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Thermochemical integration key to improving the efficiency of bio-ethanol production

A recently concluded CRF study has revealed the important role of combustion in the efficient operation of cellulosic ethanol plants for producing biofuels. Unlike 'first-generation' ethanol derived from the fermentation of sugar or starch sources (such as corn), future production of ethanol in the United States is expected (and indeed is federally mandated) to increasingly utilize lignocellulosic biomass such as crop residues, fast-growing wood, or herbaceous energy crops. Lignocellulosic biomass sources generally do not compete with the production of food crops and also offer much lower effective carbon emissions than current bio-ethanol and biodiesel sources. Research and development of this 'second-generation' ethanol process is largely focused on making improvements to the biochemical processes that convert cellulose and hemicellulose polysaccharides to sugars that are fermented to ethanol.

However, as shown in Figure 1, typical lignocellulosic biomass sources only contain 60–70% polysaccharides, so optimization of second-generation bio-ethanol production also requires that the remainder of the biomass, predominately lignin, be effectively utilized.

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Characterizing the development of thermal stratification in HCCI engines

Homogeneous charge compression ignition (HCCI) engines can deliver high efficiencies—comparable to a diesel engine or higher—and ultra-low NO_x and particulate emissions. They also offer the potential for lower cost than diesel engines and do not require expensive diesel-emissions aftertreatment for a significantly lower overall package price. HCCI is therefore well suited for future transportation engines; however, the limited power output of these engines is a barrier to their widespread implementation. This load limitation occurs mainly because the cylinder-pressure rise rate (PRR) with combustion increases with increased fueling, eventually becoming so rapid that it causes excessive noise (knock) and even engine damage.

Although the name HCCI implies a homogeneous charge, the charge is never fully homogeneous in practice because heat transfer during the compression stroke combined with convective transport creates thermal inhomogeneities even if the fuel and air are well mixed. This thermal stratification causes combustion to occur sequentially as various parts of the charge reach their autoignition temperatures at different times when they are compressed by the piston. This reduces the combustion rate (and therefore the maximum PRR), allowing considerably higher fueling rates without knock than would have been possible with a fully homogeneous charge. Moreover, computational studies have shown that even modest increases in the thermal stratification, above that which occurs naturally, can allow significantly higher loads without knock. To move toward this goal, it is first necessary to understand the sources and mechanisms responsible for naturally occurring thermal stratification.

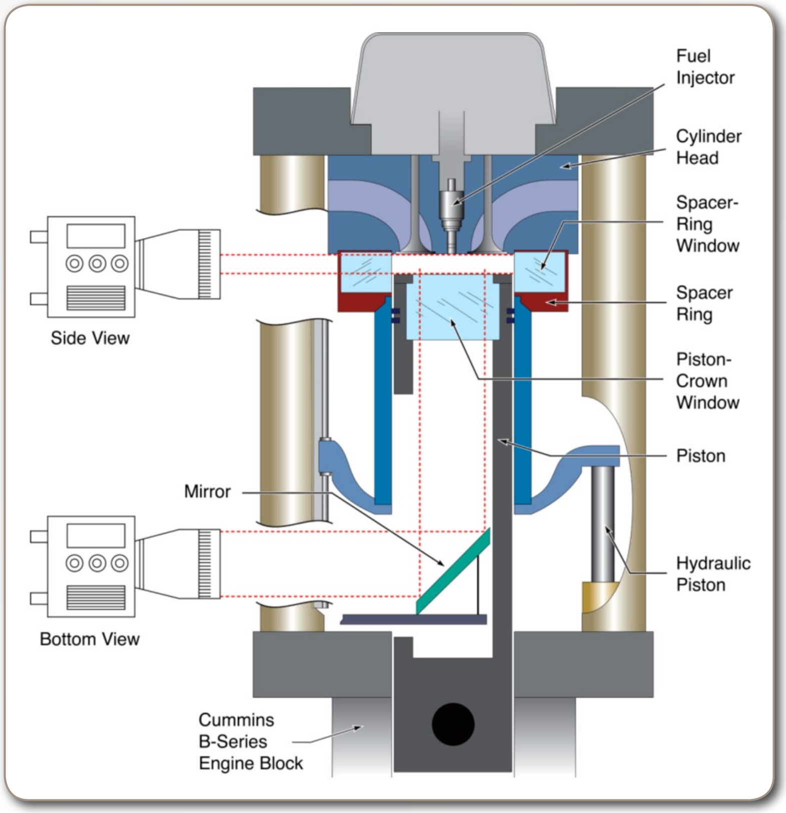

***Figure 1.** Schematic of the optically accessible HCCI research engine.*

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Newsletter

Thermochemical integration key to improving the efficiency of bio-ethanol production

