>
<tr>
<td>ALAMI(I)</td>
<td>( \int_0^{y_i} (1/\lambda_c(y))dy )</td>
<td>-</td>
<td>calculated in the main program</td>
</tr>
<tr>
<td>ALAMV</td>
<td>( \psi_v )</td>
<td>-</td>
<td></td>
</tr>
<tr>
<td>A, A1, A2, A21, A22, A31, A32</td>
<td>dummy variables</td>
<td>cm(^2)</td>
<td></td>
</tr>
<tr>
<td>AT</td>
<td>bed cross section</td>
<td>-</td>
<td></td>
</tr>
<tr>
<td>BC</td>
<td>( B_{cw} )</td>
<td>defined by Eq. (4-9)</td>
<td>-</td>
</tr>
<tr>
<td>BCI</td>
<td>( B_{cf} )</td>
<td>defined by Eq. (4-10)</td>
<td>-</td>
</tr>
<tr>
<td>CC</td>
<td>( C_c )</td>
<td>defined by Eq. (4-8)</td>
<td>-</td>
</tr>
<tr>
<td>DY(i)</td>
<td>increment of ( y; y_i - y_{i-1} )</td>
<td>-</td>
<td></td>
</tr>
<tr>
<td>EC</td>
<td>( (A_t/W_b) &lt; K^* y^3 &gt; )</td>
<td>-</td>
<td></td>
</tr>
<tr>
<td>L</td>
<td>total number of grids on ( y )-coordinate</td>
<td>-</td>
<td></td>
</tr>
</tbody>
</table>
(Cont.)

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

Original page is of poor quality
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 

\[
(Y - \text{FLOAT}(N-1) - \text{DZAV} \cdot \text{GT} \cdot 0.01 \cdot \text{DZAV}) \cdot N = N+1. \]

This statement avoids the computation for infinitesimal difference in height \((Y - \text{FLOAT}(N) \cdot \text{DZAV})\) 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.
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 \( \text{SO}_2 \) concentrations in the bubble phase and emulsion phases, bubble diameter and sulfur dioxide capture 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

Bed dia. = 73 cms.
Excess Air = 17.4%
Coal feed rate = 14.7 \( \frac{g}{sec} \)
\( d_p = 84 \mu \)

**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.

<table>
<thead>
<tr>
<th>Variable</th>
<th>NCB DATA</th>
<th>COMPUTED RESULTS</th>
</tr>
</thead>
<tbody>
<tr>
<td>Combustion Efficiency</td>
<td>92.8%</td>
<td>92.84%</td>
</tr>
<tr>
<td>Average Bed Temp.</td>
<td>1470°F (799°C)</td>
<td>1457°F (791.5°C)</td>
</tr>
<tr>
<td>Outlet gas concentration</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Oxygen</td>
<td>4.3% v</td>
<td>4.6% v</td>
</tr>
<tr>
<td>Carbon dioxide</td>
<td>13.9% v</td>
<td>16.36% v</td>
</tr>
<tr>
<td>Sulfur dioxide</td>
<td>400 ppm</td>
<td>374 ppm</td>
</tr>
<tr>
<td>Sulfur capture efficiency</td>
<td>83%</td>
<td>81.69%</td>
</tr>
</tbody>
</table>
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, \( u_0/u_{mf} \) 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, because 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 \( (\eta_s) \) is shown in Figure 16. The decrease is \( \eta_s \) 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
TAPERED BED WITH FIXED BED AT TOP

\[d_p = 0.1 \text{ cm}\]
\[u_{mf} = 20 \text{ cm/s}\]
\[H_{LF} = 67.056 \text{ cm}\]
\[\text{Excess Air} = 17.4\%\]

FIGURE 1. TEMPERATURE PROFILE IN THE TAPERED BED (LEVEL II MODEL).
\[ \frac{C_a}{S} = 2.2 \]

Excess Air = 17.4%

\( T_{\text{avg.}} = 791^\circ C \)

\( D_p = 84 \mu \)

**Figure 14.** Concentration profile of \( SO_2 \) in the uniform bed.
FIGURE 15. EFFECT OF CALCIUM TO SULFUR RATIO IN FEED ON SULFUR CAPTURE EFFICIENCY.

Excess air = 17.4%

$u_0 = 33 \text{ cm/s}$

Av. Bed Temp. = 795°C
EXCESS AIR = 17.1%
Ca/S = 2.2

\[ \eta_S = 1 - \frac{\text{moles } \text{SO}_2 \text{ in flue gas}}{\text{total sulfur input}} \]

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 ($\eta_C$) 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 $\eta_C$ 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 $\eta_C$ due to higher oxygen concentration. The combustion efficiency at extremely large excess air ratio will be expected to drop.
FIGURE 17. BUBBLE DIAMETER ALONG THE BED HEIGHT FOR THE UNIFORM FLOW.
Figure 18. Effect of excess air on combustion efficiency in the uniform bed.

\( \eta_c \), combustion efficiency

Conc. of carbon in the bed, % wt.
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 elutiation 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 \( \text{SO}_2 \)-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 SO₂-limestone reactions which are
used to calculate the sulfur retention efficiency and the SO₂ 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. Further-
more, 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 discrepancies 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 \( \text{SO}_2 \)-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.


