

## **Department of Chemistry**



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Chemical Characterization and Mechanism of Crop Oil Pyrolysis to Produce Fuel and Chemical By-Products

Research interests focus on the development of analytical separation methods. The areas of interest target understanding of the origins of air pollution and its relation to climate changes and health, the detailed characterization of biofuels, and determination of biologically active species.

Website: http://www.und.edu/dept/chromatography/home.html

## Abstract

The world's current and future demands for fuel, chemical, and polymer products from petroleum are prompting the search for new accessible and economically feasible renewable equivalents, such as crop oil. Further, novel crop oil-based polymers and coatings have properties that differ from the petroleum derived materials they are replacing, hindering acceptance. Our team has conducted an extensive study of TG pyrolysis (conducted at 420–430 °C in the absence of catalysts, which constitutes the novelty of this work compared to previous work conducted by the others) in order to understand the chemical mechanisms that lead to the production of shorter chain FAs, alkanes, alkenes, and other chemicals which could be used to replace petroleum-based products.

Typical analytical methods applied in petroleum industry are often applied to the biofuel research; however due to significant differences in the composition of petroleum products and biofuels these methods are not fully compatible and require significant development and validation to be suitable for biofuels and their intermediates. The developed protocol of detailed gas chromatographic analysis coupled with mass spectrometry and flame ionization detection allowed not only for accurate quantification, but furnished full elutable molar speciation and homology plus partial isomer profiles for cyclopentanes, cyclopentenes, cyclohexanes, cyclohexenes, aromatic, and polycyclic aromatic (PAH) hydrocarbons as well as for linear and branched alkanes/alkenes and FAs. The developed method for estimation of undetermined and unresolved analytes allowed for mass balance closure. For batch TG cracking mass balance closed successfully whereas for flow reactors 20–30% of a non-GC-elutable fraction was discovered. Application of this protocol to the liquid fraction of TG cracking products enabled insights into the chemistry of TG pyrolysis. Analysis of TG pyrolysis products' patterns has been developed as an essential tool to decipher the cracking process mechanism.