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HYDRODYNAMICS OF CIRCULATING FLUIDIZED BEDS: KINETIC THEORY APPROACH

by

Dimitri Gidaspow, Rukmini Bezburuah and J. Ding
Department of Chemical Engineering
Illinois Institute of Technology, Chicago, IL 60616

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ABSTRACT

Rigorous methods of kinetic theory were used to derive particular phase viscosities and granular conductivities. This new kinetic theory predicted flow behavior and oscillations in a complete loop of a CFB. The results were compared to computations with imposed gas phase turbulence in the riser. The computations were repeated for production of synthesis gas from char.

The hydrodynamics of solids processing plants, such as circulating fluidized bed combustors that are being built to burn high sulfur coals is not well understood. As an aid for better design for such systems, a particulate multiphase Navier-Stokes' equation solver was developed. Particulate viscosities and solids pressures can be computed by a subroutine that solves a fluctuating kinetic energy equation for the particles.

Kinetic Theory Model

Savage (1) and Jenkins and Savage (2) have shown how to obtain constitutive equations and conservation laws for granular flow. Ding and Gidaspow (3) extended their approach to gas-particle flow. Since Ding and Gidaspow used a Maxwellian distribution their approach was restricted to dense flow. Recently Gidaspow extended this approach to cover dilute and dense particle-fluid flow. The mathematics is very similar to that described in detail in the classical text on kinetic theory by Chapman and Cowling (4). A summary of the techniques and the results is presented below.

Starting with the Boltzmann integral-differential equation for the frequency of particle velocity distributions, f, the dense phase transport theorem shown below was obtained by the authors cited above.

$$\frac{\partial}{\partial t}(n < \psi >) + \nabla \cdot (n < \vec{c}\psi > + P_c) = < n\vec{F}_s \frac{\partial \psi}{\partial \vec{c}} > + N_c \qquad (1)$$

where $\vec{F}_s$ is the body and the drag force acting on the system, $n = \int f dc$ and $< \psi > = \frac{1}{n} \int \psi f d\vec{c}$

$$P_c = -\frac{1}{2} g_o(\epsilon_s) d_p^3 \int\int\int (\psi_1 - \psi_1') f_1 f_2 \vec{k} (\vec{c}_{12} \cdot \vec{k}) d\vec{k} d\vec{c}_1 d\vec{c}_2 \qquad (2)$$

$$-\frac{1}{4} g_o(\epsilon_s) d_p^4 \int\int\int (\psi_1 - \psi_1') f_1 f_2 \nabla ln(\frac{f_2}{f_1}) \vec{k} (\vec{c}_{12} \cdot \vec{k}) d\vec{k} d\vec{c}_1 d\vec{c}_2$$

and

$$N_c = \frac{d_p^2}{2} \int \int \int (\psi_2' + \psi_1' - \psi_2 - \psi_2 - \psi_1)(\vec{c}_{12} \cdot \vec{k}) f^{(2)} d\vec{k} d\vec{c}_1 d\vec{c}_2 \qquad (3)$$

The particle conservation of mass and momentum equations are obtained by setting $\psi = m$ and $\psi = m\vec{c}$, respectively as done by Ding and Gidaspow and previous authors. The new part of the theory was to note that for the first perturbation upon the Maxwellian distribution the collision integral given by Equation (2) consists of two integrals which became as shown below.

$$Pc = Pc_1 + Pc_2 \qquad (4)$$

$$Pc_1 = \frac{2(1+e)}{5} g_o \rho_p \epsilon_s^2 (2 < \vec{C}\vec{C} > + C^2 I) \qquad (5)$$

$$Pc_2 = 2\epsilon_s \mu_{sc} \overset{o\ s}{\nabla} \vec{v} + \epsilon_s \zeta_s \nabla \cdot \vec{v} I \qquad (6)$$

where $\overset{o\ s}{\nabla}$ is the rate of shear tensor, [S] and μ_{sc} is the coefficient of viscosity, simply called viscosity by Ding and Gidaspow (3). For a Maxwellian distribution the first integral does not contribute to the viscosity since the non-diagonal terms of $< CC >$ vanish. The expressions for the viscosity and the granular conductivity given here have been generalized to the first perturbation for the frequency distribution. They are thus valid for dilute and dense flow. Equation (T1.5C) gives this shear viscosity. The standard dilute phase viscosity is given by Equation (T1.5d). Note that the kinematic viscosity is simply a product of the mean free path times a random velocity.