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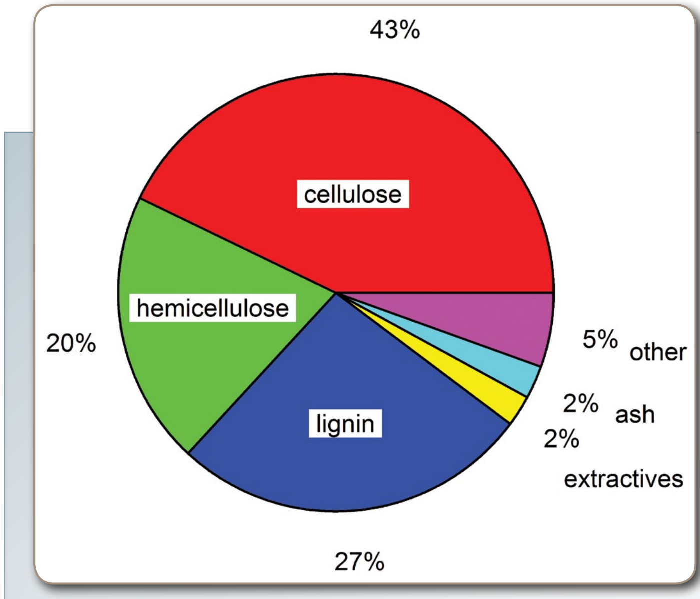

Figure 1. Typical composition of a softwood tree, in this case hybrid poplar.

The research project, funded under Sandia's Laboratory Directed Research and Development (LDRD) program, evaluated the combustion properties of practical lignin residues produced by several alternative approaches to bio-ethanol production ("Combustion properties of biomass lignin residues determined," *CRF News*, March/April 2011) and also analyzed efficiency losses in a representative bio-ethanol plant configuration.

Andy Lutz and postdoctoral researcher Kwee-Yan Teh analyzed the energy and exergy balances of a prototypical lignocellulosic biochemical ethanol plant design in which the lignin residue is burned to produce steam that is required for heating during the feedstock pretreatment and ethanol distillation processes. A schematic of the modeled system is shown in Figure 2. The performance parameters for each of the primary system processes were taken from a 2009 National Research Council study that evaluated current state-of-the-art technology as well as possible process improvements that may be attainable in the future.

The results of the energy and exergy analyses for the current state-of-the-art cellulosic ethanol plant performance are shown in Figure 3. The energy balance shows an ethanol production energy efficiency of 30%, with extensive heat losses accounting for most of the process inefficiency. The exergy analysis, which provides a more detailed evaluation of system inefficiencies, reveals that the lignin residue combustion steam cycle itself is the ultimate source of most of the inefficiency. However, extensive steam production is currently needed in cellulosic ethanol plants to provide the necessary heating for process components such as biomass pretreatment and ethanol distillation, so this exergy loss is somewhat unavoidable.

