COMSOL NEWS

A MULTIPHYSICS SIMULATION MAGAZINE

Multiphysics simulation spurs INNOVATIVE MECHATRONICS design at KOSTAL

Page 12

SIMULATION DELIVERS RELIABLE HIGH-POWER ELECTRICAL PRODUCTS AT ABB

Page 4

MIELE IS REVOLUTIONIZING THE COOKING APPLIANCES INDUSTRY WITH MULTIPHYSICS

Page 8

COMSOL

Simplicity, Effectiveness, and Accuracy: It's All in the Multiphysics Approach

This issue of COMSOL News is no exception to what we all have come to expect from the users of COMSOL Multiphysics: It's just stunning how simulation is empowering engineers and researchers to optimize and verify their designs across such a wide array of disciplines. Multiphysics simulation is key to delivering innovative solutions and capturing the concept behind many breakthrough ideas and products.

As you flip through COMSOL News, you will discover how engineers at ABB designed a tap changer capable of economically and reliably performing 1 million operations over 30-plus years, or how Miele is manufacturing safe and energy-efficient induction stoves where you can cook everything from the perfect pancake to your home-made pasta.

Mechatronics is also greatly benefiting from the multiphysics approach to simulation: the next time you use a satellite navigation system or adjust the ambient light of your car, you may be touching the next generation of capacitive sensors designed by KOSTAL.

Many other amazing user stories covering electrical, mechanical, fluid, and chemical applications are brought to you with this issue of COMSOL News. It's been an honor and a great learning experience to work with such passionate and knowledgeable users and I'd like to thank them for telling their stories and sharing their point of view on modeling and simulation.

Whether you're researching a new concept, designing a better product, or optimizing a process, I'm sure these user stories will give you insight into situations where multiphysics simulation is mission-critical and COMSOL Multiphysics is a smart choice to get the job done.

Enjoy,

Valerio Marra
Technical Marketing Manager
COMSOL, Inc.

INTERACT WITH THE COMSOL COMMUNITY
You can comment on this year's stories via
Discussion Forum: comsol.com/community/forums/
Facebook: facebook.com/multiphysics
Twitter: twitter.com/COMSOL_Inc

CONTENTS

ON THE COVER

Simulation of the electrostatic interaction between a dummy finger and a capacitive sensor in a roof module from a premium car line.

COMSOL NEWS

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

© Copyright 2013 COMSOL. COMSOL News is published by COMSOL, Inc. and its associated companies. COMSOL, COMSOL Multiphysics, Capture the Concept, COMSOL Desktop, and LiveLink are either registered trademarks or trademarks of COMSOL AB. All other trademarks are the property of their respective owners, and COMSOL AB and its subsidiaries and products are not affiliated with, endorsed by, sponsored by, or supported by those trademark owners. For a list of such trademark owners, see http://www.comsol.com/tm

ALTASIM
TECHNOLOGIES
REALIZING TOMORROW'S TECHNOLOGY

AltaSim Technologies' team of engineers provide innovative and cost effective solutions for new product development, improved product performance and innovative manufacturing technologies. Our unique S3 Process enables us to harness our engineering technology and advanced computational and multiphysics analysis capabilities. You are able to explore, develop and apply alternative solutions - without the delays and expense associated with traditional testing and evaluation. Contact us today. We'll show you how a great opportunity can become a reality.

(614) 861-7015 | www.altasimtechnologies.com

©2011 Altasim Technologies, Inc. All rights reserved.

Dielectric Stress Simulation Advances Design Of ABB Smart Grid-Ready Tap Changers

Designed in Alamo, Tennessee, ABB's new on-load tap changer is the fastest, most robust such device in the power industry. Powerful simulation technology and rigorous testing help deliver reliable and safe tap changers to the market more efficiently.

BY EDWARD BROWN

Why Power Control? For any source of electric power, the output voltage will sag as the load current increases. Electronics can correct this effect on low-power sources; power on the order of thousands of kilowatts, however, requires a different kind of control. With various power sources contributing to the grid, a large inconsistency between voltages would be destabilizing. Consumers of power rely on fairly stable voltage so that their electrical devices will operate properly. The market for regulating utility power is expanding because of the demand for increased energy efficiency. As transformers are a critical element in delivering reliable and cost-efficient power distribution, significant engineering efforts are going into making these components smart grid–ready. Tennessee-based transformer components expert ABB in Alamo has conducted detailed electrostatic simulation and design validation in its high-power test lab to develop the fastest, most accurate tap changer in the world.

