Conversion and Fouling

Background

Coal and biomass gasification is an approach to cleaner power generation and other uses of these resources. Currently, the service life of gasifiers does not meet the performance needs of users. Gasifiers fail to achieve on-line availability of 85-95 percent in utility applications and 95 percent in applications such as chemical production. The inability to meet these goals has created a potential roadblock to widespread acceptance and commercialization of advanced gasification technologies.

Gasifier output is a hot gas mixture consisting primarily of hydrogen and carbon monoxide (CO), known as synthesis gas (syngas). The syngas cooler is one of the key components identified as negatively impacting gasifier availability. Ash originating from impurities in gasifier carbon-containing feedstock is at the root of many problems, attacking or fouling syngas components and causing unplanned shutdowns for repair, replacement, or cleaning. Gaps in the understanding of how fuel properties impact carbon conversion, slag viscosity, and downstream fouling and the potential advantages of fuel flexibility on availability rates and sustainability using different feedstocks are additional factors contributing to lower efficiency and capacity factor.

To address these issues the Gasification Program is using an integrated approach to leverage the U.S. Department of Energy (DOE) National Energy Technology Laboratory (NETL)-Regional University Alliance (RUA) and URS partners’ capabilities to combine theory, computational modeling, laboratory experiments, and industrial input to develop physics based methods, models, and tools to support the development and deployment of advanced gasification based devices and systems.

Project Description

Accurate physical models to predict the rates of slag buildup in a gasifier or ash deposition in a syngas convective cooler are currently not available. Demonstration plants are currently experiencing problems such as lower carbon conversion and plugging of syngas coolers with fly ash, which reduce the thermal efficiency of a gasifier, place additional strain on solids handling and greywater circuits, and reduce the overall reliability of the gasifier. Molten ash chemistry and viscosity are crucial aspects of carbon feedstock ash impacting slag properties in a gasifier and refractory corrosion. The roles of iron sulfide (FeS) and oxides of trace elements on plastic viscosity are well understood. Studies on fouling caused by ash deposition are plentiful in the combustion community, but there are far fewer such studies under gasification. The published literature suggests that iron sulfides (FeS, FeS₂) play a primary role in ash deposition and agglomeration because they may become “sticky” at convective syngas cooler (CSC) temperatures. More recent reports suggest that other compounds may behave in a similar fashion, although there are no studies that quantify how ash deposition occurs as a function of carbon feedstock.

Researchers will develop reduced order models (ROMs) with higher fidelity computational fluid dynamics models coupled to the ROMs to enable more accurate prediction of gasifier performance. The proposed devolatization and char kinetics subtasks will attempt to identify the factors responsible for the formation of fly ash.
particles by using the traditional mineral processing approach of particle partitioning, and by superimposing kinetics of char and mineral transformations. In the slag viscosity and unburnt carbon effort, slag viscosity will be investigated using a high-temperature rotating-bob viscometer and a temperature gradient furnace in which slag infiltration in a controlled atmosphere can be studied. Particle deposition testing will initially be conducted at temperatures relevant to the convective syngas coolers in order to generate ash particle chemistry; ash adhesion probabilities as a function of particle size, temperature, and velocity; surface temperature; and contact angle. Ash particles from the High Pressure Entrained Flow Reactor (HPEFR) at Pennsylvania State University (Penn State) will be generated from coal and petcoke feedstocks that are separated into multiple size and density fractions, each containing various amounts of mineral matter, which will be used to determine the characteristics of the fly ash particles. The effect of FeS and other coatings on particle deposition will also be investigated in the latter stages of the project, and a comprehensive model for ash deposition at CSC conditions will be generated.

