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.

\[
\frac{\partial}{\partial t}(n < \psi >) + \nabla \cdot (n < \tilde{\psi} > + P_e) = n \bar{F}_s \frac{\partial \psi}{\partial c} + N_e \tag{1}
\]

where \( F_s \) is the body and the drag force acting on the system, \( n = \int f dc \) and \( < \psi > = \frac{1}{n} \int \psi f dc \)

\[
P_e = -\frac{1}{2} g_o(\epsilon_s) d^3_p \int \int (\psi_1 - \psi_1') f_1 f_2 \bar{k}(\tilde{c}_{12} \cdot \bar{k}) d\bar{k} d\tilde{c}_1 d\tilde{c}_2 \tag{2}
\]

\[
-\frac{1}{4} g_o(\epsilon_s) d^4_p \int \int (\psi_1 - \psi_1') f_1 f_2 \nabla \ln \left( \frac{f_2}{f_1} \right) \bar{k}(\tilde{c}_{12} \cdot \bar{k}) d\bar{k} d\tilde{c}_1 d\tilde{c}_2
\]
The particle conservation of mass and momentum equations are obtained by setting $\psi = m$ and $\psi = \bar{m}\bar{c}$, respectively as done by Ding and Gida 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.

$$P_c = P_{c1} + P_{c2}$$

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

$$P_{c2} = 2 \epsilon_s \mu_{sc} \nabla \cdot \vec{v} + \epsilon_s \zeta_s \nabla \times \vec{v} \cdot \nabla$$

where $\epsilon$ is the rate of shear tensor, $[S]$ and $\mu_{sc}$ is the coefficient of viscosity, simply called viscosity by Ding and Gida and previous authors. 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 $\psi = \frac{1}{2} m \bar{c}^2$ into Equation (1). The result is the fluctuating energy equation for the granular temperature $\theta$ given by Equation (T1.6). The conductivity given by Equation (T1.6c) was obtained from Equation (2) and the collisional dissipation $\gamma$ due to the non-elasticity of the particles was obtained from Equation (3). The restitution coefficient $\epsilon$ 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°K. At the riser bottom a mixture of 40% O$_2$ and 60% H$_2$O 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 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$_r$ radial distribution function
h$_v$ volumetric heat transfer coefficient
h enthalpy
$\Delta H^\circ$ standard heat of reaction
$K_e$ 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

Greek Letters

$\Theta$ two phase drag coefficient
$\gamma$ collisional energy dissipation
$\gamma_{nm}$ stoichiometric coefficient of species $n$
ed gas and solid volume fractions
$\eta$ effectiveness factor for reaction $i$
$\kappa$ conductivity of granular temperature
$\mu$ shear viscosity
$\zeta$ bulk viscosity
$\rho$ density