<table>
<thead>
<tr>
<th>Variable</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>A</strong></td>
<td>matrix defined by Eq. (3-4)</td>
</tr>
<tr>
<td><strong>A_{HE}</strong></td>
<td>total heat exchange area $\text{cm}^2$</td>
</tr>
<tr>
<td><strong>A_t</strong></td>
<td>cross sectional area of bed $\text{cm}^2$</td>
</tr>
<tr>
<td><strong>a_{HE}</strong></td>
<td>specific heat transfer area based on outside area of tubes and volume of bed minus internals $\text{cm}^2/\text{cm}^3$ (bed)</td>
</tr>
<tr>
<td><strong>B</strong></td>
<td>matrix defined by Eq. (3-5)</td>
</tr>
<tr>
<td><strong>B_{cf}</strong></td>
<td>$B_{cw} \frac{n_{cf}}{n_{cw}}$</td>
</tr>
<tr>
<td><strong>B_{cw}</strong></td>
<td>$d_{cm} \rho ch_{C} / (2M_c \theta \bar{k}<em>{c0} C</em>{O2})$</td>
</tr>
<tr>
<td><strong>B_Z</strong></td>
<td>constant defined by Eq. (3-64)</td>
</tr>
<tr>
<td><strong>C_c</strong></td>
<td>constant defined by Eq. (4-8)</td>
</tr>
<tr>
<td><strong>C_i</strong></td>
<td>concentration of gaseous species i $\text{mol}/\text{cm}^3$</td>
</tr>
<tr>
<td><strong>c_{gm}</strong></td>
<td>molar heat capacity of gas $\text{cal/gmol} \cdot ^\circ \text{K}$</td>
</tr>
<tr>
<td><strong>c_{gmf}</strong></td>
<td>molar heat capacity of gas at feed temperature $\text{cal/gmol} \cdot ^\circ \text{K}$</td>
</tr>
<tr>
<td><strong>c_s</strong></td>
<td>heat capacity of solid $\text{cal/g} \cdot ^\circ \text{K}$</td>
</tr>
<tr>
<td><strong>c_{sf}</strong></td>
<td>heat capacity of solid at feed temperature $\text{cal/g} \cdot ^\circ \text{K}$</td>
</tr>
<tr>
<td><strong>D_B</strong></td>
<td>bubble size $\text{cm}$</td>
</tr>
<tr>
<td><strong>D_{Bo}</strong></td>
<td>initial bubble size $\text{cm}$</td>
</tr>
<tr>
<td><strong>D_{Bm}</strong></td>
<td>maximum bubble size $\text{cm}$</td>
</tr>
<tr>
<td><strong>D_t</strong></td>
<td>bed diameter</td>
</tr>
<tr>
<td><strong>d_A</strong></td>
<td>ash particle size $\text{cm}$</td>
</tr>
<tr>
<td><strong>d_c</strong></td>
<td>particle diameter of coal or char $\text{cm}$</td>
</tr>
<tr>
<td><strong>d_{cm}</strong></td>
<td>maximum diameter of coal particles $\text{cm}$</td>
</tr>
<tr>
<td><strong>d_k</strong></td>
<td>particle diameter of additives (limestone or dolomite) $\text{cm}$</td>
</tr>
<tr>
<td><strong>EAR</strong></td>
<td>excess air ratio</td>
</tr>
</tbody>
</table>
$E_z$ axial dispersion constant of solids \( \text{cm}^2/\text{sec} \)

$F_{Bm}$ molar flow rate of gas through bubble phase \( \text{gmol/sec} \)

$F_{Em}$ molar flow rate of gas through emulsion phase \( \text{gmol/sec} \)

$F_m$ total molar flow rate of gas \( \text{gmol/sec} \)

$F_{mf}$ molar flow rate of inlet gas \( \text{gmol/sec} \)

$F_{mth}$ theoretical feed rate of inlet gas \( \text{gmol/sec} \)

$F_r$ Froude number

$f_\ell$ 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 \( \text{cm/sec}^2 \)

$h_j$ maximum height of jets above distributor \( \text{cm} \)

$I_t$ total number of cells

$k^*$ specific elutriation rate constant \( g/\text{cm}^2\cdot\text{sec} \)

$K_{BE,i}$ gas exchange coefficient in \( i \)th cell \( 1/\text{sec} \)

$K_{mBE,i}$ modified gas exchange coefficient (Eq. 3-59) \( 1/\text{sec} \cdot \text{cm}^3 \)

$K_{sBE,i}$ solids exchange coefficient in \( i \)th cell \( 1/\text{sec} \)

$k_c$ overall surface reaction rate constant \( \text{cm/sec} \)

$k_{cf}$ film diffusion coefficient \( \text{cm/sec} \)

$k_{cR}$ chemical reaction constant \( \text{cm/sec} \)

$k_{c0}$ value of $k_c$ for the maximum particle size \( \text{cm/sec} \)

$k_i$ overall surface reaction rate constant of reaction \( i, (i=3,4 \text{ or } 5) \) \( \text{cm/sec} \)

$k_{vi}$ overall volume reaction rate constant of reaction \( i, (i=1 \text{ or } 2) \) \( 1/\text{sec} \)

$L_f$ fluidized bed height \( \text{cm} \)

