COMSOL NEWS

THE MULTIPHYSICS SIMULATION MAGAZINE

Modeling and Simulation for
EVERYONE

P. 4

COMSOL

HOW DO I CREATE THE BEST DESIGN AND SHARE MY SIMULATION EXPERTISE?

That is the question that engineers, designers, and researchers often ask themselves. This issue of *COMSOL News* is dedicated to them, as we discuss the paradigm shift happening in the simulation industry, which began with the release of COMSOL Multiphysics® version 5 and the Application Builder.

As you will find out if you jump directly to page 4, sharing your simulation expertise in an easy and efficient way is now possible using the Application Builder. Experts can now build simulation apps—specialized user interfaces to access their models. These COMSOL users are motivated by their relentless drive for innovation and are leveraging new modeling tools that are customizable, adaptable, and accurate in their handling of the physics involved. They are also sharing their work in such a way that anyone can benefit from it. That's when the ability to build a simulation app fuels the shift towards "modeling and simulation for everyone".

And how can we create the best design? With the right tools, of course, and by learning from our peers. In this edition of *COMSOL News*, we cover the work of simulation experts from a wide range of industries. Food processing at Nestlé, building physics and architectural design at Newtecnic, corrosion protection in automotive applications at Daimler, laser-matter interaction at Lawrence Livermore National Laboratory, 3D printing at TNO, and many more.

We appreciate the generosity of COMSOL users who have shared their modeling work and best practices. It has been inspiring to work with them and we hope you will find the stories here useful. ❖

Enjoy!

Valerio Marra
Technical Marketing Manager
COMSOL, Inc.

INTERACT WITH THE COMSOL COMMUNITY

BLOG comsol.com/blogs
FORUM comsol.com/community/forums
LINKEDIN linkedin.com/company/comsol-inc.
FACEBOOK facebook.com/multiphysics
TWITTER twitter.com/comsol_inc
GOOGLE+ plus.google.com/+comsol

We welcome your comments on *COMSOL News*; contact us at info@comsol.com

COMSOL NEWS
2015

CONTENTS

FEATURED

TNO
VIRTUAL MATERIAL DESIGN IN 3D PRINTING MAKES HEADWAY WITH MULTISCALE MODELING

22

DAIMLER AND HZG
DEFENDING AUTOMOTIVE COMPONENTS AGAINST CORROSIVE DESTRUCTION

14

Simulation of hybrid material car components and joints enables innovative design for corrosion protection in automotive applications.

MTC
OPTIMIZING SHAPED METAL DEPOSITION TECHNIQUES WITH SIMULATION APPS

5

Researchers at the Manufacturing Technology Centre use simulation apps to explore the 3D metal printing technique shaped metal deposition (SMD).

36

FRAUNHOFER ISE
BETTER WAYS TO HEAT AND COOL BUILDINGS

Modeling and Simulation for
EVERYONE

by **SVANTE LITTMARCK**

Scientists like Newton, Maxwell, and others have given us the mathematical models, the "laws of science", that make it possible to accurately predict how physical objects and systems will develop in space and time given certain boundary conditions and initial conditions. Applied mathematicians have invented numerical methods that can generate numbers and graphics to accurately describe the solution to those laws.

This makes it possible for us to simulate, modify parameters, and ultimately make a better—if not the best—design.

The physics, the math, the computational tools, and the engineering community are all in place to achieve wonders using simulation. Sending exploration vehicles to the surface of Mars that report back to Earth and creating communication devices like cell phones and GPS are just two examples.

Many breakthrough technological innovations have seen daylight in the last several decades. But many areas that would benefit greatly from simulation remain almost untouched by the powerful computational tools available today. Why is this?

➔ THE OBSTACLES

It is a fact that current computational tools are so complicated to use that there are very few engineers trained to do it—at least compared to the number of potential beneficiaries. The setup of mathematical models needs to be done by a mathematician or a physicist. Model simplifications are necessary in order to save computational time, memory, and solution data management. Negligible phenomena should be ignored. The phenomena that should be ignored depend on the application and what is to be achieved. Understanding which physics phenomena to include, which to leave out, and how to model their effects requires a modeling expert.

Once the model is set up, solving the equations numerically means replacing the continuous differential equations with discretized difference equations and points in space and time. The discretization must be done in such a way that the solution to the difference equation converges to the solution of the differential equation. Otherwise, it has no physical meaning. Additionally, in order to obtain an accurate solution, the discretization must be fine enough. There are theories for good default numerical solver settings for many physics areas, but they are not all the same. Sometimes, it takes a numerical analysis expert to define the solver settings.

As a result, the typical user of a simulation package is someone who holds a PhD or an MSc and has several years of experience in modeling and simulation. The user also underwent thorough training to use the specific package. He or she typically works as a scientist in a big organization's research and development department. It is up to that person to employ his or her expertise to create and validate the model and the simulation results.

This all means that a small group of people is servicing a much larger group of people working in product development, design, or production. Simulation models are oftentimes so complicated that the person who implemented the model is the only one who can safely provide the input data needed to get useful output. Hence, we have a bottleneck.

➔ THE SOLUTION

In order to make it possible for this small group to service a much larger group, there is an obvious solution: Create a simulation package that makes it possible for the simulation expert to build an intuitive and specific user interface for his or her otherwise general model—a ready-to-use application. The application should include user documentation, checks for "input within bounds", and predefined reports at the click of a button. A simulation application with these capabilities makes it possible for a user to avoid accidental input errors while keeping the focus on relevant output details. The application can then be shared with a larger group of users.

Making this happen is easy compared to the achievements listed in the beginning of this article. It is happening as you read this. The spread of simulation applications will be immediate. No design engineer will want to be left behind. No company can afford to let their competitor get an advantage through earlier adoption. Eventually, consumers will be running simulation applications to make better purchase decisions. ❖

Svante Littmarck, co-founder and CEO of the COMSOL Group.

Optimizing 3D Printing Techniques with Simulation Apps

by **ALEXANDRA FOLEY**

Taking a new technology concept from research in its infancy to a qualified solution ready for industrial use requires rigorous testing and validation. Additive manufacturing (3D printing), for example, first appeared in the early 1980s with a Technology Readiness Level (a method of measuring a technology's maturity for industry use that was proposed by NASA in the 1970s) of TRL 1, and it took decades before it exploded on the industrial markets as a hot new manufacturing technique set to change the world.

➜ SIMULATING SHAPED METAL DEPOSITION

Organizations such as the Manufacturing Technology Centre (MTC) in Coventry, UK help to bridge the gap between concept and industry by providing the resources necessary to bring a design from fundamental research (TRL 1–TRL 3) to commercial use (TRL 7–TRL 9). One current endeavor at the

MTC is research into the additive manufacturing technique known as shaped metal deposition (SMD).

"SMD has multiple advantages over powder-based additive manufacturing technologies," says Borja Lazaro Toralles, Research Engineer in the MTC's Manufacturing Simulation theme, who has used COMSOL Multiphysics® software to design a model and simulation app of the SMD process (see Figure 1). "Among the benefits of SMD are higher deposition rates, the possibility of building new features upon preexisting components, or even the use of multiple materials on the same part."

Unlike other additive manufacturing techniques that use lasers to melt a thin layer of powder, SMD deposits a sheet of molten metal—which in some cases can be as expensive as titanium—that is built up layer-by-layer on a surface in a process that is similar to welding. "One of the challenges of this is that thermal expansion of the molten metal can deform the cladding as it cools, resulting in a final product that is
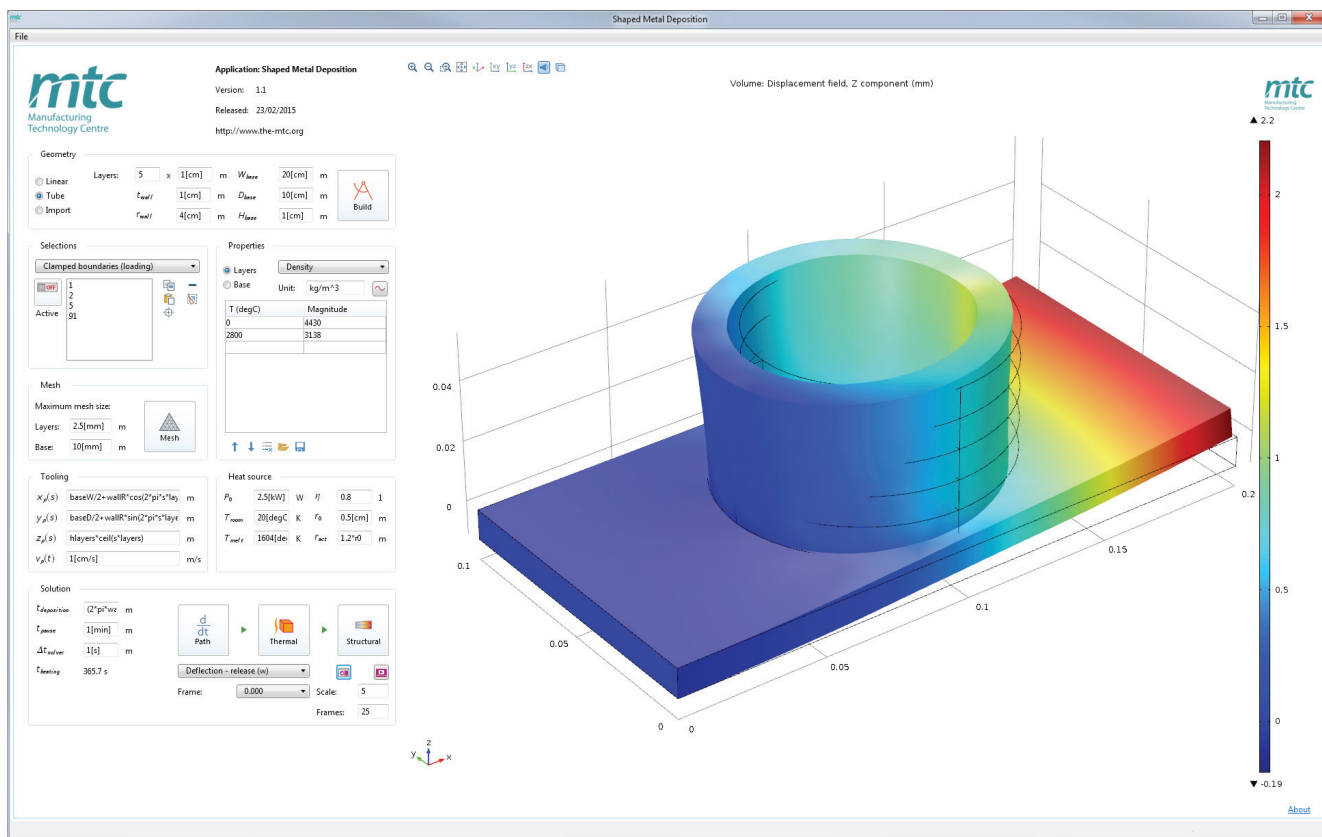

FIGURE 1. Shaped metal deposition (SMD) simulation app created using the Application Builder available in COMSOL Multiphysics. The app computes the residual stresses generated during the manufacturing process and predicts the final deflection of the part.

different than what was anticipated," describes Lazaro Toralles. "In order to predict the outcome of a proposed design, we need either to minimize the deformations or alter the design to account for them." Figure 2 shows an example of a part manufactured using SMD, where deformation occurs after six layers of deposited molten metal have been added. A model of the part, also shown in Figure 2, is used to predict the part's deflection during manufacturing, allowing the designer to update the design accordingly.

➜ COMMUNICATING COMPLEXITY WITH SIMULATION APPS

The MTC has leveraged the Application Builder in order to more efficiently communicate complex design ideas across multiple simulation and process departments, and to allow app users to easily explore the outcome of proposed designs (see Figure 1). Were it not for the simulation app, the testing and validation of a design would be significantly more time consuming and costly using physical testing alone, due to the materials used in SMD.

Simulating SMD involves solving a time-dependent coupled thermomechanical analysis that predicts residual thermal stresses and deformation, which arise from SMD thermal cycles.

"We built an app using the Application Builder that allows the user to predict whether the deposition process will produce parts that fall within their established tolerances," says Lazaro Toralles. "If not, then the app provides a user-friendly and cost-efficient way to simulate multiple variations to the input until the results achieve an acceptable final deformation."

With this app, users can easily experiment with various geometries, heat sources, deposition paths, and materials without concern for the underlying model complexities. Two predefined parametric geometries are included in the app, and a custom geometry can also be imported.

Currently, the app is being used by members of the team at the MTC who do not have the simulation experience to independently explore different parts and projects for their customers. "Were it not for the app, our simulation experts would have to test out each project we wanted to explore, something that would have decreased the availability of skilled resources," says Lazaro Toralles. "Using the Application Builder, we can now provide user-friendly app interfaces to other MTC teams." The MTC will also offer an app program for their customers.

"The use of simulation apps will help us to deploy technologies at higher TRLs for their practical use in an industrial environment," Lazaro Toralles concludes. "The Application Builder provides us with a powerful development platform through which we can package complex multiphysics models and make them accessible to the wider public." ❖
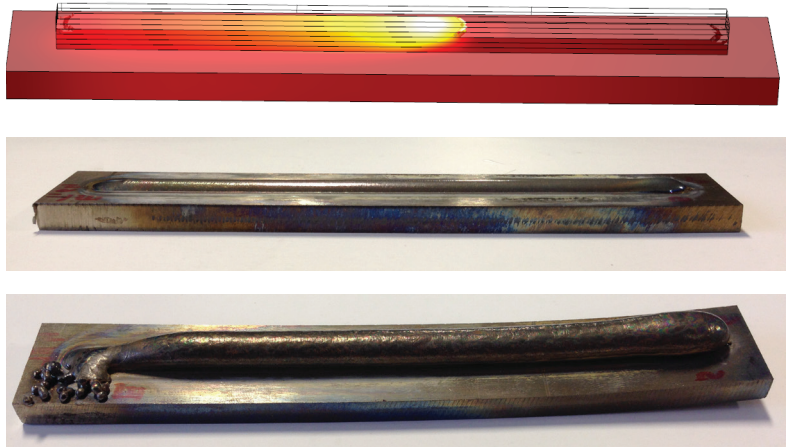

FIGURE 2. During the SMD process, thermal cycling induces residual stresses on the manufactured parts. Top: Simulation of the SMD part. Middle: The part after just one deposited layer, with no noticeable deformation. Bottom: After six deposited layers, deformation is visible to the naked eye.
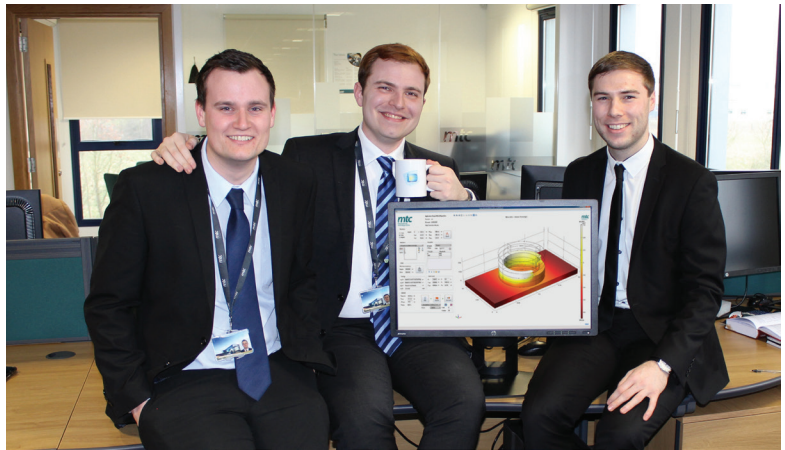
The MTC team comprising Adam Holloway (left), Borja Lazaro Toralles (center), and Willem Denmark (right) have implemented the COMSOL model, carried out experimental validation, and finally created the SMD COMSOL application.

ABOUT THE MANUFACTURING TECHNOLOGY CENTRE

The MTC provides a unique environment for developing cutting-edge technologies into manufacturing processes by bringing the UK's leading academics, engineers, and industry professionals together to develop and demonstrate new technologies on an industrial scale. This allows clients to develop new manufacturing processes in a safe, neutral industrial setting without the constraints of a commercial production environment. Their members include over 80 organizations, including BAE Systems, GKN, HP, GM, Airbus, and Rolls Royce.

APPLICATION BUILDER AND COMSOL SERVER™: A REVIEW

by **WILLIAM T. VETTERLING**

COMSOL Multiphysics® software version 5.0 introduces something new to the modeling enterprise: The Application Builder, and its counterpart, COMSOL Server™. The Application Builder allows the modeler to sweep away the detail-oriented tools that were used to produce a model and to fashion a more approachable application—an app—that is intuitive and easy to use.

The app may have a simple interface constructed with an assortment of buttons, lists, menus, graphics, and text to make its operation straightforward. It may be launched from within the COMSOL Multiphysics program. But, importantly, it may also be lifted entirely from that feature-rich environment with the help of a worldwide COMSOL Server license. In the latter case, the app may be run as a standalone application, or as a web resource within a browser.

There are many scenarios in which the Application Builder will find potential uses. With an app, modeling results may be presented in the form of live, real-time examples rather than static summaries in charts and graphs. Likewise, apps may be constructed for use in lectures or demonstrations. Companies may offer simulation apps demonstrating their product's performance, to be used in place of data sheets, or may produce licensable apps as products in their own right.

In brief, the Application Builder is a new line of communication between the professional modeling expertise of the model builder, and the science and engineering expertise of model users.

→ HOW TO BUILD AN APP

Creating an app is easy enough to try. I began with a functioning COMSOL Multiphysics model that I wanted to turn into an app. I chose to use a simple 3D model of the current distribution and heating of a multi-pixel thick-film thermal print head such as might be used in a fax machine (see Figure 1).

Voltage may be applied to selected electrodes of the print head to heat corresponding portions of a resistive film, and the purpose of the model is to discover the final temperature distribution in the film.

To implement the model as an app, I used the Application Wizard. The wizard starts with a COMSOL® software model and assembles lists of elements from the model that are suitable for use as inputs and outputs, modeling operations, and graphics.

I selected the number of electrodes and their width as inputs, a command that constructs the geometry and another that executes the model as operations, and plots of the
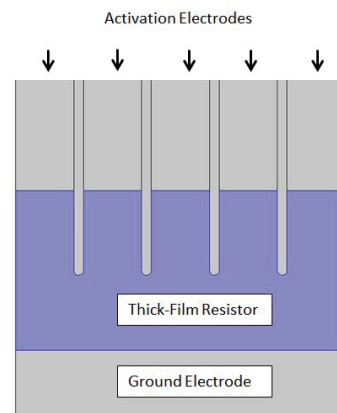

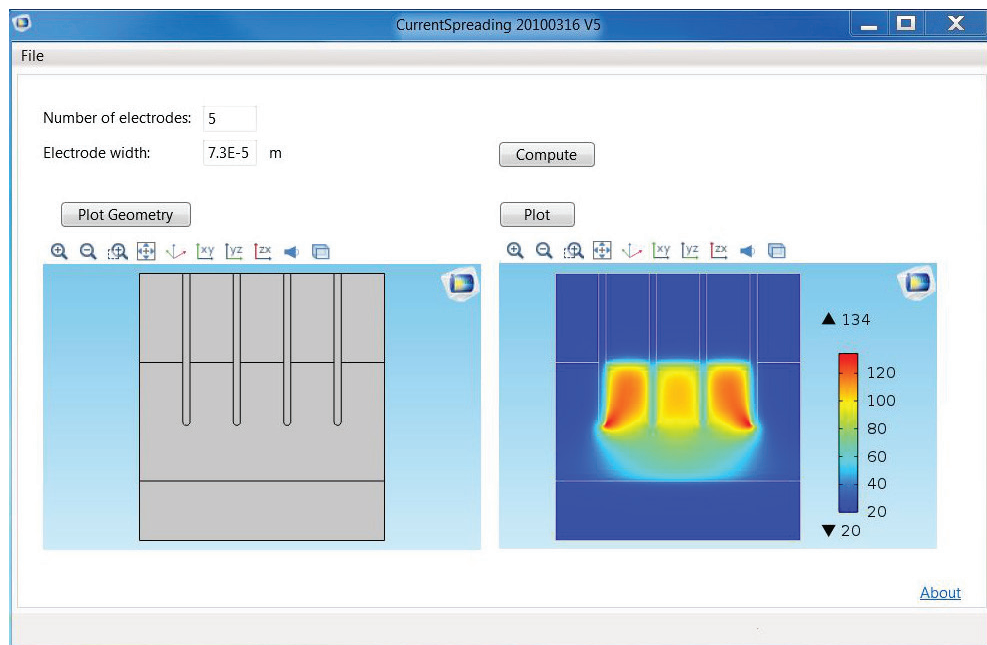**FIGURE 1.** Idealized print head schematic.

FIGURE 2. A screenshot of the app I built using the Application Wizard.

Abridged piece, originally published in February 2015 on the *Physics Today* website.

COMSOL NEWS | 7

object geometry and the surface temperature as graphics.

With these selections, the result was a working app that has input or display boxes for the input/output data, buttons for the actions, and display panels for the graphics. The app components, or widgets, are displayed on a canvas, and can be dragged with the mouse to suitable locations for an attractive interface. A *Test Application* button allows me to launch the new app and test its features from within the COMSOL design environment. Figure 2 shows the app I built from my model using the Application Wizard.

➜ FULL POWER AHEAD

The Application Wizard is quick and produces a user-friendly version of a model in just a few minutes, but it does not exercise the full power of the Application Builder. If I want to build something a bit more impressive, an array of tools can help assemble fully featured apps. For that purpose, the Application Builder has two sub-tools: the Form Editor and Method Editor.