A conservation equation for this random velocity can be obtained by substituting $\psi = \frac{1}{2}m\vec{c}^2$ into Equation (1). The result is the fluctuating energy equation for the granular temperature θ given by Equation (T1.6). The conductivity given by Equation (T1.6c) was obtained from Equation (2) and the collisional dissipation γ due to the non- elasticity of the particles was obtained from Equation (3). The restitution coefficient "e" is the normal restitution coefficient. There also exists a tangential restitution coefficient associated with particle rotation that was not considered in the theory developed so far.

CFB LOOP

The equations shown in Table 1 were solved for the loop shown in Fig 1. Fig 2 shows that 8 sec. after start-up, there is the expected dense flow in the downcomer, strong downflow at one wall of the riser, a reasonable value of the solids granular temperature and viscosity. Such reasonable viscosities and particle oscillations were achieved by adjusting the value of the restitution coefficient until the viscosity matched Miller's (5) measurements, as shown in Figure 2. Miller has also observed the fluctuations of the particle velocities, as computed in Fig. 4. The discharge velocity from the standpipe to the riser is shown in Fig. 5. The 1 m/sec velocity is of the order of discharge velocity from hoppers. The new kinetic theory model computations do not differ greatly from Ding's (6) earlier computations using the turbulent viscosity shown in Table 1 and dense kinetic theory (e.g. Fig. 5). Time averaged values of the mass fluxes, solids concentrations and velocities are given in Figs. 6 to 9. At 2 m/sec there is a strong asymmetry caused by the inlet geometry. As expected, the bed is denser near the inlet. A color video shows the turbulent structure of the particles as a function of time.

COAL REACTIONS

Ding's (6) turbulence model and dense kinetic theory were used to simulate the reactions of char particles for the conditions given in Fig. 1. Char was assumed to consist of 88% carbon. The CFB was initially filled with the N_2 at 1300^0K. At the riser bottom a mixture of 40% 0_2 and 60% H_20 entered at 700^0K, at a pressure of 3.71 atm. Table 2 summarizes the energy and the species equations while Table 3 gives the principal reactions.

Figure 10 shows typical mole fractions profiles in the reactor 15 seconds after start-up. The oxygen was all consumed near the inlet. Fig. 11 shows some hot spots. Fig. 12 shows that the exit compositions reach a near steady state 10 seconds after start-up.

ACKNOWLEDGEMENT

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NOTATION

c	fluctuating velocity of particle
C	fluctuating minus hydrodynamic velocity
C_d	drag coefficient
d_p	particle diameter
D	diffusivity
e	coefficient of restitution
g	gravity
g_o	radial distribution function
h_v	volumetric heat transfer coefficient
h	enthalpy
ΔH^0	standard heat of reaction
K_{eq}	equilibrium constant of reaction
$K_{r,i}$	rate constant of reaction i
k_g, k_s	thermal conductivities of the gas and solid
M	molecular weight
Nu	gas particle Nusselt number
p	pressure

P	pressure tensor
q	flux vector of fluctuating energy
R_e	Reynolds number
r_i	reaction rate
$\overset{=}{S}$	deformation rate tensor
T_g, T_s	temperature of gas and solid
v_g, v_s	gas and solid velocity vector
Y_n	weight fraction of gas of species n
t	time

Greek Letters

β	two phase drag coefficient
γ	collisional energy dissipation
γ_{nm}	stoichiometric coefficient of species n
ϵ, ϵ_s	gas and solid volume fractions
η	effectiveness factor for reaction i
κ	conductivity of granular temperature
μ	shear viscosity
ζ	bulk viscosity
ρ	density
θ	granular temperature $= \frac{1}{3} < C^2 >$

