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LOW GRADE COAL UTILIZATION AND PROPERTY ANALYSIS

DP/ROK/82/029

Technical report: Fluidized-Bed Combustion

Prepared for the Government of the Republic of Korea
by the United Nations Industrial Development Organization,
acting as executing agency for the United Nations Development Programme

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INTRODUCTION

I accepted a one month appointment from the United Nations Industrial Development Organization (UNIDO) to assist the Korea Institute of Energy and Resources (KIER), ministry of Energy and Resources, in the development of a fluidized-bed combustion boiler for utilizing low grade Korean anthracite. Specifically, my duties called for accomplishing the following tasks:

- o Evaluation of the fluidized-bed combustion (FBC) modelings for high-ash anthracite
- o Investigation of the effect of coal particle size distribution on the performance of fluidized-bed coal combustors
- o Characterization of freeboard combustion in FBC's.

The work was to be accomplished in consultation with the Korean authorities at the Institute.

Upon my arrival at the KIER on March 30, 1987, my job description was somewhat modified. The new job description (Attachment 1) called for my assistance in the following areas:

- o Evaluation of FBC model for high-ash anthracite coal as well as for bituminous coal
- o Comments on the freeboard model for Korean high ash anthracite coal in FBC
- o Heat transfer in FBC
- o Flow transition velocities in the circulating fluidized bed
- o Basic design of a fluidized-bed coal gasifier -- a versatile laboratory-scale unit
- o Concepts of the iso-kinetic sampling probe for collection of particulate samples and of a sensitive pressure transducer for measuring the very low static pressure in the dilute phase above a large fluidized-bed reactor.

The purpose of this preliminary report is to briefly outline the accomplishments and provide a short summary on comments and recommendations. A more detailed report, if requested, will be provided at a later date.

ACCOMPLISHMENTS

1. Evaluation of FBC model

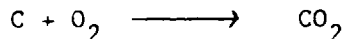
Substantial effort has been made at KIER to develop an FBC math model and, as a result, progress has been made and some model elements have been developed. Difficulties have been experienced in developing model elements for particle size distribution. This is a very important issue because, in a bed continuously fed with coal, a spectrum of particle sizes is present. The combustion rate of a single particle is related to the particle diameter; therefore, to obtain the overall reaction rate, the particle size distribution must be calculated.

The KIER model is basically derived for the investigation of the governing combustion mechanism in fluidized beds. Therefore, the model concentrates on the burning of individual carbon particles and no attention is paid to other processes in an FBC such as sulfur capture. This is quite understandable since Korean coal has a very low sulfur content and SO₂ emission is of no concern. In developing this model, other simplifying assumptions have been made in order to make a model solution obtainable.

The KIER model was discussed in great detail with emphasis on the assumptions made and the empirical relations proposed to predict various parameters. KIER's model is patterned after an earlier work by T. P. Chen and S. C. Saxena which was recently somewhat modified by B. W. Overturf and G. V. Rekilis to include the influence of the grid region. In general KIER's model is based on the following assumptions:

- o Fluid Dynamics
 - Davidson and Harrison two-phase model
 - Particulate phase well mixed
 - Bubble phase in plug flow regime
 - No jet region effect
- o Fuel Particles
 - Spherically shaped coal particles
 - Fuel particles do not change in density
 - Attrition of particles negligible
- o Combustion Process
 - All combustion reactions take place in the particulate phase
 - Char combustion is governed by chemical kinetics

- The reaction considered for char combustion is:



- Reaction rate a function of dp and unreacted core size
- o Additional Assumptions
 - Bed weight consists of both bed and freeboard material
 - Uniform temperature within a particle

As stated earlier, population balance was an area of major concern to KIER researchers, and, at their request, I concentrated on this subject. In pursuing this, I performed the following:

- o Outlined and elaborated on the solids population balance which was originally developed by T. P. Chen and S. C. Saxena. Attachment 2 is a summary of this effort.
- o Summarized equations required and steps to be followed to achieve a complete mass balance. In addition, identified functions which need to be defined/specified in advance of obtaining a complete mass balance. For each function, suggestions were made for the required estimation procedures. The results are shown in Attachment 3.
- o Developed a more simplified model element for particle size distribution. The major simplifying assumption in this model was the statement that elutriated particles have the same size distribution as the bed material. Similar assumptions have been commonly made in the past by others. This simplified model is presented in Attachment 4.

2. Freeboard Model

KIER is in the process of developing a model to characterize freeboard combustion. All three fluidized-bed combustors at KIER are designed for over-bed feeding. As a result, a high percentage of unburned carbon particles are elutriated, and consequently freeboard combustion characteristics are of great importance to their situation. Considerable effort is currently being made at KIER in order to develop a freeboard model and experimentally verify it.

The proposed model is at early stages of development, but a road map has been established to accomplish this task. Currently, as a first step, an entrainment mechanism for solid particles has been worked out and a work scope has been developed to complete the model.

The entrainment model and the future work scope were reviewed and evaluated. This was followed by extensive discussions of both theoretical work and the proposed experimental work. Detailed comments and suggestions were offered to the lead investigator. Also, freeboard model was the subject of a four-hour group discussion.