$L_{mf}$ minimum fluidization height \( \text{cm} \)
atomic or molecular weight of species $i$ \( g/mol \)

number of holes in distributor

number of ash particles held up in the bed

number of char particles held up in the bed

number of char particles held up in $i$th cell

number of adsorbent particles held up in the bed

number mass velocity vector of char particles \( 1/cm^2\cdot sec \)

number of ash particle withdrawn per unit time \( 1/sec \)

number of char particles elutriated per unit time \( 1/sec \)

number of coal particles fed to the bed per unit \( 1/sec \)

number of coal particles withdrawn per unit time \( 1/sec \)

downward flow of particles \( 1/sec \)

upward flow of particles \( 1/sec \)

number of char particles transferred from emulsion phase to wake phase per unit time \( 1/sec \)

number rate of limestone particles fed to the bed \( 1/sec \)

number rate of limestone particles withdrawn from the bed \( 1/sec \)

number of char particles transferred from wake phase to emulsion phase in the $i$th cell per unit time \( 1/sec \)

average pressure in the bed \( atm \)

lower heating value of coal on dry basis adjusted for CO \( cal/g \)

heat of calcination of limestone \( cal/g \)

gas constant \( 82.05 \, cm^3\cdot atm/gmol/°K \) or \( 1.987 \, cal/gmol.°K \)

dimensionless shrinking rate of char \( 1/sec \)

ratio of cloud sphere volume to bubble volume

reaction rate vector for reactions 1-8 \( gmol/sec\cdot cm^3 \) (emulsion)

total formation rate vector for gaseous species \( gmol/sec\cdot cm^3 \) (emulsion)

total formation rate vector for solid phase species \( gmol/sec\cdot cm^3 \) (emulsion)

terminal Reynold's number
reaction rates defined by Eqs. (3-88) \( \text{g/mol/sec} \cdot \text{cm}^3 \) (emulsion)

rate of reaction \( i \) \( \text{g/mol/sec} \cdot \text{cm}^3 \) (emulsion)

rates of reaction \( i \) in emulsion phase and in bubble phase \( \text{g/mol/sec} \cdot \text{cm}^3 \) (emulsion)

formation rates of species \( M_{gj} \) or \( M_{sj} \) by reaction \( i \) \( \text{g/mol/sec} \cdot \text{cm}^3 \) (emulsion)

rates of sulfur capture in bubble phase and in emulsion phase \( \text{g/mol/sec} \cdot \text{cm}^3 \) (emulsion)

rate of \( i \)th reaction for one particle \( \text{g/mol/sec} \)

reaction rate per char particle \( \text{g/mol/sec} \)

reaction rate per limestone particle \( \text{g/mol/sec} \)

internal surface area of calcined limestone \( \text{cm}^2 / \text{g} \)

local bed temperature \( \text{°K} \)

temperature of feed gas \( \text{°K} \)

temperature of \( i \)th compartment \( \text{°K} \)

temperature of feed solids \( \text{°K} \)

temperature of cooling water \( \text{°K} \)

overall heat transfer coefficient of cooling tubes based on outside tube diameter \( \text{cal/cm}^2 \cdot \text{sec} \cdot \text{°K} \)

superficial gas velocity \( \text{cm/sec} \)

bubble rising velocity \( \text{cm/sec} \)

minimum fluidization velocity \( \text{cm/sec} \)

terminal velocity \( \text{cm/sec} \)

volume of bed (total including tubes) \( \text{cm}^3 \)

volume of bed excluding tubes \( \text{cm}^3 \)

volumetric flow rate of solids in bubble-wake phase excluding voids \( \text{cm}^3 / \text{sec} \)