Vacuum Reactance Load Tap Changer at ABB's Alamo, Tennessee Facility.

Tap Switching

The control technique used in very high-power applications is tap switching. It evolves from the fact that voltage is stepped up to hundreds of kilovolts to minimize the size and cost of power lines and is then stepped down for consumer use by means of substation transformers. The output voltage is related to the input by the ratio of secondary to primary turns. A tap changer varies that ratio by switching the point at which either the input or output circuits are connected (i.e., it changes the ratio of secondary to primary turns). ABB has been manufacturing tap changers to control large amounts of power since 1910. Bill Teising, research and development engineering supervisor at ABB in Alamo, is heading a team of researchers who are using modern technology to update this amazing device. About the team's new vacuum reactance load tap changer (VRLTC™), Teising says, "The concept of switching is old, but the mechatronics applied to design, operate, and monitor the VRLTC are new."

Inside A Tap Changer

The VRLTC is made up of three major components. First, there are the actual tap-changing components: switches and vacuum interrupters. Second, there is a military specification–rated digital servo motor drive system that operates these components. The use of a servo drive system lets the VRLTC operate at speeds greater than one tap change per second without requiring a mechanical brake. By delivering very high tap change speeds, the VRLTC provides rapid voltage regulation for critical demand-response applications. The final component includes the proprietary Tap Logic Monitoring System (TLMS™) and a multiturn absolute encoder. The TLMS commands, monitors, and controls the entire tap change operation. The multiturn absolute encoder provides angular position data to the TLMS, eliminating the need for unreliable cam switches. The high-voltage transformer with the tapped windings is contained in a tank filled with transformer oil, which provides both high-voltage insulation and cooling. The VRLTC tap changing mechanism is housed in a smaller oil-filled steel tank that is welded or bolted to the transformer tank. Molded epoxy barrier boards hold the electrodes that connect to the transformer taps on one side and the switching mechanism on the other. The vacuum interrupter of the VRLTC is used to interrupt load current, allowing the selector mechanism to move to the next tap position.

In traditional load tap changers, switching without the vacuum interrupters causes arcing to take place in the oil. The by-products from arcing deteriorate the oil and create additional maintenance requirements. In the VRLTC, the arcing currents are contained within the vacuum interrupter.

As a result, the VRLTC can perform 500,000 tap changes before an inspection is required. The front of the VRLTC is shown in Figure 1.