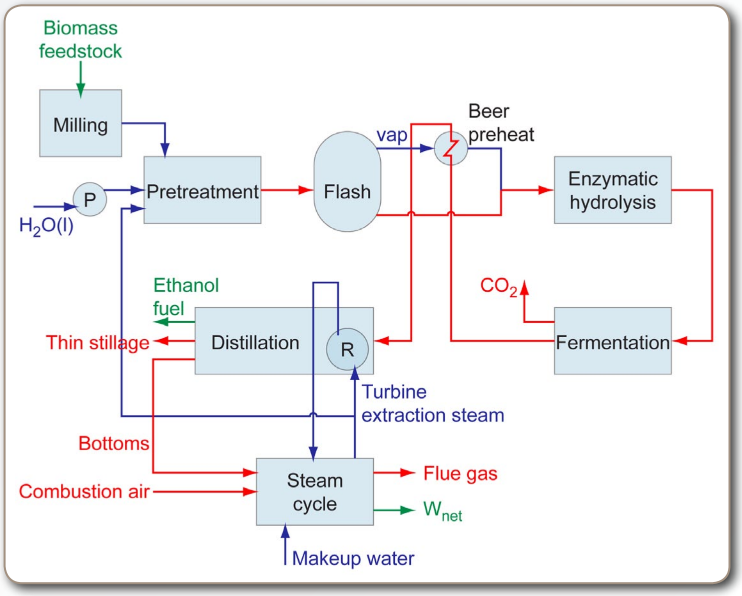

Figure 2. Schematic of the modeled, prototypical lignocellulosic biochemical ethanol plant, utilizing separate enzymatic hydrolysis and fermentation steps.

Future bio-ethanol process efficiency improvements are expected to occur in reducing the temperature of pretreatment (thereby lowering its demand for steam) and in the development of low-energy approaches to ethanol distillation such as membrane vapor permeation technology. With these innovations, the exergy analysis reveals a significant opportunity to improve the overall process efficiency through enhanced utilization of the lignin residue, for example by generating additional fuel products via pyrolysis or gasification.

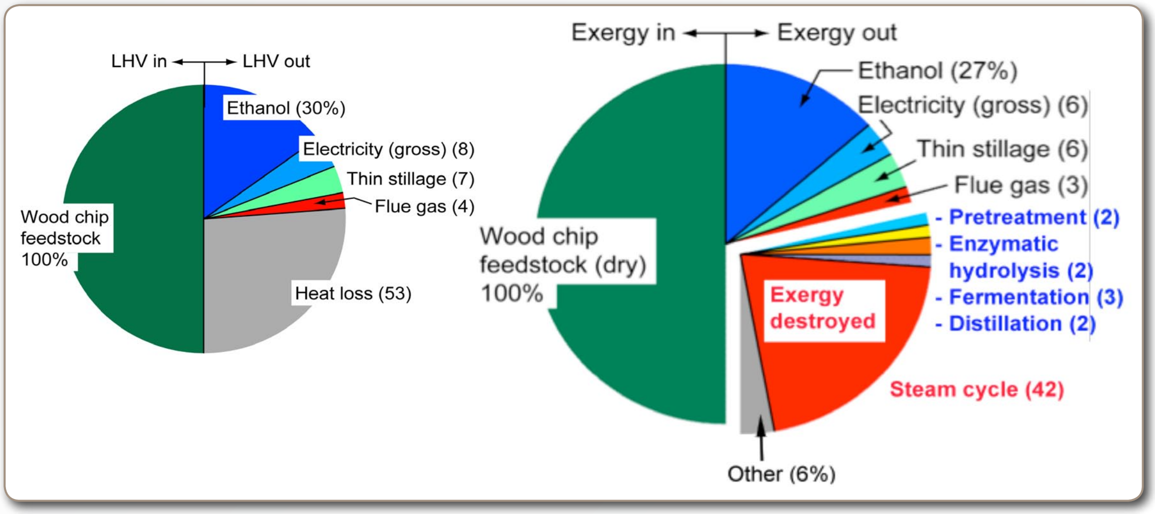

Figure 3. Energy inputs and outputs (on the basis of lower heating value, left pie chart) and exergy inputs and outputs (right pie chart) for the conventional technology biochemical process design case.

COMBUSTION RESEARCH FACILITY VISITOR PROGRAM

Darwin Arifin and Torrie Aston, visitors with Tony McDaniel

Torrie and Darwin are part of an ongoing collaboration between the CRF and students from the University of Colorado, Boulder.

