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COMPUTATION OF HYDRODYNAMICS
USING KINETIC THEORY

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Predictive Models of Circulating Fluidized Bed Combustors

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ABSTRACT

The overall objective of this investigation is to develop experimentally verified models for circulating fluidized bed (CFB) combustors.

The report presented in the form of paper submitted for presentation at the next international fluidization conference presents the results of our computations for the CFB at a higher velocity. A review of the whole project was given at the Morgantown Energy Technology Center on December 3, 1991.

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HYDRODYNAMICS OF CIRCULATING FLUIDIZED BEDS: KINETIC THEORY APPROACH

by

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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.

$$\frac{\partial}{\partial t}(n \langle \psi \rangle) + \nabla \cdot (n \langle \bar{c} \psi \rangle + P_c) = \langle n \bar{F}_s \frac{\partial \psi}{\partial \bar{c}} \rangle + N_c \quad (1)$$

where $\bar{F}_s$ is the body and the drag force acting on the system, $n = \int f d\bar{c}$ and $\langle \psi \rangle = \frac{1}{n} \int \psi f d\bar{c}$

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

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

and

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

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.

$$P_c = P_{c1} + P_{c2} \quad (4)$$

$$P_{c1} = \frac{2(1+e)}{5} g_o \rho_p \epsilon_s^2 (2 < \vec{C}\vec{C} > + C^2 I) \quad (5)$$

$$P_{c2} = 2\epsilon_s \mu_{sc} \overset{o}{\nabla} v + \epsilon_s \zeta_s \nabla \cdot \vec{v} I \quad (6)$$

where $\overset{o}{\nabla}$ 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 $< \vec{C}\vec{C} >$ 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 for inlet velocities of 2 and 5 m/s. Fig 2 shows that for an inlet velocity of 5 m/s there is the expected dense flow in the downcomer, strong downflow at both walls of the riser, reasonable values of granular temperature and solids viscosity. Such reasonable viscosities and particle oscillations were achieved by adjusting the value of restitution coefficient until the viscosity matched Miller's (5) measurements as shown in Fig 3. Miller has also observed the fluctuations of the particle velocities, as computed in Fig 4. Flow in the CFB usually oscillates with a frequency of order of $\frac{1}{4}$ Hertz. Such a low frequency compared to the high gas turbulence frequency is due to the very low granular sonic velocity. The discharge from the standpipe to the riser shown in Fig 5 is essentially this critical or sonic velocity. After start-up it oscillates around 1 m/sec, which is of the order of the discharge velocity from

hoppers. Time averaged values of the solids velocities and volume fractions are shown in Figs 6 and 7. At the very low velocity of 2 m/s there exists a very pronounced asymmetry which tends to disappear at higher operating velocities. At 5 m/s Fig 8 shows the expected high particle density at the inlet and a nearly developed profile higher up in the riser. As also shown in Fig 8, these trends agree with Ding's (6) earlier computations using a turbulent viscosity and dense kinetic theory shown in Table 1. A color video shows turbulent structure of the particles as a function of time. Cluster like dense regions are discharged from the stand-pipe and move up in the riser.

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°K. At the riser bottom a mixture of 40% O_2 and 60% H_2O entered at 700°K, at a pressure of 3.71 atm. Table 2 summarizes the energy and the species equations while Table 3 gives the principal reactions.

Figure 9 shows typical mole fractions profiles in the reactor 15 seconds after start-up. The oxygen was all consumed near the inlet. Fig. 10 shows some hot spots. Fig. 11 shows that the exit compositions reach a near steady state 10 seconds after start-up.

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NOTATION

c fluctuating velocity of particle	u_g, u_s gas and solid velocity vector
C fluctuating minus hydrodynamic velocity	Y_n weight fraction of gas of species n
C_d drag coefficient	t time
d_p particle diameter	<u>Greek Letters</u>
D diffusivity	β two phase drag coefficient
e coefficient of restitution	γ collisional energy dissipation
g gravity	γ_{nm} stoichiometric coefficient of species n
g_o radial distribution function	ϵ, ϵ_s gas and solid volume fractions
h_v volumetric heat transfer coefficient	θ granular temperature = $\frac{1}{3} \langle C^2 \rangle$
h enthalpy	η effectiveness factor for reaction i
ΔH^0 standard heat of reaction	κ conductivity of granular temperature
K_{eq} equilibrium constant of reaction	μ shear viscosity
$K_{r,i}$ rate constant of reaction i	ξ bulk viscosity
k_g, k_s thermal conductivities of the gas and solid	τ stress
M molecular weight	ρ density
Nu gas-particle Nusselt number	ψ mass, momentum or energy
p pressure	
P pressure tensor	
Pr Prandtl number	
q flux vector of fluctuating energy	
Re Reynolds number	
r_i reaction rate	
$\dot{S}$ deformation rate tensor	
T_g, T_s temperature of gas and solid	

