COMPUTATION AND MEASUREMENTS OF MASS TRANSFER AND DISPERSION COEFFICIENTS IN FLUIDIZED BEDS

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PROJECT PUBLICATIONS

DISPERSION COEFFICIENTS


MASS TRANSFER COEFFICIENTS

• Chalermsinsuwan, B., P. Piumsomboon, and D. Gidaspow, “Kinetic theory based computation of PSRI riser- Part I: Estimate of mass transfer coefficient”, Chemical Engineering Science, 64 (2009a) 1195-1211

• Chalermsinsuwan, B., P. Piumsomboon, and D. Gidaspow, “Kinetic theory based computation of PSRI riser- Part II: Computation of mass transfer coefficient with chemical reaction”, Chemical Engineering Science, 64 (2009b) 1212-1222


IMPROVED FUTUREGEN CONCEPT


Kinetic Theory Model

- **Continuity Equation for Phase k**
  \[
  \frac{\partial (\rho_k \varepsilon_k)}{\partial t} + \nabla \cdot (\rho_k \varepsilon_k \nu_k) = \dot{m}_k
  \]

- **Momentum Equation for Phase k**
  \[
  \frac{\partial (\rho_k \varepsilon_k \nu_k)}{\partial t} + \nabla \cdot (\rho_k \varepsilon_k \nu_k \nu_k) = \varepsilon_k \rho_k \ddot{g} + \nabla \cdot [\tau_k] + \sum_{l=1}^{N} \beta(v_l - v_k) + \dot{m}_k \ddot{v}_k
  \]
  acceleration of phase ‘k’ = buoyancy + stress + drag force + phase change

- **Constitutive Equation for Stress (Above Min. Fluidization)**
  \[
  [\tau_k] = [-P_k + \xi_k \nabla \nu_k \mathbb{I}] + 2\mu_k [S_k]
  \]
  \[
  [S_k] = \frac{1}{2} \left[ \nabla \nu_k + (\nabla \nu_k)^T \right] - \frac{1}{3} \nabla \cdot \nu_k [I]
  \]
Solid Phase Stress

- Solid-phase Pressure

\[ P_s = \rho_s \varepsilon_s \theta \left[ 1 + 2(1+e)g_o \varepsilon_s \right] \]

\( \text{kinetic} \quad \text{collision} \)

- Solid-phase Bulk Viscosity

\[ \lambda_s = \frac{4}{3} \varepsilon_s^2 \rho_s d_s g_o (1+e) \sqrt{\frac{\theta}{\pi}} \]

- Solid-phase Shear Viscosity

\[ \mu_s = \frac{2 \mu_{s_{\text{dil}}}}{(1+e)g_0} \left[ 1 + \frac{4}{5} (1+e)g_o \varepsilon_s \right] + \frac{4}{5} \varepsilon_s^2 \rho_s d_s g_o (1+e) \sqrt{\frac{\theta}{\pi}} \]

- Radial distribution function

[Bagnold(1954)]

\[ g_o = \left[ 1 - \left( \frac{\varepsilon_s}{\varepsilon_{s,\text{max}}} \right)^{1/3} \right]^{-1} \]

- Solid-phase dilute viscosity

\[ \mu_{s_{\text{dil}}} = \frac{5 \sqrt{\pi}}{96} \rho_p d_p \theta^{1/2} \]
• Fluctuating Energy Equation \( (\theta = \frac{1}{3} < C^2 >) \)

\[
\frac{3}{2} \left[ \frac{\partial}{\partial t} (\varepsilon_s \rho_s \theta) + \nabla \cdot (\varepsilon_s \rho_s \nu_s \theta) \right] =\tau_s : \nabla \nu_s - q - \gamma_s + \beta_A < C_g \cdot C_p > - 3\beta_A \theta
\]

- Collisional Energy Dissipation

\[
\gamma_s = 3\left(1 - e^2\right)\varepsilon_s^2 \rho_s g_o \theta \left(\frac{4}{d_s} \sqrt{\frac{\theta}{\pi}} - \nabla \cdot \nu_s\right)
\]