volumetric solids exchange rates from bubble-wake phase to emulsion phase and from emulsion phase to bubble-wake phase respectively \( \text{cm}^3 / \text{sec} \)
<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>$v_d$</td>
<td>volumetric down flow rate of solids in emulsion phase excluding voids</td>
<td>cm$^3$/sec</td>
</tr>
<tr>
<td>$v_E$</td>
<td>volumetric flow rate of solids in emulsion phase excluding voids</td>
<td>cm$^3$/sec</td>
</tr>
<tr>
<td>$v_e$</td>
<td>volumetric elutriation rate</td>
<td>cm$^3$/sec</td>
</tr>
<tr>
<td>$v_f$</td>
<td>volumetric feed rate excluding voids</td>
<td>cm$^3$/sec</td>
</tr>
<tr>
<td>$v_{net}$</td>
<td>volumetric net flow rate excluding voids</td>
<td>cm$^3$/sec</td>
</tr>
<tr>
<td>$v_u$</td>
<td>volumetric upward flow rate of solids in emulsion phase excluding voids</td>
<td>cm$^3$/sec</td>
</tr>
<tr>
<td>$v_w$</td>
<td>volumetric withdrawal rate of solids excluding voids</td>
<td>cm$^3$/sec</td>
</tr>
<tr>
<td>$W_b$</td>
<td>total weight of bed material</td>
<td>g</td>
</tr>
<tr>
<td>$w_B$</td>
<td>solids mass flow rate in bubble-wake phase</td>
<td>g/sec</td>
</tr>
<tr>
<td>$w_{BE,WEB}$</td>
<td>solids mass exchange rates from bubble-wake phase to emulsion phase and from emulsion phase to bubble-wake phase</td>
<td>g/sec</td>
</tr>
<tr>
<td>$W_c$</td>
<td>total weight of char in the bed</td>
<td>g</td>
</tr>
<tr>
<td>$w_{cf}$</td>
<td>coal feed rate, dry basis</td>
<td>g/sec</td>
</tr>
<tr>
<td>$w_d$</td>
<td>solids down flow rate in emulsion phase</td>
<td>g/sec</td>
</tr>
<tr>
<td>$w_e$</td>
<td>elutriation rate of unburned char</td>
<td>g/sec</td>
</tr>
<tr>
<td>$W_E$</td>
<td>solids mass flow rate in emulsion phase</td>
<td>g/sec</td>
</tr>
<tr>
<td>$w_f$</td>
<td>feed rate of solids</td>
<td>g/sec</td>
</tr>
<tr>
<td>$w_{kf}$</td>
<td>limestone feed rate, uncalcined basis</td>
<td>g/sec</td>
</tr>
<tr>
<td>$w_{mix}$</td>
<td>upward and downward flow rate due to backflow of solids</td>
<td>g/sec</td>
</tr>
<tr>
<td>$w_{net}$</td>
<td>net flow rate of solids</td>
<td>g/sec</td>
</tr>
<tr>
<td>$w_u$</td>
<td>solids upward flow rate in emulsion phase</td>
<td>g/sec</td>
</tr>
<tr>
<td>$w_w$</td>
<td>withdrawal rate of solids</td>
<td>g/sec</td>
</tr>
<tr>
<td>$w_{W}$</td>
<td>mass flow rate of wake</td>
<td>g/sec</td>
</tr>
<tr>
<td>$X_C$</td>
<td>mass fraction of carbon in char</td>
<td>-</td>
</tr>
<tr>
<td>$X_h$</td>
<td>mass fraction of water in coal</td>
<td>-</td>
</tr>
</tbody>
</table>
\[ X_{if} \quad (i=A,C,H,N,O,S) \quad \text{mass fraction of ash, carbon, hydrogen, nitrogen, oxygen, sulfur and in coal (dry basis)} \]
\[ X_{Ca} \quad \text{mass fraction of calcium in limestone} \]
\[ X_{vf} \quad \text{mass fraction of volatiles, dry basis} \]
\[ X_{VM} \quad \text{mass fraction of volatiles dry ash free basis} \]
\[ x \quad \text{mass fraction of carbon in the bed} \]
\[ x_B \quad \text{mass fraction of carbon in bubble-wake phase} \]
\[ x_E \quad \text{mass fraction of carbon in emulsion phase} \]
\[ x_f \quad \text{mass fraction of carbon in solids feed} \]
\[ Y(y) \quad \text{function defined by Eq. (4-6)} \]
\[ Y_B, Y_E \quad \text{mole fractions of oxygen in bubble and emulsion phases} \]
\[ Y_B', Y_E' \quad \text{mole fractions of } SO_2 \text{ or } H_2O \text{ in bubble and emulsion phase} \]
\[ y = \frac{d_c}{d_{cm}} \quad \text{dimensionless diameter of char particle} \]
\[ y_{j,f} \quad \text{mole fraction of gaseous species } j \text{ in the feed stream} \]
\[ Y_{Bj}, Y_{Ej} \quad \text{mole fractions of gaseous species } j \text{ in bubble phase and in emulsion phase} \]
\[ Y_B, Y_E \quad \text{mole fraction vectors of gases in bubble phase and emulsion phase} \]
\[ Z \quad \text{height above distributor} \quad \text{cm} \]
\[ Z_f(y) \quad \text{function defined by Eq. (19)} \]
<table>
<thead>
<tr>
<th>Greek Symbols</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\beta$</td>
<td>adjusting factor of elutriation rate constant</td>
</tr>
<tr>
<td>$\varepsilon'$</td>
<td>emissivity</td>
</tr>
<tr>
<td>$\varepsilon_B$</td>
<td>volume fraction of bubbles</td>
</tr>
<tr>
<td>$\varepsilon_c$</td>
<td>volume fraction of clouds and bubbles</td>
</tr>
<tr>
<td>$\varepsilon_{mf}$</td>
<td>volume fraction of bed at $u_o = u_{mf}$</td>
</tr>
<tr>
<td>$\varepsilon_{tube}$</td>
<td>volume fraction of internal tubes</td>
</tr>
<tr>
<td>$\varepsilon_W$</td>
<td>volume fraction of cloud and wake</td>
</tr>
<tr>
<td>$\eta_c$</td>
<td>combustion efficiency of coal</td>
</tr>
<tr>
<td>$\eta_S$</td>
<td>efficiency of sulfur capture</td>
</tr>
<tr>
<td>$\theta$</td>
<td>time</td>
</tr>
<tr>
<td>$\theta_c$</td>
<td>mean residence time of solids</td>
</tr>
<tr>
<td>$\theta_c$</td>
<td>mean circulation time of particles</td>
</tr>
<tr>
<td>$\lambda_c$</td>
<td>$= k_c/k_{c0}$</td>
</tr>
<tr>
<td>$\lambda_L$</td>
<td>reactivity of limestone defined by Eq. (e-63)</td>
</tr>
<tr>
<td>$\mu$</td>
<td>viscosity of gas</td>
</tr>
<tr>
<td>$\xi_{AE}$</td>
<td>weight fraction ash particles elutriated from bed</td>
</tr>
<tr>
<td>$\xi_{CO}, \xi_{H2}, \xi_{H2S}$</td>
<td>parameters defined by Eq. (3-42)</td>
</tr>
<tr>
<td>$\rho_A$</td>
<td>density of ash</td>
</tr>
<tr>
<td>$\rho_{cf}$</td>
<td>density of coal</td>
</tr>
<tr>
<td>$\rho_{ch}$</td>
<td>density of char</td>
</tr>
<tr>
<td>$\rho_g$</td>
<td>density of gas</td>
</tr>
<tr>
<td>$\rho_L$</td>
<td>density of lime or calcined dolomite</td>
</tr>
<tr>
<td>$\rho_{lf}$</td>
<td>density of limestone or dolomite</td>
</tr>
<tr>
<td>$\rho_s$</td>
<td>density of solids</td>
</tr>
</tbody>
</table>

