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Simulation of Coal Gasification in a Fluidized Bed

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Many commercial processes for fossil fuel conversion are currently based on fluidized-bed technology. There has been extensive development of "bubbling" fluidized-bed coal combustors and gasifiers, both atmospheric and pressurized. Recently, the use of circulating fluidized bed coal combustors has rapidly expanded (Basu and Fraser, 1991). These boilers have several advantages over more conventional technology: fuel flexibility, high combustion efficiency, high heat release rate, good load-following capabilities, efficient SO_2 capture, and low NO_x emissions. Advanced "clean coal" concepts, such as Integrated Gasification and Combined Cycle, incorporate fluidized reactors for coal gasification and/or sulfur capture. Fluidized "risers" are used universally in petroleum refineries for many purposes, primarily, the catalytic cracking of the heavy oil fraction (Squires, 1986; Avidan, Edwards, and Owens, 1990).

Most mathematical descriptions of fluidized beds are based on semi-empirical equations, usually related to the "two-phase" theory of fluidization (see, e.g., Davidson Clift and Harrison, 1985; Manno and Reitsma, 1990; Olofsson, 1980). In this context, "phase" refers to the spatially separate "bubble phase" or "emulsion phase." The motion of the bubbles through the emulsion, their frequency, size, etc., and the exchange of gas between the bubbles and the emulsion are represented by correlations. These concepts have been extended to describe fluidized beds combustors (Grace, 1986). In this literature, the meaning of the word "phase" is very different from the jargon of the present theory, in which the fluid and the granular material are represented as interpenetrating "phases".

These equations also differ from the equations which are the basis for computer codes currently used for the modeling of entrained coal gasifiers and combustors (Smith, Fletcher and Smoot, 1980; Hill and Smoot, 1993), in which the motion of the particles is described in a Lagrangian sense; such codes are only appropriate for the description of lightly loaded reactors. In fluidized beds, the particles can occupy over half the volume, locally, and the particle interactions dominate the rheology of the mixture.

In this analysis of coal gasification, a more fundamental approach is used. A set of multiphase (Eulerian) fluid dynamic equations, obtained either by a suitable averaging technique (Anderson and Jackson, 1976; Drew, 1971) or the formulations of continuum mechanics (Drew, 1983), is used to describe the conservation of mass, momentum, and energy for three interpenetrating phases. The particles, like the fluidizing gas, are described as interpenetrating continua. Different particle types are treated as distinct phases; in this study, the feed coal and the bed char are represented as seperate phases in order to account for their different histories. Constitutive laws account for the exchange of momentum between phases ("drag") and interphase energy transfer. The stresses within the granular phases are determined by a formulation based on the kinetic theory, characterized by a "granular temperature". A computer code, based on this multiphase hydrodynamic model, has been developed at the Morgantown Energy Technology Center (METC) for the detailed simulation of gas and particle dynamics in heavily loaded coal conversion processes (Syamlal, Rogers, O'Brien, 1994; Syamlal, 1995).

In these simulations, three phases were included: a gas phase with eight species (O_2, CO, CO_2, CH_4, H_2, H_2O, N_2, Tar) and two solids phases (fresh feed coal and reacted bed char) each composed of pseudo-species (Fixed Carbon, Volatile Matter, Moisture, Ash, and Sorbent). The reaction scheme allows: the vaporization of H_2O; transformation of the volatile matter to fixed carbon and light gases (CO_2, CO, CH_4, H_2) plus tar; subsequent decomposition of the tar to light gases and fixed carbon; and (reversible) oxidation/gasification of the fixed carbon by O_2, CO_2, H_2O, H_2. In order to account for the total production of CO_2 and the correct heat balance, the granular phases were also assumed to contain sorbent, $CaCO_3$ and $CaMg(CO_3)_2$. Reactions were included to describe formation of CaO and MgO, with the release of CO_2. No attempt was made to include sulphur chemistry.

Gas phase reactions were included to allow the combustion of CO, CH_4, and H_2 to CO_2 and H_2O. The evolved tar could kinetically convert to CO, CH_4, H_2 (which can further combust), CO_2 and fixed carbon. Also, the water-gas equilibrium is imposed: $CO + H_2O \Leftrightarrow CO_2 + H_2$. These reactions are summarized in Figure 1.

Under normal operating conditions, a bed of char would accumulate by conversion of feed coal or some light-off procedure. However, simulation of this build-up would require too much computational time. However, the history of the fresh feed coal is quite distinct from that of the bed char. In order to simulate this quasi-steady situation in a reasonable calculation, the initial condition specified a bed of a second granular phase, char at the nominal operating condition, whose composition corresponded to that of the devolatilized, calcined feed coal. A psuedo-reaction was introduced which, after a long time, "converted" the feed coal phase into the char phase.