The Form Editor is primarily used to generate the page layouts that comprise an app. It offers a wide selection of graphical user interface widgets, and users specify sequences of actions associated with each of them. Examples include buttons, check boxes, combo boxes, radio buttons, text boxes, sliders, and tables. The Form Editor also offers a progress bar, a message log, an equation widget displaying formatted LaTeX equations, and a results table.

The second sub-tool is the Method Editor, which is essentially a Java® programming environment that allows users to combine the COMSOL® interface with Java® programs and libraries in order to add additional functionalities.

The Method Editor also has capabilities related to modeling. As a Java® programming environment, it can, of course, implement Java® code, classes, and libraries from any source. However, it can also interact with the COMSOL model tree and the *COMSOL API* in a number of useful ways. For example, a recording feature allows users to turn on the recorder, carry out operations in the model tree (such as creating a graph, or specifying a mesh), and then turn off the recorder to find the equivalent Java® code added to the method.

➜ FURTHER EMBELLISHMENTS

After attending a COMSOL workshop on the Application Builder and reading *Introduction to Application Builder*, I spent a day embellishing the original app. The new app, shown in Figure 3, has a toolbar at the top and has the tasks of geometry definition, model execution, and display of results divided into separate pages. The first of the tabbed windows allows specification of the print head pixel count and dimensions, and then draws the print head (the geometry is also constructed and resized to fit in the graphics window).

The second tab of the app, which is shown in Figure 3, has two functions. The selection box produces a drawing of the geometry in the graphics window. This is a live drawing, and clicking any of the electrode boundaries results in the application or removal of a voltage on that boundary. Clicking the *Compute* button carries out the meshing and solving operations during which a progress bar appears on
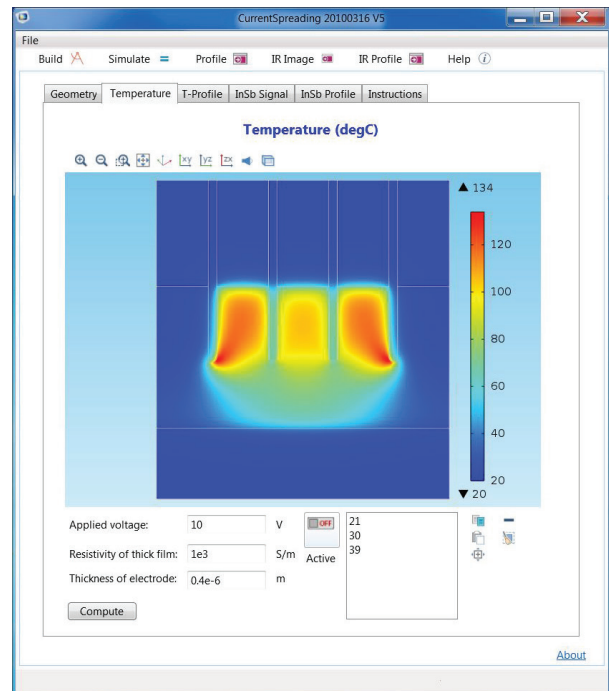

FIGURE 3. Apps built using the Application Wizard can be embellished later with forms and other enhancements.

the lower right to track the progress.

On completion, the model sounds a chime and prepares several report pages with further results: One is a 1D cut through the 2D surface temperature data to show the temperature profile through the centers of the pixels, while two others normalize the temperature data and apply the typical response curve of an indium antimonide detector.

This is the distillation of my few hours with the Application Builder. Creating an easy-to-use interface is not an onerous task, and there is satisfaction, even for a skilled model builder, in seeing the clutter removed before setting about using a model productively.

The major contribution of the new tools added in COMSOL Multiphysics 5.0 is the ability to integrate the development into a single tool, to greatly simplify the interaction with the API, and to provide a standalone server that is separate from the detail-oriented model development tools. This change promises to make the user interface a more natural and commonplace part of the model development process, and to engage a much wider audience in the use and appreciation of multiphysics models. ❖

William T. Vetterling is a research fellow and manager of the Image Science Laboratory at Zink Imaging, as well as a co-author of the Numerical Recipes *series of books and software.*

Monika Weber, Founder and CEO of Integrated Microfluidic Devices, was the Grand Prize Winner of the 2011 Create the Future Design Contest.

Mark Wagner, President of Sensorcon, Inc. Grand Prize Winner of the 2012 Create the Future Design Contest.

The team at SunFriend Corporation (l-r): Leonard Egan, Siddharth Potbhare, Karin Edgett, and Shahid Aslam (not pictured — Tariq Aslam). Winners of the 2011 Consumer Product Category.

The Future Starts With
You

Bill Zebuhr, Co-CEO and CTO of Aquaback Technologies. Sustainable Technologies Category Winner of the 2012 Create the Future Design Contest.

Salim Nasser (left), CTO and Co-Founder of Rowheels, Inc., was the Grand Prize Winner of the 2010 Create the Future Design Contest.

Create
THE
Future
DESIGN CONTEST 2015

Your future starts here:
www.createthefuturecontest.com

SPONSORED BY

COMSOL

MOUSER ELECTRONICS

ANALOG DEVICES

CATEGORY SPONSORS

Maplesoft
Mathematics • Modeling • Simulation
A Cybernet Group Company

imagineering inc.
Contract Manufacturing since 1985.

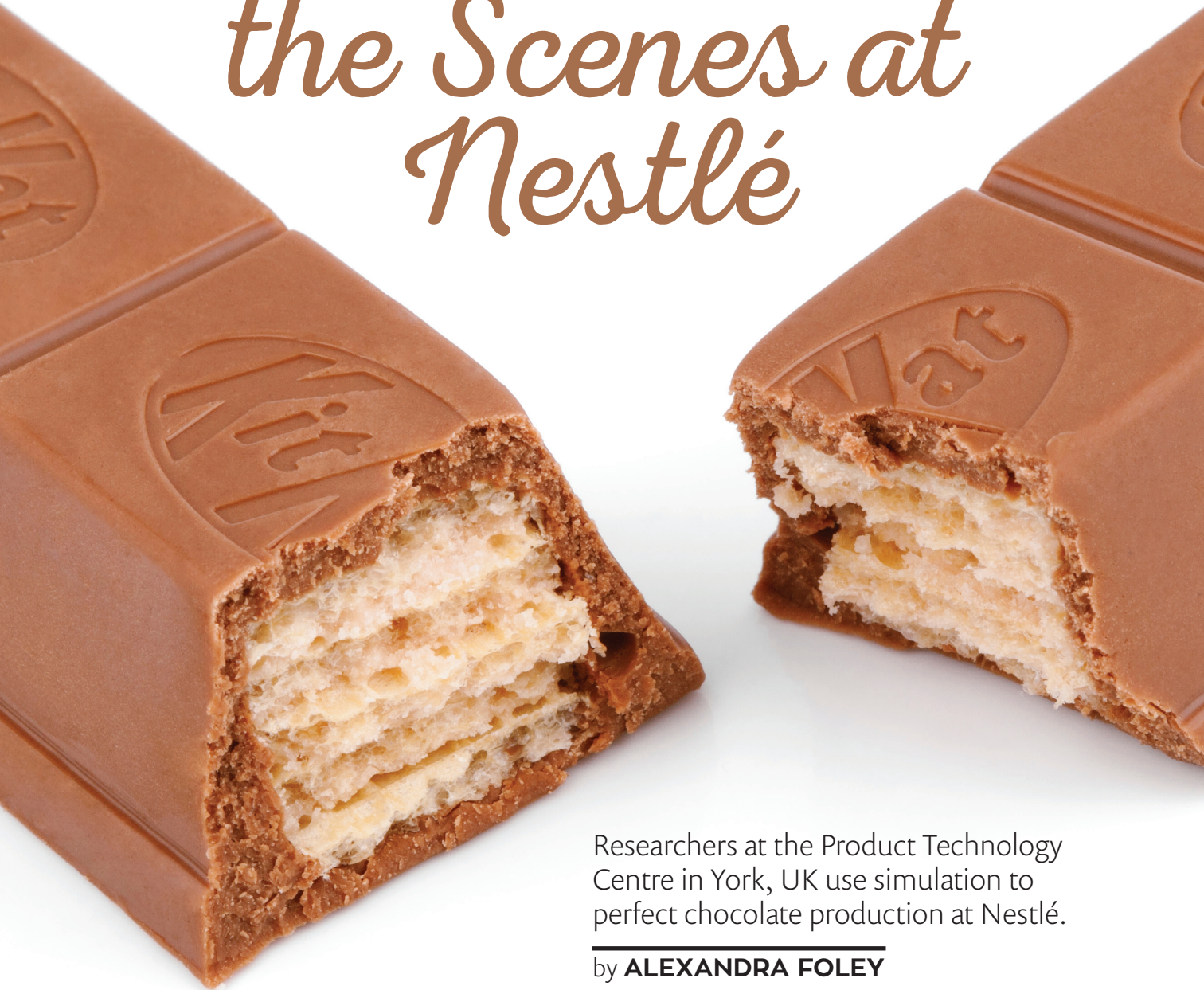PRIZE SPONSOR

orbotix

The Sweet Side of Simulation Behind the Scenes at Nestlé

Researchers at the Product Technology Centre in York, UK use simulation to perfect chocolate production at Nestlé.

by **ALEXANDRA FOLEY**

At Nestlé, the research, design, and manufacturing that goes into producing one perfect bar of chocolate candy is a mesmerizing process, not entirely different from the spectacular world of Willy Wonka's chocolate factory. While there may not be umpa-lumpas overseeing candy production, a lot of thought and quite a bit of simulation goes into perfecting the process.

Engineers at Nestlé's Product Technology Centre in York, UK (PTC York) work, among other things, on the research and development of three different products: a chocolate depositor for making candy bars; a wafer baking plate; and an extruder, used to cook and sort cereals at the same time. At PTC York, which is home to the research and development of Nestlé's confectionery products, engineers rely on multiphysics simulation to optimize and streamline the production process.

→ CHOCOLATE R&D

Candy bars, such as Kit Kat®, Aero®, Crunch, and solid milk chocolate bars are produced using a chocolate depositor that fills a mold with molten chocolate. Chocolate enters the depositor via an arm at the top and exits into a mold through each of the nozzle tips (see Figure 1).

"Ensuring that the amount of chocolate in every bar is consistent means that the flow rate and pressure of the chocolate exiting each nozzle must be the same," says William Pickles, a process engineer at Nestlé. "Not only do we need to make sure that each chocolate bar is the same weight for cost effectiveness and standardization, but we are also committed to guaranteeing that the calorie information on the package is correct as well. This allows us to deliver products with exact nutritional content that fit in with our customers' balanced diets." In order to achieve this standardization, the uniformity in flow and pressure between each nozzle tip must be precise to within a narrow margin.

To achieve this consistency, Nestlé uses a combination of modeling and simulation tools. The chocolate depositor shown in Figure 1 was first designed using SOLIDWORKS® software and the geometry was then imported
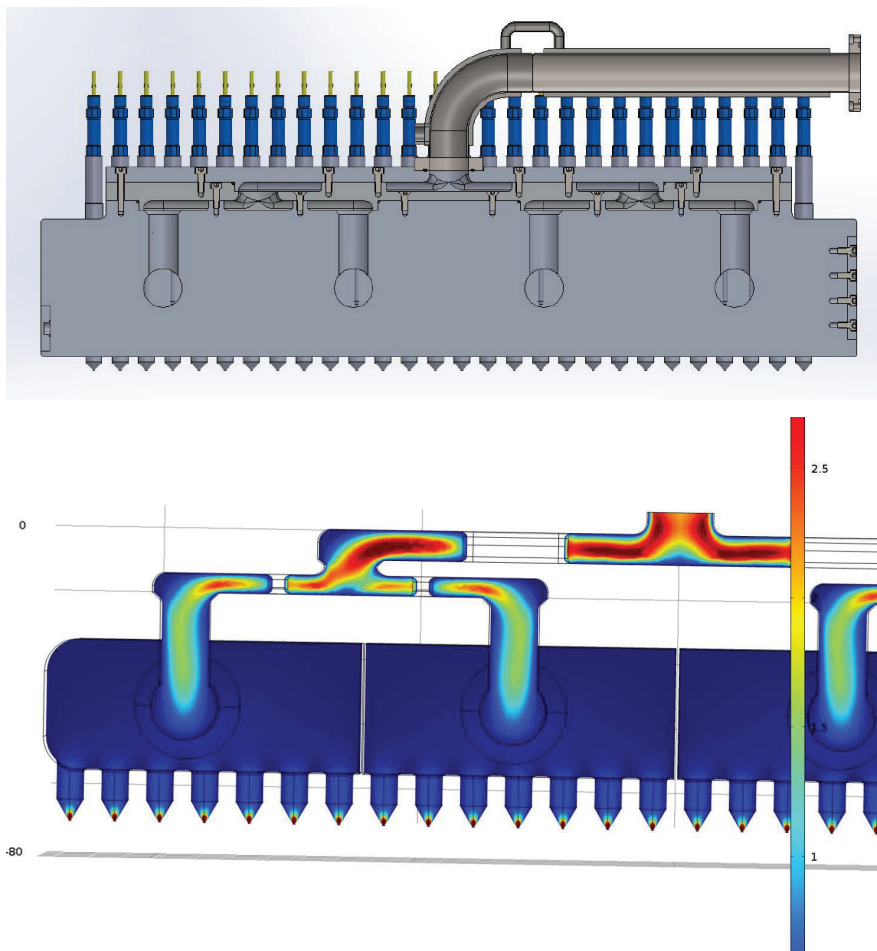
FIGURE 1. Top: SOLIDWORKS® software geometry of the depositor. Bottom: COMSOL Multiphysics® simulation showing the magnitude of chocolate flow in the depositor's nozzles and flow channels.

FIGURE 2. Probes located at each of the nozzle tips and in the flow channels demonstrate that the chocolate flow rate and pressure within the depositor and nozzles vary within specifications. Streamlines show the direction of chocolate flow.

SOLIDWORKS is a registered trademark of Dassault Systèmes SolidWorks Corp.

COMSOL NEWS | 11

a.

b.

c.

← Batter
← Baking plate

← Flames

FIGURE 3. Two wafer-baking plates (a) are used to bake Kit Kat® wafers. The top and bottom plates compress the batter (b), while the flame underneath the plates bakes the wafer (c).
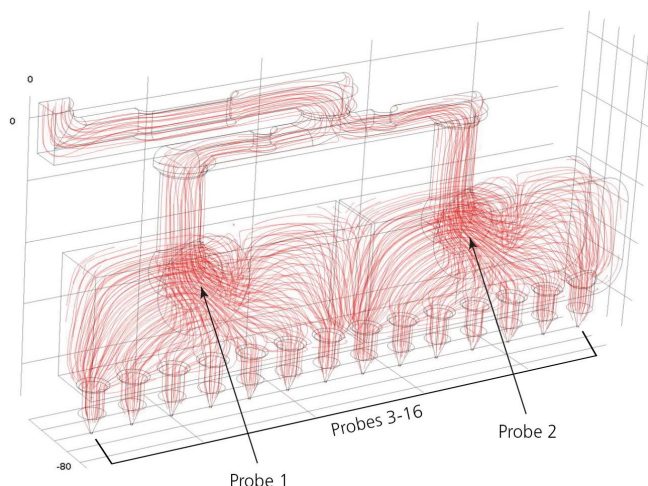
"Every chocolate manufacturer has their own special recipe that produces chocolate with unique characteristics. We were able to fully model Nestlé's signature chocolate using COMSOL Multiphysics."
—**WILLIAM PICKLES, PROCESS ENGINEER AT NESTLÉ**

into the COMSOL Multiphysics® simulation software for analysis. Simulation was used to perform fluid flow optimization, test mechanical stress, and analyze the thermal properties for a particular geometry.

"Every chocolate manufacturer has their own special recipe that produces chocolate with unique characteristics," says Pickles. "We were able to fully model the non-Newtonian behavior of Nestlé's signature chocolate by setting up a simulation where an experimental curve relating the shear rate to the shear stress of the fluid was imported into the software. This way, we were sure that we were modeling chocolate with the same fluid properties as the real product."

Using simulation, the team identified areas of high and low flow rates and

determined the differences in flow between each of the depositor needles. Numerical probes in the flow channels and at the tips of the nozzles were used to analyze conditions at certain locations of the geometry.

"By optimizing the depositor design, we were able to achieve a flow rate through each of the nozzles that is consistent to within a tenth of a percent of the desired value," says Pickles. These results of this simulation are shown in Figure 2.

➔**SIMULATION SAVES THE CRUNCH**
What would a Kit Kat® be without the well-known snap of the wafer baked inside? When baking a wafer, uneven heating can cause different moisture concentrations within the wafer, ruining its crunchy texture or even causing it to spontaneously snap.

The wafer baking process at Nestlé uses two baking plates that compress the batter between them (see Figure 3). During baking, the plates are passed above a series of about 40 flames.

"We are using simulation to optimize the baking plate design by looking at the flow of hot air below and around the plates to ensure that we have an
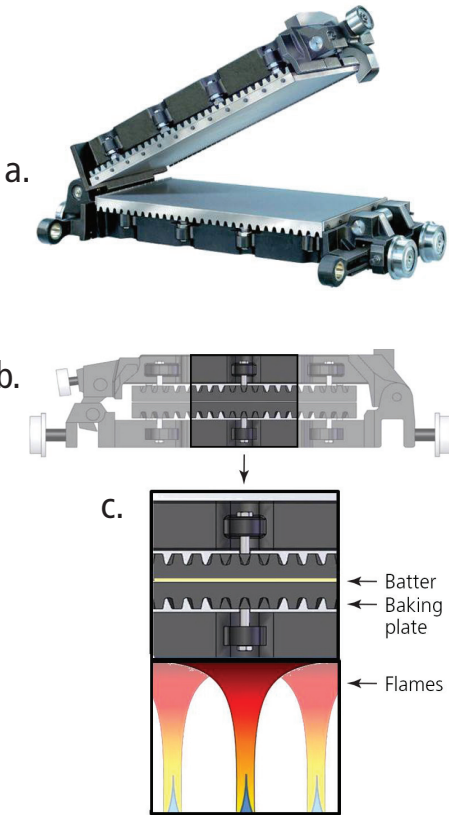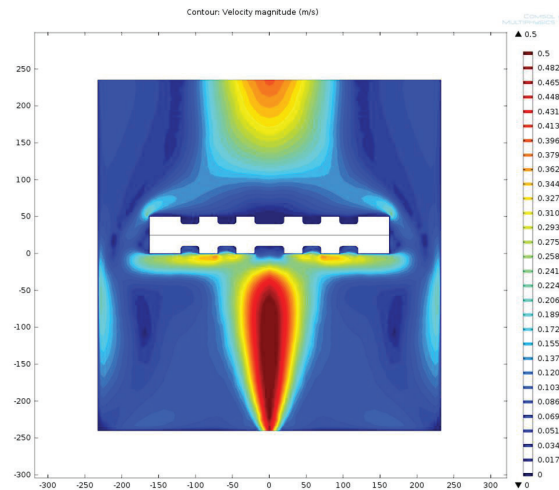

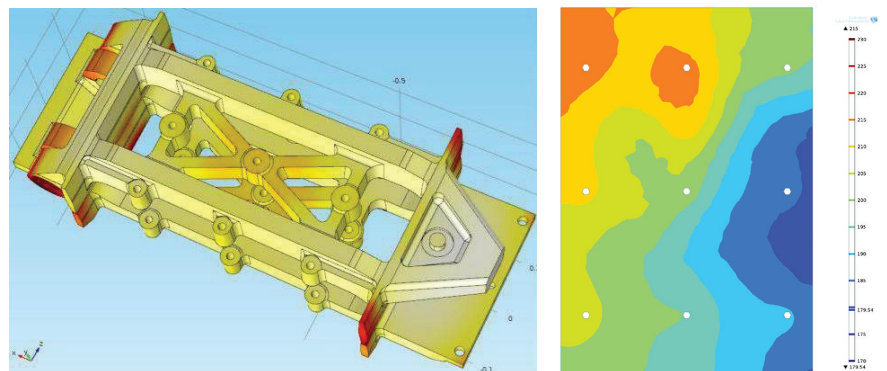**FIGURE 4.** Airflow around the baking plates.

FIGURE 5. Left: Temperature distribution in the baking plates' supporting frame. Right: Temperature profile at the surface of the top baking plate, where warmer spots can be seen at the location of the bolts (white circles).

even temperature profile across the plates' surfaces," describes Pickles. "Our aim for this study is to correct burner power and orientations to give the best wafer, while simultaneously reducing the amount of fuel we use." This fits with Nestlé's policy of continually seeking to improve efficiency in all of its manufacturing processes.

The flames underneath the baking plates were modeled as jets of hot air, where heating proceeds via convection. Figure 4 shows the profile of the flame underneath the baking plate and the airflow around the plate.

"We were able to validate our model against baking plates used in experiments, and we found that our simulation results were in very good agreement," says Pickles. The results also show how warmer spots occur due to increased heat conduction through the bolts holding the baking plates together (see Figure 5).

"The next step will be to optimize this design to distribute the heat as evenly as possible across the top of the plate and minimize temperature peaks," says Pickles.

→ COOKING WHILE EXTRUDING

Cereals such as Cheerios®, Trix®, Nesquik®, and many others are made at Nestlé using an extruder. "The high-temperature extruder used at Nestlé to make certain types of cereals works by forcing dough through a die. The pressure and friction created during this process causes the dough to cook through viscous heating," says Pickles, referring to the extruder shown in Figure 6. "Extruders are common because they are a compact, cost-effective way of manufacturing products."

