**The Importance of Reaction Mechanisms in Combustion**

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**Abstract**

Despite accelerating electrification efforts, the United States Energy Information Agency projects that, for the foreseeable future, liquid hydrocarbons and biofuels will continue to provide greater than 95% of transportation energy needs through 2050. Moreover, outside of the U.S., the European Union has set a target of 27% for renewable energy in the transportation sector, as proposed in the *2030 Framework for Climate and Energy*, which is stated to be met only by partially or completely replacing fossil fuels with biofuels. Building on the global recognition that combustion-derived energy will remain critical to the transportation sector, continued development of advanced combustion technologies plays a meaningful role in sustainably meeting rising energy demands and also in the mitigation of air quality and climate impacts.

Underpinning this effort is the need to understand fundamental chemistry and physics of fuel-engine interactions for the purpose of enabling predictive modeling capabilities to accelerate the pace of new technology creation. As one major example, advanced compression-ignition strategies offer a means for achieving low-emission, high-efficiency combustion. These strategies, which include gasoline direct-injection, among others, rely extensively on predictive chemical kinetics of hydrocarbons and biofuels. Accordingly, understanding fundamental reaction mechanisms of classes of molecules such as *n*-alkanes, cycloalkanes, and oxygenated hydrocarbons remains essential.

Results from several recent studies on hydrocarbon and biofuel oxidation mechanisms are discussed in the context of two primary topics: ignition and pollutant formation. Examples include understanding the balance of products that form from hydroperoxy-substituted carbon-centered radicals (Q̇OOH) as a function of with O2 concentration, analysis of stereochemical effects on cyclic ether reactions for the purpose of minimizing mechanism truncation error, and a recent discovery that shows a connection between the formation of organic aerosol within the low-temperature combustion region that arises from peroxy radical-mediated chemical kinetics. The results are followed with a perspective on some research questions that support continued progress on sustainable energy and on the importance of reaction mechanisms in combustion.