Multiphase Interactions in Riser-Section of CFB: Towards Realistic Model for Analysis and Prediction

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Needed research efforts and issues

- **Hydrodynamics of fluidization**  
  - Its understanding is critical to design, scale-up and prediction – more so in riser reactors.  
  - How to maximize fluid-particle contact: steam/coal, air-$\text{O}_2$/coal, steam/oil, etc.

- **Segregation in riser-section**  
  - A real performance limitation. More effort is needed to provide concrete understanding of factors at play.  
  - How to deal with inherent poly-dispersed systems.
Known facts

- Riser hydrodynamics is complicated with a lot of unknowns
- Complex reactions kinetics: coal gasification, char combustion, cracking/coke-burning, etc.
- Complicated interconnections between riser and regenerator
- Many operating constraints.

(Han et al., 2000; Gururajan et al., 1992)
Mass transfer and reactions

- Optimizing useful reactions
  - Noting that hydrodynamics influences T & P distribution which provide some indication to efficiency of operation.
  - EVEN with the limitations, riser reactors are more efficient and handle more throughput than other types of reactors.

- Future goal: Environmentally benign energy production
  - Coal gasification route minimizes pollutants.
Flow regimes with increasing gas flow rate: dense to dilute flows (Hetsroni, 1982)

- **Particle fluidization** – rather uniform
- **Bubbling fluidization** – bubbles observed
- **Slugging flow** – large bubbles
- **Turbulent regime** – clusters move irregularly
- **Fast fluidization (riser)** – clusters move up tube and out with downward motion near wall

Note: There is a wealth of information on particle fluidization. Otherwise excellent data and results in a given flow regime can erroneously be used all across (for lack of filtered data)!
Where are we? A lot has been accomplished

- A full description of the fluid-particle processes in the fluidized state is at hand.
- OR at least the limitations of the results at hand are well understood.
- Significant advances in simulation tools and experimentation.
- BUT: realistic closure and constitutive equations remain a challenge. This includes need to understand particle kinetics in riser.
Taking inventory of governing equations – vector forms are fairly standard*

1. Mass balance (for each phase)
2. Momentum balance (for each phase)
3. Energy balance (for each phase)
4. Pseudo steady-state energy balance

*Gidaspow (1994; 2004); Bogere (1996); Jackson (2004) & many others

Region mixture balance: obtained when the balances for the two phases are added (providing a consistency-check – valuable during experimental stage).
\[
\frac{\partial}{\partial t} \left( \varepsilon_g \rho_g \right) + \nabla \cdot (\varepsilon_g \rho_g \mathbf{v}_g) - E^s_{im} - S^s_{im} = 0
\]

\[
\frac{\partial}{\partial t} \left( \varepsilon_s \rho_s \right) + \nabla \cdot (\varepsilon_s \rho_s \mathbf{v}_s) + E^s_{im} + S^s_{im} = 0
\]

\[
\frac{\partial}{\partial t} \left( \varepsilon_g \rho_g \mathbf{v}_g \right) + \nabla \cdot (\varepsilon_g \rho_g \mathbf{v}_g \mathbf{v}_g) = -\varepsilon_g \nabla P_g + \nabla \cdot \mathbf{\tau}_g - F^g_d + \varepsilon_g \rho_g g + E^s_{iM} + S^s_{iM}
\]

\[
\frac{\partial}{\partial t} \left( \varepsilon_s \rho_s \mathbf{v}_s \right) + \nabla \cdot (\varepsilon_s \rho_s \mathbf{v}_s \mathbf{v}_s) = -\varepsilon_s \nabla P_g + \nabla \cdot \mathbf{\tau}_s + F^g_d + \varepsilon_s (\rho_s - \rho_g) g - E^s_{iM} - S^s_{iM}
\]

\[F^g_d = \beta (\mathbf{v}_g - \mathbf{v}_s)\]

\[
\frac{3}{2} \left[ \frac{\partial}{\partial t} \left( \varepsilon_s \rho_s \theta \right) + \nabla \cdot (\varepsilon_s \rho_s \theta \mathbf{v}_s) \right] = \mathbf{\tau}_s : \nabla \mathbf{v}_s + \nabla \cdot (\kappa_s \nabla \theta) - \gamma_s
\]
Terms that require closure and material functions

- Fluid and solid phase stress tensors, fluid and solid pressure, fluid-drag, bulk solid viscosity, solid viscosity, granular conductivity, collisional energy dissipation, drag coefficient

- Excess terms accounting for mass and momentum exchange between the phases – should amount to something in coal gassification
To account for particle size distribution, additional balances and closure are needed

- Balances of the size moments are needed
- Balances of the mixed moments (first order with respect to the velocities)
- Closure schemes higher-order moments.
Problem at hand

- To simulate flow patterns of poly-dispersed systems in coal conversion processes: riser.
- This entails simulation of particle size distribution (PSD) evolution, when the particles change size or density due to heterogeneous reaction (e.g., coal conversion or gasification process).
- First we will need clear understanding of multiphase interactions in riser.
Setting the stage for specialization of the hydrodynamic model to some application

- Examine constitutive equations/closure for:
  - Particle-particle collisions;
  - Fluid-particle interactions;
  - Particle-wall interactions
  - Particle-particle segregation
  - Fluid flow behavior and description.