- Conductivity of Fluctuating Energy \( (q = -\kappa \nabla \theta) \)

\[
\kappa = \frac{2}{(1+e)g_o} \left[ 1 + \frac{6}{5} (1+e)g_o \varepsilon_s \right]^2 \kappa_{dil} + 2\varepsilon_s^2 \rho_s d_s g_o (1+e) \sqrt{\frac{\theta}{\pi}}
\]

- Dilute Phase (Eddy Type) Granular Conductivity

\[
\kappa_{dil} = \frac{75}{384} \sqrt{\pi \rho_s d_s \theta^{1/2}}
\]
• **Gas-Solid Drag Coefficients**

- Based on Ergun equation, for $\varepsilon_g < 0.8$

$$
\beta = 150 \frac{\varepsilon_s^2 \mu_g}{\varepsilon_g (d_p \phi_s)^2} + 1.75 \frac{\rho_g \varepsilon_s |v_g - v_s|}{d_p \phi_s}
$$

- Based on single sphere drag, for $\varepsilon_g > 0.8$

$$
\beta = \frac{3}{4} C_d \frac{\rho_g \varepsilon_s \varepsilon_g |v_g - v_s|}{d_p \phi_s} \varepsilon_g^{-2.65}
$$

where,

$$
C_d = \frac{24}{\text{Re}_p} \left[ 1 + 0.15 \text{Re}_p^{0.687} \right] \quad \text{for} \quad \text{Re}_p < 1000
$$

$$
C_d = 0.44 \quad \text{for} \quad \text{Re}_p > 1000
$$

$$
\text{Re}_p = \frac{\varepsilon_g \rho_g d_p |v_g - v_s|}{\mu_g}
$$
Wei et al. (1998) FCC riser

Jiradilok et al. (2006), Chem. Eng. Sci. 61, 5544-5559
COMPUTED ENERGY SPECTRUM COMPARED TO SINGLE PHASE TURBULENT FLOW

\[ \frac{\bar{v}_y E_y(n)}{v_y' n_\Lambda_f} \]

10
1
0.1
0.01
0.001

Wall Region
Central Region
Single Phase Flow

Energy Spectrum, \( E_y(n) \) m²s⁻¹

Gravity Wave
Energy Containing Range
Kolmogorov Range

Jiradilok et al. (2006), Chem. Eng. Sci. 61, 5544-5559
IIT riser with splash plate and fluidized downcomer to obtain high flux

Particle image velocity measurement system with probe and typical streak images captured by the CCD camera. (Gidaspow et al. (2004))
Due to particle oscillations, “laminar”

\[
D_{\text{Particles oscillations}} = \frac{\text{Granular Temperature}}{\text{Friction Coefficients}}
\]

For Brownian motion: \( D = \frac{RT}{\text{Avagadro number}} \times \frac{1}{\text{Friction Coefficient}} \)

Due to cluster or bubble, “turbulent”

\[
D_{\text{Turbulent}}(a) = \frac{v'(a)v'(a)T_L}{2} = \text{Turbulent} \times \frac{\text{Characteristic Kinetic energy}}{\text{Time}}
\]

where, \( \frac{v'(a)v'(a)}{2} \) Reynolds normal stress in x or y direction

\[
T_L = \int_0^\infty \frac{v'(t)v'(t+t')}{v'^2} dt'
\]

Lagrangian integral time scale

\[
T_L \approx T_E
\]

Eulerian integral time scale approximately equals Lagrangian integral time scale

Radial Gas Dispersion Coefficients

![Graph showing radial gas dispersion coefficients with data points and lines from various studies, such as Jiradilok et al., 2007 - Turbulent riser h = 2.0 m, 4.0 m, and 6.0 m, and This study - h = 3.5 m, 7.0 m, and 10.5 m. Other studies include Leckner et al., 2000, Wei et al., 2001, Werther et al., 1992, Rhodes et al., 1993, Leckner et al., 2002, Adamez et al., 1997.](image)
Axial Solids Dispersion Coefficients

![Graph showing axial solids dispersion coefficients against gas velocity. The graph includes data from various sources such as Du et al. (2002), Thiel and Potter (1978), Aviden and Yerushalmi (1985), Wei et al. (1995, 1998), Gidaspow et al. (2004), Jiradilok et al. (2006), and IIT Riser NETL unit, Cork particles, and FCC particles. The x-axis represents gas velocity (m/sec) ranging from 0.01 to 10, while the y-axis represents axial solids dispersion (m$^2$/sec) ranging from 0.001 to 100. The graph compares experimental and computational results for bubble and cluster computations.]
IIT 2-D FLUIDIZED BED
H = 69.85 cm