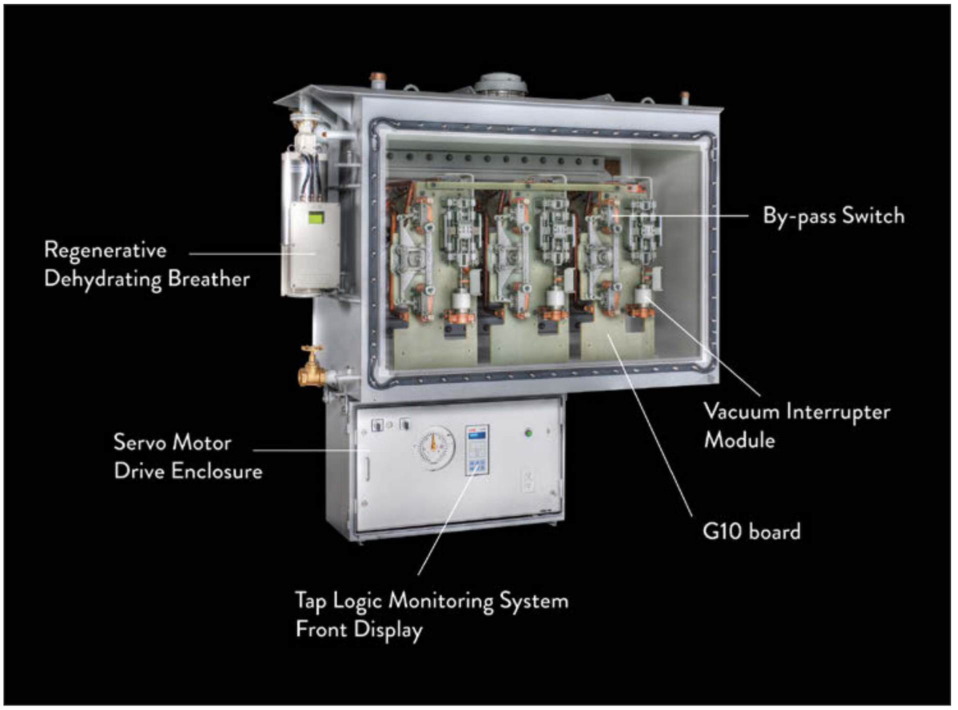


FIGURE 1: Frontal view of the VRLTC. Selector assembly is installed behind G10 diverter boards.

Simulation Of Tap Changer Insulation

One major innovation is not readily visible but is perhaps the most important of all. The epoxy barrier boards that hold the connecting electrodes and the G10 glass-reinforced epoxy laminate board that holds the switches and vacuum interrupters are constantly stressed by thousands of volts. These dielectric materials cannot be allowed to deteriorate: The life of the tap changer is seriously affected by the ability of these insulating materials to withstand high voltage. It is possible that although there might not be an immediate problem, the insulation can deteriorate over time. There are two different failure modes with solid insulation: breakdown through the material, which is called puncture or strike, and breakdown across the surface of the insulation, which is called creep. Surface failure can take place over a period of time, with a phenomenon called treeing where you can see tracks develop along the surface, eventually leading to dielectric failure. Designing to prevent these kinds of failure modes is very difficult. Traditional methods have used a combination of rules of thumb and overkill in terms of insulation thickness and spacing of the components. Even then, future behavior was still hard to predict. A more rigorous approach to the high-voltage design is to turn to simulation to compute the voltage stress on and in the insulation. Voltage potential between conductors in contact with an insulator creates an electric field in the insulator material (the dielectric). The intensity of the field at any given location is a function of the amplitude of the voltage differentials and the geometry of the structure. Every dielectric material has a maximum stress level beyond which it will fail — it will start to conduct current. This is called the dielectric strength of the material. The VRLTC design team has addressed the dielectric stress problem by building a model of the geometry in

> "The concept of switching is old, but the mechatronics applied to design, operate, and monitor the VRLTC are new."

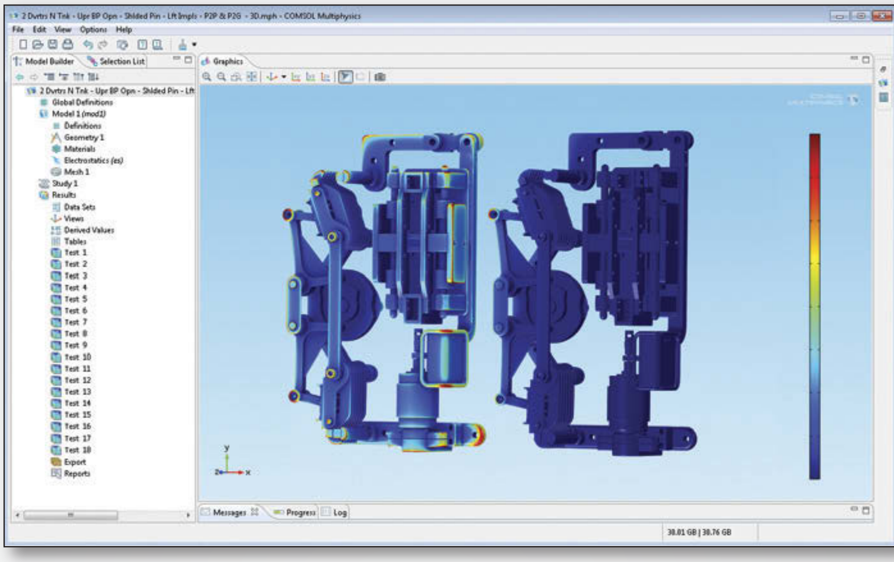


FIGURE 2: Dielectric stress simulation using COMSOL Multiphysics of the bypass switches (shown in the open position) and vacuum interrupter assemblies when applying a voltage across two adjacent phases. The assembly on the right is grounded.

