



ABSTRACTS

Friday, October 22, 2010

Session 4A: Chemicals from Lignin

**AN OVERVIEW OF OPPORTUNITIES FROM LIGNIN COUCHED IN THE MISSION OF THE U.S.
DEPARTMENT OF ENERGY**

John Holladay

Pacific Northwest National Laboratory
902 Battelle Blvd, MSIN P8-60
509-375-2025

john.holladay@pnl.gov

In December 2009 the U.S. Department of Energy Office of the Biomass Program sponsored a workshop on “Bioproducts from Lignocellulosic Resources.” This presentation we provide an overview of the workshop focusing on opportunities to produce fuels and chemicals from lignin couched into the Department of Energy mission and goals.

Lignin presents many challenges for use in the biorefinery. Chemically it differs from sugars by having a complex aromatic substructure. Unlike cellulose, which has a relatively simple substructure of glucose subunits, lignin has a high degree of variability in its structure which differs according to the biomass source and the recovery process used. In addition to its structural variability lignin is also reactive and to some degree less stable thermally and oxidatively compared with other biomass streams. Some technology is available for lignin use now. Thermochemical processes can be used with many lignin streams in the near to medium term. Also some of the macromolecular opportunities, identified as medium-term, exist today. However, medium- and long-term opportunities will require transcending some significant barriers.¹

(1) “Top Value-Added Chemicals from Biomass, Volume II—Results of Screening for Potential Candidates from Biorefinery Lignin” Holladay, J. E.; White, J. F.; Bozell, J. J.; Johnson, D. DOE Report number PNNL-16983. October 2007.

UTILIZATION OF SUSTAINABLE RESOURCES FOR PRODUCTION OF CARBON FIBER MATERIALS FOR STRUCTURAL AND ENERGY EFFICIENCY APPLICATIONS

Frederick S. Baker

Oak Ridge National Laboratory
Materials Science and Technology Division
One Bethel Valley Road
Oak Ridge, Tennessee 37831-6087, USA

bakerfs@ornl.gov

U.S. DOE Vehicle Technologies-funded work at Oak Ridge National Laboratory (ORNL) is directed to the development of more energy-efficient, cost-effective processes for production of carbon fiber for use in lightweight composite materials for vehicles. Carbon fiber has the potential for substantial weight savings in vehicles because of its remarkable high strength, high modulus, and low density. Body-in-white modeling indicates that over 60% of the steel in a vehicle could be replaced with carbon fiber-reinforced composite materials without impacting vehicle crash worthiness; each 10% reduction in vehicle weight translates into an increase in fuel economy of 6-8% as well as lower greenhouse gas emissions. However, carbon fiber is currently too expensive for large scale automotive use, which necessitates a large reduction in the cost of commercial grade fiber from about \$15-20/lb (\$33-44/kg) to \$5-7/lb (\$11-15/kg). This presentation will highlight the utilization of lignin as a precursor material for production of low cost carbon fiber for automotive use. In addition, new work on the utilization of lignin-based carbon fiber for production of high surface area electrode materials for electrical energy storage (supercapacitors) and high energy efficiency systems for capture of greenhouse gases and volatile organic compounds (VOCs) will be introduced. The talk will conclude with a discussion of the main features of a \$50 million Carbon Fiber Technology Center to be constructed at ORNL, which will contain both conventional (thermal) and advanced (plasma) processing lines for conversion of low cost precursor materials, such as lignin, into carbon fiber for qualification testing by the automotive, wind turbine, and other interested industries; to meet this need, the conventional line will have a nameplate capacity of 25 ton/year of finished carbon fiber.

PARTICLE PYROLYSIS FOR BIO-RENEWABLE CHEMICALS FROM LIGNOCELLULOSIC BIOMASS

Paul J. Dauenhauer

University of Massachusetts, Amherst
686 North Pleasant Street
Amherst, MA 01003

dauenhauer@ecs.umass.edu

The production of chemicals from lignocellulosic biomass by pyrolysis or gasification occurs through thermal degradation of biopolymers and subsequent catalytic upgrading. Overall process viability depends upon the selection of products from pyrolysis reactions that are capable of being catalytically upgraded to chemical feedstocks such as aromatics. We examine the decomposition of lignin and carbohydrate biopolymers within woody biomass to understand the chemistry that selects for the broad array of chemical species observed within pyrolysis products (bio-oils). Degradation of both lignin and carbohydrates is shown to occur through an intermediate liquid which subsequently evaporates or re-reacts to produce a solid char byproduct. Vapors and gases boil within the intermediate molten biomass droplet resulting in violent bubble collapse and evaporation from the active phase. A residual lignin matrix remains which exhibits steady structural collapse and significant reduction in size from the initial particle dimensions. The integration of high temperature particle pyrolysis with heterogeneous catalysts must account for the interaction of the intermediate liquid and the inorganic catalyst particle. Carbohydrate biopolymers are observed to exhibit highly variable wetting characteristics when in contact with inorganic surfaces, thereby significantly varying the particle heat transfer rate, reaction temperature, and selection of chemical products.