$U_g = 46.67 \text{ cm/s}$

$t = 1/250 \text{ s}$
Comparison of laminar and turbulent granular temperatures in IIT 2-D circulating fluidized bed and IIT riser

<table>
<thead>
<tr>
<th>System</th>
<th>Radial Position</th>
<th>Laminar due to individual particle oscillations</th>
<th>Turbulent due to cluster oscillations</th>
</tr>
</thead>
<tbody>
<tr>
<td>2-D CFB, 75 µm FCC particles</td>
<td>Center</td>
<td>1.27 x 10^{-2}</td>
<td>6.73 x 10^{-3}</td>
</tr>
<tr>
<td>2-D CFB, 75 µm FCC particles</td>
<td>Right Wall</td>
<td>6.67 x 10^{-3}</td>
<td>2.54 x 10^{-3}</td>
</tr>
<tr>
<td>IIT Riser, 1093 µm</td>
<td>Wall</td>
<td>9.48 x 10^{-2}</td>
<td>2.61 x 10^{-2}</td>
</tr>
</tbody>
</table>

Mixing is on the level of particles
GRANULAR TEMPERATURES

Gas Velocity (cm/sec) vs. Granular Temperature (cm$^2$/sec$^2$)

- 10 nm silica particles
- No bubbles
- No core-annular flow in IIT 2 story riser

IIT riser (1093 µm particles)
IIT 2-D bubbling bed (75 µm FCC)

- Gidaspow and Huilin (1996) 75 µm FCC
- Polasenski and Chen (1999) 74 µm FCC
- Cody et al. (1996) 70 µm FCC
- Jung (2003) 42 µm
- Tartan and Gidaspow (2004) 530 µm
- Cody et al. (1996) 420 µm
- Cody et al. (1996) 297 µm
- Jiradilok et al. (2005) 75 µm FCC
- Bubbling beds with a jet, 42 µm
  - This study, Experiment, IIT riser, Wall (1093 µm particles)
  - This study, Experiment, 2-D CFB, Right Wall (75 µm FCC)
  - This study, Experiment, 2-D CFB, Center (75 µm FCC)
  - Driscoll et al. (Riser) 10 nm (2006)
- Kashyap et al. (2008) 10 nm, 0.70 kV/cm
- Kashyap et al. (2008) 10 nm, 1.40 kV/cm
- Kashyap et al. (2008) 10 nm, 1.05 kV/cm

- Polasenski and Chen (1997) 94 µm FCC
- Cody et al. (1996) 63 µm
- Campbell and Wang (1991) 500 µm
- Polasenski and Chen (1997) 283 µm
- Jung (2003) 530 µm
- Bubbling beds, 530 µm
  - This study, Simulation, IIT riser, Wall (1093 µm particles)
  - This study, Experiment, 2-D CFB, Center (75 µm FCC)
  - Driscoll et al. (Riser) 10 nm (2006)
- Kashyap et al. (2008) 10 nm, 0 kV/cm
- Kashyap et al. (2008) 10 nm, 1.05 kV/cm

This study, Simulation, IIT riser, Wall (1093 µm particles)
This study, Experiment, 2-D CFB, Center (75 µm FCC)
Driscoll et al. (Riser) 10 nm (2006)
Kashyap et al. (2008) 10 nm, 0 kV/cm
Kashyap et al. (2008) 10 nm, 1.05 kV/cm
AXIAL SOLID DISPERSION COEFFICIENTS

Gas Velocity (m/sec)

Axial Solids Dispersion (m^2/sec)

- Fan et al. (2002)
- Thiel and Potter (1978)
- Aviden and Yerushalmi (1985)
- Wei et al. (1998)
- Wei et al. (1995)
- This study (Simulation, wall); 4.5 m; 14 m/s
- This study, IIT riser, 1093 µm
- This study, 2-D Bed, Center, 75 µm FCC
- This study, 2-D Bed, Right Wall, 75 µm FCC
- Experiment (laminar)
- Simulations (laminar)
- Experiment (turbulent)
- Simulations (turbulent)