Units:
- g/cm$^3$
- gm/cm·sec
<table>
<thead>
<tr>
<th>Variable</th>
<th>Description</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\rho_{Nc}$</td>
<td>number of char particles per unit volume of bed</td>
<td>1/cm$^3$</td>
</tr>
<tr>
<td>$\rho_{Nz}$</td>
<td>number of adsorbent particles per unit volume of bed</td>
<td>1/cm$^3$</td>
</tr>
<tr>
<td>$\phi$</td>
<td>size distribution density function of char particles</td>
<td>-</td>
</tr>
<tr>
<td>$\phi_B$, $\phi_E$</td>
<td>size distribution density functions of char particles in bubble-wake phase and in emulsion phase</td>
<td>-</td>
</tr>
<tr>
<td>$\phi_e$</td>
<td>size distribution density function of elutriated char particles</td>
<td>-</td>
</tr>
<tr>
<td>$\phi_f$</td>
<td>size distribution density function of char particles fed to the bed</td>
<td>-</td>
</tr>
<tr>
<td>$\phi_k$</td>
<td>distribution density function of adsorbent conversion</td>
<td>-</td>
</tr>
<tr>
<td>$\phi_{k_f}$</td>
<td>conversion distribution density function of adsorbent fed to the bed</td>
<td>-</td>
</tr>
<tr>
<td>$\phi_w$</td>
<td>size distribution density function of withdrawn char particles</td>
<td>-</td>
</tr>
</tbody>
</table>

\begin{align*}
\psi_V &= \int_0^1 \phi y^3 \, dy \\
\psi_{Ve} &= \int_0^1 \phi_e y^3 \, dy \\
\psi_{Ww} &= \int_0^1 \phi_w y^3 \, dy
\end{align*}

**Subscripts**

- B: bubble or bubble phase
- b: bulk density or bed
- C: carbon
- c: coal, char, cloud or circulation
- ch: char
- d: downward flow
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
l  Z = L_f
APPENDIX I

Mean Residence Time of Absorbent Particles, $\theta$

The number of absorbent particles, char particles and ash particles are indicated by $N_k$, $N_c$ 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:

$$(1 - \varepsilon_{mf})V_{mf} = \frac{\pi}{6} N_k \bar{d}_k^3 + \frac{\pi}{6} \bar{d}_{cm}^3 N_c \psi_{vw} + \frac{\pi}{6} \bar{d}_A^3 N_A$$  \hspace{1cm} (I-1)

Substituting the definition of $\theta$, namely

$$\theta = \frac{N_k}{n_{kf}} = \frac{N_c}{n_{cw}} = \frac{N_A}{n_{Aw}}$$  \hspace{1cm} (3-31)

we get

$$\theta = \frac{(1 - \varepsilon_{mf})V_{mf}}{\frac{\pi}{6} (n_{kf} \bar{d}_k^3 + n_{cw} \bar{d}_{cm}^3 \psi_{vw} + n_{Aw} \bar{d}_A^3)}$$  \hspace{1cm} (I-2)

By the use of the relations,

$$\frac{\pi}{6} n_{kf} \bar{d}_k^3 = \frac{w_{lf}}{\rho_{lf}}$$

$$\frac{\pi}{6} n_{cw} \bar{d}_{cm}^3 \psi_{vw} = \frac{(1 - n_c) \psi_{cf}}{\rho_{cf}} - \frac{\pi}{6} \bar{d}_{cm} n_{ce} \psi_{ve}$$

and

$$\frac{\pi}{6} n_{Aw} \bar{d}_A^3 = \frac{n_c \psi_{cf} X_{Af} (1 - \varepsilon_{Ae})}{\rho_A}$$

we have

$$\theta = \frac{(1 - \varepsilon_{mf})V_{mf}}{\frac{w_{lf}}{\rho_{lf}} + \left( \frac{\pi}{6} \right) \bar{d}_{cm} \psi_{vw} n_{cw} + \frac{n_c \psi_{cf} X_{Af}}{\rho_A} (1 - \varepsilon_{Ae})}$$  \hspace{1cm} (3-32)
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, \( dV \),
\[ dV = dX_1 \, dX_2 \, \ldots \, dX_m \]  \hspace{1cm} (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:
\[ \left( \frac{dX_i}{d\theta} \right)^* = R_i(x) \hspace{1cm} (i = 1 \text{--} m) \]  \hspace{1cm} (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.
\[ dV = \left( \frac{dX}{d\theta} \right)^* = \frac{dX_1}{d\theta} \cdot dX_2 \cdot \ldots \cdot dX_m \hspace{1cm} (II-3) \]