Pickles is working on designing the housing for a viscometer that can be placed within the extruder to measure the viscosity of the dough entering the die. This will ensure consistent quality of the dough so that it will cook in a predictable manner. "For our design, we needed to make sure that the viscometer housing could withstand the high pressure within the device," says Pickles.

In the original extruder design, the pressure was too high for the viscometer housing to withstand.

"We redesigned the housing, which helped to reduce the pressure. We were then able to make sure that the die design didn't exceed the yield stress so that the viscometer could safely be housed inside it," says Pickles. Additionally, simulation was used to check that the displacement of the extruder was consistent, as varying displacement of the device would cause the cereal being produced to have uneven shapes and sizes (see Figure 7).
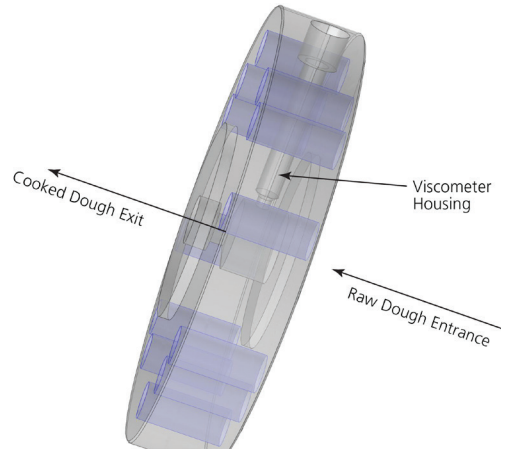
FIGURE 6. Extruder geometry.

→ BETTER, SAFER PRODUCTS WITH MULTIPHYSICS SIMULATION

At Nestlé, simulation is a big part of the design process, from producing chocolate to wafers to cereals and everything in between. "Since Nestlé products are going to be consumed by our customers, we need to be able to ensure that our designs will hold up in the real world," concludes Pickles. "We are confident in the results obtained from our simulations, and we know that they can be trusted to help us produce the best and safest designs possible. This in turn allows us to consistently deliver tastier and healthier products." ❖

FIGURE 7. Viscometer housing and die simulation results. Left: Contour of von Mises stress. Right: Slice plot of the total displacement.

Defending Automotive Components Against Corrosive Destruction
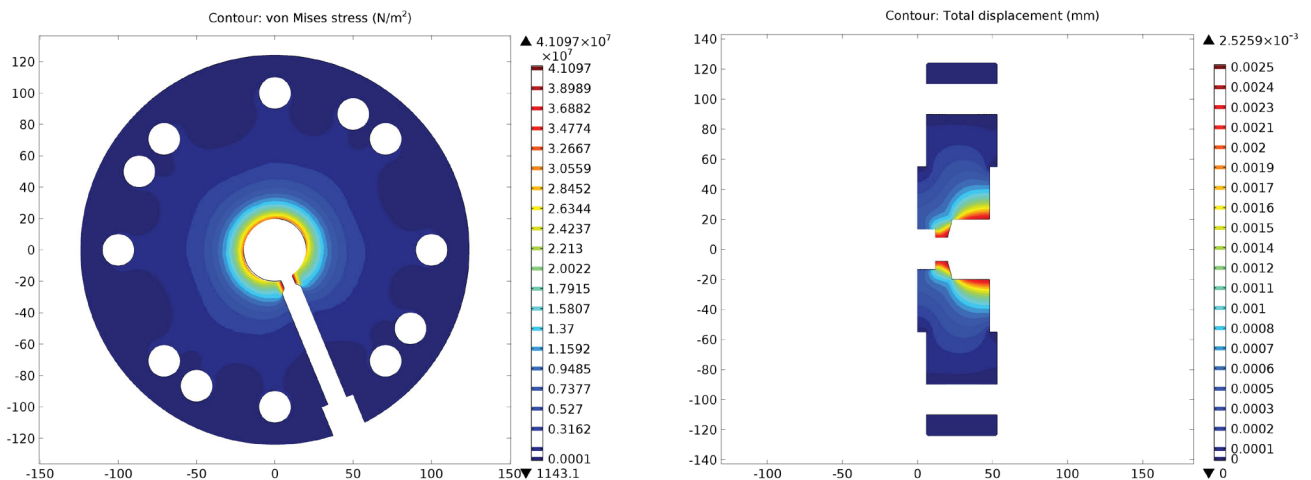
Simulation of hybrid material car components and joints enables innovative design for corrosion protection in automotive applications.

by **LEXI CARVER**

FIGURE 1. Left: Clean rivet. Top right: Rivet showing magnesium hydroxide deposit (white growth) due to corrosion. Bottom right: Magnification of a rivet in a test sheet.

Glance at a bridge's support beams while stuck in traffic, examine the door of an airplane while waiting to board, or check around the hood of your car, and you will see the small, round heads of rivets holding different surfaces together. Found in metal-bodied vehicles and support structures across the transportation industry, these rivets usually go unnoticed despite their role in joining components that withstand enormous mechanical stress. Some cars contain over 2,000 of them.

As automotive design trends move toward lightweighting and the use of multiple metals, so do the questions surrounding a destructive, invisible culprit whose handiwork is often only noticed once it is too late: corrosion.

➔ THE CLASH OF METAL-ON-METAL: GALVANIC CORROSION

Galvanic corrosion is an omnipresent process that costs the automotive industry billions of dollars each year. Caused by chemical reactions between different metals coming into contact with one another, this type of corrosion in some cases is visible as a white powdery growth that forms on the surface of metal parts (see Figure 1, top right). Bubbling paint and deteriorating aluminum are telltale signs that metallic ions are being exchanged and degrading the surface of the metal.

Different metal combinations react differently to environmental influences, and a number of factors such as joining techniques, material properties, and surface roughness affect the chemical reactions occurring on rivets and the sheets they bind together. Hence, understanding the underlying electrochemistry is essential to developing robust corrosion protection.

Eager for faster testing and better protection methods, engineers at Helmholtz-Zentrum Geesthacht (HZG) and Daimler AG joined forces to investigate corrosion prevention using multiphysics simulation. HZG is a German institute focusing on materials, medical technology, and coastal research; Daimler AG is the manufacturer of the highly-revered Mercedes-Benz automobiles. The two
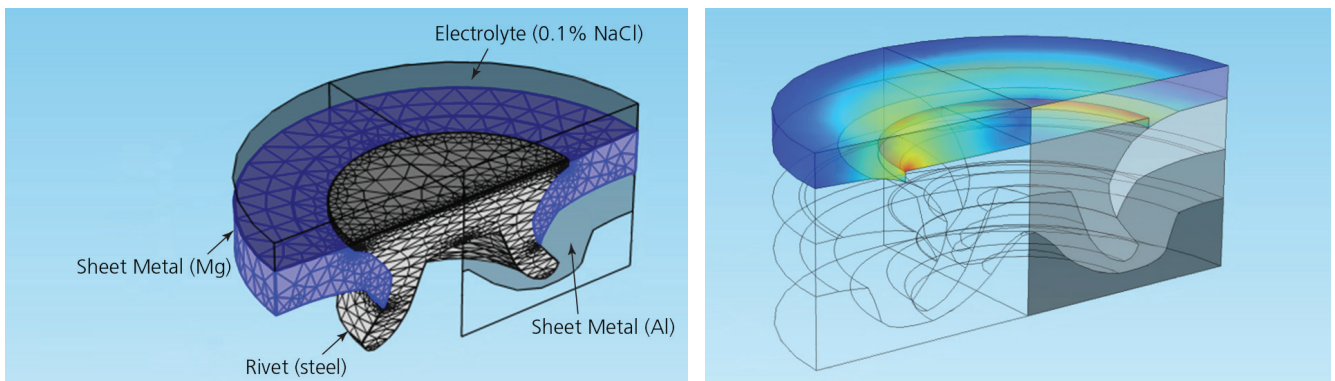

FIGURE 2. Left: Geometry depicting half of a punch rivet joint in COMSOL Multiphysics® software. Right: Simulation results show the current density at the surface of the rivet and sheet metal. The simulation mathematically models current flow at the rivet-sheet interface; the highest current density occurs at the sharp edge.
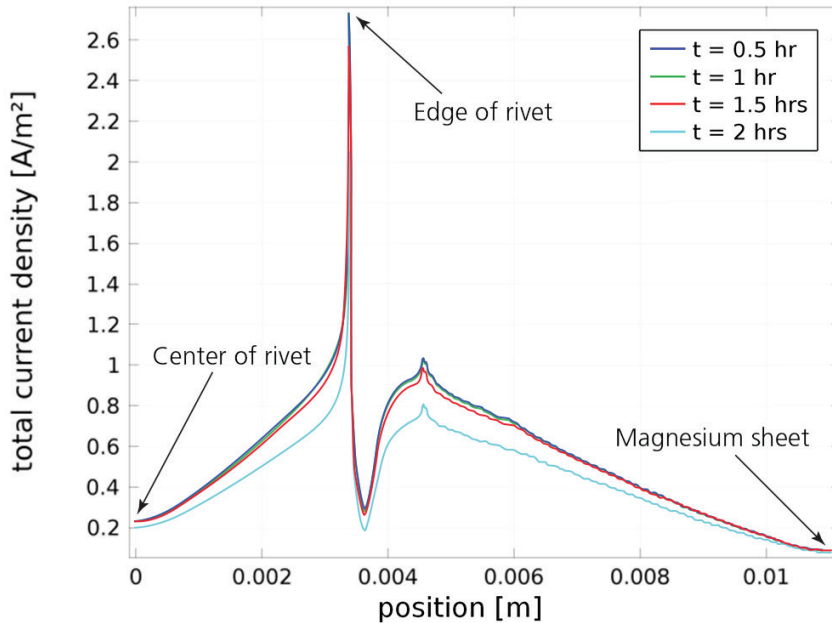
FIGURE 3. COMSOL® software plot showing the localized current density at different positions on the surface of the rivet joint.

and the sheets experiences corrosion, the magnesium sheet begins to degrade more rapidly than the other metals. The chemical reaction produces magnesium hydroxide $(Mg(OH)_2)$ that forms a weak barrier film on the surface. Growth in this deposit layer actually increases resistance to further corrosion, hindering its own progress. A complete stop cannot be reached because of the porosity of the $Mg(OH)_2$, however, and the growth continues deeper into the metals.

In order to determine the electric current distribution and analyze the chemical response, Höche needed to account for this non-constant growth and the influencing material properties. Using the Chemical Reaction Engineering Module and Batteries & Fuel Cells Module, two add-ons to the COMSOL® software, he treated the rivet and the sheet metal like a set of electrodes. This allowed him to assess how the anode/cathode area ratio, the electrolyte exposure duration, and the changes in electric current due to $Mg(OH)_2$ buildup contributed to magnesium degradation.

"Since the porosity directly affects the barrier properties, the resulting surface topology is influenced by the downward degradation velocity and the opposing growth of the deposit. Basic galvanic current density computations

→ MULTIPHYSICS MODELING OFFERS INSIGHT INTO CORROSION KINETICS

To study galvanic corrosion kinetics, including material loss, surface conditions, and the long-term behavior of the interacting metals, Dr. Daniel Höche, scientist at HZG, created a simulation of a steel punch rivet joint using the COMSOL Multiphysics® software. The rivet is plated with an aluminum-zinc alloy that acts to cathodically protect the steel. The software allowed Höche to analyze the electrochemical interactions at the surface and edges of the rivet, predict the decay of the adjoined sheets, and adjust the geometry to minimize corrosion.

His model consists of the rivet, bonded metal sheets of aluminum and magnesium, a 0.1% NaCl electrolyte layer on the surface representing the outside environment, and a galvanic couple at the interface between the rivet and the sheets (see Figure 2). He also added a corner bur in the rivet
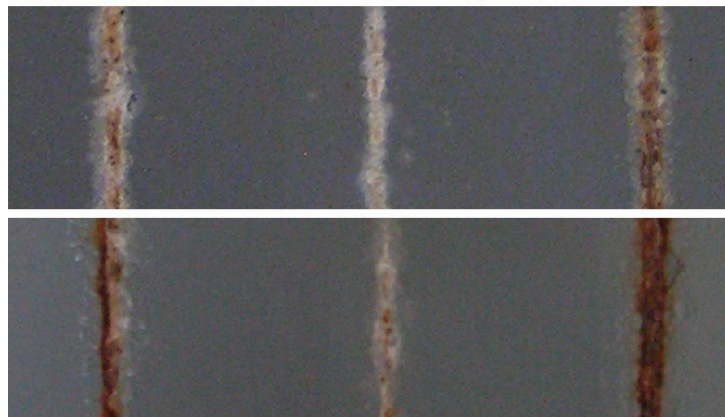
geometry to simulate the presence of a sharp edge, which increases gradients in the electrolyte potential. This in turn increases current flow and hastens the electrochemical reactions that cause galvanic corrosion.

As the interface between the rivet

FIGURE 4. A corrosion test on a galvanized steel sheet showing visible corrosion in the scratched layers (view from above). Bösch created several initial scratches of varying depths and widths in order to analyze the influence of the scratch size on the delamination process. Results are shown after one week (top) and five weeks (bottom).

teams sought ways to streamline rivet design and development, minimize physical testing, and reduce the need for subsequent steps such as surface treatment.
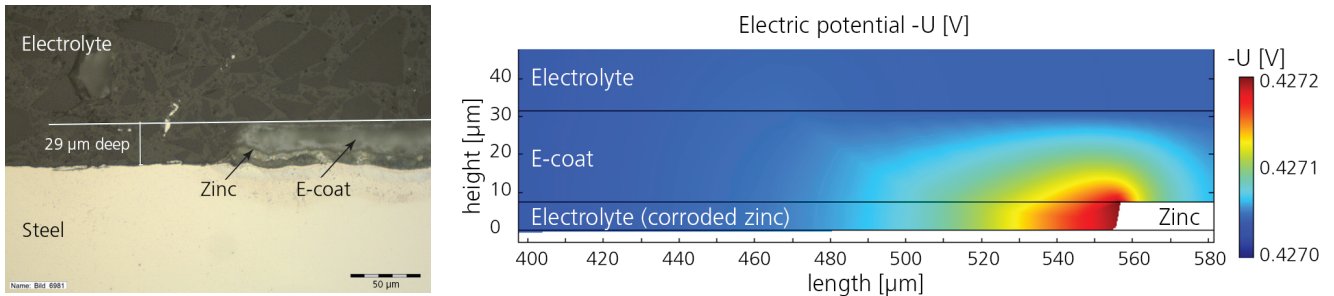
FIGURE 5. Left: Close-up of a cross-section of the test sheet where a scratch has destroyed part of the e-coat and zinc layers. Right: The COMSOL Multiphysics® software results showing the electric potential in the e-coat and electrolyte. The white region indicates the remaining zinc after much of it has already been consumed.

were modified by these layer growth aspects," Höche commented. "This led us to study time-dependent variations in the electrochemical response of the electrodes."

The model includes chemical reaction rates, known electrochemical properties of the metals, and a time-dependent function with an exposure period of 24 hours. His results report the electric potential and the current density when the rivet joint is exposed to the electrolyte, and reveal the surface coverage (the proportion of the sheets and rivet surfaces covered by $Mg(OH)_2$) at different times after immersion begins. The current density varies over distance from the center of the rivet, showing where corrosion will occur most rapidly (see Figure 3).

DIGGING DEEPER: THE RISKS OF DELAMINATION

In addition to galvanic corrosion occurring at the rivet-sheet interface, other automotive components are in danger of being destroyed by the elements. Minor, seemingly superficial imperfections, such as a scratch in the coating or paint on a panel, open the door to corrosion

Left: Dr. Daniel Höche, scientist at HZG.
Right: Nils Bösch, researcher at Daimler AG.

and allow moisture and environmental electrolytes access to electrically conductive surfaces. In car paneling, small impairments can create a galvanic couple that causes delamination—the debonding of coatings on the metal sheets—which significantly weakens the corrosion protection.

To analyze this additional risk, Höche worked with Nils Bösch, researcher at Daimler AG, to study delamination on a zinc-plated steel test sheet electrocoated with a layer of cathodic paint called an e-coat (see Figure 4). "Due to a scratch extending down to the steel surface, you can get a galvanic couple between the zinc and the steel and the zinc corrodes," explained Bösch. "This results in a crevice that grows continuously between the e-coat and the steel in the horizontal direction, rather than vertically through the layers." This behavior is quite similar to the process of crevice corrosion, which digs between two surfaces, creating fissures in the metal. Stress fractures at the base of these cracks can eventually cause part failure, even though the obvious damage and overall material loss may appear small.

Höche and Bösch used parametric sweeps in COMSOL to study the electric potential in the electrolyte and the e-coat for different e-coat barrier properties. Their model reported the corresponding horizontal growth of the crevice as it consumes the zinc (see Figure 5).

Their study to understand how the size of these surface defects impacts the rate of zinc consumption is ongoing. So far, the model indicates that the width of these defects has a greater influence than the depth: a smaller cathode/anode

ratio and more limited diffusion is present in the narrower scratches, which slows the corrosion process compared to a wider impairment. The existing results are being used to further investigate coating flaws for their negative influence on corrosion protection.

LAYING THE GROUNDWORK FOR LONGER-LASTING STRUCTURAL SUPPORT

Although corrosion is an omnipresent process that cannot be avoided entirely, it can be minimized through expert design and careful analysis. Höche and Bösch reduced the sharp edges in the rivet joint and honed the geometry to minimize the exposed area while maintaining mechanical stability. They also recommended an e-coat for the sheet metal that, based on the parametric study, would exhibit the lowest electric current and therefore the least decay in the paneling. Their COMSOL models offered indispensable insight into the relevant electrochemical behavior, providing the engineers at HZG and Daimler AG the tools for optimizing their rivet joints for the best corrosion defense.

"This kind of computer-aided analysis enhances the developments in lightweight design and enables identification of possible corrosion problems early in the design cycle," Höche concluded. "Despite the dangerous enemy that corrosion is to the automotive rivet, control of magnesium corrosion through knowledge-based processing and careful geometric design has come within our reach." ❖

SIMULATING LASER-MATERIAL INTERACTIONS

Lawrence Livermore National Laboratory researchers use multiphysics simulation to develop techniques to repair fused silica optics.

by **CHRIS HARDEE**

Tunable and precise, lasers are used extensively in everything from common household devices to state-of-the-art research facilities. Prominent everyday uses include automotive parts, barcode scanners, DVD players, and fiber-optic communications. Lasers are, perhaps, less well known as precision heat sources. However, it is this particular characteristic that makes them a very effective tool for material processing applications, where they are used to manipulate or alter specific substances such as glass, metals, or polymers with nanometer-scale accuracy.

Understanding the interaction of lasers with materials is the key to designing and optimizing laser systems for any application. It is these complex laser-material interactions that Manyalibo Matthews, deputy group leader in the Materials Science Division of the Lawrence Livermore National Laboratory (LLNL), studies. His research pertains to the repair and maintenance of fused silica optics in the most expansive laser system in the world.

➜ USING LASERS TO REPAIR HIGH-POWER SYSTEM OPTICS

California-based LLNL oversees the National Ignition Facility (NIF), home to the world's largest and most energetic laser. The giant machine—with 192 separate beams and 40,000 optics that focus, reflect, and guide those beams—can amplify emitted laser-pulse energy by as much as ten billion times and direct it towards a target about the size of a pencil eraser. The laser produces temperatures, pressures, and densities that are similar to those found in the cores of stars, supernovae, and large planets. Astrophysics and nuclear researchers use the giant laser to better understand the universe, utilizing such technologies as inertial confinement fusion (ICF), where hydrogen fuel is heated and compressed to the point where nuclear fusion reactions take place.

However, repeated use of this powerful laser can damage the optics within the system. "The optics can be quite expensive," says Matthews. "The high-power laser light generated by the NIF can damage some of the fused silica optics, creating little pits in the surface—similar to the ding you get when a rock hits your car's windshield. We do everything we can to repair and recycle the damaged ones." An example of two damaged optic surfaces before and after repair is shown in Figure 1.

Although the energy deposited by repeated laser use is damaging to the optics over time, lasers can also aid in their repair. In contrast to the giant laser system in the NIF, which spans three football fields, the lasers used to repair damaged optics are smaller, tabletop systems that are integrated with beam- and pulse-shaping components to produce a damage mitigation system. Matthews' recent research at LLNL focuses on novel techniques for optic
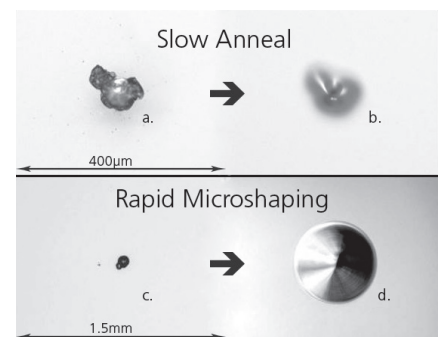

FIGURE 1. Examples of optics damaged by repeated exposure to high-peak-power laser pulses. Damaged optic surfaces are shown in (a) and (c) and the corresponding repaired site is shown in (b) and (d). A slow annealing process was used to repair the damaged site in (a), while the rapid microshaping technique currently employed at NIF was used to repair the site in (c) so that it is optically benign.

repair and more broadly encompasses laser interactions with fused silica or glass[1].

➜ SIMULATING LASER-GLASS INTERACTIONS

Matthews and his team have used simulation to explore three techniques for repairing damaged optics: infrared (IR) pulsed laser microshaping/micromachining, slow annealing, and laser chemical vapor deposition (L-CVD)[2].