The hydrodynamic simulation showed the reactor operated in a jetting/bubbling mode. A gas jet penetrated a considerable distance into the bed, and then detached as "bubbles" which rose

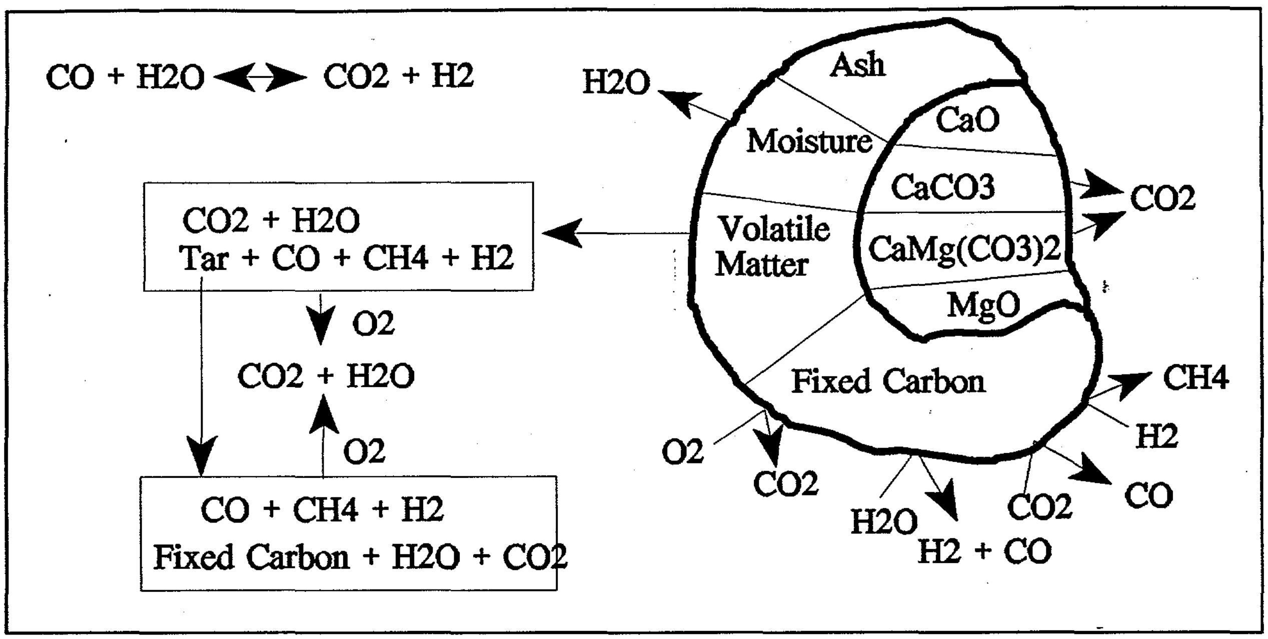

Figure 1

to the top of the column. The reaction scheme indicated that the feed coal did not begin to devolatilize until it had traversed this region, because of the time required to heat up. Thus, volatiles were not released in the jetting region of the bed, but higher in the bed. The oxygen fed with the coal, however, reacted immediately with the recirculating hot char. The net effect of the char reaction scheme was to create CO, which burned in the region where the jet detached, creating a fairly stable "flame". The tar reaction scheme indicated that none of the tar escaped the bed.

Anderson, T.B. and R.G. Jackson, "A Fluid Mechanical Description of Fluidized Beds", *Industrial and Engineering Chemistry Fundamentals*, **6**, No.4, 527-539, 1967.

Avidan, A. A., M. Edwards, and H. Owens, "Innovative Improvements Highlight FCC's Past and Future," *Oil and Gas J.*, **88**, 33-58, 1990.

Basu, P., and S. A. Fraser, Circulating Fluidized Bed Boilers: Design and Operations, Butterworth-Heinemann, Boston, 1991.

Davidson, J.F., R. Clift, and D. Harrison, editors, Fluidization, 2nd ed., Academic Press, London, 1985.

Drew, D.A., "Continuum Modeling of Two-Phase Flows," in Theory of Dispersed Multiphase Flow, ed. R.E. Meyer, Academic Press, New York, 173-190, 1983.

Drew, D.A. and L.A. Segel, "Averaged Equation for Two-Phase Flows", *Studies in Appl. Math*, **50**, 205, 1971.

Grace, J.R., "Modelling and Simulation of Two-Phase Fluidized Bed Reactors," Chemical Reactor Design and Technology, ed. H.I. de Lasa, Martinus Nijhoff Publishers, Dordrecht, 245-289, 1986.

Hill, S.C., and L.D. Smoot, "A Comprehensive Three-Dimensional Model for Simulation of Combustion Systems: PCGC-3," *Energy and Fuels*, **7**, 874-883, 1993.

Manno, V. P., and S.H. Reitsma, "An Annotated Bibliography of Fluidized Bed Combustion Modeling Information," *Powder Technology*, **63**, 23-34, 1990.

Olofsson, J. Mathematical Modelling of Fluidised Bed Combustors, IEA/ICTIS/TR-14, IEA Coal Research, London, November, 1980.

Smith, P.J., T.H. Fletcher, and L.D. Smoot, "Model for Coal-Fired Reactors," Eighteenth Symposium (International) on Combustion, The Combustion Institute, Pittsburgh, PA, 1285, 1980.

Squires, A.M., "The Story of Fluid Catalytic Cracking," in Circulating Fluidized Bed Technology, ed. P. Basu, 1-19, Pergamon Press, Toronto, 1986.

Syamlal, M., W. Rogers, T. J. O'Brien, "MFIX Documentation: Theory Guide," DOE/METC-94/1004 (DE94000087), 1994.

Syamlal, M., "MFIX Documentation: User's Manual," DOE/METC-95/1013 (DE95000031), 1995.