IIT 2-D bubbling bed (75 µm FCC)

IIT riser (1093 µm particles)
OZONE DECOMPOSITION REACTION EXPERIMENTAL SETUP
Ozone decomposition reaction \( \rightarrow \)
\[
2O_{3(g)} \rightarrow 3O_{2(g)}
\]

Conservation of species equation in the code:
\[
\frac{\partial}{\partial t} (\varepsilon_g C_i) + \nabla \cdot (\varepsilon_g C_i v_i) = k_{\text{reaction}} \varepsilon_s C_i
\]

A one dimensional approximation leads to:
\[
v_y \varepsilon_g \frac{dC_{O_3}}{dY} = -KC_{O_3} \varepsilon_s
\]

where, “\( K \)” is the overall rate constant given by the additive resistance concept as
\[
\frac{1}{K} = \frac{1}{k_{\text{mass transfer}} a_v} + \frac{1}{k_{\text{reaction}}}
\]

Sherwood number,
\[
Sh = \frac{k_{\text{mass transfer}} d_p}{D}
\]
## PARTICLE CLUSTER DIAMETER

<table>
<thead>
<tr>
<th>Method</th>
<th>Height (m)</th>
<th>Minimum</th>
<th>Maximum</th>
<th>Averaged</th>
</tr>
</thead>
<tbody>
<tr>
<td>This study</td>
<td>3.5</td>
<td>0.0064</td>
<td>0.0232</td>
<td>0.0101</td>
</tr>
<tr>
<td></td>
<td>7.0</td>
<td>0.0040</td>
<td>0.0238</td>
<td>0.0095</td>
</tr>
<tr>
<td></td>
<td>10.5</td>
<td>0.0027</td>
<td>0.0150</td>
<td>0.0087</td>
</tr>
<tr>
<td></td>
<td>Averaged</td>
<td>0.0027^a</td>
<td>0.0238^b</td>
<td>0.0095</td>
</tr>
<tr>
<td>Harris's correlation</td>
<td>3.5</td>
<td>0.0033</td>
<td>0.0151</td>
<td>0.0092</td>
</tr>
<tr>
<td></td>
<td>7.0</td>
<td>0.0035</td>
<td>0.0149</td>
<td>0.0092</td>
</tr>
<tr>
<td></td>
<td>10.5</td>
<td>0.0034</td>
<td>0.0165</td>
<td>0.0099</td>
</tr>
<tr>
<td></td>
<td>Averaged</td>
<td>0.0033^a</td>
<td>0.0165^b</td>
<td>0.0095</td>
</tr>
<tr>
<td>Gu's correlation</td>
<td>3.5</td>
<td>0.0028</td>
<td>0.0154</td>
<td>0.0091</td>
</tr>
<tr>
<td></td>
<td>7.0</td>
<td>0.0030</td>
<td>0.0149</td>
<td>0.0089</td>
</tr>
<tr>
<td></td>
<td>10.5</td>
<td>0.0029</td>
<td>0.0175</td>
<td>0.0102</td>
</tr>
<tr>
<td></td>
<td>Averaged</td>
<td>0.0028^a</td>
<td>0.0175^b</td>
<td>0.0094</td>
</tr>
</tbody>
</table>

![Graph showing natural logarithm of time-averaged ozone molar concentration against riser height (m).](image)
EXAMPLE OF SHERWOOD NUMBER AND MASS TRANSFER COEFFICIENT

For PSRI riser Challenge Problem 1, overall mass transfer coefficient, $K = 30.81 \text{ s}^{-1}$

(Chalermsinsuwan, B., P. Piumsomboon, and D. Gidaspow, “Kinetic theory based computation of PSRI riser- Part II: Computation of mass transfer coefficient with chemical reaction”, Chemical Engineering Science, 64 (2009) 1212-1222)

The mass transfer coefficient is calculated from equation:

$$\frac{1}{K} = \frac{1}{k_{\text{mass transfer}} a_v} + \frac{1}{k_{\text{reaction}}}$$

With

$$d_p = 76 \times 10^{-6} \text{ m}$$

$$a_v = \frac{(3 \times 4\pi(\text{particle radius}^2))}{(4\pi(\text{particle radius}^3))} = \frac{3}{\text{particle radius}} = \frac{3}{(d_p/2)} = \frac{3}{((76 \times 10^{-6})/2)} = 78947.37 \text{ m}^{-1}$$

$$k_{\text{reaction}} = 39.60 \text{ s}^{-1}$$

Note that the overall resistance, $1/K$, and the reaction resistance, $1/k_{\text{reaction}}$, are close to each other. This implies that the mass transfer resistance is small.