In a first research cycle, they focused on the basic underlying physics and

material science of how fused silica behaves when exposed to laser light at varying temperatures.

There were several milestones in their temperature-tiered campaign: The first was to understand the thermal-elastic response of the material up to the glass transition temperature of 1,300 K, where fused silica exhibits a sudden increase in elastic response and becomes less resistant to flow. They continued by examining the molecular relaxation of glass under viscous flow between the glass transition and the
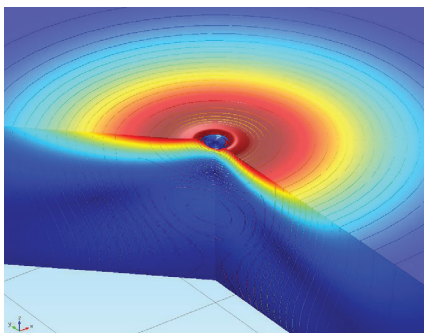

FIGURE 2. Simulation results showing Marangoni flow of laser-heated glass. This effect occurs when laser heating leads to gradients in temperature-dependent surface tension, which causes material to flow radially outward, forming what looks like ripples or layers.

evaporation point at ~2,200 K. The final objective was to investigate the evaporation and redeposition of the material over temperatures between 2,200 and 3,400 K.

To explore specific techniques for repairing the damaged optics, Matthews turned to the COMSOL Multiphysics® software. "I decided to use COMSOL to get a better understanding of what was going on," says Matthews. "All the necessary physics were already available in the software, so I could readily try out ideas and avoid the time and effort that would be needed to develop my own code from scratch."

According to Matthews, COMSOL has been instrumental in helping them understand how lasers interact with fused silica, as well as in refining their specific repair methods. "A high-power laser system can't tolerate much surface roughness in the optics. Controlling flatness to such high standards required extensive simulation," he says. His simulations include heat transfer in fluids, chemical reactions, and structural mechanics, as well as mass transport and fluid flow.

➔IR-PULSED LASER MICROSHAPING
While the simple approach of slow annealing was first used to mitigate

optic damage (see top panels of Figure 1), experimentation and simulation showed that surface rippling caused by thermocapillary flow, or Marangoni shear stress, leads to unwanted light modulation when such surfaces are placed into a laser beam. A simulation showing the laser-induced temperature profile and material displacement due to Marangoni shear stress is shown in Figure 2.

To counter this effect, Matthews and colleagues explored the use of shorter (10's of microseconds compared with minutes) laser pulses to precisely "machine" away material into a shape that is less prone to downstream light modulation when placed in the laser system. In Rapid Ablation Mitigation (RAM), an IR laser is used to heat the substrate just beyond the evaporation point, which precisely removes a small amount of material, leaving behind a smooth, fractureless surface. This nano-ablation of material is repeated thousands to millions of times to produce a smooth, conical-shaped pit, which is "optically benign" in that it does not produce downstream light modulation (see bottom panel of Figure 1).

"Despite the long history of IR-laser processing of silica optics," Matthews says, "few attempts have been made to understand the energy coupling and heat flow in order to optimize the process. We were able to answer many of these questions by simulating a wide range of laser parameters and material properties in COMSOL."

Results from the simulations for temperature and material behavior in the ablated regions compared well with the team's experiments. "What we learned in our research is far-reaching," Matthews says, "and can be applied beyond the repair of damage in our high-energy, pulsed-laser systems to virtually any system that requires laser polishing, annealing, and microshaping of silica surfaces[1]."

➔LASER CHEMICAL VAPOR DEPOSITION FOR LARGE REPAIRS
The third approach the LLNL team studied for repairing damaged optics was laser-based chemical vapor deposition (L-CVD). In this additive
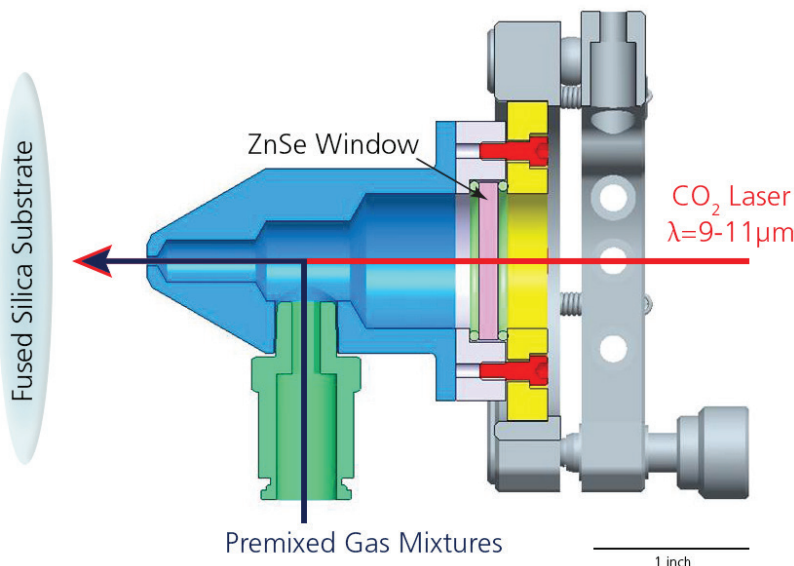

FIGURE 3. Schematic showing the optically coupled gas nozzle used for laser-based CVD processing, which allows gas flow to enter through a lateral port while IR laser light enters axially through a ZnSe window.

Fused Silica Substrate

ZnSe Window

CO_2 Laser
λ=9-11μm

Premixed Gas Mixtures

1 inch

process, a silica precursor gas is "flowed" onto the surface through a nozzle. A focused CO_2 laser beam, coupled into the nozzle through a window (see Figure 3), decomposes the precursor and deposits solid SiO_2 glass into the damage pit. L-CVD is being explored to repair large defects on optic surfaces with nanoscale precision that are difficult to fix using IR microshaping or other subtractive approaches. Ultimately, the optic performance can be entirely restored.

"Using simulation, we experimented with how beam intensity, position, and pulse duration affected the amount of material deposited onto the optic," explains Matthews. Simulation can determine the concentration and flow of the silica as it decomposes, as well as the location of deposited material (see Figure 4).

The team found that the laser power was a critical process parameter for avoiding the unwanted features that are common in many L-CVD deposition profiles, such as the well-known "volcano" feature.

"To date, we know of no other approach that additively repairs damage by replacing lost material with high-grade substrate material," says Matthews. "Successful application of such a method could reduce processing costs, extend optic lifetime, and lead to more damage-resistant optics for high-power laser applications in general. In addition, L-CVD can offer advantages over conventional methods for other material systems beyond silica glass. The ability to simulate the transient flow, reaction, and heat transport are critical to exploring new applications."

➔ FROM GLASS REPAIR TO MANUFACTURE

While the L-CVD process is still exploratory for optics refurbishment, the team has implemented CO_2 laser-based surface microshaping at NIF, optimized using multiphysics simulation, as part of the facility's optics mitigation program. Through 2014, over 130,000 damage sites have been repaired using IR microshaping and other techniques, and the optics are continuously being recycled back into the NIF, enabling its routine use.
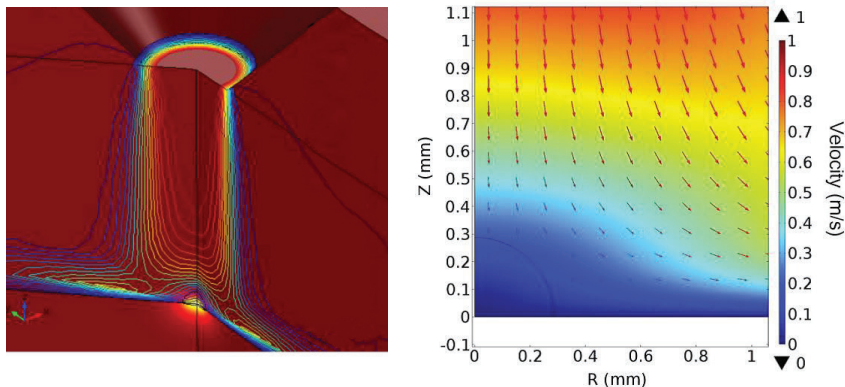
Their laser-material interaction

FIGURE 4. Simulation of velocity and temperature fields for L-CVD. Left: Velocity contours associated with the L-CVD precursor flow from a 3 mm diameter nozzle and the temperature field induced by laser heating at the air-glass interface. Right: Velocity streamlines of the vaporized silica where diffusion-dominated transport of the glass in the lower left corner can be seen (dark blue).

research, however, does not stop at optics repair. Mathews and his team are also supporting a laboratory-wide Additive Manufacturing Initiative by further developing an additive process for 3D printing known as selective laser melting (SLM)[3]. "I'm really excited about this research," says Matthews. "Figuring out how to optimize the 3D printing system could have a huge impact on this rapidly growing industry, which could benefit tremendously from a model-based approach, which was largely trial-and-error in the past." ❖

REFERENCES

[1]M. J. Matthews, S. T. Yang, N. Shen, S. Elhadj, R. N. Raman, G. Guss, et al., "Micro-Shaping, Polishing, and Damage Repair of Fused Silica Surfaces Using Focused Infrared Laser Beams," Advanced Engineering Materials, vol. 17, p. 247, 2015.

[2]M. J. Matthews, S. Elhadj, G. M. Guss, A. Sridharan, N. D. Nielsen, J.-H. Yoo, et al., "Localized planarization of optical damage using laser-based chemical vapor deposition," in SPIE Laser Damage, 2013, pp. 888526-888526-9.

[3]N. E. Hodge, R. M. Ferencz, and J. M. Solberg, "Implementation of a thermomechanical model for the simulation of selective laser melting," Computational Mechanics, vol. 54, pp. 33-51
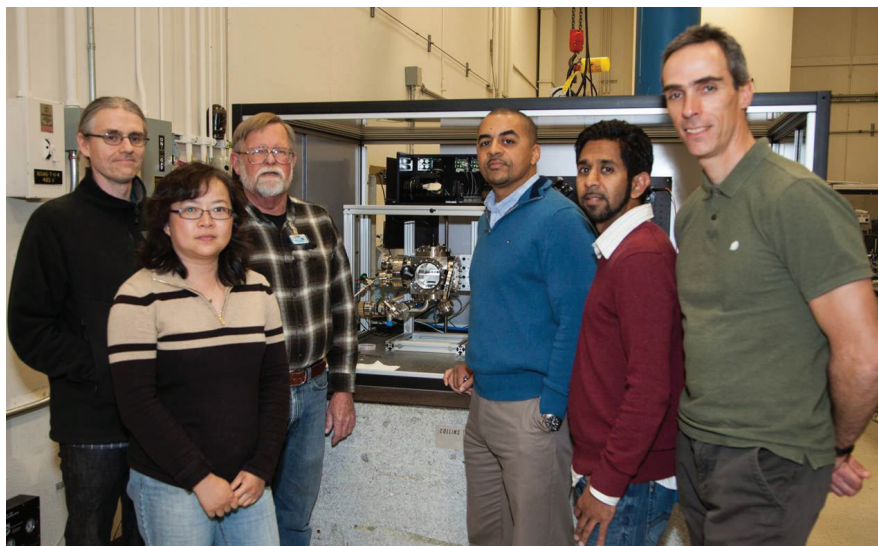
Optical damage mitigation and laser materials processing research team at LLNL (from left to right): Gabe Guss, Nan Shen, Norman Nielsen, Manyalibo Matthews, Rajesh Raman, and Selim Elhadj. The apparatus in the background is used to study the dynamics of metal powder melting under high-power laser irradiation, a topic important to the field of metal-based additive manufacturing (3D printing).

Simulations for Solar

EMIX uses multiphysics simulation to optimize its cold crucible continuous casting process for the manufacture of photovoltaic-quality silicon.

by **CHRIS HARDEE**

The massive semiconductor industry is built on a firm foundation of micro-thin wafers of silicon. Those wafers serve as the basic building block of integrated circuits (IC), where the innate conducting properties of the elemental metal create the communication pathways for all modern computers and electronics.

Yet another technology in which silicon plays a key role is in the manufacture of photovoltaics (PV). In this growing alternative energy application, silicon-wafer-based solar cells are used to convert photons from the sun into earth-bound electricity. Solar energy is seen by many as a power source that has great potential. However, solar manufacturers must find ways to decrease the cost per unit of power generated before the technology will be truly competitive with more mature fossil-fuel technologies.

"Depending on the price of polysilicon, about 30% of the final sale price of a solar cell is a function of the cost of the silicon alone," says Dr. Julien Givernaud, a research engineer at EMIX, part of the French subsidiary of Grupo FerroAtlántica. Givernaud works on the optimization of the inductive cold crucible and associated equipment used to purify silicon for photovoltaics. "Lowering silicon production costs while increasing its purity is critically important in this industry."

→MANUFACTURING PV-QUALITY SILICON

In nature, silicon is the second most abundant element by mass in the earth's crust. For photovoltaic applications, metallurgical silicon (which is 99.9% pure) must be processed into a higher-purity grade containing no more than one part-per-million impurity (99.9999%). Purity is important because it directly influences the amount of electricity a solar cell can produce from incoming sunlight—a measure called the photovoltaic conversion efficiency.

There are a number of competing manufacturing processes that transform silicon from its natural state to solar-cell ready. "Our continuous cold crucible casting, or 4C process, is a very innovative method for manufacturing PV-quality silicon," says Givernaud, who uses the COMSOL Multiphysics® software to optimize production parameters. The company holds several patents and an exclusive worldwide operating license for the technology.
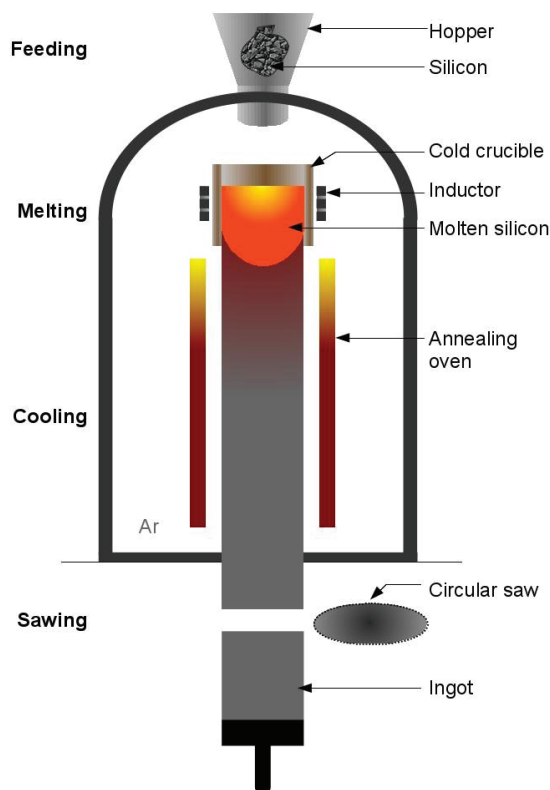

FIGURE 1. The schematic illustrates the cold crucible continuous casting (4C) process used to make silicon for photovoltaic applications. Silicon stock is fed into the system's hopper at the top, then heated, cooled, and cut into ingots.

In the 4C process, silicon feedstock is fed into a water-cooled crucible where it is inductively heated to its melting temperature of 1,414 °C. It is then electromagnetically mixed in the crucible where Lorentz forces prevent contact between the crucible and the silicon melt, and the strong stirring homogenizes species concentrations at the solid-liquid interface, enhancing crystallization conditions. This results in high purity (see Figure 1).

Following mixing, the melt is then "pulled down" through the open-bottom crucible, where it cools and solidifies using a carefully controlled annealing process. The continuously produced silicon rod is next sawed into ingots, which are sold to PV manufacturers who, in turn, slice them into the 200-micrometer-thick sections used to make solar cells.

→SIMULATION IMPROVES PHOTOVOLTAIC PRODUCTION EFFICIENCY

While relatively simple in concept, EMIX's 4C process involves numerous manufacturing variables. This is where simulation comes in. Givernaud has performed countless calculations using simulation to examine, for example, the cooling method, the pull rate, crucible and coil shapes, and the characteristics of the furnaces. He has also analyzed the effect of the

electromagnetic field, the shape of the solid-liquid interface, and the effect of elastic stresses on crystallization behavior.

Engineers at EMIX have been using multiphysics simulation for eight years—almost as long as they have been in the PV silicon business—to evaluate the production process. "COMSOL Multiphysics is easier to use than the FEA tool in my previous job," says Givernaud. "I create all of my geometries directly in COMSOL. The model is very easy to mesh. It's simple to switch between physics, and the solver is very fast and efficient. All-around, it's an intuitive and powerful tool."

Givernaud's most recent modeling studies have involved both multiscale electromagnetic and 3D continuous casting simulations. His electromagnetic simulations permitted the estimation of inductance and impedance, as well as the optimization of the crucible design to improve electrical efficiency (see Figure 2). The continuous casting simulations allowed for the input of parameters such as electromagnetic power, crystallization rate, height of the crucible cooling zone, and after-heater temperatures. The combined results of these studies have led to a compromise between high production rates and low stresses in the ingots.

In the various simulations, the Heat Transfer in Fluids and Laminar Flow interfaces in COMSOL were used to calculate phase change in the silicon as it solidified in the crucible. Calculations for a cylindrical test crucible, when validated, will be applied to a larger crucible utilized in the commercial process.

"There has been very good agreement between our simulations and experiments for the pilot process," says Givernaud. "Simulation helped us to reach good crystallization parameters, improve the electrical efficiency of the industrial size crucible, and reduce the number of tests on the pilot furnace." He further adds that the latest series of simulations have, in theory, demonstrated energy savings of approximately 15% and pulling-rate increases of about 30%, which makes the 4C method far more productive than other standard silicon crystallization processes.

Industry-wide, manufacturers are striving to reduce silicon-wafer cost and improve purity for PV applications. Increased share in a growing solar marketplace will be the reward for the companies that develop the most commercially viable solutions. "Multiphysics simulation has helped us to identify some processes that will be tested soon on the industrial scale," says Givernaud, who expects that EMIX will break new ground with innovations the company has been working on. ❖

> "COMSOL Multiphysics is easier to use than the FEA tool at my previous job…All around, it's an intuitive and powerful tool."
>
> —JULIEN GIVERNAUD, RESEARCH ENGINEER AT EMIX

The R&D team at EMIX stands in front of a silicon production furnace (from left to right): Julien Givernaud, Elodie Pereira, Nicolas Pourade, Florine Boulle, Alexandre Petit.
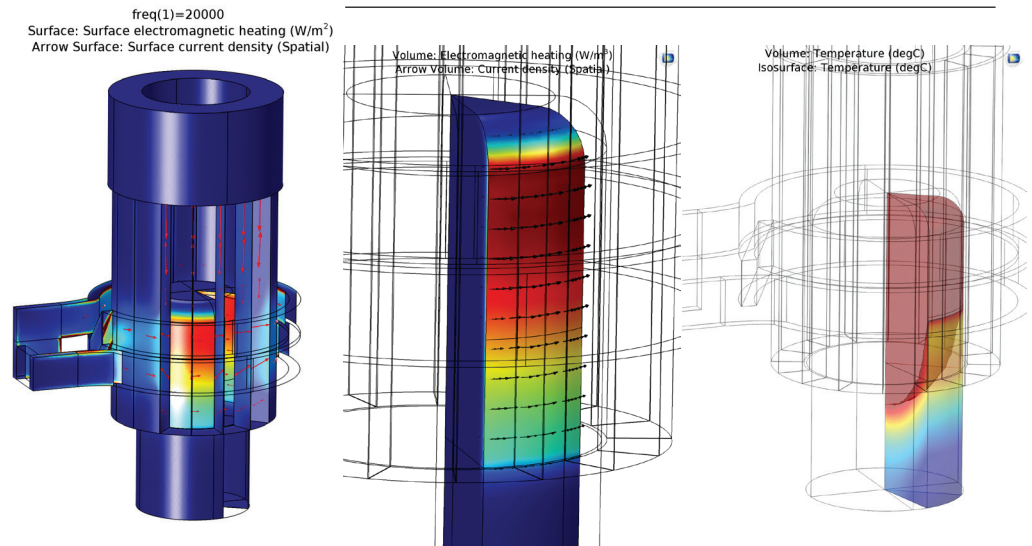

FIGURE 2. The model of the cold crucible has been used to predict the electromagnetic heating of the crucible (left) and molten silicon (center) and the triple-point liquid/solid/gas interface (right) where red/yellow represents the melt and blue/green represents the solid phase.

VIRTUAL MATERIAL DESIGN IN 3D PRINTING MAKES HEADWAY WITH MULTISCALE MODELING

Researchers at the Netherlands Organization for Applied Scientific Research (TNO) are using multiphysics simulation, multiscale modeling, and topology optimization to explore multimaterial 3D printing.

by **LEXI CARVER**

In recent years, 3D printing (additive manufacturing) has become a major player in research, design, and manufacturing work. Now the technology is also showing promise in the realm of material design. It will soon be commonplace to create prints with multiple materials and varying properties over a single object—a capability that will create a wealth of new applications with integrated products featuring highly tailored material properties.

Additive manufacturing often uses small periodic microstructures in a repeating pattern to create the shape being built. A single microstructure is called a unit cell, and these may be as simple as triangles or honeycombs, or more complicated, with cross-struts and multiple voids between walls. Recent developments in 3D printing indicate that capabilities for multimaterial printing at the microlevel, where these microstructures can be combined and tailored to the designer's needs, are rapidly expanding. This kind of fine control will allow engineers to choose the proportion and arrangement of each material included, giving them the freedom and flexibility to "design" performances that are impossible to achieve with a single material.