Brian Fisher, post-doc with Chuck Meuller

Brian Fisher worked as a post-doctoral research fellow in the Alternative Fuels Optical Engine Laboratory with Chuck Mueller. Their work focused on gaining an improved understanding of how fuel, injection-system, and in-cylinder thermodynamic properties affect the maximum distance that liquid-phase fuel penetrates into the combustion chamber of a heavy-duty, direct-injection, diesel-cycle engine. Brian is leaving Sandia to join the Department of Mechanical Engineering at the University of Alabama in Tuscaloosa as an assistant professor.

Sebastian Kaiser, visitor with Dick Steeper

Sebastian, the principle investigator in Sandia's Hydrogen Engine lab, took a distinguished German academic position last year. He has returned to complete the hydrogen research project. He is also involved with the Engine Combustion Network, an international effort initiated by Lyle Pickett to advance engine research through cooperative experiments and simulations. Sebastian is building up a new engine lab at the University of Duisburg-Essen.

Peter Lillo, visitor with Lyle Pickett

Peter Lillo finished his B.S. in Mechanical Engineering at U.C. Berkeley and joined Sandia as a student intern. Peter worked with Chuck Mueller, Chris Polonowski, and Brian Fisher last summer to study the behavior of flame lift-off length in diesel engines. Since January, he has conducted research with Lyle Pickett on locating the position of diesel ignition as a function of ambient gas temperature. His work supports activities of the Engine Combustion Network (www.sandia.gov/ECN) for the "Spray A" condition. Peter will continue engine research studies this fall at the University of Michigan, beginning a PhD program advised by Prof. Volker Sick.

Photos by Daniel Strong

Of blackboards and computer screens: scientific programming in the 21st century

Since he was a college student, Damian Rouson has been fascinated by the intersection of science and computing. Computers have transformed scientific research, yet the fields still exist in separate planes. He takes on the challenge of rendering computer languages, so vital to scientific advancements, more expressive and easier to read in a new book *Scientific Software Design: The Object-Oriented Way*, published by Cambridge Press this spring.

Everyone is familiar with old black-and-white photographs of physicists working out difficult theories at a blackboard. To the layman, those cryptic equations strewn across the board look like gibberish, but to fellow scientists it is a perfectly understandable code. These scientists used common mathematical expressions that provided a concise, expressive, and clear way of communicating the intricacies of their abstract theories.

The 21st-century equivalent of the blackboard could be the computer screens that are so much a part of today's world. Complex computer programs are used in most of today's scientific research. However, the commonly understood mathematical symbols from 50 years ago have given way to incredibly complex computer languages that often look like gibberish even to fellow scientists. Most computer languages such as Fortran and C++ are not expressive: code written in these languages is hard to decipher even to fellow researchers.

Photo by Daniel Strong

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Damian Rouson
Jim Xia
Xiaofeng Xu

SCIENTIFIC SOFTWARE DESIGN
The Object-Oriented Way

Characterizing the development of thermal stratification in HCCI engines

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To address this challenge, CRF researchers John Dec and Nicolas Dronniou, previous CRF researcher Wontae Hwang, and visiting researcher Jordan Snyder from Stanford University have been working to provide a fundamental understanding of the in-cylinder processes related to thermal stratification. Using an HCCI engine modified for optical access (see Figure 1), they applied planar imaging thermometry to obtain two-dimensional temperature maps (T-maps) in various parts of the charge. The thermal imaging diagnostic is based on the temperature sensitivity of planar laser-induced fluorescence (PLIF) of toluene tracer added to the fuel and excited by a 266-nm UV laser. As indicated in Figure 1, two optical configurations were used: (1) a horizontal laser sheet with the PLIF image acquired through the piston-crown window (bottom view), and (2) a vertical laser sheet with the PLIF image acquired through a side window at the top of the cylinder wall (side view).

Because previous research ("Imaging thermal stratification in HCCI engines," *CRF News*, March/April 2006) has shown that the most critical thermal stratification for controlling the PRR is that occurring within the bulk gas, the researchers first studied the development of bulk-gas thermal stratification using the bottom-view optical configuration. Figure 2 shows a temporal sequence of T-map images in the mid-plane of the combustion chamber during the latter part of the compression stroke. Initially, the bulk-gas temperature is nearly uniform, but beginning at about 330–340 crank angle (CA) degrees some colder regions begin to appear. The number of these cold pockets and their temperature difference from the hotter regions continue to increase through the remainder of the compression stoke. As a result, when autoignition occurs near the end of the compression stroke, significant thermal stratification is present in the central bulk gas, as evident in the 360° top dead center (TDC) image in Figure 2.

