Study paves way for new biofuels models, technologies

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Biofuels hold promise as environmentally friendly sources of renewable energy, but which ones should industry and policy leaders focus their efforts on developing? A new study involving researchers from North Carolina State University offers detailed insights into how biofuel chemicals react when burned. Their data and new computer models pave the way for development of new biofuels and technologies to maximize energy efficiency while minimizing environmental and human health risks.

"Biofuels are a sensible choice as a renewable energy source, but of course there are complications," says Dr. Phillip Westmoreland, a co-author of the study, professor of chemical and biomolecular engineering and director of the Institute for Computational Science and Engineering at NC State. "All of the biofuels have pros and cons, and you can't manage or plan for use and risks unless you understand them enough."

The new paper helps define these risks by finding the network of chemical steps that take place when biofuels are burned. An invited overview for *Angewandte Chemie*, one of the world's premier chemistry journals, the paper draws on landmark research conducted by Westmoreland and his co-authors from research institutions in the United States, Germany and China.

"By studying individual chemicals that make up biofuels, we were able to explain what emissions result from burning real biofuels," Westmoreland says. "We can measure the individual intermediates and

chemical reactions, helping us craft models that reveal what chemicals are emitted, and in what amounts, by various biofuels. These models can be used to design new engines, new fuels and new policies that foster environmentally sustainable and efficient energy solutions.

"This is important for regulation, where policy makers are weighing the environmental and health costs versus the energy benefits of different biofuels, but it is also essential to decision makers in the business community. Industry does not want to invest in developing biofuels and related technologies that can't pass policy muster, and this research will help them make educated investment decisions."

The paper draws on information the researchers have collected about the chemicals produced when biofuels are burned, and how those chemicals change during the combustion process. These insights stem from the use of a novel experimental apparatus the researchers built at Lawrence Berkeley National Laboratory and a second system in Hefei, China - which provide unprecedented detail as to exactly what is happening at a molecular level when biofuels are burned.

More information: The paper, "Biofuel combustion chemistry: from ethanol to biodiesel," is the featured cover article in the May 3 issue of Angewandte Chemie.

Provided by North Carolina State University