

ABSTRACT SYMPOSIUM NAME: Advances In Biomass-Derived Fuels and Chemicals

ABSTRACT SYMPOSIUM PROGRAM AREA NAME: ENFL

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TITLE: Characterization of the combustion of terpene biofuels with the help of high-resolution mass spectrometry

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ABSTRACT BODY:

Abstract: Because of their high-energy density, terpenes could be used as drop-in liquid fuels for ground or air transportation. Two potential terpene fuels, limonene and α -pinene, were oxidized at atmospheric pressure, in a jet-stirred reactor, in the cool flame regime, under fuel-lean conditions and short residence time. Gas samples of the reacting mixtures were collected, analyzed online by FTIR and dissolved in cool acetonitrile for analysis by high-resolution mass spectrometry (Orbitrap). Direct flow injection or chromatographic separation by ultra-high-performance liquid chromatography and +/- heated electrospray ionization and +/- atmospheric pressure chemical ionization were used to characterize the products of oxidation of limonene and α -pinene. Reaction with 2,4-dinitrophenylhydrazine was used to assess the presence of carbonyl groups in the products. H/D exchange by adding D₂O to reaction samples were used for probing the presence of hydroxy and hydroperoxy groups in the products. A large set of oxidation products, including highly oxygenated organic products with five and more oxygen atoms, was observed. Aromatic and/or polyunsaturated products were detected. Van Krevelen plots, computed oxidation state of carbon, aromaticity index, and degree of unsaturation in products were used to rationalize the results and propose reaction pathways.

