Title: GASIFICATION TRANSPORT: A MULTIPHASE CFD APPROACH & MEASUREMENTS

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Grant Number: DE-FG26-06NT42736
Performance Period: 2/15/06 – 2/14/09

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. A joint paper with Ronald Breault of NETL explaining the five-orders of magnitude difference in dispersion coefficients was accepted for publication in Chemical Engineering Science.

We are completing a second paper "Simulations of the NETL Morgantown riser cork data" on the comparison of the dispersion coefficients measured at NETL to our hydrodynamic calculations. We are measuring velocities, stresses and dispersion coefficients of FCC particles in the IIT riser.

- **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 per cent 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 per cent, 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.

This concept was illustrated using carbon nanoparticles as the fuel, in a paper available online in the Journal of Power Sources by Gidaspow and Jiradilok (2007). The nanoparticle gasifier-fuel cell computational fluid dynamics CFD modeling was now extended to gasification of 200 mesh carbon particles using a kinetic theory based bubbling bed model. Concentration, temperature and current density profiles have been computed. The computed efficiency for power generation is of the order of 70% of the enthalpy of carbon combustion. The details will be presented at the Clearwater Coal Conference, June 13, 2007.

FUTURE WORK

We plan to compare our measurements to the simulations of velocities, stresses and dispersion coefficients of FCC particles in the IIT fluidized bed.

We also plan to measure the dispersion coefficients at NETL and to compare them to the CFD calculations.

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," Accepted for publication in Chemical Engineering Science
2. Gidaspow D. and V. Jiradilok, "Nanoparticle gasifier fuel cell for sustainable energy future," Article in press in Journal of Power Sources, 2007
3. Jiradilok, V., D. Gidaspow, R.W. Breault, and L.J. Shadle, "Simulations of the NETL Morgantown riser cork data," Paper under review.
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, 2007

LIST OF PATENTS

1. D. Gidaspow, Nanoparticle gasifier fuel cell: Patent application, Illinois Institute of Technology, September 2006.

STUDENTS

Ph.D. candidates: Mayank Kashyap and Jing Huang