ACS PRF Annual Narrative Progress Report

1. **PRF#** 58973-ND4
2. **Project Title**: Microwave Driven Pyrolysis: Comparative Heating Rates and Reactive Plasma Assessments
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Update on Personnel

Though our project was awarded in 2018, it took a full cycle of our graduate admissions to identify and recruit a graduate student for the project, now beginning this fall semester. The student, admitted to our Ph.D. program track is presently engaged in learning the analytical methods and receiving instrument training as will be needed for characterization of the char, gas and liquid products to be produced in this project while preparing tests.

Project Goals

It is proposed that MW heating accomplished pyrolysis, curtailing the cracking to C_1-C_4 gases. Using hydrogen and methane to cap radicals and promote methylation reactions improves the yield and quality of liquid products by microwave pyrolysis of coal. Therein lie two project goals.

1. Benchmark the MW heating rate by product distribution similarity using model compounds and materials.
2. Quantify the extent of upgrading that occurs by overall product yield, product classes (light gases, benzene-toluene-xylene (BTX) compounds and tars) and chemical composition (aliphatic versus aryl hydrogen, sp^2/sp^3 carbon).

Outcomes will include identification of underlying reaction and conversion process in microwave driven coal pyrolysis under reactive atmospheres.

Project Impacts

Personnel – This project has stimulated advancements into coal-derived chemicals and uses. Development of greener processes for their extraction while improving their quality has sparked the research interest the graduate student on this project.

Societal – Use of microwave plasma both catalyzes reactions in a novel way and allows very rapid (thousand degrees per second) heating of gas, which is not possible with conventional heating technologies (boilers, furnaces, heat exchangers, inductive heaters). Since microwaves can be powered by renewable (wind or solar) electricity and decomposition does not use oxygen, the entire process can be completely free of CO_2 emissions. This enables modular, small-scale, low-capital deployment of chemical conversion plants, making the chemical industry more efficient, effective, flexible, and, ultimately, more competitive.

Interim Progress Sept. 2019 – Temperature

A hallmark of plasma processes is the non-equilibrium chemistry. Specifically, the system is not at thermodynamic equilibrium with hot atoms and energized radicals formed by continuous electron impact and ionization. This energetic plasma environment can however be described by temperature, but not a single global average. Instead different degrees of freedom may be characterized by separate and different temperatures. Nevertheless, temperature is the most important metric by which to gauge plasma intensity and associated reactions.

Temperature is of particular interest, given its relevance to carbon aerosol formation. Black body temperature – a MATLAB algorithm was written to determine the black body temperature of the forming carbon aerosol, assuming unity for emissivity. Essentially the spectral emission profile between 650 – 900 nm is fit to a Planck function and adjusted for scaling, after background subtraction. A particularly novel feature is the smart feature of the code that ignores Ar* emission lines automatically, so as to avoid spurious temperature determination. Figure 1 illustrates the spectral fit over a portion (650 nm – 850 nm) of the observed spectrum using this algorithm, for illustration, before and after removing Ar* emission. In summary, temperature can serve as a tangible physical reference by which to gauge carbon product structure against reaction conditions.

Fig. 1