3. Heat Transfer in FBC

This subject was treated at a group discussion. At this session experimental work at KIER involving both operations with and without fly ash recycle was discussed in great detail. In addition, heat transfer rates in general and bed-to-wall heat transfer coefficients in particular, were covered. Comments and suggestions were made regarding estimation of heat transfer coefficients, their reliabilities and values commonly used. Also, ideas on how to improve efficiencies of FBC systems at KIER were discussed, and some suggestions were made.

4. Circulating Fluidized Beds

A cold model circulating bed has been designed and built at KIER. Some preliminary experimental results have been obtained. However, due to limitations on fan power and the limited recycle line capabilities, full-range pressure profiles have not been obtained. Thus, no information on transition velocities has been experimentally established.

Data obtained at KIER were reviewed and then discussed in a group meeting. Techniques commonly practiced to obtain full-range pressure profiles in circulating beds were reviewed. KIER's circulating bed and its limitations were discussed at length, and possible solutions were explored.

5. Fluid Bed Gasifier

At KIER's request this topic was not discussed. However, information on references regarding various gasifier concepts including fluidized-bed gasifiers, were provided.

6. Iso-Kinetic Sampling

Information on an iso-kinetic sampling probe and a very sensitive pressure transducer which I designed and built sometime ago was provided to KIER's staff members. The probe was designed to collect samples

iso-kinetically in the freeboard of fluidized beds and simultaneously measure static pressure. The ultimate goal was to establish concentration and pressure profiles in order to determine the so called Transport Disengaging Height (TDH). The pressure transducer was capable of detecting very small pressure changes in the freeboard.

In addition to the above topics, test planning procedures and metal loss from heat exchanges in fluidized beds were also discussed in some detail.

COMMENTS AND RECOMMENDATIONS

The available fluidized-bed models, at best, are capable of describing the qualitative performance of fluidized-bed combustors. All models at present time are at an initial stage and, therefore, require substantial improvements and refinements. In general:

- o Most models are based on small particle size and low velocities. Knowledge of flow regime in a large-particle fluidized bed is insufficient.
- o Most models consider only vertical solid circulation. Knowledge of horizontal solid circulation is required for tube bundle design in large FBC boilers.
- o At present, no accurate method exists to obtain elutriation rate constants. This parameter is quite essential for predicting combustion efficiencies.
- o The influence of distributor plate design on bed dynamics is an area of uncertainty.
- o Most models ignore the burning of volatiles. Since unburned CO oxidizes in the freeboard, it is essential to predict the extent of this reaction.
- o Most flue gas emission models ignore calcination. Furthermore, the effect of SO₂ diffusion into the solid product and also the effect of impurities in the acceptor are not well understood.
- o Knowledge of heat transfer mechanism is lacking. Most empirical relations which are commonly used are system specific.
- o Until recently little attention was paid to the freeboard phenomena. Consideration of freeboard is quite important since CO burnout and NO_x reduction take place there. Most models ignore chemical reactions in the freeboard.

The development of math models for accurate quantitative analysis requires a more comprehensive knowledge of processes and phenomena occurring not only in the bed itself, but also in the freeboard. An important area of model evolution is the verification of the models in terms of comparison between predicted and experimental data. In the evaluation of a model, large deviations can be caused by inaccurate or incomplete experimental data. Therefore, the need for a data base containing suitable data is obvious.

In summary, I recommend the following:

- o KIER is in an excellent position (with three different combustor sizes) to develop an extensive data base comprehensive enough for comparison of various model elements. This would be a great contribution to the field of FBC technology.
- o With some modifications to the existing equipment (including additional instrumentation) KIER is in a very good position to conduct basic studies in:
 - Fluid dynamics
 - Elutriation
 - Freeboard reactions

I am quite pleased to see that researchers at KIER are quite aware of what is needed and work is already in progress in areas such as freeboard characterization and basic FBC modeling. In both areas the researchers are emphasizing experimental verification of their models and as a result experimentation and theoretical analyses are moving ahead at the same time.

ATTACHMENT 1

Job Description

JOB DESCRIPTION OF DR. NAZEMI

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CHOI

1. Evaluation of FBC model for high ash anthracite coal as well as for bituminous coal (with Choi; Mar. 30 - Apr. 18)
 - Review and discuss the solution of models
2. Comment on the freeboard model for Korean high ash anthracite coal in FBC (Group meetings with 2 Parks, Bak and Choi; 2 days of Mar. 27 - Apr. 2)
 - Evaluation of the freeboard combustion model
 - Estimation of carbon hold-up in the freeboard including carbon elutriation and attrition
 - Fine coal combustion kinetics in the freeboard
 - Estimation of the relative combustion proportions taking place in the bed and freeboard
 - Gas analysis in freeboard region (O₂, CO₂, CO)
 - Selection of experimental parameters
- ✓ 3. Heat transfer in FBC (Group meetings with 2 Parks and Bak; 1 day of Apr. 3 - 9)
 - Effect of fly ash recycle on the in-bed heat transfer coefficient
 - What is the most reliable correlation for the in-bed heat transfer coefficient in design aspect
- ✓ 4. Flow transition velocities in the circulating fluidized bed (Group meeting with Lee and Choi; 1 day of Apr. 3 - 9)
 - Measurement of FTV
 - Determination of FTV
 - Prediction of FTV
5. Basic design of a fluidized bed coal gasifier—a versatile lab. scale unit (Group meeting with Bak and Choi; 2 days of Apr. 10 - 18)
 - Consider the P & I diagram
 - Determine the over-all configuration of gasifier
 - Determine the basic design parameter of gasifier
6. Concepts of the iso-kinetic sampling probe for collection of particulate samples and of a sensitive pressure transducer for measuring the very low static pressure in the dilute phase above a large fluidized bed reactor (2 Seminars for each topic; 2 days of Mar. 30 - Apr. 21)

