

U.S. DEPARTMENT OF ENERGY  
OFFICE OF FOSSIL ENERGY  
NATIONAL ENERGY TECHNOLOGY LABORATORY



## COAL PARTICULATE PARTITIONING DURING GASIFICATION

### Background

The goal of this project is to better understand the impact of the non-homogeneous nature of coal on coal gasification systems and to develop better modeling tools to improve reliability and efficiency of coal gasifiers. It is well known that the mineral and organic components in coals, known as macerals, vary widely in their composition, distribution, and occurrence. These components have different physical and chemical makeup. When ground to the fine sizes required for advanced gasification systems, some of these components will separate to form particles enriched in individual minerals or macerals which respond completely different than the aggregate or average coal particles. These outliers can lead to process inefficiencies, fouling, and other reliability problems. Coals will be fractionated by hardness and density and those fractions will be characterized, gasified, and the resulting information will be used to develop validated computer models.

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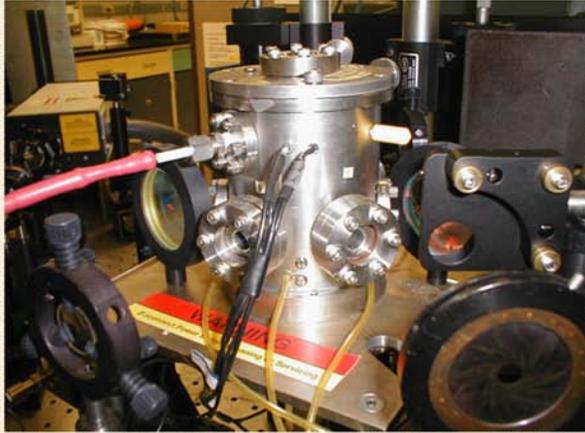
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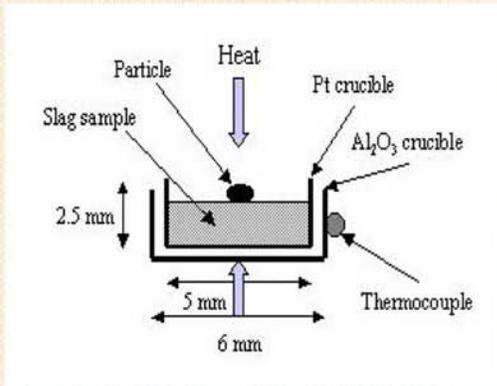
### Accomplishments

A project was initiated at the end of FY2006 to improve the understanding of slag formation during coal gasification as a response to coal outlier particles. A team of experts in relevant disciplines have been assembled as part of the National Energy Technology Laboratory's (NETL) Collaboratory of Multiphase Flow Research. This team comprises researchers from NETL, West Virginia University, Carnegie Mellon University, Pennsylvania State University, SRI International, Niksa Energy Associates, REM Engineering Services, and Leonardo Technologies, Inc. including experts in coal science, high temperature mineral chemistry, high pressure gasification, hydrodynamics, single particle characterization, computational fluid dynamics, and coal partition modeling.

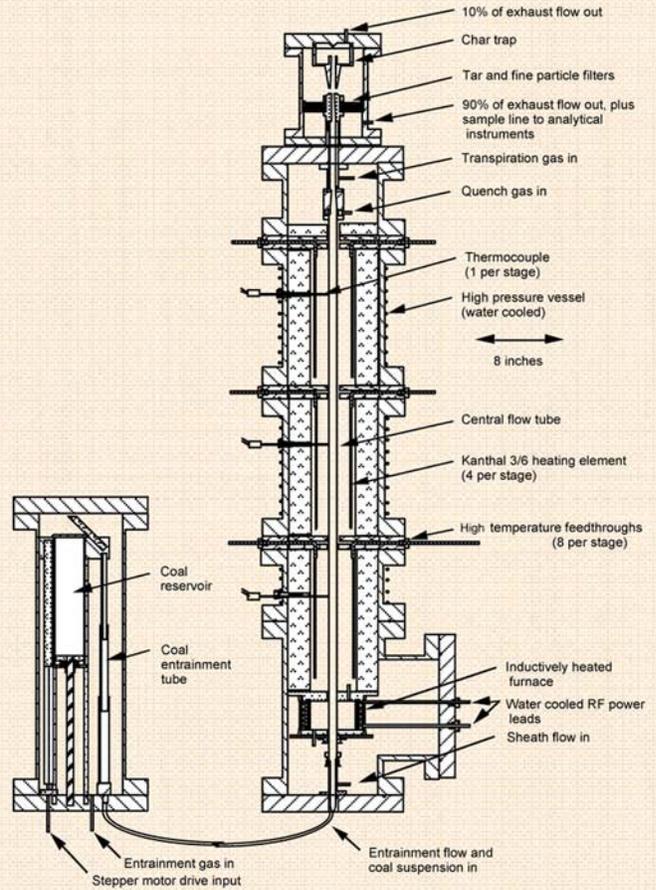




**NETL's Electrodynamic Balance Facility**



**CMU Hot stage microscopy**



**SRI High P Gasifier**

Figure 1. Experimental facilities at NETL, SRI, and CMU used to characterize individual coal particles, gasify coal fractions, and characterize the interactions of gasified char and minerals with slag.