LITERATURE CITED

### TABLE 1: KINETIC THEORY MODEL FOR MULTIPHASE FLOW

<table>
<thead>
<tr>
<th>1. CONTINUITY EQUATION FOR PHASE k (= g, s)</th>
<th>2. MOMENTUM EQUATION FOR PHASE k (= g, s; l = g, s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>[ \frac{\partial}{\partial t} (r_k \rho_k) + \nabla \cdot (r_k \rho_k \mathbf{v}_k) = \dot{m}_k, \sum \dot{m}_k = 1 ]</td>
<td>[ \frac{\partial}{\partial t} (r_k \rho_k \mathbf{v}_k) + \nabla \cdot (r_k \rho_k \mathbf{v}_k \mathbf{v}_k) = r_k \rho_k \nabla \cdot \mathbf{v}_k ]</td>
</tr>
<tr>
<td>(T.1.1)</td>
<td>(T.1.2)</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>3. CONSTITUTIVE EQUATION FOR STRESS</th>
</tr>
</thead>
<tbody>
<tr>
<td>[ \tau_k = [-P_k + \xi_k \nabla \cdot \mathbf{v}_k] / 2 + 2G_k \dot{\varepsilon}_k^S ]</td>
</tr>
<tr>
<td>[ \Omega_k = \frac{1}{2} (\nabla \mathbf{v}_k + (\nabla \mathbf{v}_k)^T) - \frac{1}{3} \nabla \cdot \mathbf{v}_k \mathbf{I} ]</td>
</tr>
<tr>
<td>(T.1.3a)</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>4. GAS PHASE STRESS</th>
</tr>
</thead>
<tbody>
<tr>
<td>[ \tau_g = 2\alpha \mu_g \varepsilon_\tau ]</td>
</tr>
<tr>
<td>(T.1.5)</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>5. SOLID PHASE STRESS</th>
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</thead>
<tbody>
<tr>
<td>Kinetic Theory Model (Gidaspaw's 1991 extension of Savage's 1983 and Ding and Gidaspaw's, 1990 expressions for dilute and dense flow)</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Solids Phase Pressure</th>
</tr>
</thead>
<tbody>
<tr>
<td>[ P_s = \rho_s v_s^2 (1 + 2(1 + \epsilon)g_s) ]</td>
</tr>
<tr>
<td>(T.1.5a)</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Solids Phase Bulk Viscosity</th>
</tr>
</thead>
<tbody>
<tr>
<td>[ \mu_s = \frac{2\mu_{sol}}{(1 + \epsilon)g_s} \left[ 1 + \frac{4}{5}(1 + \epsilon)g_s \right] ]</td>
</tr>
<tr>
<td>(T.1.5b)</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Solids Phase Shear Viscosity</th>
</tr>
</thead>
<tbody>
<tr>
<td>[ \mu_s = \frac{2\mu_{sol}}{(1 + \epsilon)g_s} \left[ 1 + \frac{4}{5}(1 + \epsilon)g_s \right] ]</td>
</tr>
<tr>
<td>(T.1.5c)</td>
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</tbody>
</table>

<table>
<thead>
<tr>
<th>Solids Phase Dilute Viscosity</th>
</tr>
</thead>
<tbody>
<tr>
<td>[ \mu_{sol} = \frac{3\sqrt{2}}{5\sigma \rho_s d_p g_s} ]</td>
</tr>
<tr>
<td>(T.1.5d)</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Radial Distribution Function</th>
</tr>
</thead>
<tbody>
<tr>
<td>[ g_s = \frac{3}{5} \left[ 1 - \left( \frac{r_s}{r_{max}} \right) \right]^{-1} ]</td>
</tr>
<tr>
<td>(T.1.5e)</td>
</tr>
</tbody>
</table>

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<thead>
<tr>
<th>6. FLUCTUATING ENERGY (( \Theta = \frac{1}{4} &lt; c^2 &gt; )) EQUATION</th>
</tr>
</thead>
<tbody>
<tr>
<td>[ \frac{3}{2} \left[ \frac{\partial}{\partial t} (r_c \rho_c \Theta) + \nabla \cdot (r_c \rho_c \mathbf{v}_c \Theta) \right] = \dot{e}_c : \mathbf{v}_c ]</td>
</tr>
<tr>
<td>(T.1.6)</td>
</tr>
</tbody>
</table>

| - Collisional Energy Dissipation \( \gamma \) |
| - Flux of Fluctuating Energy \( q \) |
| - Conductivity of Fluctuating Energy \( \kappa \) |

<table>
<thead>
<tr>
<th>7. GAS - SOLID DRAG COEFFICIENTS</th>
</tr>
</thead>
<tbody>
<tr>
<td>For ( \epsilon_s &lt; 0.8 ) (based on Ergun equation)</td>
</tr>
<tr>
<td>[ \beta = 150 \frac{c_s^2 d_s^2}{d_p^2} + 1.75 \rho_s \left[ \frac{g_s - \mu_s}{d_p} \right] ]</td>
</tr>
<tr>
<td>(T.1.7a)</td>
</tr>
</tbody>
</table>

| For \( \epsilon_s > 0.8 \) (based on empirical correlation) |
| \[ \beta = \frac{3}{4} \left[ \frac{c_d}{C_4} \right] \left( r_s \rho_s |\mathbf{v}_s - \mathbf{v}_d| \right) \epsilon^{-1} \] |
| (T.1.7b) |

where

| \[ C_4 = \frac{24}{\kappa} \left[ 1 + \frac{0.15 \rho_s g_s}{\mu_s} \right] \] for \( \kappa p < 1000 \) |
| (T.1.7c) |

| \[ C_4 = 0.44 \] for \( \kappa p > 1000 \) |

| \[ \beta = \frac{c_d}{C_4} \left( r_s \rho_s |\mathbf{v}_s - \mathbf{v}_d| \right) \epsilon^{-1} \] |
| (T.1.7d) |