Researchers at the Netherlands Organization for Applied Scientific Research (TNO) have begun investigating virtual material design, relying on multiphysics simulation and multiscale modeling to determine how specific properties could be effectively designed into a 3D-printed object. Work at the research institute spans many subjects, including safety and security,

energy, and manufacturing—the techniques used for optimizing material and topology in 3D-printed designs have been extended to their other areas of research, such as lightweight mechatronics, free-form solar cells, and lighting products.

➔ **THE STORY OF STRESS, STRAIN, AND STIFFNESS IN ANISOTROPIC MATERIALS**

Anisotropic materials behave differently depending on the direction they are loaded; however, with current methods of material production, control over the anisotropy is limited. Hence, any advantages are difficult to exploit for product design purposes.

Marco Barink, researcher at TNO, set out to develop a procedure for designing manufacturable anisotropic structures using stiffness and topology optimization techniques. He began using the COMSOL Multiphysics® software to investigate a single unit cell intended to have twice the stiffness in one planar direction as the other (see Figure 1). "We were aiming for a desired stiffness matrix, so we applied a strain in COMSOL and then optimized it to find the desired stress," he explained. "We can tell COMSOL to make the material twice as stiff in one direction as another, and analyze the material behavior for a given geometry." He verified the simulation results using a printed sample that he tested for the expected material behavior. After determining that his results were accurate, he performed a second optimization study for a highly anisotropic material. In this case, the simulation could control not only the spatial distribution of the material, but also the orientation of
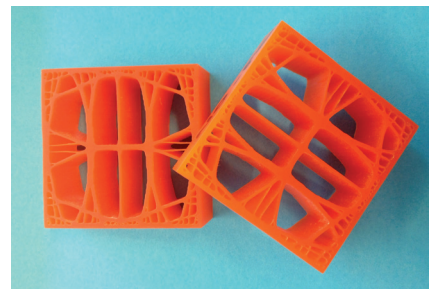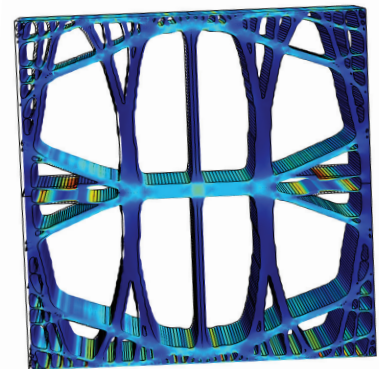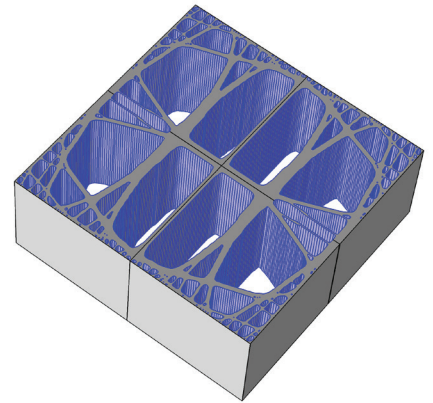

FIGURE 1. Top: Geometry of a unit cell. Middle: Simulation results showing mechanical stress for an optimized design with one planar direction having half the stiffness of the other. Bottom: 3D-printed samples.
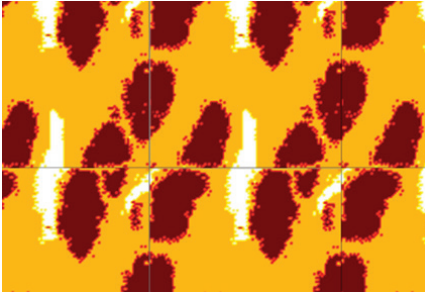
FIGURE 2. Barink's simulation results showing optimized material composition (with three materials) for the desired anisotropic thermal conductivity. The simulation shows regions of high conductivity (white), low conductivity (orange), and a nonconductive material and voids (red). Several unit cells are arrayed periodically.

the anisotropic fibers.

With the larger goal in mind of designing properties beyond those available in a single material, the next step was to extend the simulation to structures comprising different material combinations, or multimaterials. Barink defined an anisotropic multimaterial cell in COMSOL, then optimized the local distribution of each material over a whole structure composed of a pattern of these cells (see Figure 2). He used the software to adjust the composition and arrangement until he reached the desired overall thermal conductivity.

➔MULTISCALE MODELING AND COMPUTATIONAL HOMOGENIZATION

Each of these unit cells, in reality, would only be a tiny region in a final piece. After optimization at the microlevel, the TNO team began to study material optimization for larger-scale devices. "We've found that this microscale strategy works well for relatively small volumes," said Erica Coenen, a research engineer at TNO. "However, to design real-life products, these need to be scaled up while maintaining feasible computation times. This is where so-called multiscale modeling comes in, giving the designer the tools to efficiently simulate at both the micromaterial scale and the product scale simultaneously."

Coenen implemented tools in

COMSOL to extract parameters for the effective structural behavior of a single multimaterial cell. This effective behavior is used in a full-scale model, or macromodel, of a whole device. "We succeeded in creating a fully-coupled multiscale simulation—the macromodel contains homogeneous properties without any substructure details, and the micromodel contains the heterogeneous multimaterial microstructure. Many micromodels run within a single macromodel," she explained. "We can consider multiple micromodels at once, solving for highly nonlinear and temperature-dependent behavior, based on local conditions from the macromodel."

Coenen and Barink applied a simplified version of this method to one of the major research topics at TNO, the development of large, flexible organic LEDs (OLEDs), which require the deposition of organic semiconductors onto flexible substrates. For good light homogeneity, these devices require careful design of the metal grids used in their transparent front-end electrodes; visible differences in light output create lighter and darker areas, which are undesirable for a final product.

But directly modeling an OLED with a metal grid proved challenging in the past, due to large differences in the dimensions of different components. The honeycomb shapes that form the grid are only a few millimeters wide, and their metal edges 10 – 100 microns thick. Against the backdrop of the
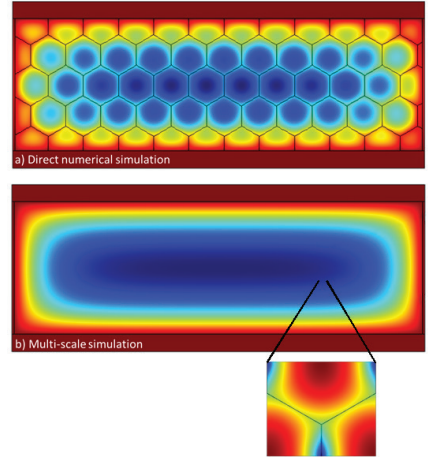

FIGURE 3. Simulation results in the COMSOL® software showing the light output of an OLED. Top: Model including the hexagonal grid. Bottom: Macromodel with homogenized material properties.

comparatively large complete OLED (tens of centimeters wide), the different length scales are difficult to account for in a single model.

"Multiscale modeling is really the way to go forward," Barink commented. With a new COMSOL study, they analyzed the grid shape to determine the ideal layout for improving light distribution. Combining a macromodel of the entire OLED with a micromodel of the honeycomb grid, they solved for effective light output and optimized the spacing and honeycomb dimensions (see Figure 3). Their updates to the existing
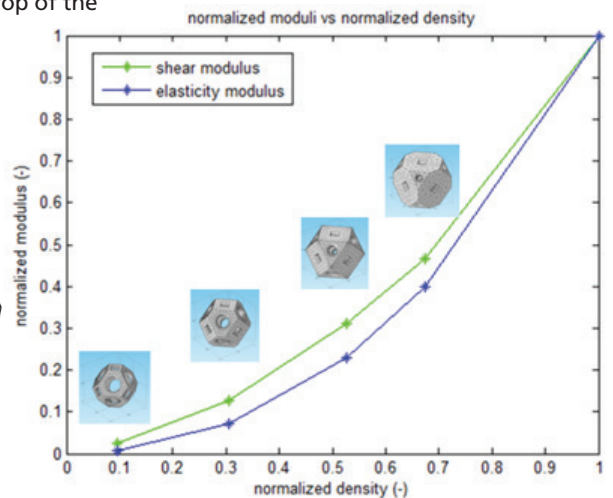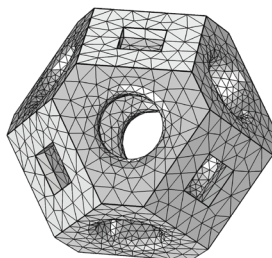

FIGURE 4. Left: Meshed model of a cell optimized for metal 3D printing. Right: Overview of the homogenized material properties for different cell designs.

design resulted in a 12% improvement in homogeneity without compromising efficiency in the OLED.

→ BRINGING IT ALL TOGETHER: FROM SINGLE CELL TO COMPLETE PART

Coenen and Barink had demonstrated that topology optimization is a powerful tool for generating designs for additive manufacturing, given the capabilities of developing products that cannot be manufactured using conventional techniques. But even such a flexible manufacturing technology has some limitations. In one form of 3D printing called selective laser melting (SLM), the printer melts layers of powder into the desired shape. Unused powder must be removed from the object afterward, and large overhangs are usually avoided in SLM designs as they may warp. Therein lies a potential conflict: What happens when topology optimization creates an idealized design containing closed voids or large overhangs?

"To circumvent this issue, our engineers came up with a few unit cells of different densities," Barink remarked. "These cells are designed to be stiff, always printable, and contain holes so that the powder can be removed. Different unit cells combine to create the desired overall properties." They then used COMSOL to analyze the relationship between material density and mechanical stiffness (see Figure 4).

At the device level, it is not possible to handle a model with thousands of small 3D unit cells. So they combined their tested techniques: stiffness homogenization for each unit cell type followed by topology optimization at a larger level. "The homogenized properties of each unit cell serve as a separate material in the topology optimization at the device level," Barink continued.

For a concrete, less expensive example than a metal print, they applied the whole procedure to a polymer hammer handle (see Figure 5). The final design contains a combination of the different cell types, optimized by the software for the correct stiffness with minimal material use. "The hammer handle served as a demonstration of the power and
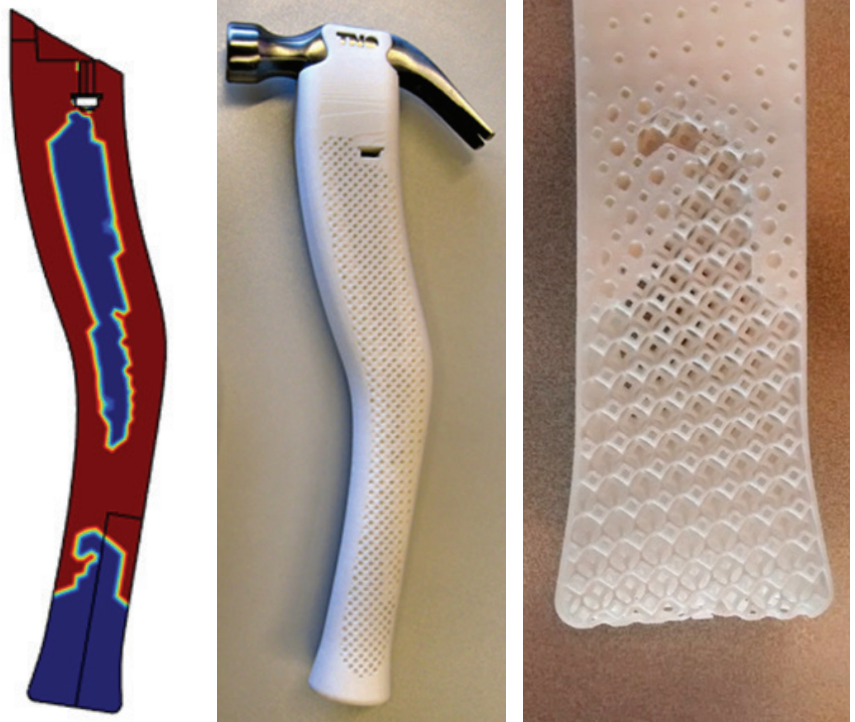

FIGURE 5. Left: Topology optimization result in the COMSOL® software. Center: The optimized hammer handle, printed in nylon. Right: Close-up of the pattern containing three different cell types: most dense cells with small holes near the top, least dense cells toward the bottom, and a few intermediate shapes in between.

versatility of the whole procedure, going from design to final product," Barink said. "From the design of unit cells, homogenization, topology optimization, generating printer input, and finally, printing, we have developed a good technique for designing a complete device with all the microlevel features. When applied to SLM designs, the techniques will address the typical production issues faced in metal printing, where stronger and more high-tech products are designed."

The team at TNO had begun with a single cell and successfully built their way to anisotropic multimaterial microstructures. The application of their techniques to multiple areas of research at TNO demonstrated the power of combining simulation and multiscale modeling with innovative product development. This glimpse into the future, where multimaterial design may become the norm in additive manufacturing, would not have been possible without simulation. ❖
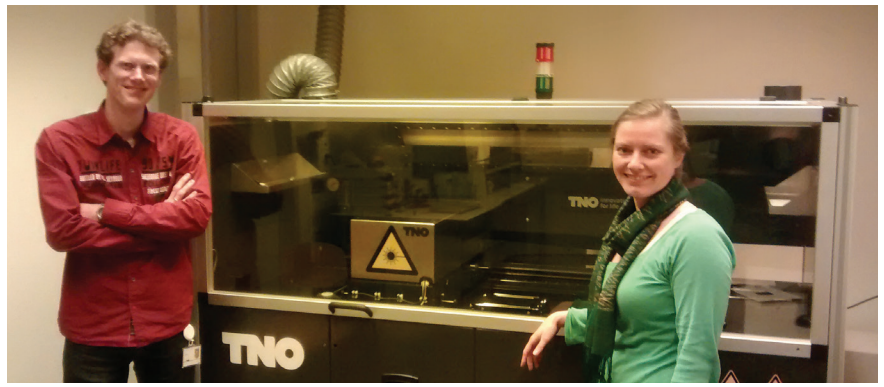
Marco Barink (left) and Erica Coenen (right) standing with the 3D printer at TNO.

OPTIMIZING THE PERFORMANCE OF COMPLEX BUILDING FAÇADES

Using multiphysics simulation to understand the interaction between environmental, geometrical, and structural variables, engineers at Newtecnic ensure that innovative building façades are both beautiful and buildable.

by **JENNIFER HAND**
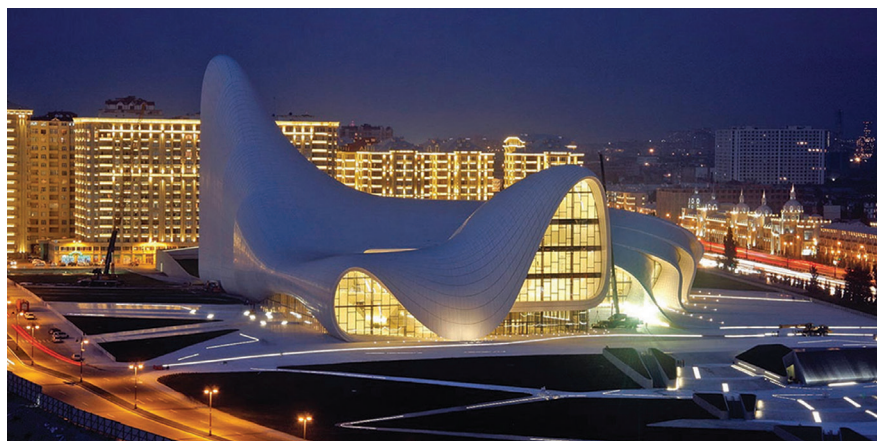
Federation Square, Melbourne, Australia

FIGURE 1. Heydar Aliyev Cultural Center, Baku, Azerbaijan.

Dynamic, textural, and symbolic; whether they ambitiously defy gravity or grow organically from the landscape, iconic buildings frequently involve complex façades. Designed not only to protect, they also regulate variables such as thermal and visual comfort.

A specialist in this area, Newtecnic designs and analyzes façade systems for use in high-profile public projects and regularly works with Zaha Hadid Architects, a practice recognized for its bold and fluid architectural forms. Newtecnic's founders and current directors, Andrew Watts and Yasmin Watts, are known for their work on prominent projects including the iconic Federation Square (Melbourne, Australia) and more recently, the Heydar Aliyev Cultural Center in Baku, Azerbaijan (see Figure 1).

Bespoke is the norm for Newtecnic, and every project requires thinking that goes far beyond conceptual design alone. Architects provide an artistic view and perhaps some surface modeling of a building design, then Newtecnic engineers build up the façade in layers, making sure that the design retains its creativity while also ensuring its structural integrity.

"Our clients want viable and economic design solutions that meet the required performance targets, can withstand environmental effects, and are easy to maintain," says Carmelo Galante, head of Research and Development at Newtecnic. "A key aspect of our work is therefore to describe the physical behavior of the façade systems we design."

From solar studies that allow optimization of the shading design in order to reduce cooling loads and maximize visual comfort, to the way in which fixing brackets for rainscreen cladding affect the integrity of the insulation, there are numerous challenges that can be resolved with the help of simulation.

➔ **BEYOND CONCEPTUAL DESIGN WITH SIMULATION**

The COMSOL Multiphysics® software has become a key tool for Newtecnic. Galante explains: "We can do everything within one simulation software. I use COMSOL to study the 3D thermal bridging effect—the way in which highly conductive materials penetrate insulation—on the overall energy efficiency of the build-up, evaluate the maximum temperature of components, and suggest the most suitable product or material. I can evaluate cladding pressures on the building structure for schematic design stages and study more complex façades in which mechanical and natural ventilation are present at the same time. I can also evaluate how
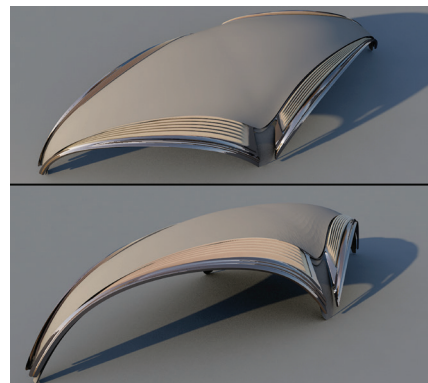
FIGURE 2. Rendering of a single shell shown from two different angles, many of which will be part of the building.
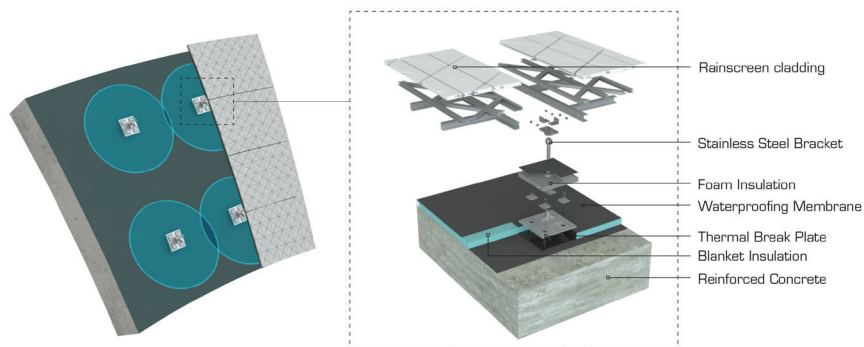
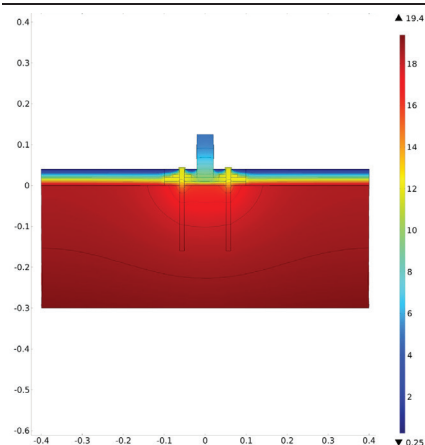**FIGURE 3.** Highlighted view of the rainscreen system with fixing brackets.

FIGURE 4. Simulation results showing isotherms and temperature profile in °C of a section taken through a bracket.

> "Simulation minimizes construction costs by allowing contractors to see exactly what they are required to build."
>
> —**FABIO MICOLI, ASSOCIATE DIRECTOR AT NEWTECNIC**

different design configurations would affect the hygrothermal performance of a façade system."

Using the CAD import functionality available in the COMSOL® software, Galante often imports complex geometries, mainly from Autodesk® AutoCAD® software and Rhinoceros® software. The use of Autodesk® Revit® software is continuously increasing at Newtecnic, and he considers the new LiveLink™ *for* Revit®, an add-on to COMSOL that allows users to interface their simulations with the Revit environment, to be a powerful asset. Galante also combines the use of COMSOL with parametric design tools such as the programming language Grasshopper®, which is used to build and analyze complex geometries by means of generative algorithms.

One current project at Newtecnic involves designing the façade system for a high-profile private building comprising a series of self-supporting concrete shells ranging from 10 to 80 m in length and reaching heights of up to 30 m (see Figure 2).

The concrete shells are clad with a rainscreen façade system made out of ceramic panels that are doubly curved in order to accurately reproduce the building geometry. Each panel is supported at its corners by adjustable fixing brackets made out of stainless steel. These brackets are attached to the concrete structure through four post-drilled anchorages, as shown in Figure 3. As the brackets penetrate the insulation layer and have a much higher thermal conductivity than the concrete structure, they create thermal bridges through the façade envelope, significantly reducing its thermal performance.

By conducting a simplified 2D study in COMSOL, Galante studied how the thermal bridge effect created by the brackets influenced the temperature distribution in the façade (see Figure 4). The results from the simulation were entered into a Grasshopper® script to evaluate three areas of interest: those influenced by one bracket, those influenced by two or more brackets, and those not influenced at all (these areas are shown in Figure 5).