Goals/Objectives
The main goal of this project is to improve the reliability, availability, and maintainability of gasification plants by developing tools to evaluate the impact of fuel properties on slag and refractory interactions. By evaluating ash deposition from carbon feedstock, plugging and fouling throughout the syngas cooling system can be reduced. To achieve this goal, four major areas of research are being pursued concurrently:

- Model Development: The modeling effort involves developing a heuristic spreadsheet-based reduced ROM with the capability to predict the effects of the distributive properties of fuels used in entrained-flow gasifiers on key gasifier performance indicators, so that the ROM may be used as a tool to investigate syngas cooler fouling and the amount of unconverted carbon.

- Devolatization and Char Kinetics: The objective of the devolatization and char kinetics effort is to measure pyrolysis kinetics for various density and size fractions of Pittsburgh #8 coal and, at high temperature and pressure, characterize the changes to char particles during pyrolysis (early stages)—including particle size, density, char reactivity in carbon dioxide (CO₂), and mineral matter transformations—and identify the critical conversion(s) at which the particle fragmentation occurs.

- Slag Viscosity and Unburnt Carbon: The slag viscosity and unburnt carbon effort is focused on measuring slag viscosities as a function of temperature and CO/CO₂ ratio for laboratory manufactured synthetic ash to determine how slag infiltrates into a refractory material subjected to a temperature gradient.

- Particle Deposition: The particle deposition effort is focused on conducting ash particle deposition experiments at conditions relevant to existing convective syngas coolers and using the data to generate a comprehensive model of ash deposition probability as a function of feedstock size and density fractions, ash particle size, particle temperature, particle velocity, surface temperature, and contact angle.

Accomplishments
Researchers at West Virginia University (WVU) have developed a rules-based partitioning spreadsheet ROM to predict gasifier performance. The ROM can be used to predict the solids mass fraction that adheres to the slag and the fraction that leaves the gasifier. A HPEFR has been commissioned at Penn State and the fuel feeder has been tested with coal particles of various sizes and very consistent flow was observed for both atmospheric and pressurized (100 pounds per square inch) flow. Researchers at Carnegie Mellon University (CMU) have completed viscosity measurements of coal/petcoke slag mixtures with good experimental reproducibility. The resultant slags are being analyzed by researchers. The ash deposition ROM developed for the industrial convective syngas cooler is being used to help determine how the High Pressure Tubular Reactor deposition studies at atmospheric pressure will relate to the actual particle deposition process at higher pressures relevant to domestic integrated gasification combined cycle (IGCC) plants.

Also at CMU, the x-ray diffraction and scanning electron microscope (SEM) analyses of the crystalline phases precipitated during viscosity measurements from the four coal, petcoke, or coal/petcoke carbon feedstock mixtures (100 percent eastern coal, 100 percent western coal, 50 percent eastern coal+50 percent petcoke, 50 percent western coal+50 percent petcoke) have been completed. An improved flowing slag film model that will account for the flux of ash into the slag film distributed over the entire slag-syngas interface is being developed. This model will be used as part of the heuristic coal partitioning model currently undergoing refinement. Predictions of the axial slag thickness distribution were obtained for a range of constant gasifier temperatures and for ash of various chemistries/viscosities. Four slags were designed for plastic flow modeling, viscosity measurements were conducted and the slags analyzed using the SEM, and the conversion of trolite (FeS) to ferrous oxide (FeO) was evaluated in a specially designed thermogravimetric analysis sample holder.

Benefits
This research will enhance the ability of researchers to predict gasifier performance, including rates of carbon conversion and fly ash generation, and to address fouling rates in syngas coolers. The impact of volatile organic oxides and iron content and its oxidation state on plastic viscosity will be established. The impacts and limitations of using various coal grades and petcoke in entrained gasifiers, in terms of optimizing slag fluidity to ensure drainage along gasifier walls and limit refractory degradation to an acceptable limit will be determined. This will reduce plugging and fouling throughout the syngas cooling system and should help gasification technology achieve wider accessibility by allowing for a greater understanding of the role fuel properties have on gasifier RAM. These benefits will support the NETL Gasification Program goals of 90 percent IGCC availability and greater cost efficiency.

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