Reference Methods for Detailed Quantitative Analysis of Bio-Oils

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Abstract

This project will develop advanced reference analytical methods to support biofuel-production process improvement, quality control, and troubleshooting. The development of reference analytical methods is critical for the nascent biofuels industry to develop cost-efficient processing for renewable energy sources. The analytical methods for bio-oils will be developed using comprehensive two-dimensional gas chromatography (GCxGC), a powerful new technology pioneered by Zoex Corporation, one of the collaborating companies, and advanced analytical cheminformatics software for GCxGC, pioneered by the principal investigator (PI) and GC Image, LLC, another of the collaborating companies. Bio-oils produced at the University of Oklahoma will be analyzed by GCxGC coupled to flame ionization detection (FID), low-resolution mass spectrometry (MS), and high-resolution time-of-flight mass spectrometry (HRToFMS). Collaborators at the University of Oklahoma use fast pyrolysis to convert solid lignocelluloses to liquid pyrolysis oil (or bio-oil), followed by catalytic conversion of the bio-oil components to hydrocarbons. This process provides fast throughput and is robust with respect to feed composition, e.g., switchgrass or other forage grasses, woodchips and byproducts, algal biomass, etc. In Year 1, the team will study GCxGC separation methods and develop analytical templates for characterizing chemical groups and individual target compounds in bio-oils and catalytically prepared finished fuels. In Year 2, the project will develop and publish reference analytical methods. Expected results include methods for producing detailed chemical information of significant value for optimizing agricultural biofuel production processes, biofuel-related conference and journal publications, strengthened collaborations with academia and private-sector researchers, and submission of competitive funding proposals.

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Biofuels can be produced from renewable, domestic sources and are potential alternatives to increasingly expensive petroleum fuels, for which supplies are limited, mostly foreign, and subject to disruption. However, research is required to develop more cost-effective sources, production methods, and uses for biofuels.

The motivation for this project is the need for methods and tools to better analyze the chemistry of biofuels. Better chemical understanding is the basis for improving biofuel feedstocks, production, quality control, and utilization, which in turn will help to make biofuels a more viable alternative energy resource. Biofuels are chemically complex, so the analytical task of characterizing and quantifying the constituent compounds to produce chemical information requires advanced instruments and informatics.

This project employs powerful new analytical instruments to provide data for comprehensive characterizations of biofuel samples. The datasets generated by these instruments are rich with information, but also large, complex, multidimensional, and multispectral. Currently, there are no reference standard methods for the instrument conditions and extracting information from the data. Project collaborators at the University of Oklahoma Center for Biomass Refining and Zoex Corporation are investigating instrumental conditions for biofuels analysis, but require data analysis methods to produce chemical information.

The specific aim of this project is to develop cheminformatic methods and software to extract chemic information from analytical data for biofuels. This requires the creation of new algorithms and of templat (analytical patterns) specifically crafted for biofuels. Project collaborators at GC Image, LLC, will collabora in method and software development and provide a path for commercialization. The methods will b demonstrated on data produced by collaborators and will be used by collaborators in their research. Th direct result will be analytical methods, supported in software, for advanced chemical analysis of biofuels. Th methods will be described in conference presentations and journal papers and will provide a basis f collaborative funding proposals to relate chemical analyses to production processes and fuel properties and innovate cheminformatics. Indirectly, the project will enable biofuels researchers and producers to advan the state-of-the-art for this important renewable energy resource.