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3. Ding, J. and D. Gidaspow, AIChE Journal, 36, 523 (1990).
4. Chapman, S. and T.G. Cowling, "The Mathematical Theory of Non-Uniform Gases," 2nd Ed., Cambridge Univ. Press (1961).
5. Miller, Aubrey, Ph.D. Thesis, Illinois Institute of Technology, Chicago 1991.
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TABLE 1:KINETIC THEORY MODEL FOR MULTIPHASE FLOW

1. CONTINUITY EQUATION FOR PHASE k(= g,s)

$$\frac{\partial}{\partial t}(\epsilon_k\rho_k) + \nabla\cdot(\epsilon_k\rho_k v_k) = \dot{m}_k, \quad \sum_k \epsilon_k = 1 \qquad (T1.1)$$

3. CONSTITUTIVE EQUATION FOR STRESS

$$\bar{\bar{\tau}}_k = [-P_k + \xi_k\nabla\cdot v_k]\,\bar{\bar{I}} + 2\mu_s\bar{\bar{S}}_k \quad (T1.3)$$

where

$$\bar{\bar{S}}_k = \frac{1}{2}\left[\nabla v_k + (\nabla v_k)^T\right] - \frac{1}{3}\nabla\cdot v_k\bar{\bar{I}} \qquad (T1.3a)$$

5. Solid Phase Stress

Kinetic Theory Model ((Gidaspow's 1991 extension of Savage,1983 and Ding and Gidaspow's, 1990 expressions to dilute and dense flow)

Solids Phase Pressure

$$P_s = \rho_p\epsilon_s\Theta\,[1 + 2(1+e)g_o\epsilon_s] \quad (T1.5a)$$

Solids Phase Bulk Viscosity

$$\xi_s = \frac{4}{3}\epsilon_s^2\rho_p d_p g_o(1+e)\left(\frac{\Theta}{\pi}\right)^{\frac{1}{2}} \quad (T1.5b)$$

Solids Phase Shear Viscosity

$$\mu_s = \frac{2\mu_{s_{dil}}}{(1+e)g_o}\left[1 + \frac{4}{5}(1+e)g_o\epsilon_s\right]^2$$

$$+\frac{4}{5}\epsilon_s^2\rho_p d_p g_o(1+e)\left(\frac{\Theta}{\pi}\right)^{\frac{1}{2}} \quad (T1.5c)$$

Solids Phase Dilute Viscosity

$$\mu_{s_{dil}} = \frac{5\sqrt{\pi}}{96}\rho_p d_p\Theta^{\frac{1}{2}} \quad (T5d)$$

Radial Distribution Function

$$g_o = \frac{3}{5}\left[1 - \left(\frac{\epsilon_s}{\epsilon_{s_{max}}}\right)^{\frac{1}{3}}\right]^{-1} \quad (T1.5e)$$

7. GAS - SOLID DRAG COEFFICIENTS

For $\epsilon_s < 0.8$ (based on Ergun equation)

$$\beta = 150\frac{\epsilon_s^2\mu_g}{\epsilon d_p^2} + 1.75\frac{\rho_g\epsilon_s|v_g - v_s|}{d_p} \quad (T1.7a)$$

For $\epsilon_s > 0.8$ (based on empirical correlation)

$$\beta = \frac{3}{4}C_d\frac{\epsilon\epsilon_s\rho_g|v_g - v_s|}{d_p}\epsilon^{-2.65} \quad (T1.7b)$$

2. MOMENTUM EQUATION FOR PHASE k(= g,s; l= g,s)

$$\frac{\partial}{\partial t}(\epsilon_k\rho_k v_k) + \nabla\cdot(\epsilon_k\rho_k v_k v_k) = \epsilon_k\rho_k g + \nabla\cdot\bar{\bar{\tau}}_k$$

$$+\beta(v_l - v_k) + \dot{m}_k v_k \qquad (T1.2)$$

4. Gas Phase Stress

$$\bar{\bar{\tau}}_g = 2\epsilon_g\mu_{ge}\bar{\bar{S}}_g \qquad (T1.4)$$

Turbulent Viscosity (Used for comparison only)

$$\mu_{ge} = \mu_t + \mu_g = \rho_g(c_t\Delta)^2(2\bar{\bar{S}}_g\cdot\bar{\bar{S}}_g)^{\frac{1}{2}} + \mu_g \qquad (T1.4a)$$

