Annual Report for the School of Energy Resources – GA Program

A New Concept for the Gasification of Wyoming Coal

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1. Background of the original proposal

Wyoming produces 36% of US coal, most of which is burned in pulverized coal boilers to produce electricity. As a result, Wyoming coal is used to generate about 20% of the United States' electrical output. This coal is sold at fuel value, minus transportation cost, resulting in a relatively low economic value because the majority of the coal is shipped out of state. Higher value products from the coal could be produced through gasification to make a synthesis gas composed of carbon monoxide and hydrogen, followed by conversion to liquid fuels or chemical products, which would result in much higher economic values for the state. Unfortunately, most coal gasification plants are designed for operation at altitudes near sea level and are less efficient at elevations near the coal mines in Wyoming. Current gasifiers are also designed for use with higher rank coals, mostly mined in the Eastern US. General Electric and the University of Wyoming are therefore designing a gasifier to operate at high altitudes (above 4000 feet) and with Wyoming coals. The gasifier design is unique for several reasons. The operation is once-through, meaning no recycle of ungasified char and coal is required, which reduces the size and complexity of the gasifier. Further, the fluidized reactor bed has reactant injection along the length of the bed, which reduces hot spots that occur when reactant injection is done at one location in the bed. This design permits use of lower cost materials of construction and allows a modular design for ease of maintenance. Finally, the air compressors required to pressurize and operate the gasifier will be based on aircraft gas turbines that are designed to operate at high altitudes, which should be easily modified for efficient operation at any elevation in Wyoming. However, many aspects of the design are unproven. The kinetics of Powder River Basin and other subbituminous Wyoming coals for gasification have not been studied in detail. Further, the variable density fluidized bed, with reactions that decrease particle sizes, is a challenging design that has not been modeled. Therefore, a significant modeling effort of the chemically reacting flow in the fluid bed is required to properly design the reactor vessel.

The fast progress in computer technology enables detailed simulations of such complicated processes as coal gasification [1]. Numerical simulations can help to avoid the development of expensive prototypes in the design phase, and they offer distinct advantages over experiments in the optimization of processes. With the exception of natural gas, fossil fuels are found either in the liquid or solid phase. Thus, accurate predictive simulation tools for two-phase turbulent reactive flows are a key element in the development and improvement of gasification devices.

2. Specific goals of the work

Phase 1 (6 months): Extension of the single-phase combustion model to two phase flows
In the first phase we will extend the existing stochastic single-phase combustion model to turbulent reacting two-phase flows [2]. This extension will account for the nontrivial interaction of the solid particles with gas-phase flow. In addition to that, one needs to model the changing particle mass, chemical composition and temperature to account for the conversion of the coal particles into gas (pyrolysis). It is worth emphasizing that the new stochastic model for turbulent reactive two-phase flows can be used for a wide class of technical applications ranging from coal gasification to liquid spray-combustion in combustion chambers. The model will be implemented in FLUENT.

Phase 2 (6 months): Wyoming coal chemistry modeling
In the second phase the model developed in phase 1 will be combined with appropriate chemical kinetics of the solid and gas phase to simulate the Wyoming coal gasification. The chemical kinetics for the Wyoming coal will be developed by Professor D.A. Bell and Professor M. Argyle on the basis of previous work and new measurements. Furthermore, numerical simulations of an already existing pilot-scale gasifier at the Western Research Institute (WRI) will be performed by using the Wyoming coal chemistry. These simulation results will be compared to experimental data of the synthesis gas composition to asses the quality of the chemical kinetics modeling.

Phase 3 (6 months): Design study of the GE/UW gasifier concept

In the third phase the design parameters of the GE/UW industrial-scale gasifier will be studied. The models developed in phases 1 and 2 will be used for numerical simulations of a preliminary design of the GE/UW gasifier. In a close collaboration with Professor M. Argyle, a detailed analysis of the simulation results will be used to verify and improve the conceptual design of the GE/UW gasifier.

Phase 4 (6 months): Optimization of the GE/UW gasifier

Once the conceptual design has been verified in phase 3, the geometry and operating conditions of the GE/UW industrial-scale gasifier will be optimized by means of numerical simulations. In particular, the CO/H_2 ratio of the synthesis gas will be optimized to increase the economic efficiency. To optimize this ratio, the controlling parameters have to be identified. Among others, these parameters may include the size of the coal particles, the operating temperature, and the coal/steam plus oxygen ratio. Simulations of the GE/UW gasifier operation will be used to determine the controlling parameters and to find optimal parameter values. Economic constraints will be included in the optimization.

3. Results

The gasification and combustion of coal involves a large number of complex physical and chemical processes. The development of a comprehensive simulation tool has to be done stepwise to correctly account for all processes. In each step the simulation predictions have to be validated against accurate experimental data. In a first step, we have extended our existing model for turbulent reactive single-phase flow to a model for dispersed two-phase flows. In dispersed two phase flows the volume occupied by the second phase (solid coal particles) is small compared to the volume occupied by the gas. This means that the solid particles affect the flow of the gas only weakly. Dispersed two phase flow conditions are found in entrained flow coal gasification and combustion reactors. In the next step, we have considered flow conditions in which the gas and solid phase occupy comparable fractions of the volume. Such flow conditions are called granular flows. In granular flows the gas velocity is strongly modified by the solid particles, this means there is a tight coupling between the gas phase and the solid phase. Mathematical modeling of granular flows is therefore more challenging than the modeling of dispersed phase flow conditions. Granular flow conditions are found in fluidized bed coal gasification facilities.

