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-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).

$$\frac{\partial}{\partial t}\left(\varepsilon_g \rho_g\right) + \nabla \bullet \left(\varepsilon_g \rho_g \mathbf{v}_g\right) - E_{im}^s - S_{im}^s = 0$$

$$\frac{\partial}{\partial t}\left(\varepsilon_s \rho_s\right) + \nabla \bullet \left(\varepsilon_s \rho_s \mathbf{v}_s\right) + E_{im}^s + S_{im}^s = 0$$

$$\frac{\partial}{\partial t}\left(\varepsilon_g \rho_g \mathbf{v}_g\right) + \nabla \bullet \left(\varepsilon_g \rho_g \mathbf{v}_g \mathbf{v}_g\right) = -\varepsilon_g \nabla P_g + \nabla \bullet \boldsymbol{\tau}_g - F_d^g + \varepsilon_g \rho_g \mathbf{g} + E_{iM}^s + S_{iM}^s$$

$$\frac{\partial}{\partial t}\left(\varepsilon_s \rho_s \mathbf{v}_s\right) + \nabla \bullet \left(\varepsilon_s \rho_s \mathbf{v}_s \mathbf{v}_s\right) = -\varepsilon_s \nabla P_g + \nabla \bullet \boldsymbol{\tau}_s + F_d^g + \varepsilon_s \left(\rho_s - \rho_g\right)\mathbf{g} - E_{iM}^s - S_{iM}^s$$

$$F_d^g = \beta\left(\mathbf{v}_g - \mathbf{v}_s\right)$$

$$\frac{3}{2}\left[\frac{\partial}{\partial t}\left(\varepsilon_s \rho_s \theta\right) + \nabla \bullet \left(\varepsilon_s \rho_s \theta \mathbf{v}_s\right)\right] = \boldsymbol{\tau}_s : \nabla \mathbf{v}_s + \nabla \bullet \left(\kappa_s \nabla \theta\right) - \gamma_s$$

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

- A pattern for analysis of multiphase-multicomponent processes first introduced into fluidization work [by MN Bogere, *Chem. Eng. Sci.*, vol. 51, 4, 603,1996] is used to interpret the transport mechanisms in risers.
- 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.

$$\mathrm{C}=\left\{\begin{array}{l}\rho_g,\varepsilon_g,\nabla\varepsilon_g,v_g,v_s,\theta_g,\nabla\theta_g,\\ \omega_{ag},\nabla\omega_{ag},\underline{\underline{\mathrm{E}}}^s,\underline{\underline{d}}^g,s_g,\nabla s_g\end{array}\right\}$$

$$Z=\left\{\begin{array}{l}\varepsilon_g,\theta_g,\omega_{1,g},\ldots,\omega_{N-1,g};\\ \text{fluid properties,solid properties}\end{array}\right\}$$

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)

$$\boldsymbol{\tau}_g = 2\varepsilon_g\mu_g\left\{\frac{1}{2}\left[\nabla\mathbf{v}_g + \left(\nabla\mathbf{v}_g\right)^T\right] - \frac{1}{3}\left(\nabla\bullet\mathbf{v}_g\right)\mathbf{I}\right\}$$

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

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

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

$$\mu_s = \frac{10\sqrt{\pi}\rho_s d_p\sqrt{\theta}}{96(1+e)g_o}\left[1 + \frac{4}{5}(1+e)g_0\varepsilon_s\right]^2 + \frac{4}{5}\varepsilon_s^2\rho_s d_p(1+e)g_o\sqrt{\frac{\theta}{\pi}}$$

$$\kappa_s = \frac{150\sqrt{\pi}\rho_s d_p\sqrt{\theta}}{384(1+e)g_o}\left[1 + \frac{6}{5}(1+e)g_0\varepsilon_s\right]^2 + 2\varepsilon_s^2\rho_s d_p(1+e)g_o\sqrt{\frac{\theta}{\pi}}$$

$$\gamma_s = 3(1-e^2)\varepsilon_s^2\rho_s g_o\theta\left(\frac{4}{d_p}\sqrt{\frac{\theta}{\pi}} - \nabla\bullet\mathbf{v}_s\right)$$

$$\beta = \frac{3}{4} C_d \frac{\varepsilon_s \rho_g \left| \mathbf{v}_g - \mathbf{v}_s \right|}{d_p} \varepsilon_g^{-2.65} \rightarrow \varepsilon_g \geq 0.8$$

$$C_d = \frac{24}{\mathrm{Re}_s} (1 + 0.15 \, \mathrm{Re}_s^{0.687}) \rightarrow \mathrm{Re}_s < 1000$$

$$C_d = 0.44 \rightarrow \mathrm{Re} \geq 1000$$

$$\beta = 150 \frac{\varepsilon_s^2 \mu_g}{\varepsilon_g^2 d_p^2} + 1.75 \frac{\rho_g \varepsilon_s \left| \mathbf{v}_g - \mathbf{v}_s \right|}{d_p \varepsilon_g} \rightarrow \varepsilon_g < 0.8$$

$E_{im}^s, E_{iM}^s, S_{im}^s, S_{iM}^s$ (?)

Conclusion

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

Questions