with $c_t = 0.1$ and $\Delta = \sqrt{(\Delta x\Delta y)}$

6. FLUCTUATING ENERGY ($\Theta = \frac{1}{3} < C^2 >$) EQUATION

$$\frac{3}{2}\left[\frac{\partial}{\partial t}(\epsilon_s\rho_s\Theta) + \nabla\cdot(\epsilon_s\rho_s v_s\Theta)\right] = \bar{\bar{\tau}}_s : \nabla v_s$$

$$-\nabla\cdot q - \gamma \qquad (T1.6)$$

Collisional Energy Dissipation γ

$$\gamma = 3(1 - e^2)\epsilon_s^2\rho_s g_o\Theta\left(\frac{4}{d_p}\left(\frac{\Theta}{\pi}\right)^{\frac{1}{2}} - \nabla\cdot v_s\right) \qquad (T1.6a)$$

Flux of Fluctuating Energy q

$$q = -\kappa\nabla\Theta \qquad (T1.6b)$$

Conductivity of Fluctuating Energy

$$\kappa = \frac{2}{(1+e)g_o}\left[1 + \frac{6}{5}(1+e)g_o\epsilon_s\right]^2\kappa_{dil}$$

$$+2\epsilon_s^2\rho_p d_p g_o(1+e)\left(\frac{\Theta}{\pi}\right)^{\frac{1}{2}} \qquad (T1.6c)$$

Dilute Phase ("Eddy Type") Granular Conductivity

$$\kappa_{dil} = \frac{75}{384}\sqrt{\pi}\rho_p d_p\Theta^{\frac{1}{2}} \qquad (T1.6d)$$

where

$$C_d = \frac{24}{Re_p}\left[1 + 0.15Re_p^{0.687}\right], \text{for } Re_p < 1000 \qquad (T1.7c)$$

$$C_d = 0.44, \text{for} \quad Re_p > 1000 \quad (T1.7d)$$

$$Re_p = \frac{\epsilon\rho_g|v_g - v_s|d_p}{\mu_g} \qquad (T1.7e)$$

TABLE 2: CONSERVATION OF SPECIES AND ENERGY

1. CONSERVATION EQUATION OF GAS COMPONENT "n"

$$\frac{\partial}{\partial t}(\epsilon\rho_g Y_n) + \nabla\cdot(\epsilon\rho_g Y_n v_g) = M_n \sum \gamma_{nm} r_n \qquad (2.1)$$

2. ENERGY EQUATIONS

Gas Phase

$$\frac{\partial}{\partial t}(\epsilon\rho_g h_g) + \nabla\cdot(\epsilon\rho_g h_g v_g) = \epsilon(\frac{\partial p}{\partial t} + v_g\cdot\nabla p)$$

$$+\epsilon\sum r_n \Delta H_n^0 + h_v(T_s - T_g) + \nabla\cdot(k_g\epsilon\nabla T_g) \qquad (2.2)$$

Solid Phase

$$\frac{\partial}{\partial t}(\epsilon_s\rho_p h_s) + \nabla\cdot(\epsilon_s\rho_p h_s v_s) = +h_v(T_g - T_s)$$

$$+\nabla\cdot(k_s\epsilon_s\nabla T_s) \qquad (2.3)$$

Gas - Particle Heat Transfer h_v
For $\epsilon \leq 0.8$,

$$Nu_p = (2+1.1Re^{0.6}Pr^{\frac{1}{3}})S_p, \qquad Re \geq 200$$

$$Nu_p = 0.123\left(\frac{4Re}{d_p}\right)^{0.83} S_p^{0.17}, \quad 200 < Re \leq 2000$$

$$Nu_p = 0.61Re^{0.67}S_p, \qquad Re > 2000$$

$\epsilon > 0.8$

$$Nu_p = (2+0.16Re^{0.67})S_p, \qquad Re \leq 200$$

$$Nu_p = 8.2Re^{0.6}S_p, \qquad 200 < Re \leq 1000$$

$$Nu_p = 1.06Re^{0.4557}S_p, \qquad Re > 1000$$

where

$$Re = \frac{d_p\rho_g|v_g - v_s|}{\mu_g}$$

$$S_p = \epsilon_s\frac{6}{d_p} \quad \text{and} \quad Nu_p = h_v d_p/k_g$$

TABLE 3. KEY REACTIONS

$$r_i = \frac{\epsilon_s(p_i - p_i^*)}{\frac{d_p\rho}{6K_{p,i}} + \frac{d_p\rho^2(1-\rho)RT}{12\rho D_{M,i}} + \frac{1}{\eta\rho^3 K_{r,i}C_c^0}}$$