## Benefits

Coal mineral behavior in an entrained gasifier (including mineral partitioning, ash chemical and physical transformations at temperature and pressure, particle fragmentation, and conversion) will be incorporated into gasifier models to determine the impact on slagging and potential flyash formation for a sample coal. We will use this to evaluate the potential for adjusting mineral preparation procedures to reduce fouling and process inefficiencies. Computer submodels will be developed for fragmentation and conversion of coals in high pressure high temperature gasifiers, drag of poly-disperse coal and char particles, mineral transformations and slagging, and wall boundary determining slag acceptance or rejection. The project offers the potential to define a research and development approach to improve the heat rate and reliability of gasification-based power systems. Models will be developed from this project including both partitioning and computational fluid dynamic (CFD) submodels for slag formation and growth. CFD tools capable of simulating individual coal size and density fractions will be developed including: trajectories, chemical and physical transformations, and incorporation or rejection from a slag layer, in a typical coal gasifier.

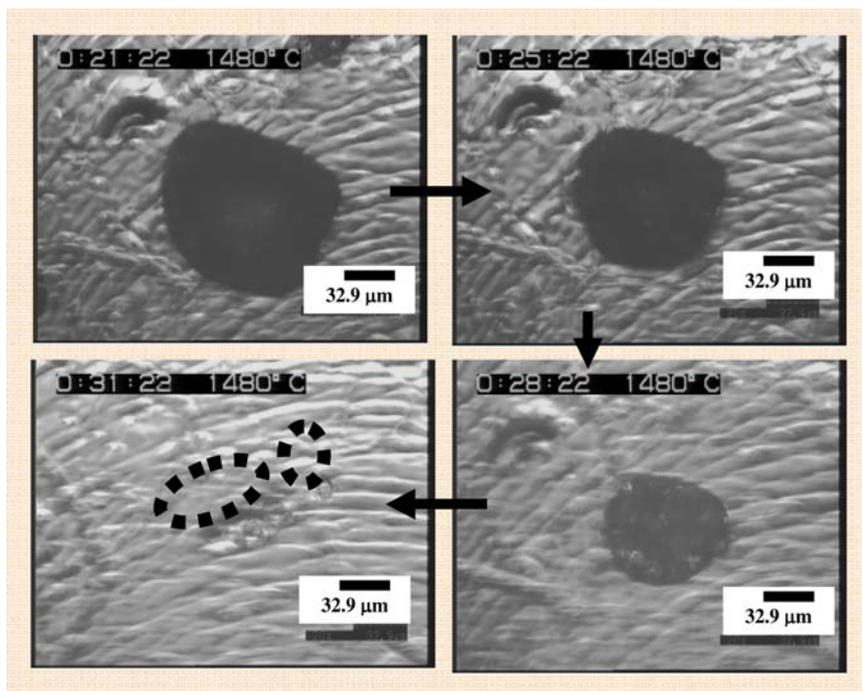


Figure 2. Mineral particle incorporation into high temperature slag.

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## Opportunities

Coal suppliers, utilities, and gasifier developers are desired who can provide coal samples and gasifier performance results to enable validation of the simulations and experimental test results. There is potential to develop a Cooperative Research and Development Agreement or other means of partnership for this type of collaboration.

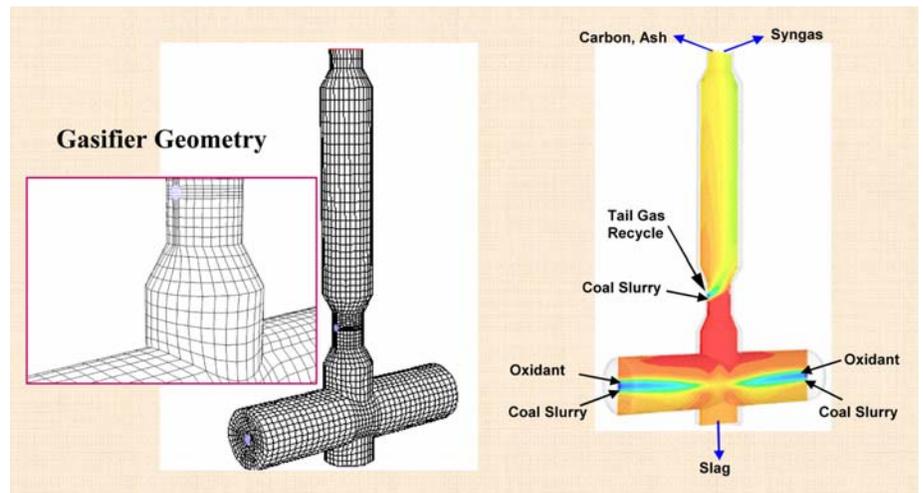


Figure 3. NETL grid and simulation results mapping temperature gradients in an entrained-flow coal gasifier.