* Pick-up time

Monday to Friday:

9:20 AM (Hotel to Office)

17:30 PM (Office to Hotel)

Saturday:

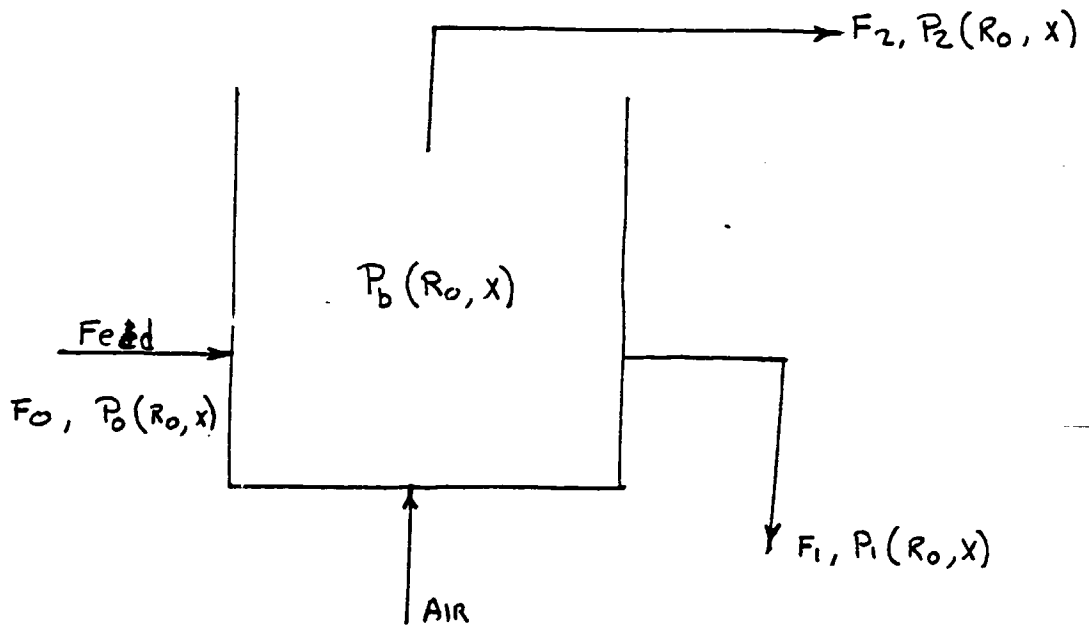
9:20 AM (Hotel to Office)

12:30 PM (Office to Hotel)

* Lunch(12:00): Institute Dining Room(Korean Food)

ATTACHMENT 2

Outline of and Elaboration
on Solids Population Balance
by Chen, T.P. and S.C. Saxena



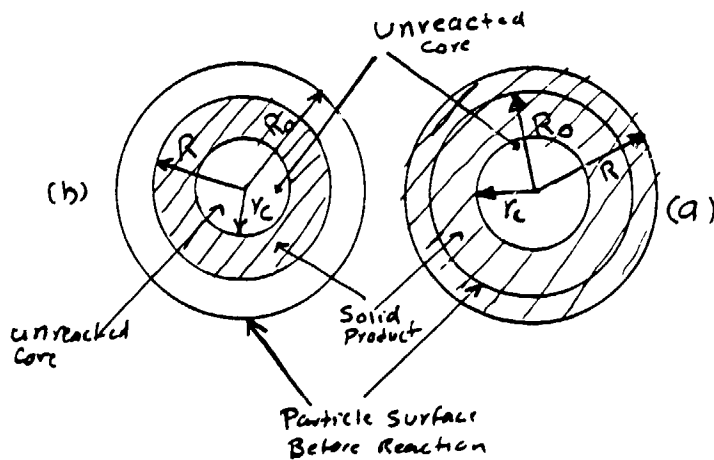
Assume backmixing of solids in the bed

⇒

$$P_1(R_0, x) = P_b(R_0, x) \quad (1)$$

We can relate entrainment to bed material through elutriation constant K

$$\therefore K(R_0, x) = \frac{F_2 P_2(R_0, x)}{W P_b(R_0, x)} \quad (2)$$



a) Growing particle

b) Shrinking particle

Let

$$Z = \frac{\text{Volume of Solid Product Formed}}{\text{Volume of Solid Reactant consumed}}$$

$$= \frac{R^3 - r_c^3}{R_0^3 - r_c^3} \quad (3)$$

if ρ_a = Density of product solid, and
 ρ_c = Density of unreacted solid

then, then the mean particle density ρ can be defined as

$$\rho = \rho_a \left(\frac{R^3 - r_c^3}{R^3} \right) + \rho_c \left(\frac{r_c}{R} \right)^3 \quad (4)$$