1. COMBUSTION REACTION

$$C + \gamma_1 O_2 \longrightarrow 2(1-\gamma_1)CO + (2\gamma_1 - 1)CO_2$$

where γ_1 is determined by

$$\frac{CO}{CO_2} = \frac{2(1-\gamma_1)}{2\gamma_1 - 1} = 10^{3.4}\exp(\frac{-12400}{RT_s})$$

$$K_{r,1} = 1.79\times10^{6}\exp(\frac{-27000}{RT_s})$$

$$\Delta H_{r,1}^0|_2 98^0 k = (-97.7)(2\gamma_1 - 1) + 2(-28.714)$$

$$(1-\gamma_1) + 2.4 \text{ and } p_{O_2}^* = 0.0$$

2. GASIFICATION REACTIONS

$$(a) C + CO_2 \longrightarrow 2CO$$

$$K_{r_2} = 930\exp(\frac{-45000}{RT_s})$$

$$K_{eq} = \frac{P_{CO}^2}{P_{CO_2}^*} = 1.22\times10^9\exp(\frac{-40300}{RT_s})$$

$$\Delta H_{r,2}^0|_2 98^0 k = 40.3$$

$$(b) C + H_2O \longrightarrow CO + H_2$$

$$K_{r_4} = 930\exp(\frac{-45000}{RT_s})$$

$$K_{eq} = \frac{P_{H_2}P_{CO}}{(P_{H_2O}^*)^2} = \exp(17.3 - \frac{16326.1}{T_s})$$

$$\Delta H_{r,4}^0|_2 98^0 k = 32.4$$

3. WATER SHIFT REACTION

$$Co + H_2O \longleftrightarrow CO_2 + H_2$$

$$r_8 = 0.775\exp(\frac{-8421.3}{T_g})p^{0.5-\frac{p}{250}}(x_{CO}x_{H_2O}$$

$$-\frac{x_{CO_2}x_{H_2}}{K_{wg}})(1 - W_c)\rho_{coal}\epsilon_s$$

$$K_{wg} = 0.027\exp(\frac{7860}{T_g})$$

$$\Delta H_8^0|_2 98^0 k = -9.84$$

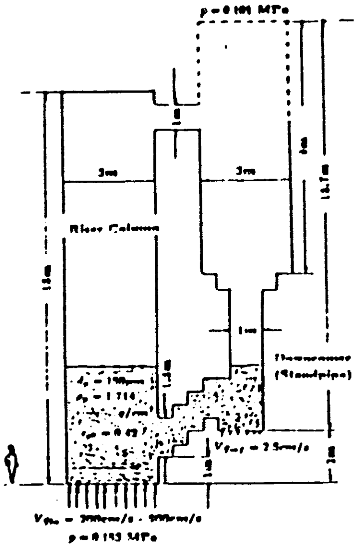

FIGURE 1. CFB Loop Including Initial and Inlet Conditions

Inlet Conditions

Diameter of particles	=	150 μm
Density of particles	=	1714 Kg/m³
Terminal velocity of particles	=	1.1 m/s
Gas flow rate at bottom of standpipe (Minimum fluidization velocity)	=	2.5 cm/s
Air inlet (riser) velocity	=	2 m/s
Initial bed height	=	4.5 m
Initial porosity	=	0.42