Also, the particles in the subspace \( dV \) are continuously leaving the neighbouring subspace \( dV'' \) (see Figure II-1).
\[ dV'' = \sum_{i=1}^{m} R_i(x + dx) \frac{1}{dX_i} \, dV \, d\theta \]  \hspace{1cm} (11-4)
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.

\[ \text{input} = N \phi \left( x \right) \sum_i R_i \left( x \right) \frac{dV}{dx_i} \, dv \delta \, ........., 1 \]

\[ + n_{in} \phi_{in} \, dV \delta \, .................. 3 \]  

\[ \text{output} = N \sum_i \phi \left( x_j = x_i, x_i = x_i + dx_i \right) R_i \left( x_i = x_i + dx_i \right) \frac{dx_i}{dx_i} \, dV \delta \, 2 \]

\[ + n_{out} \phi_{out} \, dV \delta \, .................. 4 \]  

\[ \text{accumulation} = d \left( N \phi \left( x \right) \right) \, dV \]

Since the term 2 can be rewritten as follows:

\[ \sum_i \phi \left( x_j = x_i, x_i = x_i + dx_i \right) R_i \left( x_i = x_i + dx_i \right) \frac{dx_i}{dx_i} \, dV \delta \quad j = 1 \rightarrow m, j \neq i \]

\[ = \sum_i \left( \phi \left( x \right) \frac{dx_i}{dx_i} + \frac{\partial \phi}{\partial x_i} R_i \right) \, dV \delta \]  

\[ \text{(II-7)} \]

We obtain the final expression of the population balance as

\[ \frac{\partial N \phi}{\partial \theta} = -N \sum_i \frac{\partial \phi R_i}{\partial x_i} + n_{in} \phi_{in} - n_{out} \phi_{out} \]  

\[ \text{(II-8)} \]
Mass balance

The relation between $\phi$ (density function for number fraction) and $\phi^*$ (density function for weight fraction) is given by

$$N \frac{\pi}{6} \rho_p \frac{d^3}{d^3} \phi \, dV = W \phi^* \, dV \quad (II-9)$$

because

$\phi \, dV$: fraction of the number of particles which have the state $x - x + d \, x$

$\phi^* \, dV$: weight fraction of particles which have the state $x - x + d \, x$

Therefore,

$$\phi = \frac{6 \, W}{\pi \, N \, \rho_p \, d^3} \phi^* \quad (II-10)$$

The average mass of one particle $m_p$ is calculated by

$$m_p = \frac{W}{N} = \frac{\frac{\pi}{6}}{x} \phi(x) \rho_p \frac{d^3}{d^3} \, dV$$

$$= \frac{\int \phi^*(x) \, dV}{x} \quad (II-11)$$

Then each term in the equation (II-8) can be written in terms of $\phi^*$.

$$\frac{\partial N \phi}{\partial \theta} = \frac{6 \, W}{\pi \, \rho_p \, d^3} \frac{\partial W \phi^*}{\partial \theta} \quad (II-12)$$

where the fact that $(\rho_p \, d^3)$ is not dependent on $\theta$, but only dependent on $x$ is used.

$$N \frac{\partial \phi_R}{\partial X_i} = \frac{6W}{\pi} \frac{\partial \left[ (\phi^* \, R_i \, \rho_p \, d^3) \right]}{\partial X_i} \quad (II-13)$$

$$= \frac{6W}{\pi} \frac{1}{\rho_p \, d^3} \frac{\partial \phi^* \, R_i}{\partial X_i} - \frac{\phi^* \, R_i}{(\rho_p \, d^3)^2} \frac{\partial \left( \rho_p \, d^3 \right)}{\partial X_i}$$
\[ \frac{n_{\text{in}} \phi_{\text{in}}}{n_{\text{out}} \phi_{\text{out}}} = \frac{n_{X} m_{P}}{\pi/6}, \quad \frac{\phi_{X}^{\ast}}{\rho_{P} d_{P}} = \frac{w_{X}}{\pi/6 (P d_{P})} \] (II-14)

\[ \frac{\partial W \phi^{\ast}}{\partial \theta} = - W \sum_{i} \left[ \frac{\partial \phi^{\ast} R_{i}}{\partial X_{i}} - \frac{\phi^{\ast} R_{i}}{\rho_{P} d_{P}} \right] + \frac{3 W \phi^{\ast} R_{i}}{X_{i}} + w_{\text{in}} \phi_{\text{in}}^{\ast} - w_{\text{out}} \phi_{\text{out}}^{\ast} \] (II-15)

\[ 3 \frac{W \phi^{\ast} R_{i}}{X_{i}} : \text{loss of mass due to shrinkage volume balance} \]