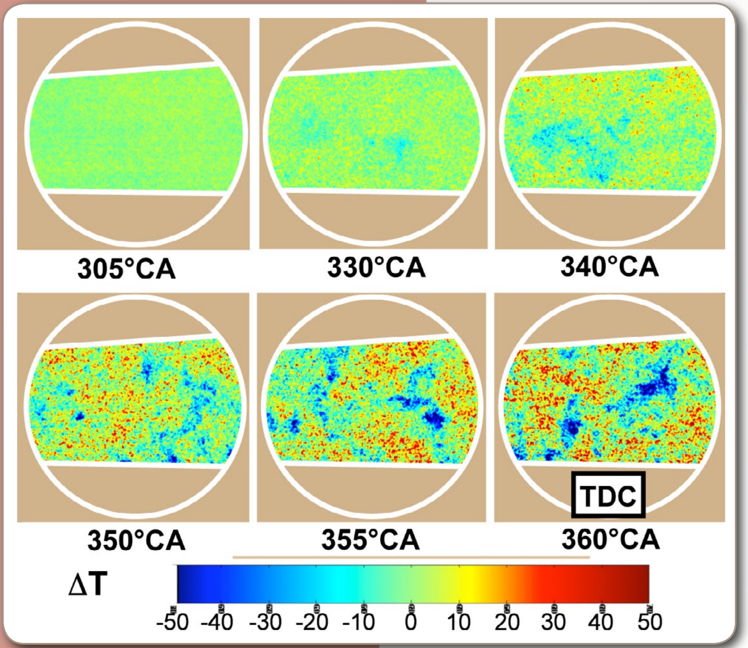

Figure 2. Temporal sequence of T-map images at the mid-plane of the pancake combustion chamber. The white lines define the limits of the laser sheet and the 70-mm diameter field of view through the piston-crown window. The crank angle after top dead center of the intake stroke is given at the bottom (360° CA = TDC compression). Each image is from a separate engine cycle and has been selected as being representative of a set of images at that crank angle. The false color of the images shows the variation in temperature relative to the mean of each image as indicated by the colorbar.

Although the mid-plane images in Figure 2 are representative of the central bulk-gas, it is also important to understand how the thermal stratification changes for the regions nearer the wall. Figure 3 shows a spatial sequence of T-map images at TDC acquired as the laser sheet was traversed from the mid-plane (z = 4 mm) to a position 0.8 mm from the cylinder-head surface. These results show that the amount of thermal stratification is similar from the mid-plane to a plane half way to the wall (z = 2 mm), but beyond this half-way position (z < 2 mm), the temperature variation within the T-maps increases significantly. The T-maps in Figure 3 also show that in this outer boundary-layer region (2 mm ≤ z ≤ 0.8 mm), the character of the thermal stratification has changed. Rather than the more round individual cold pockets in the central region, the cold zones now appear as more narrow elongated regions that are suggestive of vortex tubes, which could be responsible for transporting the colder fluid very near the wall into the bulk gases.

To further study the transport of cold near-wall gases into the central region, side-view images were acquired. Figure 4 shows an example of a typical side-view T-map acquired at TDC. This single-cycle image shows considerable thermal stratification throughout the charge; however, side-view T-maps averaged over multiple cycles show no thermal stratification beyond thin boundary-layer regions, indicating the random (turbulent) nature of the cold-gas regions that extend beyond this thin boundary layer into the bulk gas. Another key finding from Figure 4 is that virtually all the

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Thermal stratification

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cold-gas regions in the central charge are parts of larger cold-gas structures that extend from the cylinder-head or piston-top surfaces. This finding agrees well with the near-wall images of Figure 3, suggesting that the cold-gas structures in Figure 4 are cuts through vortex tubes that convect the cold near-wall gases into the central region. Continuing the development of this three-dimensional picture, these results also show that the thermal stratification in the mid-plane images in Figures 2 and 3 does not consist of isolated cold pockets, but results because these images are cut planes through the tips of the turbulent cold-gas structures in Figure 4.

