Laser Beams and 3D Printers: How Recent Experimental Advances Have Helped Reveal the Complex Chemistry of Combustion

Abstract: Under the high-temperature and high-pressure conditions of a combustion engine, hundreds of chemical species may be undergoing thousands of chemical reactions at any time. These reactions help dictate the speed at which the fuel ignites, the heat produced in the engine, how fast the flame front moves through the engine cylinder, and what pollutants are formed. Thus, in order to design new transportation engines that are more efficient and less polluting, we must first obtain a fundamental understanding of the chemistry of fuel oxidation. By integrating computational chemistry, kinetic modeling, and molecular beam mass spectrometry techniques, my group aims to clarify the often poorly understood chemical kinetics of fuels. This approach allows us to understand the kinetic pathways for fuel breakdown, focusing on the role of several key combustion radicals, which drive the chain reactions of combustion. These radicals can often exhibit unexpected behaviors and are particularly challenging to quantify. In this talk, I highlight recent experimental advances in detection of molecular combustion products, and how we implement those advances in tandem with our computational chemistry efforts to better understand the fundamental chemistry of fuels. First, we discuss how a pre-production prototype of the KMLabs Hyperion VUV™ has allowed for one of the first tunable VUV-PIMS studies of molecule isomerization within a university laboratory setting. This prototype was the key factor for the first ever experimental confirmation of the keto-enol tautomerization of acetone. Next, we highlight how through hybrid additive manufacturing and traditional manufacturing techniques, our group has developed new casting methods for silicon carbide at small scales. This has resulted in a new microreactor with which we can carefully control experimental conditions for our pyrolysis studies. And finally, we implement these techniques in a study of propionic acid, the primary reaction byproduct of an important ethyl ester biodiesel component, ethyl propanoate.

Nicole J. Labbe
Assistant Professor
Department of Mechanical Engineering
University of Colorado Boulder

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https://uark.zoom.us/j/89444434013?pwd=b003SW5ha3ZyaFRXAUpS2xPWVVVdz09

Dr. Nicole J. Labbe is an Assistant Professor of Mechanical Engineering at the University of Colorado Boulder. She received her Ph.D. in Chemical Engineering from the University of Massachusetts Amherst in 2013. Before joining the faculty at the University of Colorado in 2016, Professor Labbe was a postdoctoral associate in the Chemical Sciences and Engineering division of Argonne National Laboratory. Professor Labbe's research focuses on several areas of gas phase chemical kinetics, especially in the areas of theoretical chemistry and reaction rate theory, combustion kinetic modeling and combustion dynamics, pollution control and renewable liquid fuel design.