

Attending 2018 SACNAS – The National Diversity in STEM Conference to
Present a Research Poster on
The Role of Quinone Methides in Dimerization of Coniferyl Alcohol in Wood-Based Pyrolysis Oil

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The need for alternative energy sources is becoming increasingly important. Continued dependence on fossil fuels is problematic not only because they are a non-renewable source, but also due to the concerns surrounding increasing carbon dioxide levels in the atmosphere. My research has been directed at an alternative fuel source, “pyrolysis oil.” Pyrolysis oil is an energy-rich liquid that is produced from biomass, including wood, by heating the biomass for seconds in a reactor.ⁱ While wood-based pyrolysis oil has the potential of becoming an alternative for the consumption of fossil fuels, it is currently highly unstable, because it reacts at room temperature to form a viscous liquid making it difficult to manage.ⁱⁱ

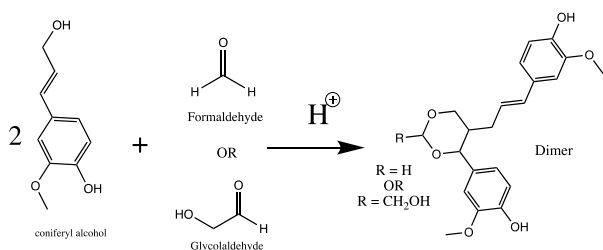


Figure 1: The dimer produced by the reaction with coniferyl alcohol and formaldehyde or glycolaldehyde in the presence of acid

This previous research concluded that coniferyl alcohol and small aldehydes, such as formaldehyde, react in the presence of acid, naturally found in the oil, to form a dimer (see Fig.1) which then continues to polymerize to form larger molecules, which explains the increase in viscosity.ⁱⁱⁱ

In the span of two years, I have worked in Professor Stemmler’s Lab. I have conducted research working with synthetic oils that simulated the reactions occurring in the authentic oil. My work showed that formic acid (an acid naturally found in wood-based pyrolysis oil) could be used to simulate reaction conditions and found clear evidence of the dimer at six hours of simulated aging, which can be translated to 1.5 months of aging at room temperature.^{iv} The research allowed us to place a timeline on how fast the aging occurs based on the oil composition, as it was highly dependent on the concentration of acid in the oil.

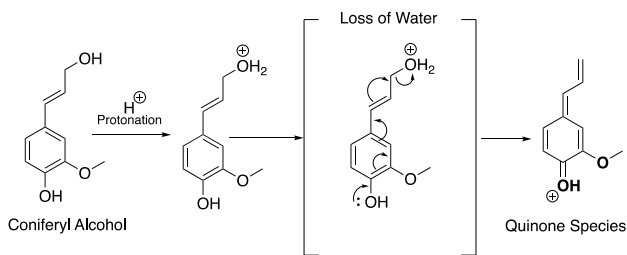


Figure 2: Coniferyl alcohol to quinone methide mechanism

During the Summer and Fall of 2018, I tested the hypothesis that quinone methides, highly reactive conjugated cation species, are important for reactivity (Figure 2). I varied the substituents on coniferyl alcohol to identify what attributes of the molecule were essential to promoting the quinone species and found that the hydroxyl (-OH highlighted in red) groups present in coniferyl alcohol promoted reactivity. Structural variants without the hydroxyl groups were not able to dimerize.

Through understanding the role of each of substituents, we can devise ways in how to treat the oil before the reaction occurs, preventing the increase in viscosity.

Presenting my research at the SACNAS meeting, was extremely rewarding and receiving feedback and constructive criticism from other researchers helped strengthen the project’s results. I was able to hear about other projects that worked with quinone methides and their reactivity, and in this way, I was able to learn about my own reactive species through a new perspective. Interestingly enough the highly reactive species is involved in many projects working towards green energy.

Overall, the conference was inspiring because of its focus on diversity in the STEM fields. By interlacing culture and science, the conference created an encouraging space for students to showcase their research and pursue careers in the STEM fields through grad school fairs and panels.

ⁱ Bridgwater, A. V. *Biomass Bioenergy* **2012**, *38*, 68-94.

ⁱⁱ Czernik, S.; Johnson, D. K.; Black, S. *Biomass Bioenergy* **1994**, *7*, 187-192.

ⁱⁱⁱ DeSisto, W. J.; Hill, N.; Beis, S. H.; Mukkamala, S.; Joseph, J.; Baker, C.; Ong, T. H.; Stemmler, E. A.; Wheeler, M. C.; Frederick, B. G.; van Heiningen, A. *Energy Fuels* **2010**, *24*, 2642-2651.

^{iv} Joseph, J.; Rasmussen, M. J.; Fecteau, J. P.; Kim, S.; Lee, H.; Tracy, K. A.; Jensen, B. L.; Frederick, B. G.; Stemmler, E. A. *Energy and Fuels*, **2016**, *30*, 4825-4840.