Particle mass can be defined as

$$m_p = \left(\frac{4}{3} \right) \pi R^3 \rho \quad (5)$$

For an spherical particle of original radius R_0 and unreacted core radius r_c , the fraction of conversion, x , is given by

$$x = 1 - \left(\frac{r_c}{R_0} \right)^3 \quad (6)$$

Combining Equations 3, 4, and 6 will give

$$R = R_0 [1 + (Z-1)x]^{1/3} \quad (7)$$

and

$$\rho = \frac{\rho_a Z x + \rho_c (1-x)}{1 + (Z-1)x} \quad (8)$$

Substitutions from eqns 7 and 8 for R and ρ into eqn. 5 will result :

$$m_p(R_0, x) = (4/3)\pi R_0^3 [\rho_c + (z\rho_a - \rho_c)x] \quad (9)$$

differentiating eqn. 9 with respect to time, t

\therefore

$$\frac{d[m_p(R_0, x)]}{dt} = (4/3)\pi R_0^3 (z\rho_a - \rho_c) \frac{dx}{dt} \quad (10)$$

The mass of a particle with size R and density ρ changes with time according to

$$\frac{d[m_p(R, \rho)]}{dt} = R_1(R, \rho, C_e) \quad (11)$$

Where R_1 = mass change of a single particle

C_e = gas concentration in the emulsion phase

Combining equations 10 and 11 will give

$$\frac{dx}{dt} = \frac{R_1(R, \rho, C_e)}{(4/3)\pi R_0^3 (z\rho_a - \rho_c)} = R_3(R, \rho, C_e) = R_3(R_0, x, C_e) \quad (12)$$

Where R_3 = Rate of solid conversion

Let the average rate of conversion of all particles with size R and density ρ be:

$$\overline{\frac{dx}{dt}} = R_4(R_0, x) = R_4(R, \rho) \quad (13)$$

Where R_4 = mean rate of solid conversion

Substituting Equ. 13 into Equ. We obtain the average mass change rate

∴

$$\frac{d[m_p(R_0, x)]}{dt} = (4/3) \pi R_0^3 (z e_a - \rho_c) R_4(R_0, x) \quad (14)$$

For a given R_0 , The material balance of particles over the interval of x to $x + \Delta x$ gives:

$$\left[\begin{array}{l} \text{Solids Entering} \\ \text{in Feed} \end{array} \right] - \left[\begin{array}{l} \text{Solids Leaving} \\ \text{in overflow} \end{array} \right] - \left[\begin{array}{l} \text{Solids Leaving} \\ \text{in entrainment} \end{array} \right] + \left[\begin{array}{l} \text{Solids growing into} \\ \text{the interval from} \\ \text{a smaller } x \end{array} \right]$$

$$- \left[\begin{array}{l} \text{Solids growing out} \\ \text{of the interval to a} \\ \text{Larger } x \end{array} \right] + \left[\begin{array}{l} \text{Solid generation} \\ \text{due to the growth} \\ \text{within the interval} \end{array} \right] = 0 \quad (15)$$

or

$$F_0 P_0(R_0, \bar{x}) \Delta x - F_1 P(R_0, \bar{x}) \Delta x - F_2 P_2(R_0, \bar{x}) \Delta x +$$

$$W P_b(R_0, x) \left. \frac{d\bar{x}}{dt} \right|_x - W P_b(R_0, x) \left. \frac{d\bar{x}}{dt} \right|_{x+\Delta x} +$$

$$\frac{W P_b(R_0, x)}{m_p(R_0, \bar{x})} \cdot \frac{d[m_p(R_0, \bar{x})]}{dt} \Delta x = 0 \quad (16)$$

Where \bar{x} = Average fraction of conversion in the interval $x \in x + \Delta x$.

Dividing through by Δx and taking limit as $\Delta x \rightarrow 0$, Equ. 16 becomes

$$F_0 P_0(R_0, x) - F_1 P_1(R_0, x) - F_2 P_2(R_0, x) - W \cdot \frac{d}{dx} \left[P_b(R_0, x) \frac{d\bar{x}}{dt} \right] + \frac{W P_b(R_0, x)}{m_p(R_0, x)} \cdot \frac{d}{dt} [m_p(R_0, \bar{x})] = 0 \quad (17)$$