Galante was then able to prepare an accurate geometry for the system, including all the components of the build-up. "It is a real advantage to be able to combine two tools," says Galante. "Grasshopper® allows me to investigate the geometry on a very large scale—that of the entire building—then I move back to COMSOL with this information and create a very detailed 3D model to capture the real physics of the system." Using this approach, Galante was able to conduct a 3D analysis to study the thermal bridge effect in the bracket and surrounding building (see Figure 6) and compute the global heat transfer coefficient (U-value) of the façade.

"Using multiphysics simulation allows me to develop a better understanding of the real situation," explains Galante.
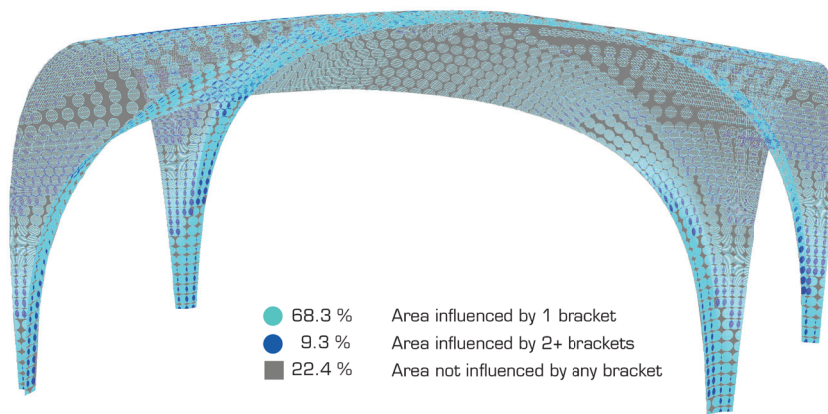

FIGURE 5. Model of one of the shells shown in Figure 2 with areas highlighted that are influenced by one bracket, two brackets, or not influenced by any bracket.
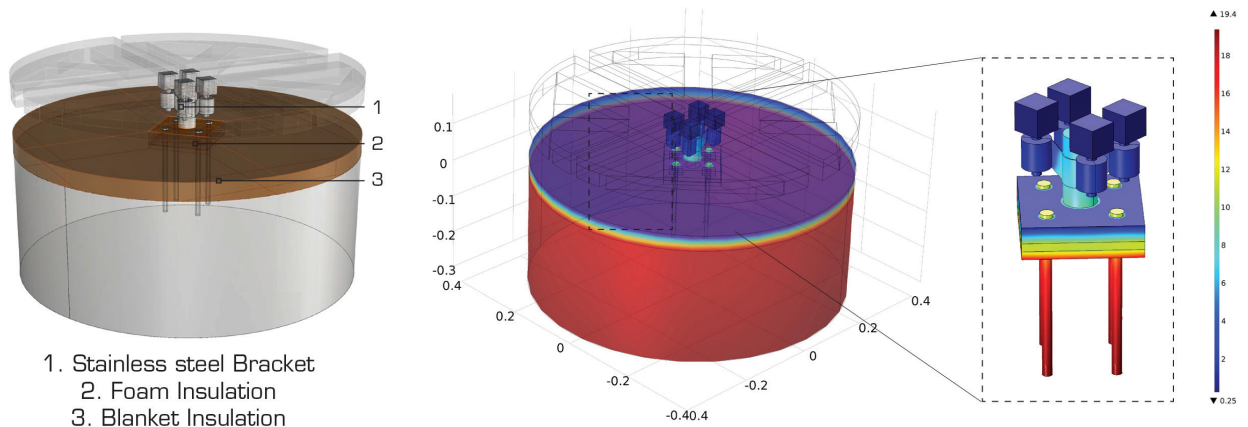
1. Stainless steel Bracket
2. Foam Insulation
3. Blanket Insulation

FIGURE 6. Left: 3D model of the brackets and surrounding insulation built in Rhinoceros® software and imported into the COMSOL Multiphysics® software. Center: COMSOL® software model showing the temperature profile in °C in the area influenced by the bracket. Right: Stainless steel bracket.

"I can combine fluid flow with heat transfer by conduction, convection, and radiation, meaning that I can thoroughly evaluate the interplay of different physical effects and confirm the performance of different structures and materials."

➔RESPONDING TO DESIGN CHANGES

Newtecnic's engineers have to respond to continually changing designs, and need to be able to validate any design updates. "Simulation allows us to do that," observes Galante. "We can demonstrate exactly what effect a design change will have, whether it relates, for example, to energy efficiency, structural performance, corrosion, or the lifecycle of a component."

For Newtecnic director Andrew Watts, it is all about answering questions such as "Is it worth changing this to make something else work?" or "If we have to change it, how much do we have to change it by?" He comments: "With simulation, we can move away from the traditional building philosophy of studying individual components that only perform one function and can instead think in terms of multi-functional components, and of the building as a whole."

Simulation is used to conduct analyses for every component of a building, and these results are fully integrated with drawings so that budget estimates are both clear and comprehensive. Fabio Micoli, Associate Director at Newtecnic,

notes the value of delivering live feedback to clients.

"Simulation minimizes construction costs by allowing contractors to see exactly what they are required to build, thereby reducing the need for contingency budgets or time for unresolved design issues and allowing the construction team to concentrate on meeting project deadlines."

➔CONTINUING IMPROVEMENT

"The digital tools that we use, such as simulation software, enable us to explore new possibilities and improve our design processes," Galante says. He and his colleagues can see potential

for expanding the use of simulation at Newtecnic, including using the new Application Builder, now part of the COMSOL Multiphysics® version 5.0. As Micoli notes, "We could, for example, enhance communication with clients by creating an application that allows an architect to modify different parameters and see exactly how changes would affect their design without knowing the underlying multiphysics simulation details."

The bottom line is that with simulation, a better understanding of building performance can be delivered to Newtecnic's clients than ever before, ensuring that an innovative architectural design puts its best face forward. ❖
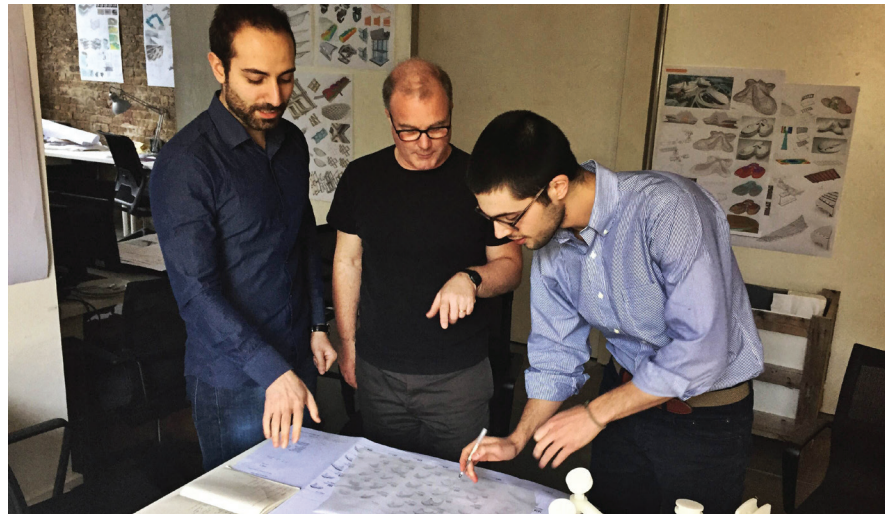
Carmelo Galante (left), Andrew Watts (middle), and Fabio Micoli (right) discuss a recent project at the Newtecnic office in London, UK.

PRECISION PERFORMANCE: THE PURSUIT OF PERFECT MEASUREMENT

Researchers at Brüel & Kjær are using simulation to achieve new levels of precision and accuracy for their industrial and measurement-grade microphones and transducers.
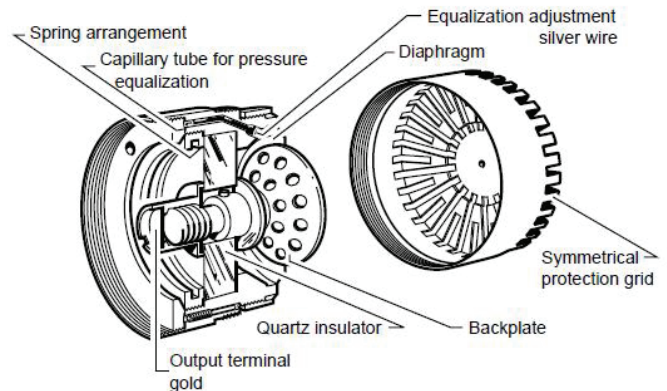
by **ALEXANDRA FOLEY**

FIGURE 1. Left: Photo of a 4134 microphone including the protective grid mounted above the diaphragm. Right: Sectional view of a typical microphone cartridge showing its main components.

There will never be a perfect measurement taken or an infallible instrument created. While we may implicitly trust the measurements we take, no measurement will ever be flawless, as our instruments do not define what they measure. Instead, they react to surrounding phenomena and interpret this data against an imperfect representation of an absolute standard.

Therefore, all instruments have a degree of acceptable error—an allowable amount that measurements can differ without negating their usability. The challenge is to design instruments with an error range that is both known and consistent, even over extended periods of time.

Brüel & Kjær A/S has been a leader in the field of sound and vibration measurement and analysis for over 40 years. Their customers include Airbus, Boeing, Ferrari, Bosch, Honeywell, Caterpillar, Ford, Toyota, Volvo, Rolls-Royce, Lockheed Martin, and NASA, just to name a few.

Because industry sound and vibration challenges are diverse—from traffic and airport noise to car engine vibration, wind turbine noise, and production quality control, Brüel & Kjær must design microphones and accelerometers that meet a variety of different measurement standards. In order to meet these requirements, the company's R&D process includes simulation as a way to verify the precision and accuracy of their devices and test new and innovative designs.

➜DESIGNING AND MANUFACTURING ACCURATE MICROPHONES

Brüel & Kjær develops and produces condenser microphones covering frequencies from infrasound to ultrasound, and levels from below the hearing threshold to the highest sound pressure in normal atmospheric conditions. The range includes working standard and laboratory standard microphones, as well as dedicated microphones for special applications. Consistency and reliability is a key
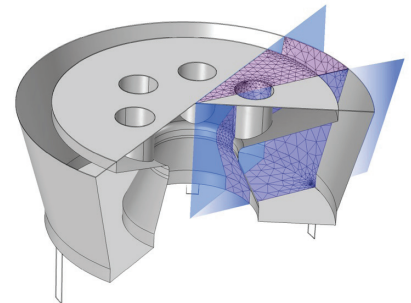
FIGURE 2. Geometry plot of the 4134 condenser microphone. The figure shows the mesh used in the reduced sector geometry, representing 1/12 of the total geometry.

parameter in the development of all of Brüel & Kjær's microphones.

"We use simulation to develop condenser microphones and to ensure that they meet relevant International Electrical Commission (ICE) and International Organization for Standardization (ISO) standards," says Erling Olsen, development engineer in Brüel & Kjær's Microphone Research

and Development department. "Simulation is used as part of our R&D process, together with other tools, all so that we know that our microphones will perform reliably under a wide range of conditions. For example, we know precisely the influence of static pressure, temperature and humidity, and the effect of other factors for all of our microphones—parameters that would have been very difficult to measure were it not for our use of simulation."

The Brüel & Kjær Type 4134 condenser microphone shown in Figure 1 is an old microphone that has been subject to many theoretical and practical investigations over time. Therefore, the 4134 microphone has been used as a prototype for developing multiphysics models of Brüel & Kjær condenser microphones. To analyze the microphone's performance, Olsen's simulations include the movement of the diaphragm, the electromechanical interactions of the membrane deformations with electrical signal generation, the resonance frequency, and the viscous and thermal acoustic losses occurring in the microphone's internal cavities.

→ MICROPHONE MODELING

When sound enters a microphone, sound pressure waves induce deformations in the diaphragm, which are measured as electrical signals. These electrical signals are then converted into sound decibels. "Modeling a microphone involves solving a moving mesh and tightly coupled mechanical, electrical, and acoustic problems—something that could not be done without multiphysics," says Olsen. "The models need to be very detailed because in most cases, large aspect ratios (due to the shape of the microphone cartridges) and small dimensions cause thermal and viscous losses to play an important role in the microphone's performance."

The model can also be used to predict the interactions that occur between the backplate and diaphragm. Among other things, this influences the directional characteristics of the microphone. "We used the simulation to analyze the bending pattern of the diaphragm," says

Olsen. For simulations such as thermal stress and resonance frequency, model symmetry was used to reduce calculation time (see Figure 2). The reduced model was also used to analyze the sound pressure level in the microphone for sounds that are at a normal incidence to the microphone diaphragm (see Figure 3). However, when sound enters the microphone with non-normal incidence, the membrane is subjected to a nonsymmetrical boundary condition. This requires a simulation that considers the entire geometry in order to accurately capture the bending of the membrane (see Figure 4).

Simulation was also used to determine the influence of the air vent in the microphone for measuring low-frequency sounds. "We modeled the microphone with the vent either exposed to the external sound field, outside the field (unexposed), or without a vent," says Olsen. "While the latter would not be done in practice, it allowed us to determine the interaction between the vent configuration and the input resistance results for different low-frequency behaviors. This is one of the most important things about simulation: We can make changes to the parameters of a model that move away from already manufactured devices, allowing us to test other designs and explore the limits of a device (see Figure 5)."
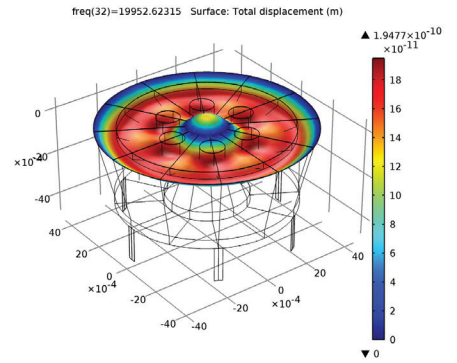

freq(32)=19952.62315   Surface: Total displacement (m)

FIGURE 3. Representation of the sound pressure level below the diaphragm for normal incidence, calculated using the sector geometry. The membrane deformation is evaluated at f = 20 kHz.
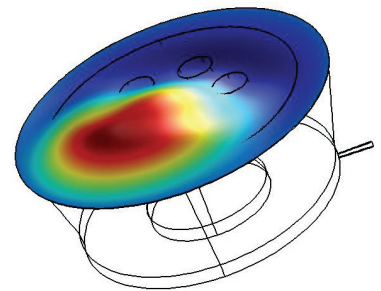

FIGURE 4. Simulation results showing the membrane deformation calculated for non-normal incidence at 25 kHz. Since the deformation is asymmetrical, this is calculated using the full 3D model.
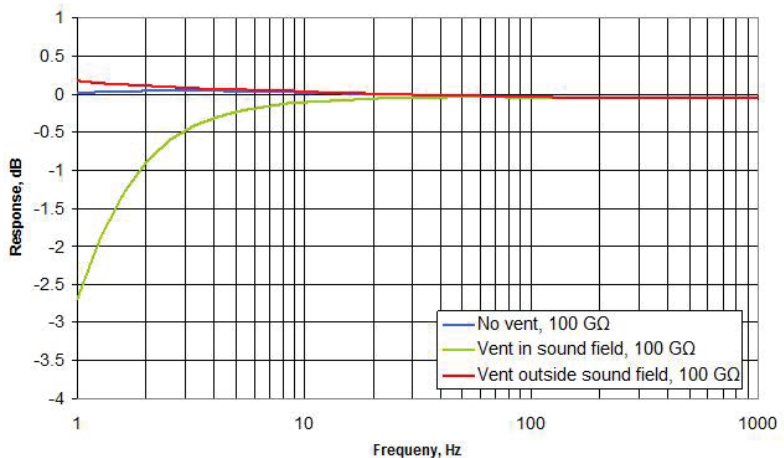

FIGURE 5. In the no-vent configuration, the sensitivity increase is due to the fact that the sound field becomes purely isothermal inside the microphone at very low frequencies. In the vent outside the sound field configuration, the curve initially follows the no-vent curve, but sensitivity increases further as the vent becomes a pressure release on the back of the diaphragm.

With simulation as part of the R&D process, Olsen and his colleagues are able not only to design and test some of Brüel & Kjær's core products, but devices can also be created based on a specific customer's requirements.

"With simulation, we can pin-point approaches for making specific improvements based on a customer's needs. Although microphone acoustics are very hard to measure through testing alone, after validating our simulations against a physical model for a certain configuration, we are able to use the simulation to analyze other configurations and environments on a case-by-case basis."

➜ VIBRATION TRANSDUCER MODELING

Søren Andresen, a development engineer with Brüel & Kjær, also uses simulation to design and test vibration transducer designs.

"One of the complications with designing transducers for vibration analysis is the harsh environments that these devices need to be able to withstand," says Andresen. "Our goal was to design a device that has so much built-in resistance that it can withstand extremely harsh environments."

Most mechanical systems tend to have their resonance frequencies confined to within a relatively narrow range, typically between 10 and 1000 Hz. One of the most important aspects of transducer design is that the device does not resonate at the same frequency as the vibrations to be measured, as this would interfere with the measured results. Figure 6 shows the mechanical displacement of a suspended vibration transducer, as well as a plot of the resonance frequency for the device.

> ❝With simulation, we can pin-point approaches for making specific improvements based on a customer's needs.❞
> —**ERLING OLSEN, DEVELOPMENT ENGINEER AT BRÜEL & KJÆR**

"We want the transducer to have a flat response and no resonance frequency for the desired vibration range being measured," says Andresen. "We used COMSOL to experiment with different designs in order to determine the combination of materials and geometry that produces a flat profile (no resonance) for a certain design. This is the region in which the transducer will be used."

When designing the transducer, a low-pass filter, or mechanical filter, can be used to cut away the undesired signal caused by the transducer resonance, if any. These filters consist of a medium, typically rubber, bonded between two mounting discs, which is then fixed between the transducer and the mounting surface.

"As a rule of thumb, we set the upper frequency limit to one-third of the transducer's resonance frequency, so that we know that vibration components measured at the upper frequency limit will be in error by no more than 10 to 12%," says Andresen.

➜ AS ACCURATE AND PRECISE AS POSSIBLE

While it may not be possible to design a perfect transducer or take an infallible measurement, simulation brings research and design teams closer than ever before by allowing them to quickly and efficiently test new design solutions for many different operating scenarios.

"In order to stay ahead of the competition, we need knowledge that is unique," says Andresen. "Simulation provides us with this, as we can make adjustments and take virtual measurements that we couldn't otherwise determine experimentally, allowing us to test out and optimize innovative new designs." ❖
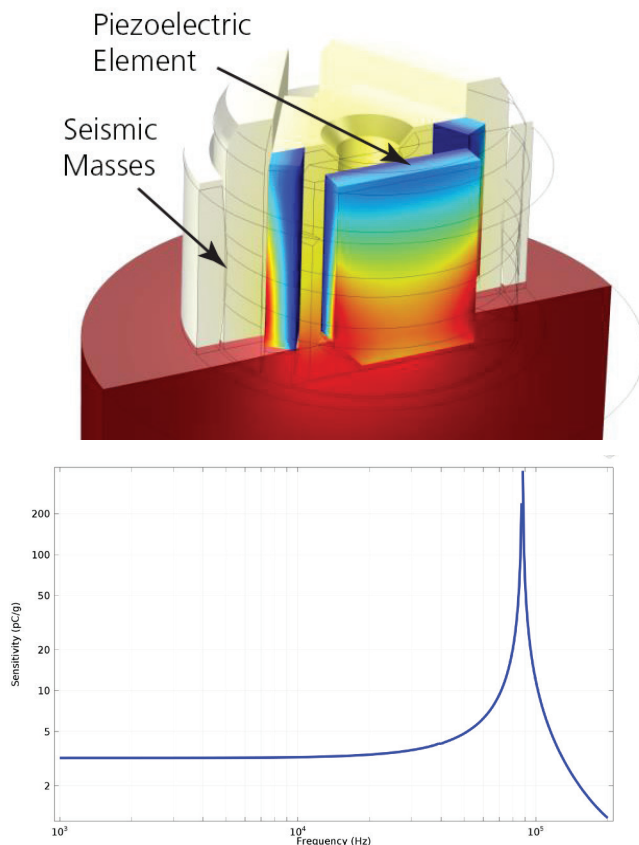

FIGURE 6. Simulation results of a suspended piezoelectric vibration transducer. Top: Mechanical deformation and electrical field in the piezoelectric sensing element and seismic masses. Bottom: Frequency-response plot showing the first resonance of the transducer at around 90 kHz. This device should only be used to measure objects at frequencies well below 90 kHz.

MAKING BIOFUEL A COST-EFFECTIVE, RENEWABLE SOURCE OF ENERGY

Researchers at the National Renewable Energy Laboratory are using multiphysics simulation to better understand and optimize the conversion process for plant-derived biofuels.

by **JENNIFER SEGUI**

Biofuels could potentially replace fossil fuels for many applications, offering an alternative source of energy to heat buildings, generate electricity, and keep the transportation industry moving.

There are many benefits to producing biofuels from plant-based materials, generally referred to as biomass. Such fuels are renewable, clean-burning, and carbon-neutral, producing no more carbon dioxide than is sequestered by its original plant source. However, biofuel availability is still fairly limited for its most common use—in vehicles. As of 2014, the U.S. Energy Information Administration reports that only 2% of retail fueling stations were offering the ethanol-based fuel E85.