- Examine scales of analysis

- Flow regime specification
Interpretation of multiphase interactions


- Some assumptions are made but there has to be a mechanism to verify those assumptions – this is the tough part when experimental data is not forthcoming.
Functional dependence of constitutive and material functions

- Established using the well-known eight axioms of constitutive theory (Eringen, 1980).
- Kinetic theory is however firmly established as viable tool for its straight-forward approach (Gidaspow, 1994; others).
- In general constitutive and material functions are expressed in functional form (Bogere, 1996).
Independent variables

- Constitutive functions are in general expressed in terms of the set $C$ of independent variables.
- Material functions are dependent on the variables in the set $Z$.

$$C = \left\{ \rho_g, \varepsilon_g, \nabla \varepsilon_g, v_g, v_s, \theta_g, \nabla \theta_g, \omega_{ag}, \nabla \omega_{ag}, \mathbf{E}_s, d^g, s_g, \nabla s_g \right\}$$

$$Z = \left\{ \varepsilon_g, \theta_g, \omega_{1,g}, \ldots, \omega_{N-1,g}; \text{fluid properties, solid properties} \right\}$$
Need for focused experiments or mechanistic models with verifiable assumptions

- Measurement of: Temperature, pressure, pressure-drop distribution, velocity, mass fraction, porosity, porosity distribution, particle size, particle size distribution, etc.
- Characterization of coal: composition, etc.
- Prediction of hydrodynamics is dependent on having some form of data on internal profiles. Allows verification of assumptions & definition of realistic constraints.
Summary: Hydrodynamic model (Tartan & Gidaspow)

- Other reviews available in a number of works: Gidaspow (1994), Jackson (2000), Agrawal et al. (2001)
\[ \boldsymbol{\tau}_g = 2\varepsilon_g \mu_g \left\{ \frac{1}{2} \left[ \nabla \mathbf{v}_g + (\nabla \mathbf{v}_g)^T \right] - \frac{1}{3} (\nabla \cdot \mathbf{v}_g) \mathbf{I} \right\} \]

\[ \boldsymbol{\tau}_s = (-P_s + \xi_s \nabla \cdot \mathbf{v}_s) \mathbf{I} + 2\mu_s \left\{ \frac{1}{2} \left[ \nabla \mathbf{v}_s + (\nabla \mathbf{v}_s)^T \right] - \frac{1}{3} (\nabla \cdot \mathbf{v}_s) \mathbf{I} \right\} \]

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

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

\[ \mu_s = \frac{10\sqrt{\pi} \rho_s d_p \sqrt{\theta}}{96(1+e)g_o} \left[ 1 + \frac{4}{5}(1+e)g_o \varepsilon_s \right]^2 + \frac{4}{5} \varepsilon_s^2 \rho_s d_p (1+e)g_o \sqrt{\frac{\theta}{\pi}} \]

\[ \kappa_s = \frac{150\sqrt{\pi} \rho_s d_p \sqrt{\theta}}{384(1+e)g_o} \left[ 1 + \frac{6}{5}(1+e)g_o \varepsilon_s \right]^2 + \frac{2}{5} \varepsilon_s^2 \rho_s d_p (1+e)g_o \sqrt{\frac{\theta}{\pi}} \]

\[ \gamma_s = 3(1-e^2) \varepsilon_s^2 \rho_s g_o \theta \left( \frac{4}{d_p} \sqrt{\frac{\theta}{\pi}} - \nabla \cdot \mathbf{v}_s \right) \]
\[ \beta = \frac{3}{4} C_d \frac{\varepsilon_s \rho_g |v_g - v_s| \varepsilon^{-2.65} }{d_p \varepsilon_g} \rightarrow \varepsilon_g \geq 0.8 \]

\[ C_d = \frac{24}{\text{Re}_s} (1 + 0.15 \text{Re}^{0.687}_s) \rightarrow \text{Re}_s < 1000 \]

\[ C_d = 0.44 \rightarrow \text{Re} \geq 1000 \]

\[ \beta = 150 \frac{\varepsilon_s^2 \mu_g}{\varepsilon_g^2 d_p^2} + 1.75 \frac{\rho_g \varepsilon_s |v_g - v_s|}{d_p \varepsilon_g} \]

\[ E_{iM}, E_{iM}^s, S_{iM}^s, S_{iM}^s (\text{?}) \]
Conclusion

- Working on a review to include the excess terms to account for the effect of mass transfer between phases for coal gasification.
Questions