In Equ. 17 substituting for $P_1(R_0, x)$, $F_2 P_2(R_0, x)$, $m_p(R_0, x) \frac{d\bar{x}}{dt}$, and $\frac{d}{dt} [m_p(R_0, \bar{x})]$ from Equations 1, 2, 9, 13, and 14

respectively, Equ. 17 becomes:

$$F_0 P_0(R_0, x) - F_1 P_b(R_0, x) - K(R_0, x) \cdot W P_b(R_0, x) - W \cdot \frac{d}{dx} [P_b(R_0, x) \cdot R_4(R_0, x)] + \frac{W P_b(R_0, x) \cdot (z P_a - P_c) \cdot R_4(R_0, x)}{P_c + x(z P_a - P_c)} = 0 \quad (18)$$

Since solid feed contains only fresh particles, i.e. $x=0 \Rightarrow F_0 P_0(R_0, x) = 0$ when equ. 18 is applied at a x other than $x=0$. Therefore Equ. 18 becomes:

$$W \cdot \frac{d}{dx} [P_b(R_0, x) \cdot R_4(R_0, x)] = \frac{W P_b(R_0, x) (z P_a - P_c) R_4(R_0, x)}{P_c + x(z P_a - P_c)} - F_1 P_b(R_0, x) - K(R_0, x) W P_b(R_0, x) \quad (19)$$

Rearrangement of equ. 19 will give

$$\frac{dP_b(R_0, x)}{dx} = \left[\frac{ze_a - e_c}{e_c + (ze_a - e_c)x} - \frac{1}{R_4(R_0, x)} \frac{dR_4(R_0, x)}{dx} - \frac{F_i}{WR_4(R_0, x)} - \frac{\kappa(R_0, x)}{R_4(R_0, x)} \right] P_b(R_0, x) \quad (20)$$

Integrating equ. 20 from $x=0$ to x gives

$$\ln \frac{P_b(R_0, x)}{P_b(R_0, 0)} = \ln \left[\frac{e_c + (ze_a - e_c)x}{e_c} \right] - \ln \frac{R_4(R_0, x)}{R_4(R_0, 0)} - \int_0^x \frac{(F_i/W) + \kappa(R_0, x)}{R_4(R_0, x)} dx \quad (21)$$

When Equ. 16 is applied to an interval containing $x=0$, $\Delta x \rightarrow 0$ and all terms except the first and fifth disappear and equ. 16 becomes (other terms disappear because solids after entrance will only undergo conversion)

$$F_0 P_0(R_0, x) \Delta x = W P_b(R_0, x) \frac{dx}{dt} \Big|_{x+\Delta x} \quad (22)$$

Substituting for $\frac{dx}{dt}$ from equ. 13, equ. 22 becomes

$$F_0 P_0(R_0, x) \Delta x = W P_b(R_0, x) \cdot R_4(R_0, x) \quad (23)$$

taking $\lim_{\substack{\Delta x \rightarrow 0 \\ x \rightarrow 0}} P_0(R_0, x) \Delta x = P_0(R_0, 0) = P_0(R_0)$

and Eqv. 23 is finalized to

$$P_b(R_0, 0) = \frac{F_0 P_0(R_0)}{W |R_4(R_0, 0)|} \quad (24)$$

Substituting for $P_b(R_0, 0)$ from Eqv. 24 into eqv. 21 we obtain

$$\begin{aligned} \ln \frac{P_b(R_0, x)}{F_0 P_0(R_0) / W |R_4(R_0, 0)|} &= \ln \left[\frac{P_c + (Z C_a - P_c) x}{P_c} \right] - \ln \frac{R_4(R_0, x)}{R_4(R_0, 0)} \\ &\quad - \int_0^x \frac{(F_1 / W) + k(R_0, x)}{R_4(R_0, x)} dx \quad (25) \end{aligned}$$

Taking antilog of both sides of eqv. 25 we obtain the following distribution function of particles in the overflow:

$$\begin{aligned} P_b(R_0, x) &= \left[\frac{F_0 P_0(R_0)}{W |R_4(R_0, 0)|} \right] \left[\frac{P_c + (Z C_a - P_c) x}{P_c} \right] \\ &\quad \exp \left[- \int_0^x \frac{F_1 / W + k(R_0, x)}{R_4(R_0, x)} dx \right] \quad (26) \end{aligned}$$

The distribution function of particles in the overflow at $x=1$ can be found to be represented by the following relation:

$$P_b(R_0, 1) = \frac{F_0}{W} \cdot \frac{P_0(R_0)}{\left[\frac{F_1}{W} + k(R_0, 1)\right]} \approx \frac{P_a}{P_c} \exp\left[-\int_0^1 \frac{\frac{F_1}{W} + k(R_0, x)}{R_0(R_0, x)} dx\right] \quad (27)$$

Thus For $0 \leq x < 1$ Equ. 26 applies
For $x = 1$ = 27 =

Integration over the entire particle size and conversion ranges will provide the relationship between bed weight and flow rate

