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Tailoring biofuels to meet the needs of current and advanced combustion engines

By Mike Janes

At a Sandia-led workshop late last year, transportation industry experts concluded that research into advanced biofuels and combustion engines needs to be much more closely coupled in order to accelerate the transition to biofuels for the transportation sector.

With an LDRD-funded project titled "Tailoring Next-Generation Biofuels and their Combustion in Next-Generation Engines" that assimilates the engine and combustion-chemistry expertise of Craig Taatjes (8353) and John Dec (8300) with that of biochemist Masood Hadi (8634), Sandia is, quite literally, putting its money where its mouth is.

"Everyone knows about the gap that has existed between biofuel developers and producers and engine combustion researchers, but it's been a hard gap to bridge," says Craig. "Sandia, however, is a unique institution, which affords us the opportunity to work side-by-side on this issue."

The issue Craig refers to is the development of a biofuel that will work well in an internal combustion engine.

The biofuel material being investigated for this project, says Masood, are types of fungi known as endophytes that live between plant cell walls. Professor Gary Strobel from Montana State University, a collaborator on the project, is an expert in such fungi, some of which have already been used to make chemicals such as Taxol (an anti-cancer drug). The cellular material in plant walls contains molecules that can be converted into hydrocarbon compounds that work well as fuels for internal combustion engines. Some of these are similar to the hydrocarbon compounds found in petroleum-derived fuels.

The beauty of the endophytic fungi, Masood says, is that there is no need for the cost-intensive industrial processes that are typically required to break down biomass. "These things can turn cellulosic material directly into fuel-type hydrocarbons themselves without any mechanical breakdown," he points out.

These fungi, in other words, are designed by nature to grow on cellulose and to digest it, forming fuel-type hydrocarbons as a by-product of their metabolic processes. Through genetic manipulation, the Sandia team hopes to first identify these pathways, and then to improve the yield and tailor the molecular structure of the hydrocarbons it produces.

"This is the only organism that has ever been shown to produce such an important combination of fuel substances," says Professor Strobel in a Society for General Microbiology press release, referring to *Gliocladium roseum*, an example of the type of endophytic fungi used in this project. "The fungus can even make diesel-fuel compounds from cellulose."

Finding a fuel-friendly mix of molecules

Masood's team, which includes Eiza Yu (8632) and Mary Tran-Gyamfi (8634), is using genetic sequencing and other molecular biology techniques to understand how changes in feedstock determine the type and amount of hydrocarbons the fungi make, with a long-term goal of engineering greater quantities of the desirable fuel species. Craig and John, meanwhile, are able to experiment with the main compounds produced in the molecular "soup" and give feedback to Masood's team on their ignition chemistry and engine performance. The ideal outcome, John says, is to "dial in" the right feedstocks combined with the right set of genes to produce the preferred blend of compounds to go into an engine.

The first step has been to learn what kinds of compounds the fungus makes naturally on its own. "There is a large spectrum of compounds present, but many of them – octane, for example – are already well understood with regards to their combustion chemistry," says Craig. "Others, we just don't know much about, so we need to do research on their ignition chemistry and how they behave in an engine." He adds that "before the biologists start modifying the fungus, the natural products will already give us specific targets to investigate from a fundamental chemistry point of view."

The team, Craig says, is working with Professor William H. Green at the Massachusetts Institute of Technology to develop an ignition chemistry model for the class of compounds made by the fungi.

John says the fungus offers good versatility with respect to the variety of fuel-like molecules it provides for possible engine experimentation.

Masood and his colleagues are doing their part to build up the understanding of the spectrum of molecules produced by the various fungi, at which point they can genetically tailor them to produce more of the "right" kinds of compounds that suit the needs of engine combustion. Initially, the team will purchase (from commercial sources) the main compounds produced by the fungus so that chemistry and engine testing can proceed simultaneously with development of the fungus and production techniques.

Eventually, the team anticipates that enough hydrocarbons will be extracted from those produced by the fungus to test in the lab, or even in an engine. “We hope, in the end, to have a biofuel that was developed in conjunction with the development of the combustion model for that biofuel,” Craig says.

John, who runs the homogeneous-charge compression ignition (HCCI) lab at Sandia’s Combustion Research Facility (CRF), says experiments on the HCCI platform offer good fundamental information on fuel auto-ignition behavior that can be related to performance in other engine types such as spark-ignition or diesel. HCCI engines can operate using a variety of fuels, making HCCI a good starting point for the experimentation and chemical measurements necessary for a project of this type.

Engine, biofuels collaboration a no-brainer

Craig, John, and Masood all say that it makes perfect sense for Sandia to invest in a project that focuses on an engine’s interaction with a new biofuel.

“Any fuel that’s going to make it in the marketplace is going to have to blend with gasoline,” John says. “A new biofuel, whether it comes from the *Gliocladium* fungus or another source, will be more useful commercially if we have first learned how it will affect combustion processes,” adds Masood.

While Craig and John both note that there are a broad range of other technical issues that engine manufacturers must test and worry about in addition to ignition chemistry, the success of this project will prove important as the industry works toward developing biofuels that can displace petroleum in the long term.

Masood says the project is unique to his team for a couple of reasons.

“This is completely out of our comfort zone, but in a good way,” he says with a smile. “Although we know how to grow things in the lab and can manipulate DNA, we’ve never worked with an endophytic fungi before. Plus, working with the combustion experts is new to us.”

On the combustion side, Craig says the usual model would be for Sandia’s engine researchers to receive a potential new fuel to work with and simply asked to “figure out” whether it was viable for a combustion engine. With this project, he says, the combustion experts are working directly with the biofuels researchers to understand from the start just what will work best as fuel for internal combustion engines. “We have a rare opportunity to decide ourselves what the fuel is going to look like and can build our own optimization loop.”

“There is a whole new range of potential fuels now with biomass,” says John. “These biofuels are going to have to be compatible with existing engines, since you’re just not going to get something into the marketplace that requires both a completely new fuel and a new engine. So the new fuels will have to work well with both existing engines and advanced engines like HCCI or low-temperature diesel combustion. Only then will you be able to sell the fuel at the pump and get your new high-efficiency, low-emissions engine into the marketplace."

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