A Simple Case

\[ \rho_{P} = \text{constant} \quad \text{and} \quad X_{1} = \frac{d_{P}}{d_{P} m} \]

\[ \frac{\partial V \phi^{\ast}}{\partial \theta} = - V \sum_{i} \left[ \frac{\partial \phi^{\ast} R_{i}}{\partial X_{i}} - \frac{3 \phi^{\ast} R_{i}}{X_{i}} \right] + v_{\text{in}} \phi_{\text{in}}^{\ast} - v_{\text{out}} \phi_{\text{out}}^{\ast} \] (II-16)

if \( \rho_{P} \) is constant the Equation (II-11) becomes

\[ m = \frac{\pi}{6} \rho_{P} \int_{x} \phi d_{P}^{3} dV = \frac{\pi}{6} d_{P}^{3} \rho_{P} \psi_{V} \] (II-18)

\[ \psi_{V} \equiv \frac{V}{\frac{\pi}{6} d_{P}^{3} \rho_{P} N} \equiv \iiint \ldots \int \phi X_{1}^{3} dX_{1} dX_{2} \ldots dX_{n} \ldots \ldots \ldots \ldots \int dV \] (II-19)

Total Number Balance

The disappearance of particle occurs only when \( d_{P} \) becomes 0:

\[ dX_{1} = \frac{dX_{1}}{d\theta} \left( -R_{1} (x) \right)_{X_{1} \rightarrow 0} d\theta \quad R_{1} < 0 \] (11-20)
Then total number of particles disappeared during $d\Phi$ is given by:

$$N \int \int \int \phi (X_1 = 0) \frac{dVdX_1}{dX_1} d\Phi = \int X_2 ... X_m$$

$$dN = n_{in} - n_{out} + N \int \int \int \phi (X_1 = 0, x) R_1 (X_1 = 0, x) dX_2 ... dX_m$$

**SUMMARY**

basic equation: $$\frac{\partial N}{\partial \Phi} = - N \sum \frac{\partial \phi R_i}{\partial X_i} + n_{in} \phi_{in} - n_{out} \phi_{out}$$

or $$\frac{\partial \psi^*}{\partial \Phi} = - W \sum \frac{\partial \phi^* R_i}{\partial X_i} - \frac{\partial \phi \psi}{\partial p} \frac{d^3}{dp^3} - \frac{\partial \phi}{\partial X_i}$$

where $R_i = (d X_i / d\Phi)^*$

Total number balance

$$\frac{dN}{d\Phi} = n_{in} - n_{out} + N \int \int \int \phi (x) R_1 (x) dX_2 ....dX_m$$
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

$\Theta$: time

$\phi$: distribution density function of x based on the number of particles

$\phi^*$: distribution density function of x based on the mass of particles

$\rho_p$: 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

\[ \frac{dY_k}{df} + B_1 \frac{Y_k}{\lambda_k} = B_2 \phi_k f \]  \hspace{1cm} (III-1)

where

\[ Y_k \equiv \phi_k \lambda_k \]

Integrating this equation by assuming initial value \( Y(0) \) and the integration constraint, \( \int_0^1 \phi_k f \, df = 1 \), we obtain

\[ Y_k(f) = \frac{B_2 + Y(0-)}{\exp \left[ \int_0^f (B_1/\lambda_k) \, df \right]} \]  \hspace{1cm} (III-2)

Therefore,

\[ \phi_k(f) = \frac{B_2 + Y(0-)}{\lambda_k \exp \left[ \int_0^f (B_1/\lambda_k) \, df \right]} \]  \hspace{1cm} (III-3)

The function \( \phi_k \) must satisfy the constraint

\[ \int_0^1 \phi_k(f) \, df = (B_2 + Y_k(0-)) \int_0^1 \frac{df}{\lambda_k \exp \left( \int_0^f \frac{B_1}{\lambda_k} \, df \right)} \equiv 1 \]

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Then,

$$B_2 + Y_{s}(0-) = \frac{1}{\int_0^1 \frac{B_0}{\lambda} \exp(\int_0^1 \frac{B_0}{\lambda} \, df)}$$  \hspace{1cm} (III-4)

Substitute Equation (III-4) into Equation (III-3) and use the relation

$$\int_0^1 \frac{1}{\lambda} \exp \left[ \int_0^1 \frac{B_0}{\lambda} \, df \right] \, df = - \frac{1}{B_0} \left[ \exp(- \int_0^1 \frac{B_0}{\lambda} \, df) - 1 \right]$$

then we have

$$\phi_{s}(f) = \frac{(B_0/\lambda) \exp \left[ - \int_0^1 \frac{B_0}{\lambda} \, df \right]}{1 - \exp \left[ - \int_0^1 \frac{B_0}{\lambda} \, df \right]} \hspace{1cm} (3-65)$$
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:
\[ N \frac{d \phi R^*}{dy} = r_f \phi_f - n_0 \phi \]  (IV-1)

2) boundary conditions for particle shrinking system (i.e. no particles beyond \( y = 1 \)):
\[ \phi(1+) = 0 \]  (IV-2)

3) integral constraint:
\[ \int_{0}^{1} \phi \ dy = 0 \]  (IV-3)

where
\[ R^* = (dy/d\theta)^* = f(y, \ldots) \]  (IV-4)
\[ y = \frac{dp}{d_{pm}} \]