The production process itself poses an important economic barrier to the widespread use of biofuels. Research at the National Renewable Energy Laboratory (NREL), supported by the Computational Pyrolysis Consortium, is directed toward gaining a better understanding of the physical processes behind biofuel conversion by developing computational models that feature the most accurate representation of biomass particle geometry to date. Such a model could then be used to improve reactor design and operation as required for the mass production of biofuel.

This work can ultimately make biofuel use more cost-effective and competitive with traditional nonrenewable fuels, some of which will be depleted in mere decades.

FIGURE 1. In preparation for pyrolysis, the woody biomass shown at left has been milled and may also undergo additional chemical treatment. Several physical processes including heat transfer, mass transfer, chemical reactions, and phase change must be taken into account to develop a complete model of pyrolysis, shown at right. The flask in the photo collects the condensed bio-oil vapors resulting from pyrolysis in a pre-commercial reactor. Photo credits: Warren Gretz, NREL 05756 (left) and Phil Shepherd, NREL 03677 (right).
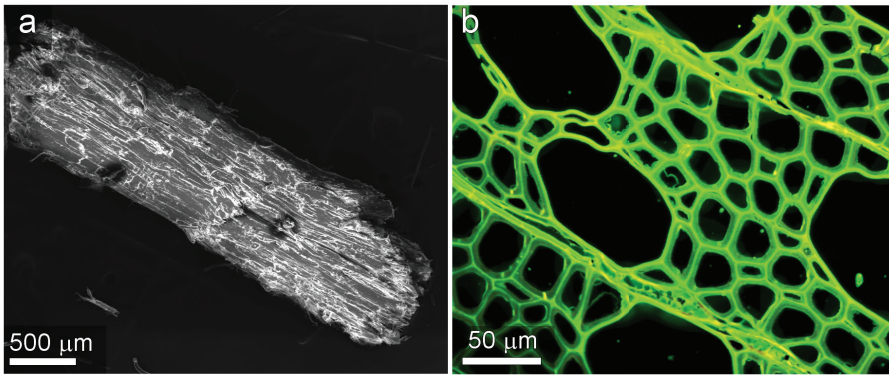
FIGURE 2. Left: A scanning electron micrograph confirms the shape and structure of a hardwood biomass particle. Right: A confocal scanning laser micrograph of a particle cross section shows the microstructure.

> "Since COMSOL has geometry tools, physics, meshing, and solvers already implemented, we can spend more time making the biomass model geometry really accurate."
>
> —**PETER CIESIELSKI, RESEARCH SCIENTIST AT NREL**

→ PRODUCING FUEL FROM PLANTS

Thermochemical processes such as pyrolysis, which is shown in Figure 1, use exposure to high temperatures to break down and convert biomass particles to liquid biofuels that can support many everyday life activities. Improving fast pyrolysis, a pre-commercial thermochemical conversion route often used for woody biomass, is one objective of the research program at NREL, and is described in more detail in the sidebar below.

Peter Ciesielski, a research scientist at NREL, and his colleagues are using multiphysics simulation to gain insight into the fundamental processes behind biomass conversion via pyrolysis, starting with investigating heat and mass transfer.

Efficient heat and mass transfer through biomass particles minimizes char formation and accelerates favorable reactions by facilitating the penetration of conversion catalysts and the escape of desired products. Ciesielski's work considers the effect of size, shape, and internal microstructure of biomass particles, which is determined by the species of wood and by the milling process used prior to pyrolysis.

→ AN ACCURATE MODEL OF BIOMASS

Computational studies designed to understand and optimize the biofuel conversion process have always used simplified biomass particle geometry that ignored internal microstructure.

Ciesielski's research aims to provide insight into the heat and mass transfer in biomass by developing a model in

COMPUTATIONAL PYROLYSIS CONSORTIUM

Ciesielski's work, supported by the Computational Pyrolysis Consortium and funded by the U.S. Department of Energy, is a collaborative effort between researchers at NREL, Oakridge National Laboratory (ORNL), and the National Institute of Standards and Technology (NIST). The collaboration brings together experts in computational modeling, biomass conversion, reactor design, and materials characterization to optimize biofuel production via pyrolysis.

To appreciate the significance of pyrolysis—first think about a fire, but take away the flame. Pyrolysis is a thermochemical conversion route that causes decomposition of biomass via exposure to high temperatures and in the absence of oxygen. Without oxygen, there is no combustion or flame. The result of pyrolysis is char, a liquid product often referred to as bio-oil, and gaseous products of the chemical reaction. Biofuels are produced from further refinement of the bio-oil.

Fast pyrolysis research at NREL takes the process one step further by using an extremely high rate of heat transfer to break down biomass, where internal temperatures reach upwards of 500°C within 1 second.
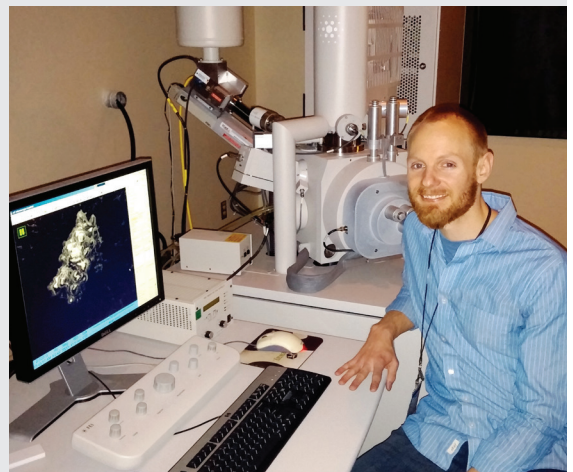
Peter Ciesielski, a research scientist at NREL, is pictured next to the scanning electron microscope used to acquire images of wood biomass for his work published in Energy & Fuels[1].

the COMSOL Multiphysics® software that takes internal microstructure into account. "Since COMSOL has the geometry tools, physics, meshing, and solvers already implemented, we can spend more time making the biomass model geometry really accurate," explains Ciesielski.

In order to generate 3D models of biomass for use in COMSOL simulations, a confluence of imaging methods was used to characterize the external morphology and size distribution as well as the internal microstructure of each type of biomass. Examples of images that were acquired for this study are shown in Figure 2.

A solid geometry was generated using the external and internal dimensions of biomass particles, determined from the images, as input to a series of Boolean geometry operations in COMSOL. The complete geometry consists of two domains, as shown in Figure 3.

➜SIMULATING PYROLYSIS: HEAT AND MASS TRANSFER

Biomass decomposition via fast pyrolysis starts with the application of high temperatures (about 500ºC) to an oxygen-free reaction vessel for a few seconds. Applying these conditions, the Conjugate Heat Transfer interface in COMSOL was used to simulate heat transfer between the outer fluid domain shown in Figure 3a, consisting of nitrogen gas, and the biomass particle. Heat transfer in the fluid domain is predominately by convection, whereas at the interface and through the biomass particle, heat transfer is by conduction only.

The simulations were run on a high-performance computing (HPC) cluster using one or two compute nodes each consisting of 24 Intel® Xeon® Ivy Bridge processors with 64 GB of RAM. The results in Figure 3b show the temperature distribution in a hardwood biomass particle 0.5 seconds into a transient simulation of conjugate heat

transfer. For a given particle size, shape, and microstructure, it is possible to determine the amount of time required for the entire particle, particularly the center, to reach optimal temperatures for decomposition.

In a separate simulation, the diffusion of sulfuric acid, a chemical used to pretreat biomass prior to its conversion to biofuel, was evaluated. The Transport of Diluted Species interface was used for transient simulations of mass transport in the microstructure and solid particle geometries where the surrounding fluid in this case was water.

The results from both the heat and mass transfer studies indicate that a solid model, particularly a spherical one, may not offer sufficient accuracy to evaluate and optimize biofuel conversion processes and that the use of a microstructured model is justified.

➜INPUT FOR LARGE-SCALE REACTOR DESIGN

While the present study focuses on heat and mass transfer in biomass, rapid phase transitions and chemical reactions are critical to fully understand and optimize biofuel production via fast pyrolysis. Ciesielski's ongoing work involves adding these to his simulations, the ability to do so being an important reason why COMSOL was chosen.

Ultimately, however, the team has bigger plans for the computational model. By performing simulations to gain a fundamental understanding of transport in biomass, effective correlations for low-order models can be determined for a range of process parameters and biomass feedstocks. These correlations can be used to optimize the design and operation of large-scale reactors for mass production of biofuel, making the process more efficient and cost-effective. ❖

REFERENCES
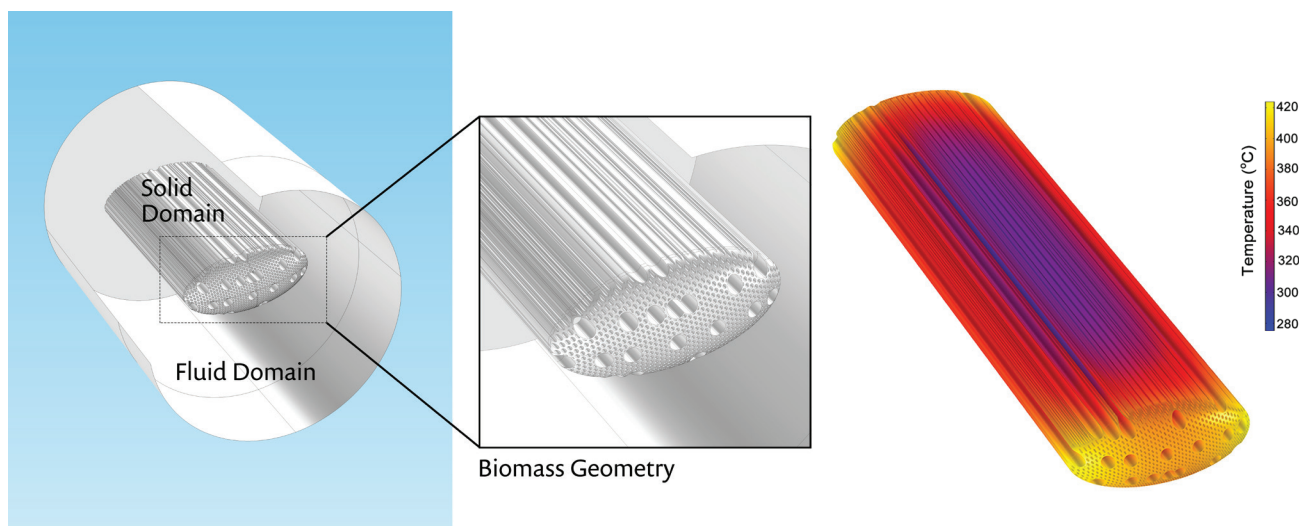[1] P. N. Ciesielski, et. al., Energy Fuels, 2015, 29(1), pp 242-254.

FIGURE 3. Left: COMSOL® software model geometry featuring a fluid domain surrounding a hardwood biomass particle. Right: The temperature distribution from a transient simulation of conjugate heat transfer is shown.

SIMULATION SOLVES THE MYSTERY BEHIND AN ELEVATOR ACCIDENT

While we can easily picture simulation as an integral part of product design related activities, other uses are equally important: Field failure analysis and forensic examination are two examples. Veryst Engineering used multiphysics simulation to investigate and determine how an elevator brake failed prematurely.

by **STUART BROWN, NAGI ELABBASI, & MATTHEW HANCOCK, VERYST ENGINEERING**

In 2007, an elevator began moving upwards while passengers were exiting, trapping and injuring an occupant. A drum brake intended to hold the elevator stationary failed, resulting in the unexpected movement. Subsequent investigation revealed that a solenoid responsible for opening and closing the brake had deteriorated, causing the brake linings to drag on the drum and wear prematurely. When the solenoid was not engaged, normal brake shoes would have pushed against the drum, preventing elevator motion. Excess brake shoe wear caused the brake to fail to hold, leading to the accident. Figure 1 shows a CAD model of the brake, where the brake arms are pivoted at the bottom and spring loaded to maintain contact with the drum.

Criminal charges were filed against the elevator maintenance firms, claiming that there was evidence in previous years that the solenoid was deteriorating and that repairs should have been performed. The question was not whether the solenoid had failed, but rather, how did it fail and at what rate—slowly or quickly?
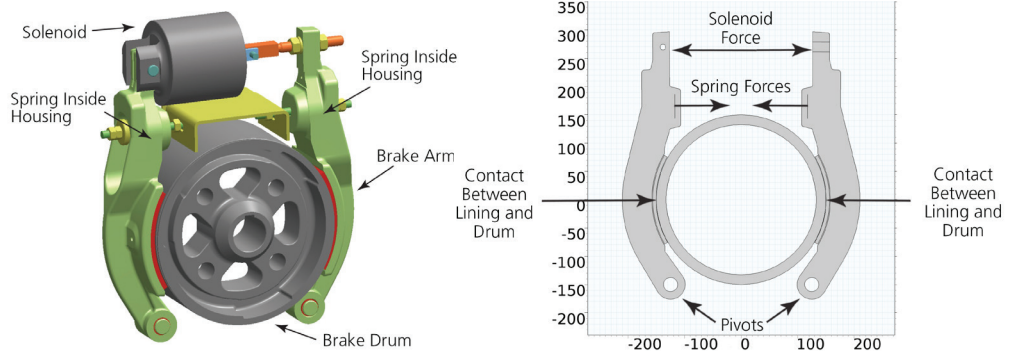
If the failure were

FIGURE 1. Left: Brake CAD geometry. Right: Brake lining wear model setup showing the brake drum, arms and pivots, the opposing spring and solenoid forces, and the contact between brake linings and the drum.

rapid, it would have been unlikely that the accident could have been anticipated. However, if the failure involved a slow deterioration, perhaps the accident could have been prevented. Many possible theories of failure were suggested. We at Veryst Engineering, a consulting firm based in Massachusetts, were hired to investigate the validity of the different failure theories, and simulation played a pivotal role in our investigation.

➔ANALYSIS OF SOLENOID FAILURE

After the accident, investigators discovered that the solenoid had approximately half the electrical resistance of an undamaged solenoid, and therefore, generated less force compared to an undamaged solenoid. Several theories were proposed to explain how this failure could have occurred.

One theory for slow failure was that thermal expansion and contraction within the solenoid due to resistive heating produced high stresses leading to slow, progressive cracking of the wires within the solenoid coil. Cracks would reduce the solenoid's electromotive force (EMF), thereby leading to brake shoe dragging. In order to test this theory, we used the COMSOL Multiphysics® software to produce a coupled

thermomechanical stress analysis of the solenoid. The model demonstrated that the stresses were not large enough to produce cracking, therefore proving that expansion and contraction due to resistive heating was not the cause of the failure.

A second theory for slow failure was that the EMF itself generated high stresses in the coil, causing it to fail over an extended period of time. We tested this by performing a coupled electromechanical analysis, which is shown in Figure 2. COMSOL® software was used to calculate the Lorentz force within the solenoid coil, demonstrating that the force throughout

the coil was practically negligible.

In contrast, one theory for rapid solenoid failure stipulated that localized heating within the solenoid resulted in shorting between adjacent coil wires. While we did not analyze this theory directly, our analysis refuting the above slow failure theories narrowed the field of possible failure modes and lent support to the rapid failure scenario.

➔ANALYSIS OF RAPID BRAKE LINING WEAR

In addition to the solenoid failure analysis, we investigated the effect of a damaged solenoid on brake lining wear. Given that the solenoid involved in the accident could not generate the force of a normal solenoid, could the brake linings have also deteriorated so quickly? After the accident, investigators discovered that the brake lining wear was extensive, and assumed that this degree of wear had to have occurred gradually.

To test whether the extensive brake wear could have occurred swiftly given a damaged solenoid, we developed a COMSOL model of the brake to calculate the local brake lining wear. The model included the brake arm pivoting as well as the opposing forces of the springs and damaged solenoid. In addition, the model included data from the extensive wear experiments performed by investigators on prototype drum brake linings, which resulted in data correlating bulk lining wear rates to brake drum temperature.

We used this temperature-wear data combined with a wear rate model commonly used in the brake industry to develop a local wear rate model. The model was implemented using both the Structural Mechanics Module and user-defined differential equations defined on the brake lining surfaces. The contact boundary condition available in COMSOL provided the local contact pressure for the model, which was used to determine the local wear rate at each point along the brake linings. The predicted brake lining wear was in turn used to specify an offset from the original brake surface in the contact boundary condition, a valid assumption provided the amount of wear is small compared to the lining thickness. The input to the wear simulation was an assumed time history of drum temperature. We validated this wear modeling approach by simulating two mechanical wear problems: wear resulting from pin-on-disc contact and wear in automotive disk brakes.

The contact boundary condition within the Structural Mechanics Module and the ability to easily implement user-defined differential equations made programming the wear process remarkably straightforward and helped us to avoid cumbersome methods such as mesh element deletion. This type of analysis would have been either impossible or prohibitively difficult using any other finite element package.

Figure 3 shows the finite element model used in the wear analysis. Figure 4 shows a comparison between the measured and predicted brake lining wear along the length of the brakes at the end of the test. The model also predicted how wear depth varied with time. The results of the wear simulation indicated that a damaged solenoid could result in high drum temperatures, leading to rapid brake lining wear.

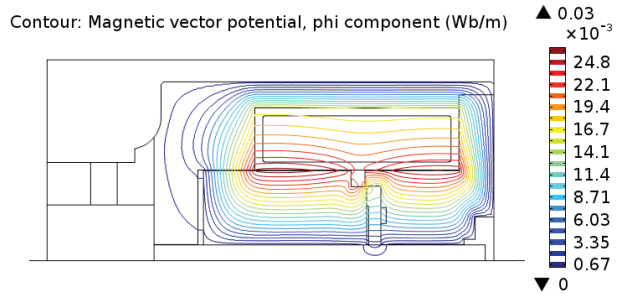In other words, the high amount of wear on the brake

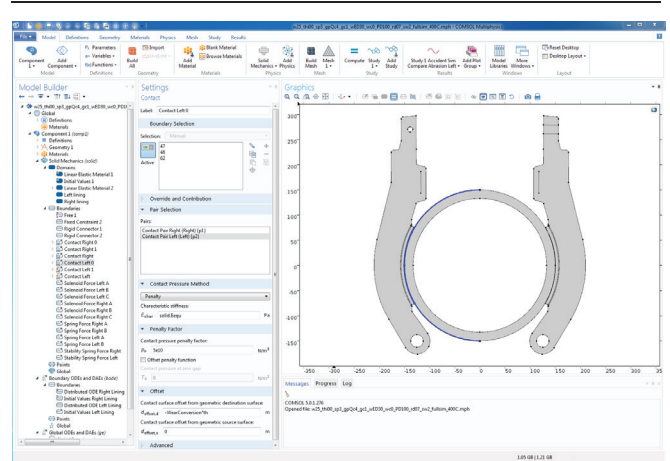**FIGURE 2.** Magnetic potential within solenoid component.

FIGURE 3. COMSOL Multiphysics® software model used to calculate brake lining wear.
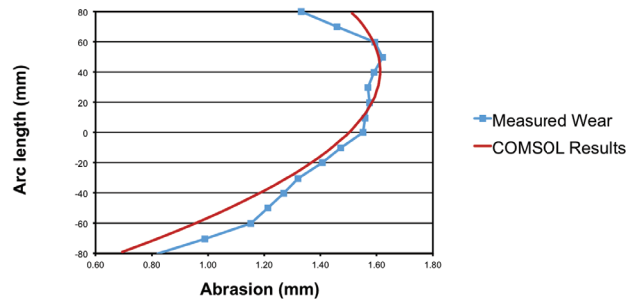

FIGURE 4. Comparison of measured lining wear with simulation prediction.

linings was entirely consistent with a rapid train of events, from the rapid deterioration of the solenoid to the rapid and extensive brake lining wear. This rapid failure theory provided an alternative, self-consistent, and scientifically sound explanation of the accident, involving no slow processes.

COMSOL Multiphysics was an essential contributor to this investigation, enabling us to quickly investigate different scenarios by allowing us to readily import and handle different geometries, include multiple physics in a single simulation, and import and use experimental data with our simulations. The simulations provided an efficient and systematic way to test and evaluate the failure scenarios, an approach that no one else had tried. ❖

BETTER WAYS TO HEAT AND COOL BUILDINGS

Multiphysics simulation helps researchers at the Fraunhofer Institute for Solar Energy Systems develop innovative adsorption-based chillers, heat pumps, and thermal storage units driven by solar, natural gas, and waste heat.

by **GARY DAGASTINE**

FIGURE 1. Example of a commercially available adsorption-based chiller.

The heating and cooling of buildings accounts for nearly 50 percent of energy consumption in Europe, spurring researchers to find alternatives to conventional technologies.

One enticing possibility is to use adsorption-based heating and cooling systems driven not by electricity, but by heat. Because heat could come from solar collectors, from waste heat generated by industrial facilities, or from combined heat and power units, this adsorption technology offers the possibility of significantly reducing electricity consumption and associated CO_2 emissions. The technology can be used not only as a highly efficient heating system that uses gas-fired heat pumps to multiply the heat delivered to a building, but also for the compact storing of energy for a long period of time.

In brief, heating and cooling systems based on this principle use a working fluid in an adsorption/desorption cycle where the fluid's state is altered from liquid to gas and vice versa numerous times (see the sidebar on page 37 for more details). With this technique, special heat exchangers can be built that act as

thermal compressors by periodically heating and cooling an adsorbent material at different temperatures and pressures. These systems can replace electrically driven mechanical compressors in heat pumps and chillers with the extra benefit of offering heat storage capacity, which can store up to three times the energy stored using traditional hot water systems.

➔ OPTIMIZING THERMAL TRANSFER AND STORAGE

The development of adsorption-based heating systems and chillers is complex. They have discontinuous operating cycles, varying peak energy fluxes, and their dynamic behavior is determined by complex and coupled heat and mass transfer phenomena.