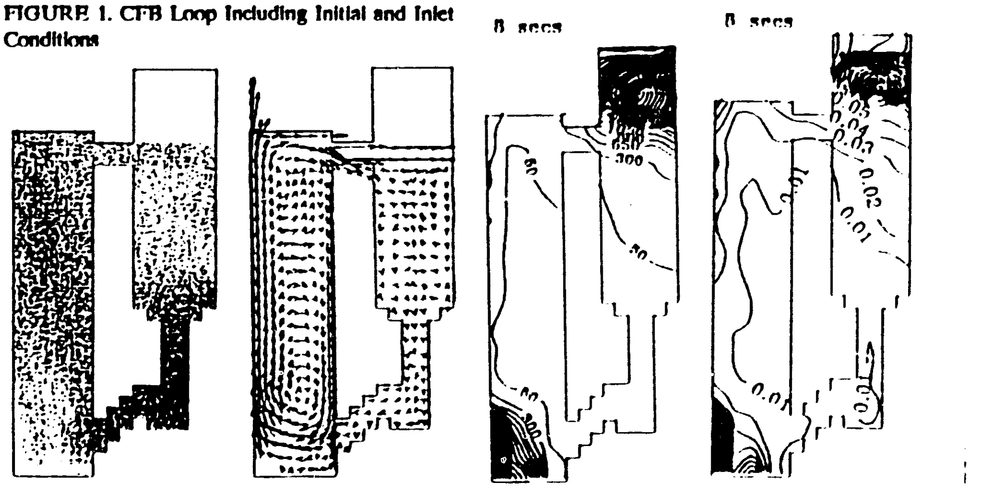

FIGURE 2. Particle Concentration, Velocities, Granular Temperatures (cm/s)² and Solid Viscosities (Poise)