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TABLE 2: CONSERVATION OF SPECIES AND ENERGY

1. CONSERVATION EQUATION OF GAS COMPONENT "n"
\[
\frac{\partial}{\partial t}(\rho u_n) + \nabla \cdot (\rho u_n u_i) = \sum_{m} \gamma_{nm} r_n
\]
(2.1)

2. ENERGY EQUATIONS

Gas Phase
\[
\frac{\partial}{\partial t}(\rho h) + \nabla \cdot (\rho h u_i) = \epsilon \left( \frac{\partial p}{\partial t} + u_i \nabla p \right) + \epsilon \sum_{m} \Delta H^0_n + h_n(T_s - T_g) + \nabla \cdot (k_v \nabla T_g)
\]
(2.2)

Solid Phase
\[
\frac{\partial}{\partial t}(\epsilon u_i h_s) + \nabla \cdot (\epsilon u_i h_s u_i) = + h_s(T_s - T_s) + \nabla \cdot (k_v \nabla T_g)
\]
(2.3)

Gas - Particle Heat Transfer \( h_g \)
For \( \epsilon \leq 0.8 \),
\[
N_{u_p} = (2 + 1.1 Re^{0.1} Pr^{0.1})S_p, \quad Re \geq 200
\]

\[
S_p = \epsilon \frac{6}{d_p} \quad \text{and} \quad N_{u_p} = h_g d_p / k_g
\]

TABLE 3. KEY REACTIONS

1. COMBUSTION REACTION
\[ C + \gamma_1 O_2 \rightarrow 2(1 - \gamma_1) CO + (2\gamma_1 - 1) CO_2 \]
where \( \gamma_1 \) is determined by
\[
\frac{CO}{CO_2} = \frac{2(1 - \gamma_1)}{2\gamma_1 - 1} = 10^{3.4} \exp(-12400 / R_T)
\]
\[ K_{\gamma_1} = 1.79 \times 10^6 \exp(-27000 / R_T) \]

\[ \Delta H^0_{\gamma_1 O_2} = 198 \times 40.3 \]

(b)C + II$_3$O $\rightarrow$ CO + II$_2$
\[ \Delta H^0_{II_3O} = 99 \times 40.3 \]

3. WATER SHIFT REACTION
\[ Co + II_3O \rightarrow CO_3 + II_2 \]
\[ \Delta H^0_{CO_3} = 99 \times 40.3 \]

2. GASIFICATION REACTIONS
(a)C + CO$_2$ $\rightarrow$ 2CO
\[ K_{s} = 930 \exp(-4500 / R_T) \]
\[ K_{ref} = \frac{P_{CO} P_{CO}}{(P_{CO})^2} \]

\[ \Delta H^0_{CO} = 198 \times 99 \times 40.3 \]

\[ \eta = 0.775 \exp(-84121.3 / T_g) \]
\[ K_{eq} = 0.027 \exp(7860 / T_g) \]
\[ \Delta H^0_{CO} = -9.84 \]

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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 = 2.5 cm/s (Minimum fluidization velocity)
- Air inlet (riser) velocity = 2 m/s
- Initial bed height = 4.5 m
- Initial porosity = 0.42

**Figure 1. CFB Loop Including Initial and Inlet Conditions**

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

**Figure 3. Effect of Restitution Coefficient on Solids Viscosity**

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FIGURE 5. Discharge from Standpipe to River

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

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FIGURE 10. Mole Fractions CO₂, Steam (b), and O₂ 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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END

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