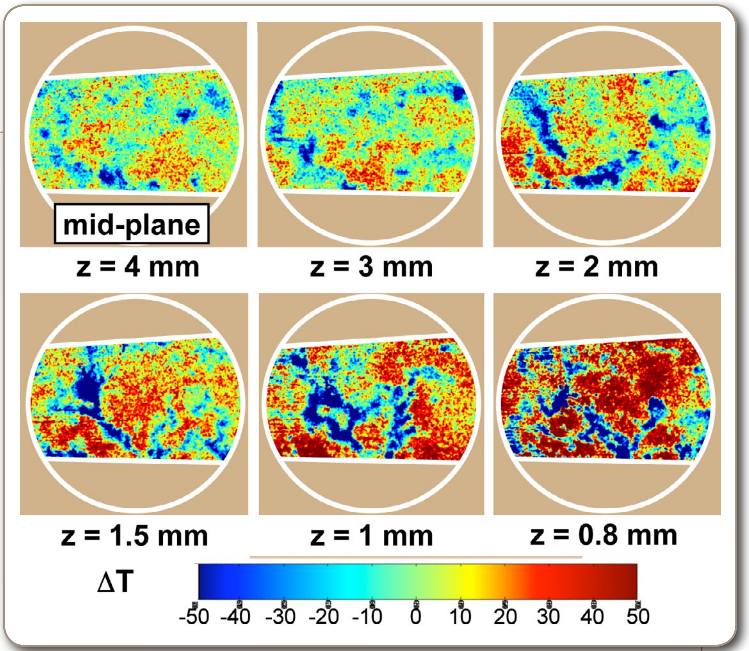

Figure 3. T-map image sequence from mid-plane to near the wall at 360° CA. The "z" value below each image gives the distance of the image plane below the cylinder head.

These combined results greatly increase understanding of the mechanisms responsible for producing thermal stratification in HCCI engines. They suggest that the thermal stratification primarily results from convective transport by large-scale turbulent vortices (eddies), and that the quest to enhance the thermal stratification to obtain higher loads without knock should focus on methods to supplement these flows. Toward achieving this, a two-pronged approach is planned in which advanced Large Eddy Simulation (LES) modeling will be applied to help guide experimental efforts.

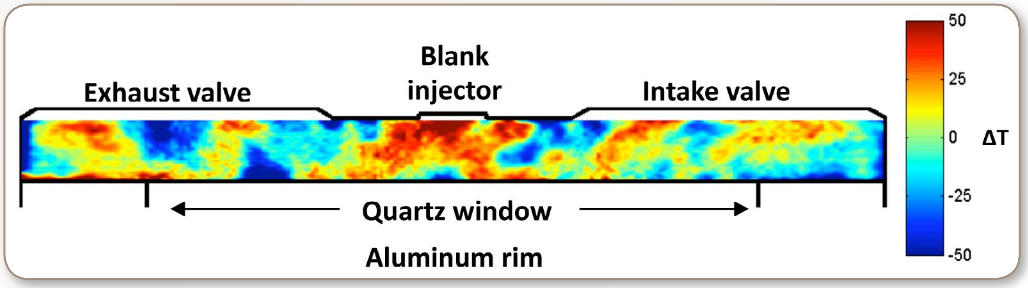

Figure 4. Side-view T-map image showing the thermal stratification in the bulk-gas and near-wall regions at TDC (360° CA).

Of blackboards and computer screens

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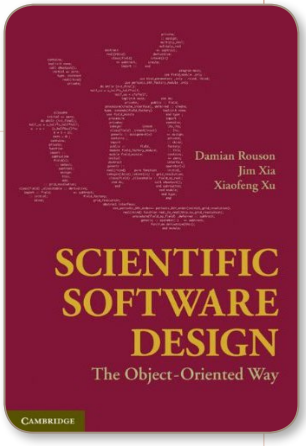


"This book comes out of my experience as a graduate student, 15 years ago," Damian explains. "I took a class in software engineering from the computer science department, and none of the examples used in the class had any relationship to science. By contrast, if you take scientists, even those who are computationally oriented, they really don't talk about the writing of the program. They talk about the mathematical algorithms and it's assumed that the translation of the basic algorithm into code—into a program—is straightforward and doesn't deserve much discussion. They don't get down to the practices for writing the code."