Evaluation of the dispersed phase model: Detailed experimental data sets which can be used for numerical model evaluations are limited to pulverized coal combustion in laboratory scale combustors [3]. The underlying physico-chemical processes in coal combustion and gasification are very similar [4]. Therefore, we have chosen an experimental data set of pulverized coal combustion for the model validation. The measurements have been performed in the Controlled Profile Reactor (CPR) at the Brigham Young University [3]. The CPR is a 0.5 MW, cylindrical, down-fired reactor with an internal diameter of 80 cm and a length of 240 cm. The significant features of the gaseous flow field are illustrated with the gaseous flow streamlines and temperature field predictions in figure 1. A large recirculation zone develops away from the centerline which stabilizes the flame. The simulation results are generally in good agreement with the measurements.

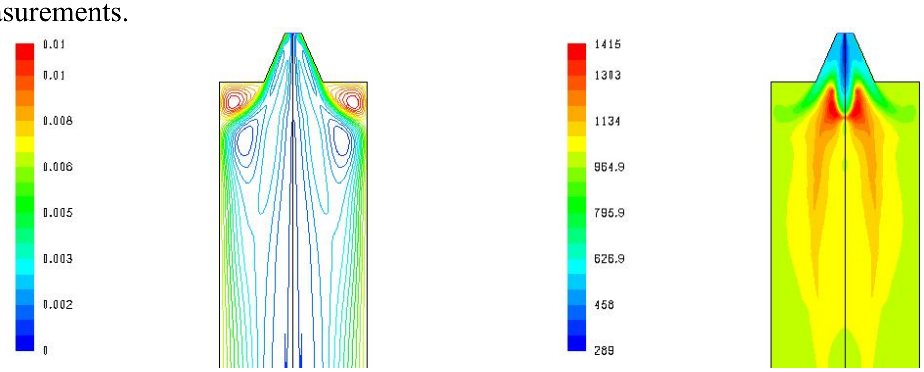

Figure 1: Velocity stream function (left) in kg/s and temperature contours in K (right).

Evaluation of the granular flow model: To validate the granular flow model we have simulated the riser section of a circulating fluidized bed (CFB) and compared the results with available measurements [5]. The CFB has a height of 14 m and diameter of 0.2 m. The solid particles have a diameter of 76 μm and a density of 1712 kg/m^3. Figure 2 (left) shows the solid volume fraction and the gas velocity vectors near the solid inlet after four seconds of flow time. The solid density is high near the wall and more dilute at the center of the riser where high values of the axial gas velocity can be observed. A comparison between the calculated time-averaged solid mass flux with the experimental data at a height of 3.9 m is shown on the left-hand side of figure 2. The computational results agree reasonably with the experimental data.

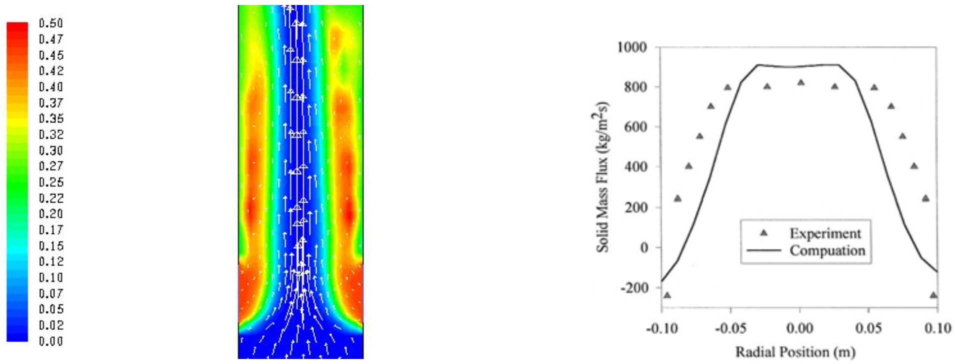

Figure 2: Volume fraction of the solid phase in the CFB (left) and comparison between the calculated and measured solid mass flux in kg/s (right).

4. Next steps

The new GE/UW-gasifier concept proposed by J. Ackerman of General Electric (GE) and UW Professor M. Argyle is based on fluidized bed conditions. The novel concept includes a variable fluidized bed density, coal particle injection along the length of the bed and a once-through operation. Due to the novelty of this gasification concept there are no empirical relations available that could help in determining the geometry and operating conditions of a laboratory scale prototype. Therefore, we will use the model for granular two-phase flow to find the dimensions and operating conditions for a laboratory scale prototype of the new gasification concept. The work will be done in a close collaboration with Professor M. Argyle. The up-scaling of the new gasifier design to an industrial scale will also be done based on numerical simulations.

5. Students supported by the grant

The grant supports UW-Mathematics Ph.D. student Michael Stoellinger who performed the model development and simulations. The student has earned 50 credit hours so far and maintained a GPA of 3.73. He has passed two out of three Qualifying Exams at the Ph.D level.

References:

1. C. Chen, M. Horio and T. Kojima, "Numerical Simulation of Entrained Flow Coal Gasifier. Part I: Modeling of Coal Gasification in an Entrained Flow Gasifier", Chemical Engin. Science 55, 3861-3874 (2000).
2. J.-P. Minier and E. Peirano, "The PDF Approach to Turbulent Polydispersed Two-phase Flows", Physics Reports 352, 1-214 (2001).
3. A.M. Eaton, L.D. Smoot, S.C. Hill and C.N. Eatough, "Components, Formulations, Solutions, Evaluations, and Application of Comprehensive Combustion Models", Prog. Energy Comb. Science 25, 387-436 (1999).
4. L. D. Smoot and P.J. Smith, "Coal Combustion and Gasification", Plenum, New York, 1985.
5. T. Knowlton, D. Geldart, J. Matsen and D. King, "Comparison of CFB Hydrodynamic Models", PSRI Challenge Problem Presented at the Eight International Fluidization Conference, Tour, France, May 1995.