Development of Kinetics and Mathematical Models for High-Pressure Gasification of Lignite-Switchgrass Blends

Cooperative Research and Development Final Report

CRADA Number: CRD-11-447

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In accordance with Requirements set forth in Article XI, A(3) of the CRADA document, this document is the final CRADA report, including a list of Subject Inventions, to be forwarded to the Office of Science and Technical Information as part of the commitment to the public to demonstrate results of federally funded research.

Parties to the Agreement: Georgia Institute of Technology

CRADA Number: CRD-11-447

CRADA Title: Development of Kinetics and Mathematical Models for High-Pressure Gasification of Lignite-Switchgrass Blends

Joint Work Statement Funding Table Showing DOE Commitment:

Estimated Costs	NREL Shared Resources
Mod 2	$ 1,629.00
TOTALS	$ 1,629.00

Abstract of CRADA Work:

NREL will work with Participant as a subtier partner under DE-FOA-0000240 titled "Co-Production of Power, Fuels, and Chemicals via Coal/Biomass Mixtures." The goal of the project is to determine the gasification characteristics of switchgrass and lignite mixtures and develop kinetic models. NREL will utilize a pressurized thermogravimetric analyzer to measure the reactivity of chars generated in a pressurized entrained-flow reactor at Participant's facilities and to determine the evolution of gaseous species during pyrolysis of switchgrass-lignite mixtures. Mass spectrometry and Fourier-transform infrared analysis will be used to identify and quantify the gaseous species. The results of the project will aid in defining key reactive properties of mixed coal biomass fuels.

Summary of Research Results:

The devolatilization and gasification of switchgrass and coal under pressurized conditions was investigated using a pressurized thermogravimetric analyzer (PTGA). Switchgrass and lignite were devolatilized at heating rates of 5-20°C/min at pressures of 5-30 bar in inert gas atmospheres. The major mass loss regions and gases evolved for each material were determined. Devolatilization of 90:10, 70:30, and 50:50 blends of lignite and switchgrass showed the devolatilization rates of the blends to be equal to the sums of the rates of the individual chars. Thus, blends of coal and biomass devolatilized independently of each other.

Chars that have been prepared by pyrolysis at high heating rates (~1000°C/s) are typically much more reactive than chars prepared at low heating rates such as chars prepared in a PTGA (~10°C/min). Therefore, for gasification experiments, we utilized switchgrass and lignite chars

that had been prepared in a pressurized entrained flow reactor at high heating rates and pressures at Georgia Institute of Technology. First, conditions under which the rate was not limited by mass transfer rates were established by varying the sample mass and the char particle size. Lignite and switchgrass and their blends were then gasified under these conditions. The blend gasified at a rate that was equal to the sum of the rates of the individual chars. This suggested no interaction between the chars during gasification.

Biomass chars normally gasify faster than coal chars. However, in this case, the lignite coal char gasified faster. For the rest of the experiments, a less reactive coal char – bituminous coal char prepared in a fixed reactor at atmospheric pressure – was selected. General Langmuir-Hinshelwood type kinetic models were developed for both the switchgrass and bituminous coal char.

$$k = \frac{k_{CO2}p_{CO2} + k_{H2O}p_{H2O}}{1 + K_{CO2}p_{CO2} + K_{H2O}p_{H2O} + K_{CO}p_{CO} + K_{H2}p_{H2}}$$

The chosen model described the gasification rates well. The parameters for the models and the activation energies were determined.

Experiments were conducted with blends of coal char and switchgrass char to test whether the addition of switchgrass char impacted the gasification rate of the coal char. In general, the gasification rates for blends were similar to the sum of the rates for the individual char gasification rates as long as both chars contained gasifiable material. However, after switchgrass char had become completely gasified and formed ash, the rate of bituminous char gasification increased by a factor of more than three. This suggested that the presence of switchgrass ash increased the rate of coal char gasification. A good contact between the switchgrass ash and coal char may be required for this effect to occur.

Subject Inventions Listing:

None

Report Date:

March 1, 2016

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