Therefore, $k_{\text{mass transfer}} a_v = 138.71 \text{ s}^{-1}$ and $k_{\text{mass transfer}} = 0.0018 \text{ m/s}$

The Sherwood number is calculated from equation:

$$Sh = \frac{k_{\text{mass transfer}} d_p}{D}$$

With

$$D = 2.88 \times 10^{-5} \text{ m}^2/\text{s}$$

Therefore,

$$Sh = 0.0046$$
COMPUTATION OF MASS TRANSFER COEFFICIENTS

• Example: Simulation of PSRI riser with $k_{\text{reaction}} = 39.6 \text{ s}^{-1}$

Apparent low mass transfer coefficients in PSRI riser with $k_{\text{reaction}} = 39.6 \text{ s}^{-1}$

For $Sh = 0.0111$, $Sh_{\text{cluster}} = 1.46$
**EFFECTIVE RATE CONSTANT**

- $k_{\text{reaction}} = 14.45 \text{ sec}^{-1}$
- $K = 3.62 \text{ sec}^{-1}$
- $k_{\text{mass \, transfer}} = 0.0000611 \text{ m/s}$
- $Sh_{\text{(bubbling)}} = 0.00016$

**Differential reactor analysis**

\[

\nu_g \, \varepsilon_g \, \frac{dC}{dY} = -KC_{\text{average}} \, \varepsilon_s
\]

\[

U_g \, \frac{(C_2 - C_1)}{(Y_2 - Y_1)} = -K \, \frac{(C_1 + C_2)}{2} \left( \frac{\varepsilon_{s1} + \varepsilon_{s2}}{2} \right)
\]
CONCLUSIONS

We have shown that the kinetic theory based CFD codes correctly compute:

(1) Dispersion coefficients
(2) Mass transfer coefficients

Hence, the kinetic theory based CFD codes can be used for fluidized bed reactor design without any such inputs
FUTUREGEN: COAL GASIFIER FUEL CELL SYSTEM WITH CO₂ SEQUESTRATION

200 Mesh coal

Steam $H₂O$

Gasifier - MCFC

ANEODE

$H₂ + CO₂ \leftrightarrow H₂O + CO₂ + 2e^-$

$CO + CO₂ \leftrightarrow 2CO₂ + 2e^-$

MOLTEN SALT ELECTROLYTE 600 - 800 °C

CATHODE

$1/2O₂ + 2e^- + CO₂ \leftrightarrow CO₂^-$

CON DENSER

Liquid – Solid Separator (Cleaning Unit)

Electricity

Fuel Cell # 2

Boiler with heat from fuel cell # 2

Advantages over Futuregen

• No Oxygen plant
• Water is reused
• 70% electrical efficiency
FUTUREGEN: IDEAL GASIFIER FUEL CELL WITH CARBON FEED

**Gasifier - MCFC**

**ANODE**

\[ \text{H}_2 + \text{CO}_3^{2-} \leftrightarrow \text{H}_2\text{O} + \text{CO}_2 + 2e^- \]

\[ \text{CO} + \text{CO}_3^{2-} \leftrightarrow 2\text{CO}_2 + 2e^- \]

**CATHODE**

\[ \frac{1}{2} \text{O}_2 + 2e^- + \text{CO}_2 \leftrightarrow \text{CO}_3^{2-} \]

**CONDENSER**

- Liquid \( H_2O \)
- \( CO_2 \) Sequestration

**BOILER**

- Air at Ambient Temperature
- \( CO_2 \)
- Steam \( H_2O \)

**Electrical Power Generation**

Air at 600 - 800 °C

\[ \text{Air} \leftrightarrow \text{H}_2\text{O} + \text{CO}_2 \]

**Fuels & Products**

- Carbon
- \( CO_2 \)
- \( CO \)
- \( OH \)
- \( H_2 \)

**Conditions**

- 600 - 800 °C