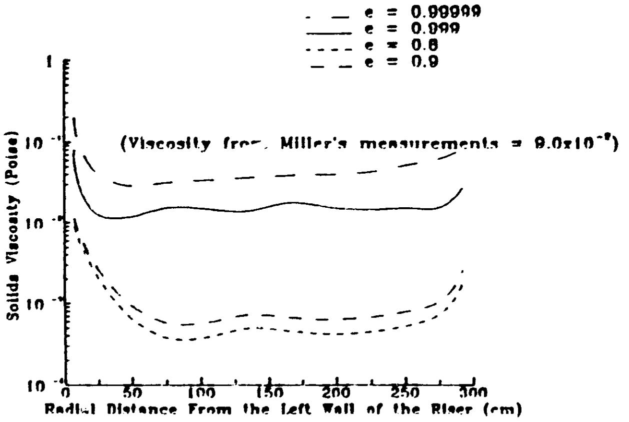

Fig. 3. Effect of Restitution Coefficient on Solids Viscosity

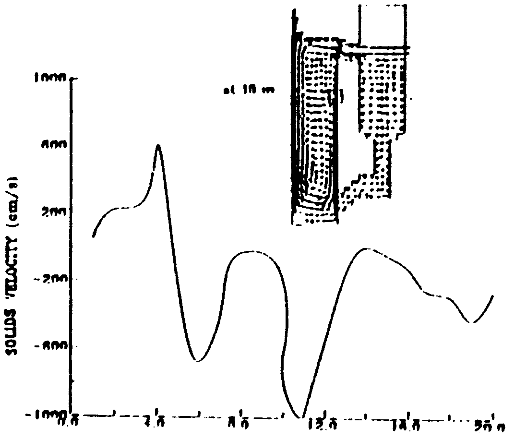

Figure 4

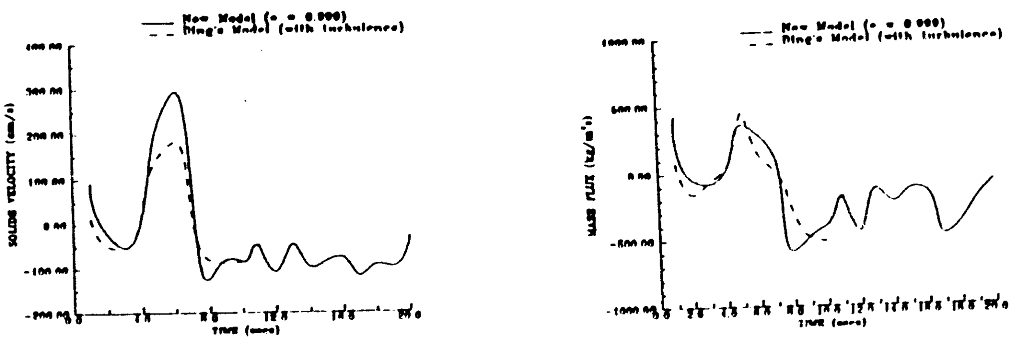

FIGURE 5. Discharge from Standpipe to Riser

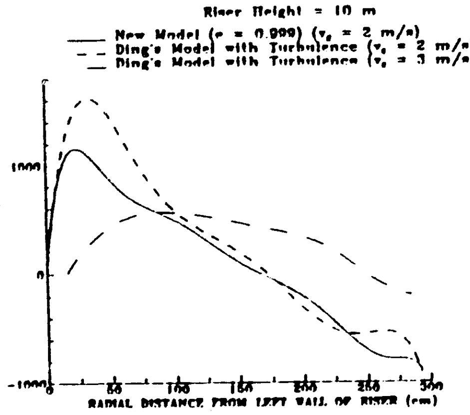

FIGURE 6. Time Averaged Radial Mass Flux Profile

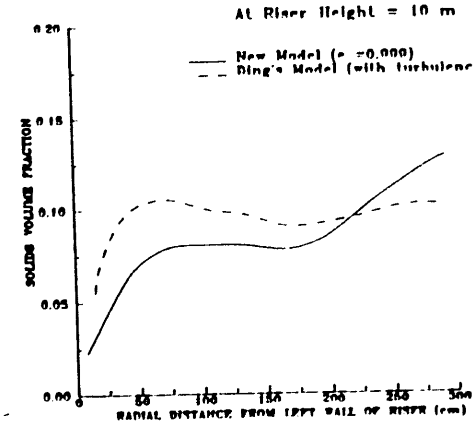

FIGURE 7. Time Averaged Radial Solids Volume Fraction Profile

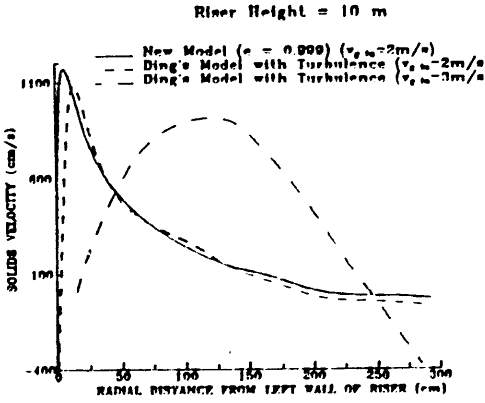