TABLE 1: KINETIC THEORY MODEL FOR MULTIPHASE FLOW

1. CONTINUITY EQUATION FOR PHASE k(= g,s)	2. MOMENTUM EQUATION FOR PHASE k(= g,s; l= g,s)
$\frac{\partial}{\partial t}(\epsilon_k \rho_k) + \nabla \cdot (\epsilon_k \rho_k v_k) = \dot{m}_k, \quad \sum_k \epsilon_k = 1 \quad (T1.1)$	$\frac{\partial}{\partial t}(\epsilon_k \rho_k v_k) + \nabla \cdot (\epsilon_k \rho_k v_k v_k) = \epsilon_k \rho_k g + \nabla \cdot \bar{\tau}_k + \beta(v_l - v_k) + \dot{m}_k v_k \quad (T1.2)$
3. CONSTITUTIVE EQUATION FOR STRESS	4. Gas Phase Stress
$\bar{\tau}_k = [-P_k + \xi_k \nabla \cdot v_k] \bar{I} + 2\mu_s \bar{S}_k \quad (T1.3)$	$\bar{\tau}_g = 2\epsilon_g \mu_{gs} \bar{S}_g \quad (T1.4)$
where	Turbulent Viscosity (Used for comparison only)
$\bar{S}_k = \frac{1}{2} [\nabla v_k + (\nabla v_k)^T] - \frac{1}{3} \nabla \cdot v_k \bar{I} \quad (T1.3a)$	$\mu_{gs} = \mu_t + \mu_g = \rho_g (c_t \Delta)^2 (2\bar{S}_g \cdot \bar{S}_g)^{\frac{1}{2}} + \mu_g \quad (T1.4a)$ <p>with $c_t = 0.1$ and $\Delta = \sqrt{(\Delta x \Delta y)}$</p>
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)	6. FLUCTUATING ENERGY ($\Theta = \frac{1}{2} < C^2 >$) EQUATION
Solids Phase Pressure	$\frac{3}{2} \left[\frac{\partial}{\partial t}(\epsilon_s \rho_s \Theta) + \nabla \cdot (\epsilon_s \rho_s v_s \Theta) \right] = \bar{\tau}_s : \nabla v_s - \nabla \cdot q - \gamma \quad (T1.6)$
$P_s = \rho_p \epsilon_s \Theta [1 + 2(1+e)g_o \epsilon_s] \quad (T1.5a)$	Collisional Energy Dissipation γ
Solids Phase Bulk Viscosity	$\gamma = 3(1-e^2)\epsilon_s^2 \rho_s g_o \Theta \left(\frac{4}{d_p} \left(\frac{\Theta}{\pi} \right)^{\frac{1}{2}} - \nabla \cdot v_s \right) \quad (T1.6a)$
$\xi_s = \frac{4}{3} \epsilon_s^2 \rho_p d_p g_o (1+e) \left(\frac{\Theta}{\pi} \right)^{\frac{1}{2}} \quad (T1.5b)$	Flux of Fluctuating Energy q
Solids Phase Shear Viscosity	$q = -\kappa \nabla \Theta \quad (T1.6b)$
$\mu_s = \frac{2\mu_{s,dil}}{(1+e)g_o} \left[1 + \frac{4}{5}(1+e)g_o \epsilon_s \right]^2 + \frac{4}{5} \epsilon_s^2 \rho_p d_p g_o (1+e) \left(\frac{\Theta}{\pi} \right)^{\frac{1}{2}} \quad (T1.5c)$	Conductivity of Fluctuating Energy
Solids Phase Dilute Viscosity	$\kappa = \frac{2}{(1+e)g_o} \left[1 + \frac{6}{5}(1+e)g_o \epsilon_s \right]^2 \kappa_{dil} + 2\epsilon_s^2 \rho_p d_p g_o (1+e) \left(\frac{\Theta}{\pi} \right)^{\frac{1}{2}} \quad (T1.6c)$
$\mu_{s,dil} = \frac{5\sqrt{\pi}}{96} \rho_p d_p \Theta^{\frac{1}{2}} \quad (T1.5d)$	Dilute Phase ("Eddy Type") Granular Conductivity
Radial Distribution Function	$\kappa_{dil} = \frac{75}{384} \sqrt{\pi} \rho_p d_p \Theta^{\frac{1}{2}} \quad (T1.6d)$
$g_o = \frac{3}{5} \left[1 - \left(\frac{\epsilon_s}{\epsilon_{s,max}} \right)^{\frac{1}{2}} \right]^{-1} \quad (T1.5e)$	
7. GAS - SOLID DRAG COEFFICIENTS	
For $\epsilon_s < 0.8$ (based on Ergun equation)	where
$\beta = 150 \frac{\epsilon_s^2 \mu_g}{\epsilon_s d_p^2} + 1.75 \frac{\rho_g \epsilon_s v_g - v_s }{d_p} \quad (T1.7a)$	$C_d = \frac{24}{Re_p} \left[1 + 0.15 Re_p^{0.687} \right], \text{ for } Re_p < 1000 \quad (T1.7c)$
For $\epsilon_s > 0.8$ (based on empirical correlation)	$C_d = 0.44, \text{ for } Re_p > 1000 \quad (T1.7d)$
$\beta = \frac{3}{4} C_d \frac{\epsilon_s \rho_g v_g - v_s }{d_p} \epsilon^{-1.65} \quad (T1.7b)$	$Re_p = \frac{\epsilon \rho_g v_g - v_s d_p}{\mu_g} \quad (T1.7e)$