The expressive style of programming outlined in the book provides a way to shorten the development time dramatically, because researchers can use familiar expressions, what they'd write on the blackboard. "That can be translated directly into code that runs on these massive platforms," says Damian. "You ultimately can get the same level of speed and scalability with the code, but you can shorten the development cycle—the time it takes you to get there."

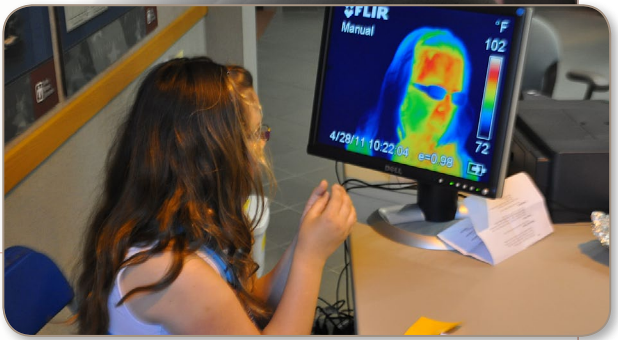
With this book, he hopes to introduce design by way of diagramming in a way that most scientific programmers don't currently use; a very up-to-date version of Fortran, also not yet in use by most scientific programmers; and the expressive style of programming. "The idea is to go behind the curtain and see how, by using some nice features of modern programming languages, you can give yourself that same level of expressiveness," he says.

Now that the book is published, Damian is moving into a new phase of research. The first was developing the style of programming itself. The second was demonstrating that it can produce publishable science—in other words, papers that focus on the science, not the code. "This third phase is showing that we can get it to scale; that we can write, not just pretty code, but fast code; and that some of what makes it pretty also makes it fast," he says.

Future scientists explore Sandia and the CRF

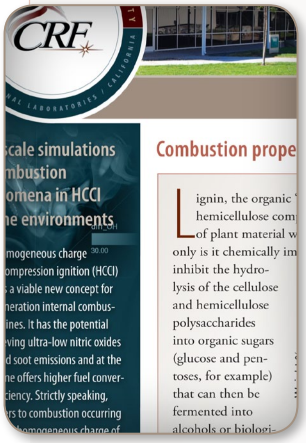
On April 28, nearly 200 daughters, sons, and family friends spent the morning at Sandia's California laboratory with their parents, getting a look at where mom and dad work and engaging in activities around the site. As always the CRF was a major player, staging several popular demonstrations and exhibits. Older children had the opportunity to build and program Lego Mindstorm robots in the mezzanine, and the "nano" spaghetti demo was a big hit. Perhaps the most exciting attraction was the opportunity to ride on the hydrogen-powered bus.

CRF staff member Isaac Ekoto (Hydrogen and Combustion Technology) and post-doc Ajith Mascarenhas (Reacting Flow Research) spoke to students at presentations arranged by the Sandia Women's Connection, which offered the chance for middle-and high-school students to meet science, engineering, and technology professionals and learn about their careers, with an emphasis on workforce diversity.



Photos by Daniel Strong

Announcing the launch of *CRF News* 2.0



After nearly 32 years of publication history, the CRF News will be moving to a new, interactive, online publishing format this fall. While this bi-monthly newsletter will no longer be printed and mailed to subscribers after the July/August issue, continually updated news, stories, technical articles, and information will be available at the CRF website: ***https://share.sandia.gov/crf/.***

If you would like to receive occasional news and updates from the CRF, please send an email with the subject: **CRF News** to ***kmcwill@sandia.gov*** to be included in our confidential subscriber database. We hope that the *CRF News* has been a good source of information and thought-provoking technical articles on a variety of subjects. Our new web-based format will be be a convenient and easy-to-use way to keep up with the latest goings-on at the CRF. Thank you for your support over the years!

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