Title: **GASIFICATION TRANSPORT: A MULTIPHASE CFD APPROACH & MEASUREMENTS**

Author(s): Dimitri Gidaspow and Veerya Jiradilok
Ph.D. student: Jing Huang
Illinois Institute of Technology
Chemical & Environmental Engineering Department
10 West 33rd Street
Chicago, IL 60616
Tel 312-567-3045
Fax 312-567-8874
Email : gidaspow@iit.edu
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ABSTRACT

OBJECTIVE

Dispersion and mass transfer coefficients needed for design of improved gasifiers for the Future Gen project to produce hydrogen from U.S. coals with sequestration of carbon dioxide are known to differ by more than five orders of magnitude. The objective of this project is to develop predictive theories for the dispersion and mass transfer coefficients and to measure them in the turbulent fluidization regime, using existing facilities. The new theories and correlations will be used in kinetic theory based CFD codes, such as the M-FIX code and in simpler non-hydrodynamic codes, with dispersion coefficients as an input, to design better gasifiers. In the past, we used our CFD code to model almost all gas-solid fluidization regimes, with particles as small as ten nanometers to rocks, as for example, found in the explosive eruption of volcanoes.(Gidaspow et al., 2004)

ACCOMPLISHMENTS TO DATE

The dispersion coefficient is a measure of the quality of mixing. We have identified two types of solids dispersion coefficients: those due to random particle oscillations, "laminar" type, and those due to cluster or bubble motion, "turbulent" type. It is an experimental fact that the radial dispersion coefficients are much smaller than those in the direction of flow. At IIT, we have developed an experimental particle image velocity technique that measures particle and Reynolds stresses. From the measured stresses, we can estimate the radial and axial "laminar" and "turbulent" dispersion coefficients.(Gidaspow et al., 2004 and Jiradilok et al., 2006) We have also developed a method of computing these dispersion coefficients based on the standard kinetic theory model in the turbulent regime of FCC particles in a riser.

The turbulent fluidization regime is characterized by the co-existence of a dense, bottom region and a dilute, top bed. A kinetic theory based CFD code with a drag corrected for clusters captured the basic features of this flow regime: the dilute and dense regions, high dispersion coefficients and a strong anisotropy. The computed energy spectrum captures the observed gravity wave and the Kolmogorov –5/3 law at high frequencies. The computed turbulent kinetic energy is close to the measurements for FCC particles. The CFD simulations compared reasonably well with the measured core-annular flow experiments at very high solid fluxes. The computed granular temperatures, solids pressures, FCC viscosities and frequencies of oscillations were close to measurements reported in the literature. The computations suggest that unlike for

the flow of group B particles, the oscillations for the FCC particles in the center of the riser are primarily due to the oscillations of clusters and not due to oscillations of individual particles. Hence mixing is not on the level of individual particles. (Jiradilok et al., 2006)

Since the beginning of the project in March 2006 we have extended the Jiradilok et al (2006) study to the computation of gas dispersion coefficients. The radial and axial gas dispersion coefficients were found to be very close to the solid dispersion coefficients in dense turbulent fluidization regime. We have also compared the dispersion coefficients to the literature survey by Ronald Breault of NETL, DOE, Powder Technology in press 2006. We are in the process of explaining the five orders of magnitude difference in dispersion coefficients.

FUTURE WORK

We plan to write a joint paper with Ronald Breault of NETL by July of this year explaining the five-orders of magnitude difference in dispersion coefficients.

In 2006, we plan to measure velocities and stresses of FCC particles in the IIT riser and compare the measurements to CFD simulations. Next we plan to measure dispersion coefficients in the IIT riser and compare the dispersion coefficients to kinetic theory model CFD calculations. We also plan to compare the dispersion coefficients measured at NETL to our hydrodynamic calculations.

LIST OF PAPERS

1. Gidaspow, D., J. Jonghwun and R.K. Singh, “Hydrodynamics of Fluidization using Kinetic Theory: an Emerging Paradigm 2002 Flour-Daniel Lecture,” *Powder Technology*, **148**, 123 (2004).
2. Jiradilok, V., D. Gidaspow, S. Damronglerd, W.J. Koves, and R. Mostofi, “Kinetic Theory Based CFD Simulation Turbulent Fluidization of FCC Particles in a Riser” *Chemical Engineering Science,* in press