TABLE 2: CONSERVATION OF SPECIES AND ENERGY

1. CONSERVATION EQUATION OF GAS COMPONENT "n"

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

2. ENERGY EQUATIONS

Gas Phase

$$\frac{\partial}{\partial t}(\epsilon \rho_g h_g) + \nabla \cdot (\epsilon \rho_g h_g v_g) = \epsilon \left(\frac{\partial p}{\partial t} + v_g \cdot \nabla p \right) + \epsilon \sum r_n \Delta H_n^0 + h_v(T_s - T_g) + \nabla \cdot (k_g \epsilon \nabla T_g) \quad (2.2)$$

Solid Phase

$$\frac{\partial}{\partial t}(\epsilon_s \rho_s h_s) + \nabla \cdot (\epsilon_s \rho_s h_s v_s) = +h_v(T_g - T_s) + \nabla \cdot (k_s \epsilon_s \nabla T_s) \quad (2.3)$$

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

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

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

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

$$\epsilon > 0.8$$

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

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

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

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

$$r_i = \frac{\epsilon_s (p_i - p_i^*)}{\frac{d p_i^0}{8 K_{p,i}} + \frac{d p_i^{02} (1 - \rho) RT}{12 \rho D_{M,i}} + \frac{1}{\eta_i \rho^2 K_{r,i} C_i^0}}$$

1. COMBUSTION REACTION

where γ_1 is determined by

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

$$K_{r,1} = 1.79 \times 10^6 \exp\left(\frac{-27000}{RT_s}\right)$$

$$\Delta H_{r,1}^0 |_{298^0 K} = (-97.7)(2\gamma_1 - 1) + 2(-28.714)$$

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

2. GASIFICATION REACTIONS

$$K_{r,2} = 930 \exp\left(\frac{-45000}{RT_s}\right)$$

$$K_{eq} = \frac{P_{CO}^2}{P_{CO_2}^*} = 1.22 \times 10^9 \exp\left(\frac{-40300}{RT_s}\right)$$

$$\Delta H_{r,2}^0 |_{298^0 K} = 40.3$$

$$K_{r,3} = 930 \exp\left(\frac{-45000}{RT_s}\right)$$

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

$$\Delta H_{r,4}^0 |_{298^0 K} = 32.4$$

3. WATER SHIFT REACTION

$$r_5 = 0.775 \exp\left(\frac{-8421.3}{T_g}\right) p^{0.5 - \frac{p}{750}} (x_{CO} x_{H_2O} - \frac{x_{CO_2} x_{H_2}}{K_{wg}}) (1 - W_c) \rho_{coal} \epsilon_s$$

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

$$\Delta H_5^0 |_{298^0 K} = -9.84$$

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Initial Conditions	
Particle Diameter	= 150 μm
Particle Density	= 1714 kg/m^3
Particle Terminal Velocity	= 1.1 m/s
Gas Flow Rate at Bottom of Standpipe	= 2.5 cm/s
Air Inlet Velocities	= 2, 5 m/s
Initial Bed Height	= 4.5 m
Initial Porosity	= 0.42
Boundary Conditions	
Mass Flux (at Outlet)	- Continuation Condition (Same as Ding & Gidaspow, 1990)
Gas Phase Velocity (at the Wall)	- No Slip
Solid Phase Velocities (at the Wall)	- Slip B.C (Same as Ding & Gidaspow, 1990)
Granular Temperature (at the Wall)	- Energy Flux is Zero

FIGURE 1. CFB Loop with Initial and Boundary Conditions.

FIGURE 2. Particle Concentration, Velocities, Granular Temperatures (cm/s^2) and Solid Viscosities (Poise) with $V_{\text{gas}} = 5 \text{ m/s}$

FIGURE 3. Effect of Restitution Coefficient on Solids Viscosity for $V_{gin} = 2$ m/s.

FIGURE 4. Solids Velocity at the Right Wall of the Riser at a Height of 10 m.

FIGURE 5. Discharge from Standpipe to Riser. for $V_{gin} = 5$ m/s.

FIGURE 6. Time Averaged (5 - 14 s) Solids Velocity Profile at a Height of 7.8 m.

FIGURE 7. Time Averaged (5 - 14 s) Radial Solids Volume Fraction Profile at a Height of 7.8 m

FIGURE 8. Area Averaged Axial Solids Volume Fraction Profiles

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

5 secs

Particle Distribution
at $V_{gin} = 2 \text{ m/s}$

5 secs

Particle Distribution
at $V_{gin} = 5 \text{ m/s}$

**Particle Density Distribution 5 seconds after
Start-up for $V_{\text{gin}} = 5 \text{ m/s}$.**

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