Annual Report for the School of Energy Resources – GA Program 2009

A New Concept for the Gasification of Wyoming Coal

Associate Professor Dr. Stefan Heinz
Ph.D Student Michael Stoellinger
University of Wyoming, Department of Mathematics

1. Background of the original proposal

Wyoming produces 36% of US coal, most of which is burned in pulverized coal boilers to produce electricity. 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.

J. Ackerman (General Electric) and UW Professor M. Argyle (Chemical and Petroleum Engineering Department) have recently suggested a revolutionary design concept for coal gasification especially suited for Wyoming coal and operation at higher elevations. The use of this concept for the gasification of Wyoming coal involves the design and construction of different gasifiers. First, a cheap laboratory-scale gasifier will be constructed to study the advantages of the new concept without large economic risks. Second, the laboratory-scale gasifier will be up-scaled to a industrial-scale gasifier that will allow an economic operation. Up-scaling means here to increase the laboratory-scale gasifier by a factor of about ten.

Numerical simulations can contribute significantly to the optimal design of the UW coal gasification [1] project. Computational studies of the effects of variations of the geometry of gasifiers, variations of operating conditions and up-scaling effects are much more efficient than corresponding experimental investigations.

2. Specific goals of the work

Phase 1: Development of a computational model for coal gasification

We will develop a computational model for coal gasification that accurately describes the complex multiphase flow conditions which are found in coal gasifiers. In addition, the model will describe the involved chemical processes such as devolatilization (release of gaseous compounds) of the coal, the heterogeneous chemical reactions between the coal char and the gasifying agent as well as the homogeneous gas phase reactions [2]. In all these processes the specifics of sub-bituminous Wyoming coal will be accounted for.

Phase 2: Model validation

The computational method will be validated by performing simulations of the Western Research Institute (WRI) gasifier and comparison of the simulation results with available measurements. The WRI gasifier is a laboratory-scale gasifier that is operated with Powder River Basin coal in Laramie, WY. Since the proposed UW gasifier will be operated with a similar coal at comparable altitude the WRI gasifier is an optimal choice for the model validation.

Phase 3: Numerical study of the laboratory-scale UW gasifier

Next, we will apply the computational model to simulations of the laboratory-scale UW gasifier. The simulations will be based on a preliminary design of a laboratory-scale UW gasifier provided by Prof. M. Argyle. We will modify the geometry and operating conditions until the feasibility of the gasifier is demonstrated.

Phase 4: Numerical study of the industrial-scale UW gasifier

Based on the results obtained in phase 3 the dimensions and operating conditions for an industrial-scale UW gasifier can be specified. We will perform simulations of the industrial-scale UW gasifier to demonstrate the feasibility of the new concept. Numerical simulations are the only mean of evaluating the performance of the industrial-scale UW gasifier at this stage.

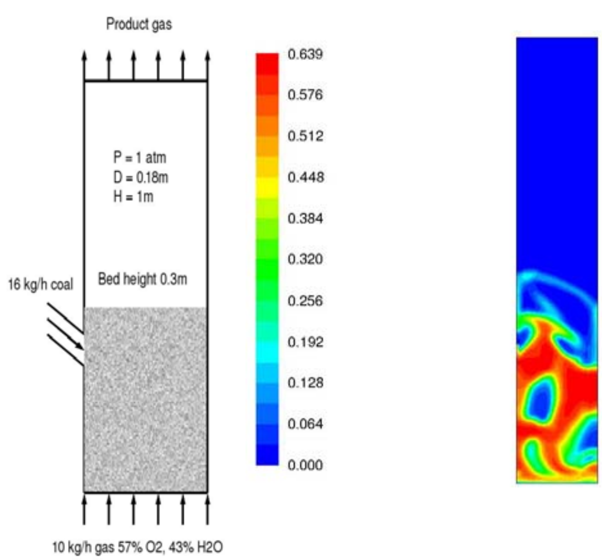
Phase 5: Analysis of the similarities between the laboratory- and industrial-scale gasifier
To be able to extrapolate experimental results obtained for the laboratory-scale gasifier to the industrial-scale gasifier one has to know how similar the processes at the two scales are. We will use the simulation results from the preceding phases to analyze the similarities between the two gasifiers. Variations of the dimensions and operating conditions of the laboratory-scale gasifier might be necessary to improve similarity. Once "sufficient" similarity has been demonstrated we will derive appropriate scaling relations between the two gasifiers. The laboratory-scale UW gasifier can be constructed then on the basis of the optimal geometry and operating conditions determined in this step.

Phase 6: Optimization of the industrial-scale UW gasifier
We will optimize the operating conditions of the industrial-scale UW gasifier by means of numerical simulations and by using experimental results for the laboratory-scale gasifier. In particular, the CO/H2 ratio of the synthesis gas will be optimized to increase the economic efficiency. Technological and economical constraints will be included in the optimization process.

3. Current results

Phase 1: Development of a computational model for coal gasification
The development of a model for dense gas-solid flow conditions has been reported in our annual report 2008 [3]. In the next step we have included all the coal specific models. The coal specific models together with the model for dense gas solid flows have been implemented in the commercial CFD code FLUENT and form a comprehensive computational model for the gasification of Wyoming coal.

