Title: GASIFICATION TRANSPORT: A MULTIPHASE CFD APPROACH & MEASUREMENTS

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ABSTRACT

OBJECTIVE

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. A second objective is to use our multiphase CFD tools to suggest optimized gasifier designs consistent with aims of Future Gen.

ACCOMPLISHMENTS TO DATE

• Dispersion coefficients

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. A literature review shows that dispersion coefficients in fluidized beds differ by more than five orders of magnitude. To understand the phenomena, two types of hydrodynamics models that compute turbulent and bubbling behavior were used to estimate radial and axial gas and solids dispersion coefficients. The autocorrelation technique was used to compute the dispersion coefficients from the respective computed turbulent gas and particle velocities.

The computations show that the gas and the solids dispersion coefficients are close to each other in agreement with measurements. The simulations show that the radial dispersion coefficients in the riser are two to three orders of magnitude lower that the axial dispersion coefficients, but less than an order of magnitude lower for the bubbling bed at atmospheric pressure. The dispersion coefficients for the bubbling bed at 25 atmospheres are much higher than at atmospheric pressure due to the high bed expansion with smaller bubbles. The computed dispersion coefficients are in reasonable agreement with the experimental measurements reported over the last half century and those measured at IIT and in the NETL riser in Morgantown (Jiradilok et al., 2007, 2008).

• Optimized gasifier designs (Gasifier – fuel cell)

For carbon capture fossil fuel electric power generation plants will have to be made more efficient. Department of Energy vision 21 concept involves coal gasification with oxygen in an entrained flow gasifier and electricity production using solid oxide fuel cells and gas turbines. The use of oxygen to supply the heat necessary for the endothermic carbon – steam reaction requires an additional 34 % moles of carbon per mole of steam. Half a century ago it was suggested that this heat can be supplied by the fuel cells. Such a concept is similar to the megawatt molten carbonate fuel cell power plants commercialized by Fuel Cell Energy, Inc. in which natural gas is internally reformed with steam, with an efficiency of larger than 50 percent and battery life of over one year.

Such a new concept for production of electricity from coal using molten carbonate fuel cells is proposed. It involves feeding fine coal particles with steam into the anode compartment of the fuel cell in which the waste heat from the fuel cell is used to produce synthesis gas which reacts electrochemically. The overall reaction is carbon plus oxygen yields carbon dioxide. Hence the reversible efficiency of this process is near 100 percent, as in the direct carbon fuel cell. The gaseous product is carbon dioxide with impurities which can be scrubbed to produce carbon dioxide for sequestration. The impurities from coal in the bubbling gasifier-fuel cell, ash and sulfur, can be potentially removed by re-circulating the electrolyte, cleaning the electrodes with pulses of steam and by filtering the electrolyte.

The computed efficiency for power generation is of the order of 70% of the enthalpy of carbon combustion (Gidaspow and Jiradilok, 2007a, 2007b).

- **Mass transfer coefficients**

It was known for half a century that the Sherwood and Nusselt numbers in fluidized beds are often three orders of magnitude lower than the classical diffusion controlled limit of two. We have shown (Chalermsinsuwan et al., 2008a, 2008b) that our kinetic theory based computer codes correctly compute low Sherwood numbers in agreement with published experimental data. For tall fluidized bed risers the computed behavior is similar to that for convective diffusion in a channel, but with a greatly reduced mass transfer. The Sherwood numbers are low due to formation of clusters, consistent with our measurements of granular temperature.

FUTURE WORK

We plan to measure mass transfer coefficients with ozone decomposition in our two dimensional bubbling fluidized bed and in our riser at IIT. We also plan to compute the low mass transfer coefficients in our bubbling bed.

LIST OF PAPERS

1. Jiradilok, V., D. Gidaspow, and R.W. Breault, "Computation of gas of solids dispersion coefficients in turbulent risers and bubbling beds," Chemical Engineering Science 62 (2007) 3397-3409

2. Gidaspow, D. and V. Jiradilok, "Nanoparticle gasifier fuel cell for sustainable energy future," Journal of Power Sources 166 (2007a) 400-410

3. Jiradilok, V., D. Gidaspow, R.W. Breault, L.J. Shadle, C. Gunther, and S. Shi, "Computation of turbulence and dispersion of cork in the NETL riser", Chemical Engineering Science 63 (2008) 2135-2148

4. Gidaspow, D. and V. Jiradilok, "Efficient Coal Gasifier-Fuel Cell with CO_2 Sequestration," The Clearwater Coal Conference, The 32nd International Technical Conference on Coal Utilization & Fuel Systems, Clearwater, Florida, U.S.A. June 13, 2007b

5. Chalermsinsuwan, B., P. Piumsomboon, and D. Gidaspow, "Kinetic theory based computation of PSRI riser- Part I: Estimate of mass transfer coefficient", Submitted for publication in Chemical Engineering Science, 2008a

6. Chalermsinsuwan, B., P. Piumsomboon, and D. Gidaspow, "Kinetic theory based computation of PSRI riser- Part II: Computation of mass transfer coefficient with chemical reaction", Submitted for publication in Chemical Engineering Science, 2008b

STUDENTS

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