CO-PRODUCTION OF HIGH VALUE OXYGENATES AND OLEFINS THROUGH INTEGRATED BIOMASS FRACTIONATION, GASIFICATION AND ADVANCED CATALYTIC CONVERSION

Mario R. Eden¹, Christopher B. Roberts¹, Sushil Adhikar² and Steven E. Taylor²

Auburn University

¹Department of Chemical Engineering

²Department of Biosystems Engineering

Auburn, AL 36849-5127, USA

edenmar@auburn.edu

The large amounts of underutilized woody biomass available (14.6 million tons annually in Alabama alone) can contribute significantly to the nation's goals for energy security and economic viability if technological advances are achieved in the thermochemical conversion platforms. In this work, we are developing viable hydrocarbon production strategies by integration of biomass fractionation technologies followed by technically well-informed application of thermochemical conversion approaches and associated catalyst structures. Our multidisciplinary team has established significant synergies in our research efforts particularly in catalyst development and characterization, chemical/fuels production and process systems engineering. This work leverages ongoing research by taking advantage of a unique set of testbeds in the Auburn University Center Bioenergy and Bioproducts consisting of biomass fractionation and several conversion technologies, most notably a pilot-scale gasification unit that will be used to produce the synthesis gas for supercritical phase Fischer-Tropsch synthesis and high value chemical co-production.

The utilization of innovative biomass fractionation technology coupled with a pilot-scale gasification unit enables systematic analysis of the downstream conversion viability and potential for value addition for each feedstock constituent, i.e. cellulose, hemicelluloses and lignin. As a specific example, we have studied a supercritical phase Fischer-Tropsch Synthesis (SCF-FTS) process developed at AU using biomass derived syngas with particular attention on the impact of novel nanoscale catalysts on reaction performance. We have demonstrated that the use of properly selected Fe-based catalysts in supercritical fluid reaction media results in a product stream consisting of more than 30% aldehyde species plus significant concentrations of 1-olefins. This affords higher value than conventional FTS approaches.

The molecular level understanding of nanocatalyst structure and performance enables informed design and optimization of biomass conversion processes. Synergistic collaboration between experts in chemical engineering and biosystems engineering allows for a systems level approach to the optimization of the biomass to hydrocarbon chemical/fuel lifecycle including design and characterization of the enabling catalysts. The Auburn University team employs a holistic methodology utilizing a systematic and flexible process integration/optimization based framework to identify product distributions and processing routes for integrated biorefineries.

GASIFICATION OF WOODY BIOMASS AT THE PILOT-SCALE

Thomas Elder and Leslie H. Groom

USDA-Forest Service-Southern Research Station
2500 Shreveport Highway
Pineville, Louisiana 71360 USA

telder@fs.fed.us

The thermochemical platform is an essential component of the biorefinery concept. In the current work this process is represented by gasification, as an efficient method that can accept a wide range of feedstocks, while resulting in a consistent product that can be utilized for energy without further modification or converted to liquid transportation fuels. The air-based gasification system in this study is of downdraft design, which has inherently low tar production levels (13-23ppm) without the need for catalytic cracking. The unit consumes $\sim 17\text{-}30 \text{ kg h}^{-1}$ of feedstock producing a synthesis gas composed of $\sim 20\%$ carbon monoxide, 12% carbon dioxide, 3% methane and 19% hydrogen, with an energy content of $\sim 6 \text{ MJ m}^{-3}$. The gas mixture from the gasifier is cooled, filtered and used directly to fuel a conventional 6-cylinder, spark-ignited engine that in turn powers a generator capable of producing 25kWe. Experimental runs have used pine and mixed-hardwood chips at a range of gas flow rates. The objective of this work is to determine the effect of feedstock and process conditions on the quality of the synthesis gas. Results indicate that carbon monoxide percentage increases with flow rate, while methane decreases with flow rate. Carbon dioxide and hydrogen are reasonably constant with flow rate. In general the hardwoods produce higher levels of carbon dioxide, hydrogen and methane, while the pine produced higher levels of carbon monoxide. The energy content of the gas was similar with feedstock, and decreased slightly with flow rate. The efficiency of the process exhibits a sharp increase at higher flow rates. Ongoing work involves determining the impact of environment on synthesis gas production and further relating process conditions to gas quality.