Phase 2: Model validation
Simulations of the WRI gasifier (see sketch in figure 1) have been performed to validate the computational model. The gasifier domain was divided into 3000 computational cells and the simulation time was about 22 hours. The comparison between the simulated and measured product gas composition shows excellent agreement: the relative errors are smaller than 12%. Figure 1 also shows a contour plot of the solid volume fraction which reveals the formation of gas-bubbles (blue regions) within the dense coal powder (red regions). The flow pattern and size of the gas-bubbles have a significant impact on the performance of the gasifier. Simulation results can be used to study these flow details that can hardly be observed in experiments.



Product gas [mol%]	Exp.	Sim.
CO	27.6	25.9
H_2	31.8	31.1
CO_2	25	24.2
H_2O	13.6	15.7
CH_4	2.5	3.1
$T[K]$	1061	1095

Figure 1: Sketch of the WRI gasifier (left), contour plot of the solid volume fraction (middle) and simulation results (right).

Phase 3: Numerical study of the laboratory-scale UW gasifier
To demonstrate the feasibility of the UW gasifier concept we have performed simulations of the laboratory-scale UW gasifier (see sketch in figure 2). The gasifier domain was divided into 6110 computational cells and the simulation time was about 48 hours. The predicted product gas composition is 29.2% CO, 34% H_2, 20% CO_2, 15% H_2O and 1.8% CH_4, T=1100K. Compared to the WRI gasifier we find a higher yield of H_2 and CO. This result is due to the higher operating pressure (p=6atm) and the specific geometry of the UW gasifier. The geometry and the higher pressure cause the formation of a larger number of small gas-bubbles (see figure 2 left). As a consequence, the fluid-solid contact time is increased which increases the formation of H_2 and CO. This simulation demonstrates the great potential of the new UW gasifier design.

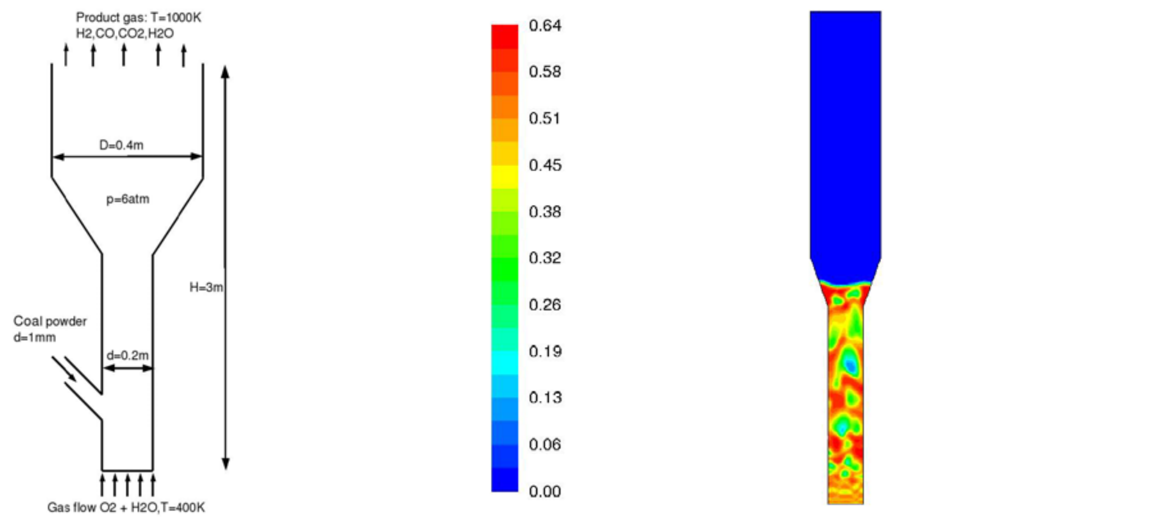


Figure 2: Sketch of the UW gasifier (left) and contour plot of the solid volume fraction (right).

4. Next steps

Phase 4: Numerical study of the industrial-scale UW gasifier
Once the dimensions and operating conditions of the industrial-scale UW gasifier have been identified we will perform simulations to demonstrate the feasibility of the industrial-scale UW gasifier concept.

Phase 5: Analysis of the similarities between the laboratory- and industrial-scale gasifier
This step will provide the final dimensions and operating conditions for the laboratory-scale UW gasifier. Moreover, the work during this phase will reveal with how much confidence results from laboratory-scale gasifier experiments can be extrapolated to the industrial-scale gasifier.

Phase 6: Optimization of the industrial-scale UW gasifier
We will perform a variety of simulations to optimize the CO/H_2 ratio of the synthesis to increase the economic efficiency of the industrial-scale UW gasifier.

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 77 credit hours so far and maintained a GPA of 3.8. He has passed the required Qualifying Exams.

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. L. D. Smoot and P.J. Smith, "Coal combustion and gasification", Plenum, New York, 1985.
3. S. Heinz, "A New Concept for the Gasification of Wyoming Coal", Annual Report for the School of Energy Resources – GA Program, 2008.