On the other hand, from the material balance
\[ w_f = w_o - 4 \pi \rho_p d_{pm}^3 N \rho_p y^2 \langle R^* \rangle \]  (IV-5)

(input) (output)

where
\[ w_o = \frac{4}{3} \pi \rho_p d_{pm}^3 \psi \ n_o \]
\[ \psi = \int_{0}^{1} \phi y^5 \ dy / \int_{0}^{1} \phi \ dy \]
\[ < y^2 R^* > = \int_{0}^{1} \phi y^2 R^* \ dy / \int_{0}^{1} \phi \ dy \]
ACTIVE PARTICLES
HOLD-UP = N PARTICLES
SIZE DISTRIBUTION OF
ACTIVE PARTICLES = \phi

\[ n_f \quad \phi_f \quad \text{ACTIVE PARTICLES} \]

\[ v_i \quad \text{INERT PARTICLES} \]

\[ n_o \quad \phi \quad \text{ACTIVE PARTICLES} \]

\[ v_i \quad \text{INERT PARTICLES} \]

INERT PARTICLE VOLUME
HOLD-UP: \( v_i \)

FIGURE IV-1 ILLUSTRATION FOR THE POPULATION BALANCE

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Equation (IV-5) can be rearranged into the form

\[w_f = a [\psi_v n_o - 3 N < y^2 R^* >]\]  

(IV-5)'

where

\[a = \frac{4}{3} \pi \rho_p d_{pm}^3\]

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

\[\int_0^1 [\text{left hand side of Equation (IV-1)}] \cdot y^3 \, dy\]

\[= N \left[y^3 R^*\right]_0^1 - 3 \int_0^1 y^2 \, dy\]  

(IV-6)

\[\int_0^1 [\text{right hand side of Equation (IV-1)}] \cdot y^3 \, dy\]

\[= n_f \psi_{vf} - n_o \psi_v \int_0^1 \phi \, dy\]  

(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:

Equation (IV-6) = - 3 N < \(y^2 R^* > \int_0^1 \phi \, dy\]  

(IV-6)'
Equating Equation (IV-6) with Equation (IV-7), we obtain the value of integration of $\phi$.

$$\int_0^1 \phi \, dy = \frac{n_f \psi_f}{n_o \psi_v - 3 N < y^2 R^*>} = \frac{w_f}{\alpha [n_o \psi_v - 3 N < y^2 R^*>]}$$

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

$$n_f - n_o = - N R^* (0) \phi (0) \quad (IV-8)$$

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 viewpoint of numerical stability and rapidness of convergence.
Nomenclature for Appendix IV

\( d_p \) diameter of active particle \( \text{cm} \)

\( d_{pm} \) maximum diameter of active particles \( \text{cm} \)

\( n \) number flow rate of active particles \( 1/\text{sec} \)

\( N \) number hold-up of active particles -

\( R^* \) shrinking rate of a single particle \( 1/\text{sec} \)

\( v_\text{i} \) volume flow rate of inert particles \( \text{cm}^3/\text{sec} \)

\( V_\text{i} \) volume hold-up of inert particles \( \text{cm}^3 \)

\( V_t \) total volume of solids in the cell \( \text{cm}^3 \)

\( w \) mass flow rate of active particles \( \text{g/sec} \)

\( y = \frac{d_p}{d_{pm}} \) dimensionless particle size -

\( \phi \) size distribution density function -

\( \rho_p \) density of particles \( \text{g/cm}^3 \)

\( \psi_v \equiv \int_0^1 \phi \frac{y^3}{\int_0^1 \phi dy} \)

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 $\phi_e^*$, the size distribution of elutriated particles on weight fraction basis, and $\phi_e$, the size distribution of elutriated particles on number fraction basis, we have,

$$dw_e = w_e \phi_e^* dy = w_e \frac{y^3 \phi_e}{\psi_{ve}} dy \quad (V-1)$$

On the other hand, the elutriation rate is given by the specific elutriation rate constant, $K^*$, in the form

$$\frac{dwe}{At} = K^* \phi_b^* dy \quad (V-2)$$

where $\phi_b^*$ is the density function of size distribution of the char particles in the bed based on the total weight of bed. $\phi^*$ is the size distribution density function based on the total weight of char particles in the bed and is related to $\phi_b^*$ by

$$W_e \phi^* dy = W_b \phi_b^* dy \quad (V-3)$$

Substituting (V-2) and (V-3) into (V-1), we obtain

$$dw_e = w_e \phi_e^* dy = \frac{At W_c}{W_b} K^* \phi^* dy \quad (V-4)$$

or by using $\phi$ and $\phi_e$,

$$dw_e = \frac{w_e \phi_e}{\psi_{ve}} y^3 dy = \frac{At W_c}{W_b \psi_v} K^* \phi dy \quad (V-5)$$

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

\[
\begin{align*}
n_e &= \frac{w_e}{(\psi_v \frac{\pi}{6} d_{cm}^3 \rho_{ch})} \\
N_c &= \frac{W}{(\psi_v \frac{\pi}{6} d_{cm}^3 \rho_{ch})}
\end{align*}
\]

We obtain the final form

\[
n_e \phi_e = \frac{k^*}{W_b} N_c \phi
\]  

(V-6)