FIGURE 8. Time Averaged Radial Solids Velocity Profile

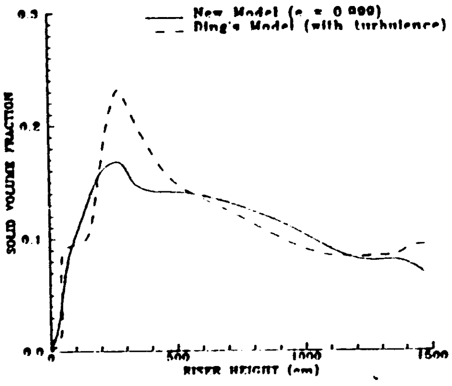

FIGURE 9. Area Averaged Axial Solids Volume Fraction Profile

DISCLAIMER

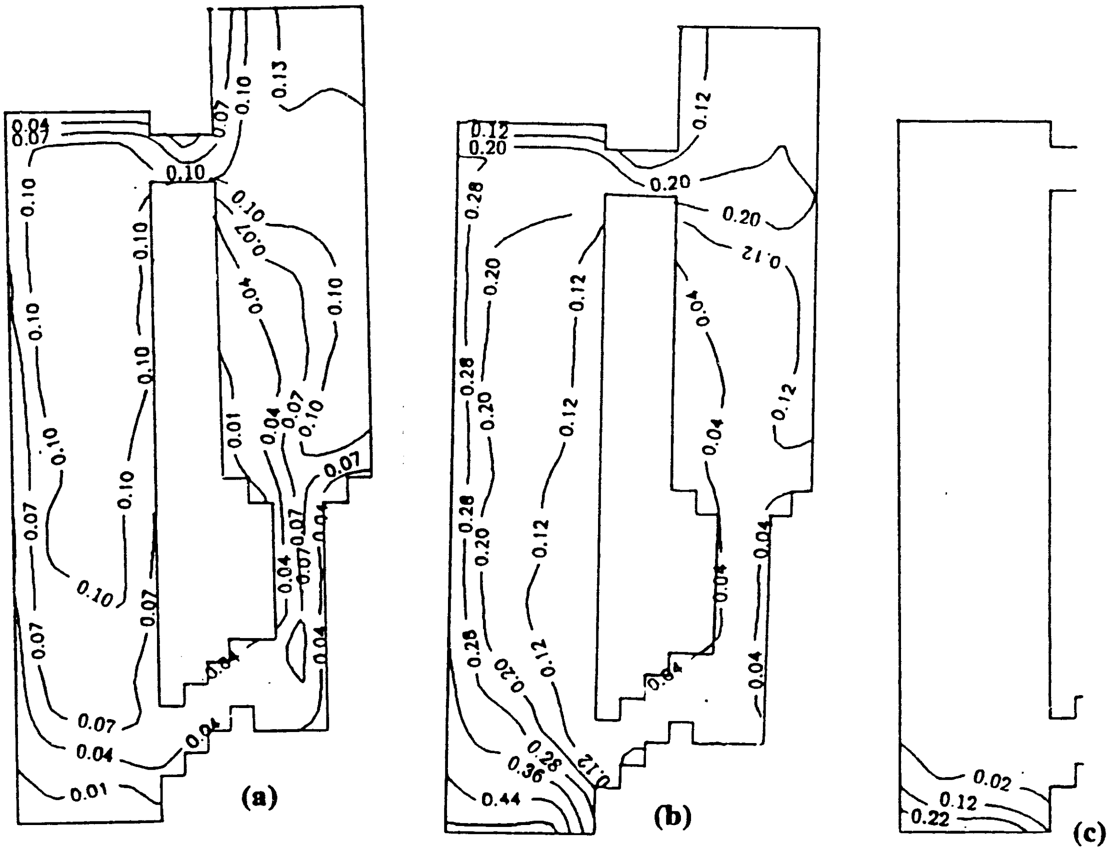

FIGURE 10. Mole Fractions CO_2, Steam (b), and O_2 in the CFB gasifier at 15 seconds.

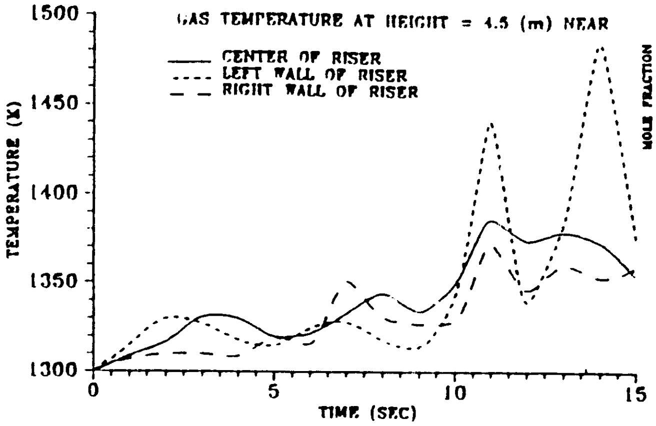

FIGURE 11. Gas Temperature

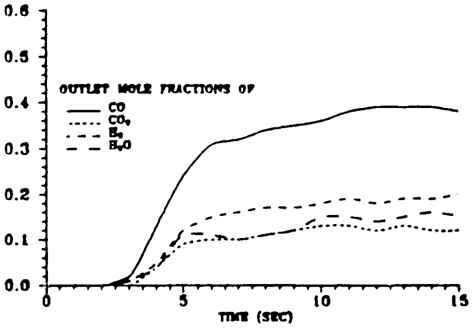

FIGURE 12. Outlet Gas Compositions for the CFB Synthesis Gas Producer

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