Although some adsorption-based systems are already commercially available (see Figure 1), to realize their full potential on a larger scale the technology must become far more efficient, more compact, and cheaper to produce.

One of the world's leading research organizations in this field is the Fraunhofer Institute for Solar Energy Systems (ISE) in Freiburg, Germany. With a staff of some 1,300 employees, it investigates all aspects of solar energy transformation, storage, and use. It is part of a network of more than

65 Fraunhofer research institutes in Germany that specialize in different aspects of applied science.

Eric Laurenz and Hannes Fugmann, researchers at Fraunhofer ISE, are part of a 20-person group led by Lena Schnabel that is developing higher-efficiency heat exchangers for adsorption systems. Laurenz studies how water vapor and heat flows through porous structures with the goal of optimizing system size and efficiency, while Fugmann conducts design studies involving non-isothermal fluid flows and heat conduction in solids in order to develop better heat
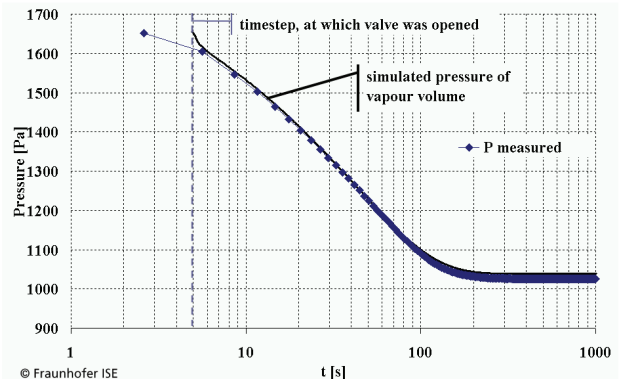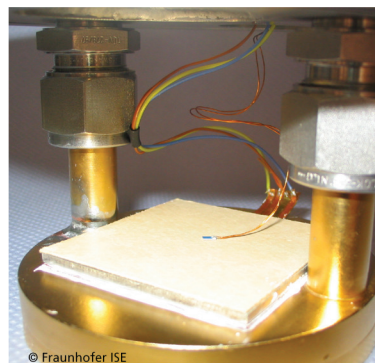

FIGURE 2. Left: Experimental setup used to validate COMSOL® software models of adsorption kinetics, consisting of a thin 50x50 mm² layer of zeolite sorbent on an aluminum carrier, placed on a cold plate in a dosing chamber and monitored with temperature and heat flux sensors. Right: Graph showing excellent agreement between simulated and measured water vapor pressure in a zeolite sorbent test setup at Fraunhofer ISE.

exchanger architectures.

"Analytical methods are inadequate for our work because of the strong nonlinear couplings between the heat and mass transfer involved," Laurenz said. "We need to use numerical tools such as COMSOL Multiphysics® to simulate the cyclic loading and unloading of the sorbent and take into account the temperature and mass distribution in both space and time. With these tools, we can make sure that the simulation will correctly capture the dynamics of adsorption and desorption."

As a general approach, the team uses a combination of simulation and well-defined, small-scale experiments to build large-scale models that can accurately predict the complex real-world behavior of the physics being investigated. With the small-scale models, the team can fully model the physical mechanisms in detail, while on the larger scales, complexity can be reduced to save on computational time. This approach can significantly reduce the need to build full-size physical prototypes, saving both time and money.

➔VALIDATING THE ADSORPTION PROCESS

One of the key objectives for improving adsorption heat exchangers is to optimize the uptake speed and capacity of the thin sorbent layers used in the system. In one investigation, simulation was used by Lena Schnabel and Gerrit Füldner to build a model that captured the heat and mass transfer interplay dynamics happening in the sorbent layer. With the help of the model, the group was able to fully understand the measurements obtained from the experimental setup shown at left in Figure 2.

"Only by comparing experimental and simulation results using parameter estimation were we able to determine the transport coefficients that could not be measured directly," describes Laurenz. "This data was then used in our more complex simulations of the system."

Schnabel's group first started using COMSOL Multiphysics nearly ten years ago. More recently, however, the group has started to use models with varying levels of detail to estimate transport parameters and to simulate the cyclic behavior of complete systems under dynamically changing operating conditions. The ability to easily simulate coupled physics in complex and dynamic systems has proven indispensable for much of their research at Fraunhofer ISE.

➔ENHANCED HEAT EXCHANGER DESIGNS

In his work to optimize heat exchanger architectures, Fugmann performs basic research on heat exchanger designs, including chillers and heat pumps. Some of his geometries are designed to increase heat transfer surface area using wire structures such as those shown in Figure 3, as opposed to the more traditional fin-and-tube heat exchanger designs. In these novel architectures, a wire structure is woven or knitted around a series of tubes, separating the two fluids in the heat exchanger. In an experimental setup for a gas-to-liquid wire heat exchanger, hot water flows within the tubes while cold air flows between the tubes and across the wires.

"We found that if we use wire structures, we can achieve a higher heat transfer coefficient with a larger surface, as

USING ADSORPTION FOR HEATING AND COOLING SYSTEMS

A schematic of the two-step cycle used to design adsorption-based chillers and heat pumps is shown in the figure below. To explain, let's look at what takes place during the heat pump mode. The cycle is composed of one adsorption and one desorption step. During the adsorption step, the working fluid is evaporated at a low temperature. At the same time, the working fluid is adsorbed by an adsorbent at a medium temperature, where the heat released can be used to heat a building.

Once the sorbent is saturated, the process is inverted and the desorption step starts. The sorbent is heated to a high temperature, thereby desorbing the working fluid. Next, the working fluid is condensed at a medium temperature, and the released heat of condensation can be used to heat a building.

In summary, for heating applications (heat pumps) the building is heated while energy is removed from the environment. Conversely, in cooling applications (chillers), the building is cooled down while heat is released to the environment. When the cycle is interrupted, the potential heat of adsorption can be stored loss free. Depending on the desired application, adsorption can be used to heat or chill a building, while the environment acts as either a heat source or sink.
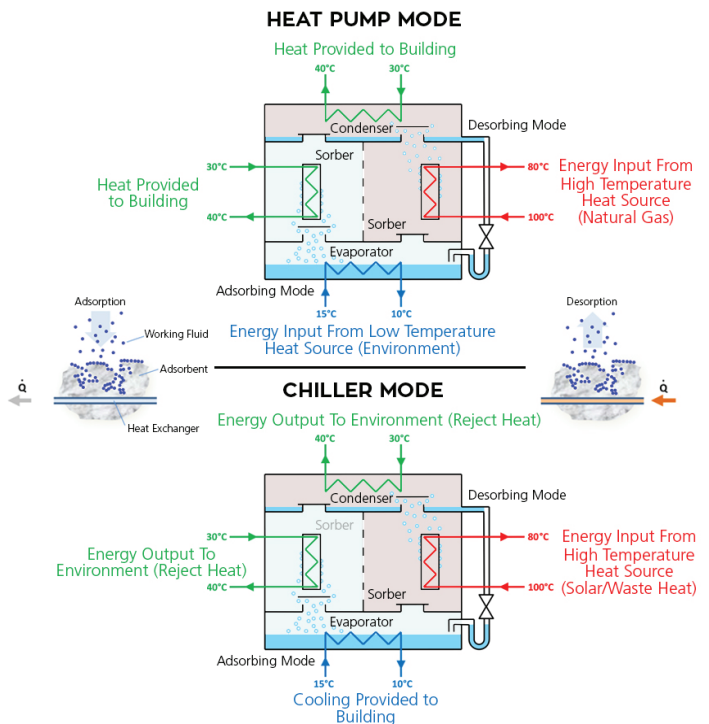
The sorber continuously switches between the adsorbing and desorbing modes during operation
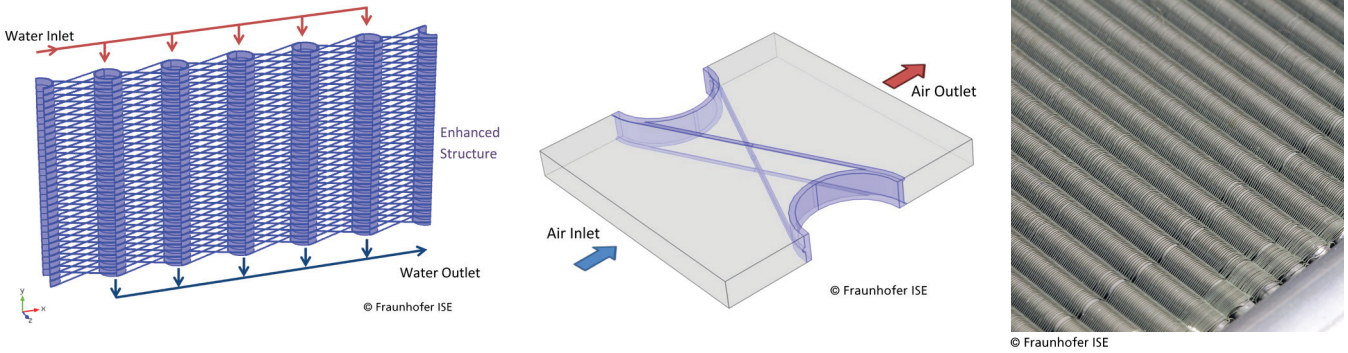
© Fraunhofer ISE

FIGURE 3. Left: Device geometry showing warm water entering the tubes. Cold air is passed across the tubes, cooling the water as it flows through the tubes. Middle: Simulated geometry showing the cold air entry and warm air exit. The wire structure and the tubes are shown in purple. Right: Device geometry used in experimental testing.

FIGURE 4. Left: Simulations showing velocity streamlines and the temperature distribution in air, in the tube wall, and in the wire connecting the two tubes (red: warm; blue: cold). Right: Simulations showing the velocity magnitude in air (red: high; blue: low).

well as significantly reduce material usage," said Fugmann. "We are able to do this without noticeably increasing the pressure drop, and the flexibility of the wire structures also gives us the ability to easily adapt the geometry depending on the operating parameters of the design."

Using COMSOL® software, Fugmann performed parametric sweeps to investigate specific pressure drops, heat transfer coefficients, material usage, and other analyses of the design's geometry. Figure 4 shows the temperature distribution and the velocity magnitude of an optimized geometry of the wire structure and the tubes.

Fugmann describes the device: "From the measurements, we found that the bonded connections between wires and tubes yield a high and dominating heat resistance. By understanding the limitations of heat transfer in the wire structures, we can further optimize the design."

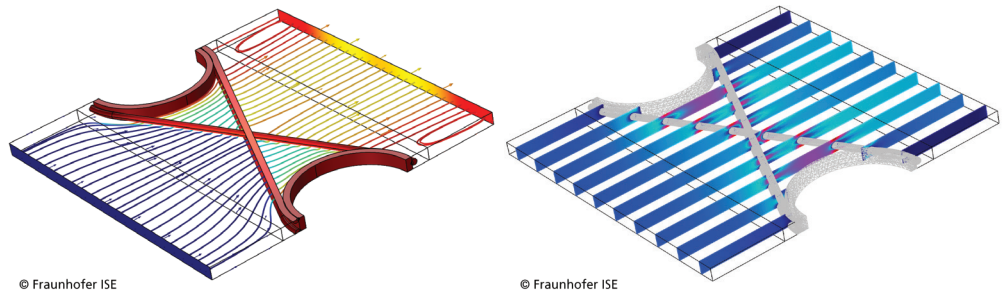Due to their higher heat exchange surface per volume, the wire structures are also analyzed experimentally and numerically at Fraunhofer ISE for use as sorptive-coated structures and as surface enlargement for heat exchangers in thermal storages.

➔ LOOKING AHEAD

"Our immediate goal is to increase knowledge and competence in these areas so that we can help both our customers and others at Fraunhofer ISE who are developing different aspects of adsorptive climate control systems," said Laurenz. "Longer-term, we look forward to the day when such technologies are in widespread use in society, helping to reduce the load on the electrical grid and conserve the earth's resources." ❖
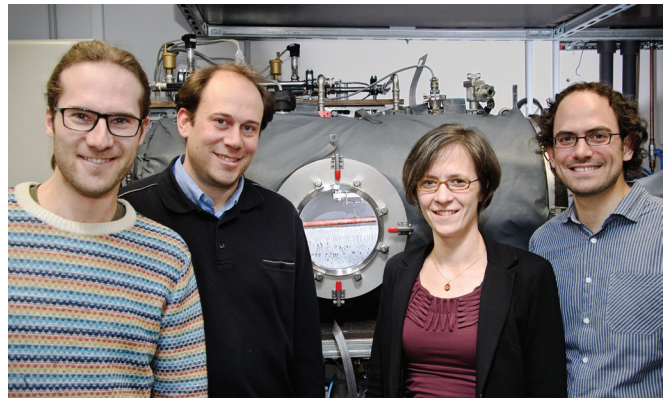
The Fraunhofer ISE team includes (from left) Hannes Fugmann, Gerrit Füldner, Lena Schnabel, and Eric Laurenz. They are standing in front of an experimental setup for the dynamic characterization of adsorption heat exchangers. The setup is used to generate experimental data for simulation-based parameter estimation.

REFERENCES
[1]Füldner, G. & Schnabel, L., 2008. Non-Isothermal Kinetics of Water Adsorption in Compact Adsorbent Layers on a Metal Support. In Proceedings of the COMSOL Conference 2008 Hannover. COMSOL Conference. Hannover.

COMSOL BLOG SHARES THE LATEST IN MULTIPHYSICS SIMULATION

The engineering community turns to the COMSOL Blog for answers to multiphysics simulation questions and fun reads.

by **FANNY LITTMARCK**

Engineers around the world are leaning on the COMSOL Blog as a go-to resource for multiphysics simulation. Readers learn about when, why, and how to best use COMSOL Multiphysics® software—directly from the experts. All blog posts are written and published in-house by application engineers and other COMSOL staff, with the occasional guest blogger. The variety of authors ensures a wide range of content, from highly technical details to lighter informative reads.

➜ FROM SUPPORT ANSWERS TO RELEASE NEWS AND EVERYTHING IN BETWEEN

The blog content mix spans over 40 topic categories, organized by physics for the most part to enable easy browsing of relevant content. Users of COMSOL Multiphysics refer to the COMSOL Blog for answers to common support questions, modeling tips, release news, COMSOL Conference updates, and more. In addition to information specific to the COMSOL® simulation software, the Trending Topics category contains popular science blog posts for all to enjoy.

While the majority of blog posts are published as stand-alone pieces, some topics are more detailed and stretch over several blog entries in a series. The most popular series is one on solvers, where Applications Engineer Walter Frei explains what happens under the hood when the COMSOL software is solving models. Other fan favorites include series on postprocessing tips, high-performance computing (HPC), the weak form, and more. A tag cloud organizes all of the series in the bottom of the right-hand sidebar on the blog and is updated as new series are launched.

➜ EXPLORE THE COMSOL BLOG

With fresh content published Monday through Friday each week and covering a variety of topics, the COMSOL Blog has something for everyone. Visit the blog now for the latest in multiphysics simulation by navigating to it directly at www.comsol.com/blogs or from any page on the COMSOL website via the Community section in the footer. ❖
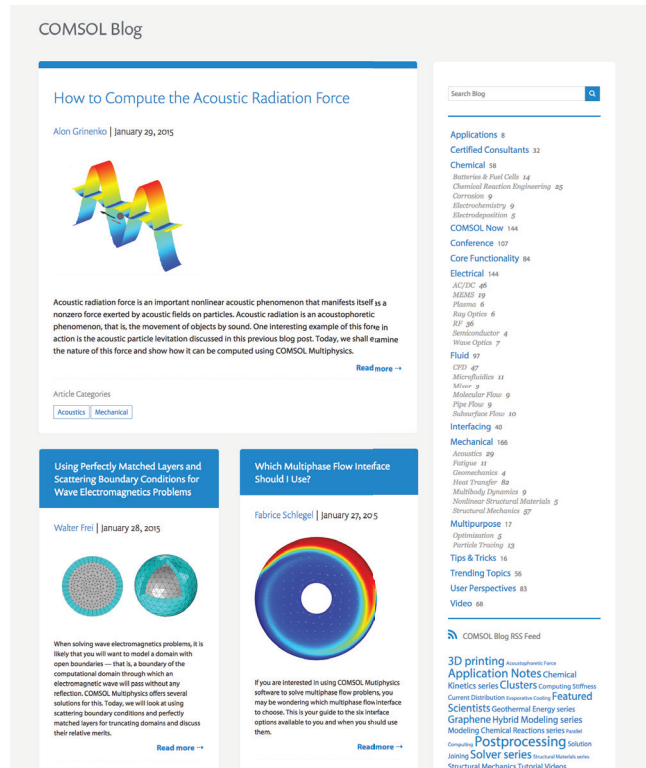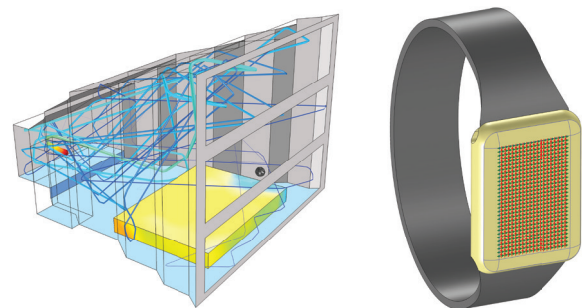

FIGURE 1. Screenshot of the COMSOL Blog.

FIGURE 2. Left: Ray path in a concert hall from the blog post "Modeling Room Acoustics with COMSOL Multiphysics". Right: Touchscreen watch from the blog post "Analyzing Capacitive Touchscreens in Consumer Electronics".

FIGURE 3. Tag cloud featuring COMSOL Blog series.

Simulation Apps Bring Us Closer to Mars

by **JIM KNOX, MARSHALL SPACE FLIGHT CENTER, NASA**

My work with mathematical modeling and computer simulations began in earnest in 1987 when I signed on with the National Aeronautics and Space Administration, better known as NASA. At the time, I was developing computer simulations to support the design of carbon dioxide (CO_2) removal systems for the International Space Station (ISS) life support system. CO_2 is a human metabolic waste, produced at a rate of a kilogram per day per crewmember. CO_2 must be removed from the crew cabin, as it will quickly become detrimental to crew health. The systems used to remove CO_2 are typically based on sorption processes, which include complex interactions of heat transfer, mass transfer, and gas flow through porous media. At this time, there were no commercial options for solving a set of coupled mathematical models such as partial differential equations (PDEs); you either force-fit the physics into a thermal analysis package or wrote your own code, complete with discretization, meshing, and solution algorithms. Unfortunately, coding CO_2 removal processes from scratch did not allow an appropriate focus on the challenging yet crucial task of understanding and capturing the underlying physics via appropriate

> **"**The Application Builder will provide the means to distribute the workload to many individuals.**"**

mathematical models. Configuration control was often simply ignored due to tight schedules, resulting in a code that would be quicker for a second party to rewrite than modify.

In the early 2000s, I decided to move CO_2 removal simulations to a platform with built-in meshing, solvers, and postprocessing capabilities, and that could solve user-defined multiphysics PDEs. The program chosen to meet these needs was the COMSOL Multiphysics® software. Along with freeing the engineer to focus on the underlying physics, a degree of configuration control was automatically achieved via a consistent user interface, thus allowing COMSOL® software users to share computer models. My team has developed simulations that are already providing a valuable debugging capability for the ISS CO_2 removal system, and will provide guidance in upgrades to that system.

As NASA looks to the next phase of human space travel, first to the vicinity of Mars, and then eventually to the Mars surface, the need for robust and efficient systems takes a quantum leap. Unlike on ISS, resupply is unavailable, and early return is impossible. Design of CO_2 removal systems thus requires a new degree of optimization, including selection of adsorbents and sorbent processes.

One facet of my current position, guiding the maturation of spacecraft CO_2 removal technologies for NASA's Advanced Exploration Systems program, is keeping abreast of parallel developments in CO_2 capture and storage. While listening to a speaker at a recent conference, I was struck by his conclusion: For this complex technology, standard figures of merit cannot be used to optimize the processes involved. Rather, computer simulations that capture the key physics of the process, including coupled heat and mass transfer in porous media, must be applied. A large number of parametric simulations are required to converge on the optimal solution. Parametric testing could also be employed, of course, but would be prohibitively expensive and time consuming, severely limiting the number of options that can be explored. Multiphysics applications have made great strides in solver robustness and speed. However, to accelerate 1D system simulations and enable multidimensional modeling of full CO_2 removal systems, further improvements in robustness, execution rate, and memory usage are highly desirable future developments.

One feature that can be applied now to increase the execution rate of parametric studies is the Application Builder in COMSOL Multiphysics. After verification of a CO_2 removal simulation against test results, the configuration can be locked down and a simulation app distributed to multiple users for parallel parametric studies. Examples of parametric variables include sorbent selections, fixed bed size, cycle times, and flow rates. The recent development of the Application Builder is very timely, as it will seamlessly facilitate this process.

In summary, early investigation of COMSOL as a platform for parametric studies towards maturation of spacecraft CO_2 removal systems appears very promising. The Application Builder will provide the means to distribute the workload to many individuals. With this approach, informed selections from a wide range of possible options can be made towards finding the best solution for a CO_2 removal system for the crew traveling to, and landing on, the Red Planet. ❖

Jim Knox is the functional area manager for maturation of CO_2 Removal systems within NASA's Advanced Exploration Systems program. He received a BS in aerospace engineering from the University of Colorado and an MS in mechanical engineering from the University of Alabama. Research using the COMSOL Multiphysics® software to simulate adsorption processes is part of his ongoing PhD dissertation.