Now, Using the following relations for the transfer of $P_b(R_0, x) \approx P_b(R, \rho)$ and $P_b(R_0, 1) \approx P_b(R, \rho_a)$

$$P_b(R, \rho) = P_b(R_0, x) \left| J_1 \left(\frac{R_0, x}{R, \rho} \right) \right|$$

$$P_b(R, \rho_a) = P_b(R_0, 1) \left| J_2 \left(\frac{R_0}{R} \right) \right|$$

When

$$J_1 \left(\frac{R_0, x}{R, \rho} \right) = \begin{vmatrix} \frac{\partial R_0}{\partial R} & \frac{\partial R_0}{\partial \rho} \\ \frac{\partial x}{\partial R} & \frac{\partial x}{\partial \rho} \end{vmatrix}$$

and

$$J_2 \left(\frac{R_0}{R} \right) = \left[\frac{dR_0}{dR} \right]$$

and considering the case when particles in the bed undergo change only in size $\Rightarrow z=0$ and eqv. 7 becomes

$$R = R_0 (1-x)^{1/3}$$

and eqv. 8 reduces to

$$\rho = \rho_c$$

one obtains the following relation for the distribution function of overflow particles

$$P_b(R_0, R) = \frac{F_0 P_0(R_0)}{W |R_0(R)|} \frac{R^3}{R_0^3} \exp \left[- \int_{R_0}^R \frac{(F_1/W) + K(R)}{R_c(R)} dz \right] \quad (28)$$

where $\frac{P_b(R_0, x)}{R_0} = P_b(R_0, R) \frac{dx}{dR}$

and $R_4(R_0, x) = - \frac{3R^2}{R_0^2} R_c(R)$

Integration of eqv. 28 over the entire ranges of R_0 and R and recognizing that

$$\int_{R_0} \int_R P_b(R_0, R) = 1$$

gives the following overall material balance

$$\frac{W}{F_0} = \int_{R_0} \int_R \frac{P_0(R_0)}{|R_0(R)|} \frac{R^3}{R_0^3} \exp \left[- \int_{R_0}^R \frac{(F_1/W) + K(R)}{R_0(R)} dR \right] dR dR_0$$

ATTACHMENT 3

Equations and Steps Required for a Complete Mass Balance

Summary of Equations Required To make a mass Balance

Step 1

Find F_1 From the following Equation :

$$\frac{W}{F_0} = \int_{R_0} \int_R \frac{P_0(R_0)}{|R_c(R)|} \frac{R^3}{R_0^3} \exp \left[- \int_{R_0}^R \frac{(F_1/W) + k(R)}{R_c(R)} dR \right] dR dR_0$$

Step 2

Calculate $P_b(R_0, R)$ from the following Equation :

$$P_b(R_0, R) = \frac{F_0 P_0(R_0)}{W |R_c(R)|} \frac{R^3}{R_0^3} \exp \left[- \int_{R_0}^R \frac{(F_1/W) + k(R)}{R_c(R)} dR \right]$$

Step 3

Calculate the overall mass change rate, M , from the following equation

$$M = \int_{R_0} \int_R \left(\frac{W P_b(R_0, R)}{(4/3) \pi R^3 \rho} \right) R_1(R, R_0, C_2) dR dR_0$$

Step 4

Calculate F_2 From the Following relation:

$$F_0 = F_1 + F_2 - M$$

Step 5

Determine $P_2(R_0, R)$ from equ.

$$K(R) = \frac{F_2 P_2(R_0, R)}{W P_b(R_0, R)}$$

The following functions need to be defined/specified in advance of implementing the above five steps:

- 1- $P_0(R_0)$, Distribution function for feed particles
- 2- $R_1(R, R_0, C_e)$, mass change rate of a single particle, $g \text{ sec}^{-1}$
- 3- $R_2(R)$, Rate of solid size change, cm sec^{-1}
- 4- $K(R)$, elutriation constant, sec^{-1}

1 - $P_0(R_0)$

The size distribution function for the feed particles can readily be established from the available information on feed particle size distribution

2 - $R_1(R, R_0, C_c)$

Since mass change in a single particle takes place due to combustion of char particles, with the assumption that the particle is non-porous sphere and is homogeneously shrinking over the entire surface and is not changing in density during burn-out time, the loss of or the change rate of mass due to heterogeneous chemical reaction is expressed

$$R_1 = M_c \pi R_0^2 \sum k_c [C_j]^{a_j}$$

Where:

M_c = Atomic weight of carbon

$\sum k_c [C_j]^{a_j}$ = The sum of all heterogeneous reaction rates per unit surface area of the particle

k_c = Over-all reaction rate constant

C_j = molar concentration of gaseous reactant j consumed in the reaction (in emulsion phase)

a_j = Stoichiometric coefficient of species j in the reaction

The overall reaction rate constant, k_c , consists of a mass-transfer rate coefficient k_m and a kinetic rate constant k_k :

$$\frac{1}{k_c} = \frac{1}{k_m} + \frac{1}{k_k}$$

k_m can be estimated from Sherwood number, Sh ,

$$Sh = \frac{k_m R_0}{D_{g,j}}$$

where $D_{g,j}$ = gas film diffusion coefficient of species j

in FBCs, $Sh = 2$ because of small particle sizes involved

The k_k is estimated from Arrhenius type expression

$$k_k = N_s \exp(-E_p/RT_s)$$

where N_s = surface reaction rate constant

E_p = activation energy

R = gas constant

T_s = particle surface temperature

3- $R_6(R)$

$$-R_6(R) = \frac{R_0^3}{3R^2} R_4(R_0, x)$$

where $R_4(R_0, x) = \overline{\frac{dx}{dt}}$ = mean rate of solid conversion

$$\frac{dx}{dt} = - \frac{R_1(R, r_0, c_c)}{\left(\frac{4}{3}\right) \pi R_0^3 \rho_p}$$

$$\Rightarrow R_c(R) = \frac{R_0^3}{3R^2} \left(M_c \cancel{R_0^2} \leq k_c [C_i]^{q_i} \right) / \left(\frac{4}{3} \cancel{\pi R_0^3} \rho_p \right)$$

$$= \frac{4}{9R^2 \rho_p} \left(M_c R_0 \leq k_c [C_i]^{q_i} \right)$$

4 - K(R)

Numerous correlations exist for estimating elutriation constant. The problem is that most of the proposed correlations are restricted to narrow particle sizes.

a) Yagi and Aochi (1955)

$$\frac{\bar{K} R}{\mu} = F_r \left[0.0015 (Re_t^0)^{0.6} + 0.01 (Re_t^1)^{1.2} \right]$$

b) Zenz and Weil (1958)

$$\frac{\bar{K}}{\rho_g u_0} = \begin{cases} (5.27) 10^{-5} \left[\frac{u_0^2}{g R \rho_p^2} (10^6) \right]^{1.87} & \frac{u_0^2}{g R \rho_p^2} \leq 581.6 \times 10^6 \\ (4.97) 10^{-3} \left[\frac{u_0^2}{g R \rho_p^2} (10^6) \right]^{1.15} & \frac{u_0^2}{g R \rho_p^2} > 581.6 \times 10^6 \end{cases}$$

c) Wen and Hashinger (1960)

$$\frac{\bar{K}}{\rho_g (u_0 - u_t)} = (1.52) 10^{-5} Fr^{0.5} Re_t^{0.725} \left(\frac{\rho_p - \rho_g}{\rho_g} \right)^{1.5}$$

d) Tanaka and Shinohara (1972)

$$\frac{\bar{K}}{\rho_g (u_0 - u_t)} = 0.045 Re_t^{0.3} Fr^{0.5} \left(\frac{\rho_p - \rho_g}{\rho_g} \right)$$

e) Highley and Merrick (1974)

$$\bar{K} = 130 \left(\frac{u_0 \rho_g}{A_t} \right) \exp \left[-10.4 \left(\frac{u_t}{u_f} \right)^{0.5} \left(\frac{u_{mf}}{u_0 - u_{mf}} \right)^{0.25} \right]$$

Where

$$Fr = \text{Froude No.} = \frac{(u_0 - u_t)^2}{gR}$$

$$Re_t = \text{Reynolds No.} = \frac{R u_t \rho_g}{\mu}$$

\bar{K} = elutriation constant expressed in mass flow rate per unit ~~in~~ bed area

Note

All \bar{K} apply to height below TDH

ATTACHMENT 4

Simplified Model Element for Particle Size Distribution

Model Element of Particle Size Distribution

In order to make an equation based on mass fractions in size intervals for shrinking char particles we make the following assumptions:

- 1 - Steady state condition
- 2 - Particles enter the bed at a rate F_0 , with size distribution $\phi_0(\delta_c)$
- 3 - The flow rate of unburned particles leaving the bed as overflow, F_1 , has equal particle size distribution, $\phi_b(\delta_c)$, to that of the bed
- 4 - Particles are lost from the bed by elutriation, at the rate of $P_{\delta_c} W_c \phi_b(\delta_p) \Delta \delta_c$, where P_{δ_c} is the elutriation rate constant in the size interval $\delta_c + \Delta \delta_c$; W_c is the total mass of char in the bed; and $\phi_b(\delta_c)$ is the size distribution function of char particles in the bed.
- 5 - Particles are completely mixed in the bed.
- 6 - Particles do not change in density during burnout
- 7 - Particles shrink due to combustion at the rate of

$$\Gamma(\delta_c) = \frac{d\delta_c}{dt}$$

Mass Balance

$$\left[\text{Char fed to the bed} \right] + \left[\text{Char particles shrinking into size interval from a larger size} \right] - \left[\text{Char lost by overflow} \right] - \left[\text{Char lost by Elutriation} \right] - \left[\text{Char particles shrinking out of size interval to a smaller size} \right] - \left[\text{Total loss of mass due to combustion of char particle in the size interval of } \delta_c \text{ to } \delta_c + \Delta \delta_c \right] = 0$$

or

$$F_0 \phi_b(\delta_c) \Delta \delta_c + W_c \phi_b(\delta_c) \Gamma(\delta_c) \Big|_{\delta_c + \Delta \delta_c} - F_1 \phi_b(\delta_c) \Delta \delta_c - P_{\delta_c} W_c \phi_b(\delta_c) \Delta \delta_c - W_c \phi_b(\delta_c) \Gamma(\delta_c) \Big|_{\delta_c} - \frac{3 W_c \phi_b(\delta_c) \Delta \delta_c}{\delta_c} \Gamma(\delta_c) = 0 \quad (1)$$

dividing through by $\Delta \delta_c$ and taking limit as $\Delta \delta_c \rightarrow 0$, equ. (1) becomes

$$F_0 \phi_b(\delta_c) + W_c \frac{d}{d\delta_c} [\phi_b(\delta_c) \Gamma(\delta_c)] - F_1 \phi_b(\delta_c) - P_{\delta_c} W_c \phi_b(\delta_c) - \frac{3 W_c \phi_b(\delta_c)}{\delta_c} \Gamma(\delta_c) = 0 \quad (2)$$

The solution to equ. (2), giving the particle size distribution $\phi_b(\delta_c)$, has been derived by Levenspiel et al (1968/1969)* for a mono-sized feed as:

* Powder Technology, 2 (2); 37-46 (Dec. 1968)

$$\phi_b(\delta_c) = \frac{F_0}{W_c \Gamma(\delta_c)} \frac{\delta_c^3}{\delta_{ci}^3} I(\delta_c, \delta_{ci}) \quad (3)$$

where the function $I(\delta_c, \delta_{ci})$ is defined as

$$I(\delta_c, \delta_{ci}) = \text{EXP} - \left[\int_{\delta_c}^{\delta_{ci}} \frac{F_1/W_c + P_{\delta_{ci}}}{\Gamma(\delta_c)} d\delta_c \right] \quad (4)$$

where δ_{ci} = initial particle diameter

For a feed of a wide size distribution, the solution to equ. (2) becomes much more complicated and is derived as:

$$\phi_b(\delta_c) = \frac{F_0 \delta_c^3}{W_c \Gamma(\delta_c)} I(\delta_c, \delta_{cm}) \int_{\delta_{ci} = \delta_c}^{\delta_{ci} = \delta_{cm}} \frac{\phi_0(\delta_{ci})}{\delta_{ci}^3 I(\delta_{ci}, \delta_{cm})} d\delta_{ci} \quad (5)$$

where δ_{cm} = largest size of particles in the feed

The carbon loading, W_c , can be derived from equ. (5) by satisfying the condition

$$\int_0^{\delta_c} \phi_b(\delta_c) d\delta_c = 1$$

$$W_c = \frac{F_o \delta_c^3}{\Gamma(\delta_c)} I(\delta_c, \delta_{cm}) \int_{\delta_{ci} = \delta_c}^{\delta_{ci} = \delta_{cm}} \frac{\phi_o(\delta_c)}{\delta_{ci}^3 I(\delta_{ci}, \delta_{cm})} d\delta_{ci} \quad (6)$$

The Shrinkage rate of a particle, $\Gamma(\delta_c)$, can be expressed in terms of mass reduction due to combustion:

$$V_c(\delta_c) = -\rho_c \frac{dV_c}{dt} = -\rho_c \frac{\pi}{2} \delta_c^2 \frac{d\delta_c}{dt}$$

$$\therefore \Gamma(\delta_c) = -\frac{d\delta_c}{dt} = \frac{2}{\rho_c \pi \delta_c^2} V_c(\delta_c) \quad (7)$$

Where =

V_c = Volume of unreacted core

ρ_c = Density of single char particle

The loss of mass due to heterogeneous chemical reaction for a single carbon particle can be expressed as:

$$V_c(\delta_c) = M_c \pi \delta_c^2 \sum k_c [C_j]^{a_j} \quad (8)$$

Where = $V_c(\delta_c)$ = mass reduction rate of a single particle of diameter δ_c

M_c = Atomic weight of carbon

$\sum k_c [C_j]^{a_j}$ = Sum of all heterogeneous reaction rates per unit surface area of the particle

k_c = Over-all reaction rate constant

C_j = Molar concentration of gaseous reactant j

a_j = Stoichiometric coefficient of species j

The overall reaction rate constant, k_c , consisting of a mass-transfer rate component and a kinetic rate component

$$\frac{1}{k_c} = \frac{1}{k_m} + \frac{1}{k_k}$$

$$\frac{1}{k_c} = \frac{1}{k_m} + \frac{1}{k_k}$$

k_m , The mass transfer coefficient can be obtained from transfer coefficient Sherwood Number, Sh

$$k_m = \frac{(Sh)(D_{oj})}{\delta_c}$$

$$k_m = \frac{(Sh)(D)}{\delta_c}$$

where D_{oj} = Gas film diffusion constant of species j

and The kinetic rate coefficient can be estimated from an Arrhenius type expression:

$$k_k = N \exp(-E/RT_s)$$

N = Surface reaction rate constant

E = Activation energy for surface reaction

R = Gas constant

T_s = Surface temperature of carbon particle

Total Combustion Rate of Char:

Combining equations (5) and 8, the total combustion rate of the bed material can be calculated

$$\therefore F_r(r_c(\delta_c), \phi_b(\delta_c)) = \int \frac{W_c \phi_b(\delta_c)}{\frac{\pi}{6} \rho_c \delta_c^3} r_c(\delta_c) d\delta_c$$

Where F_r total combustion rate