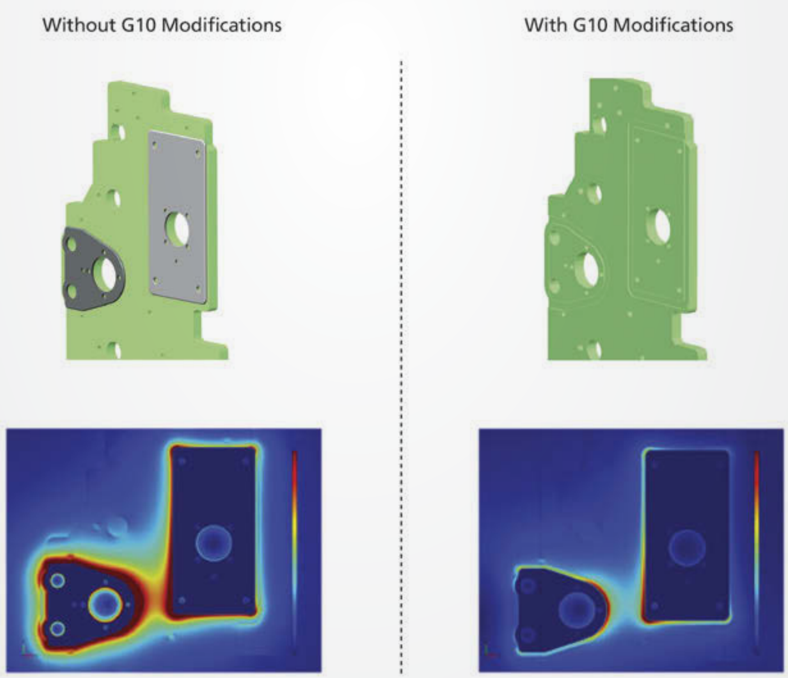


FIGURE 3: Dielectric stress simulation of G10 board with mounting plates for switching assemblies. During a tap change, there is a high voltage between the mounting plates. The simulation plots show the results with and without geometry modifications of the G10 board. These modifications significantly reduce the dielectric stress on the board, as shown in the simulation on the right.

Creo™ Parametric and then importing it into COMSOL Multiphysics. The researchers can then define the electric potentials and dielectric properties and run iterative simulations to display the pattern and amplitude of the voltage stresses throughout the dielectric. The simulation results can then be compared with the dielectric stress information they have derived from their long history with building tap changers in order to accurately predict the operational life of the VRLTC. Working with large CAD assemblies — in this case over 500 parts — at first posed a challenge to the team. How would they get this complex geometry ready for analysis? They found the tool they were looking for in LiveLink™ *for* Creo™ Parametric. Through its bidirectional link, they could move seamlessly from the geometric representation in Creo Parametric to synchronizing the corresponding geometry in COMSOL and then generating a mesh. After inspecting results from the meshing, they could go back and make the proper changes to the geometry directly in Creo Parametric. After a few iterations, they arrived at a high-quality mesh to be used in large-scale batch simulation on a powerful workstation. "LiveLink *for* Creo Parametric let us seamlessly import large CAD assemblies into COMSOL for analysis, significantly reducing the overall simulation setup time," says Teising. With the tap changer geometry in COMSOL Multiphysics, the focus turned to the dielectric stress simulation (see Figures 2, 3, and 4). Many different assemblies have been studied, including the terminal backboard, shaft drive bevel gear, tap selector, bypass switches, and vacuum interrupter assemblies. Simulation has confirmed the importance of both the geometry of the design and the spacing between component assemblies. "From running these large simulations, we could quickly visualize the impact of geometry changes on electric field magnitudes in a 3D space," Teising says.

"In COMSOL Multiphysics, we apply increasing types of test voltages to determine the level of potential dielectric breakdown," says Teising. "These simulation results are then evaluated against ABB internal dielectric design rules for allowed short-term and long-term creep and strike field magnitudes. Tommy Larsson and the team of dielectric experts at ABB in Ludvika, Sweden created these design rules to set the standard for LTC

Creo is a trademark of PTC, Inc.

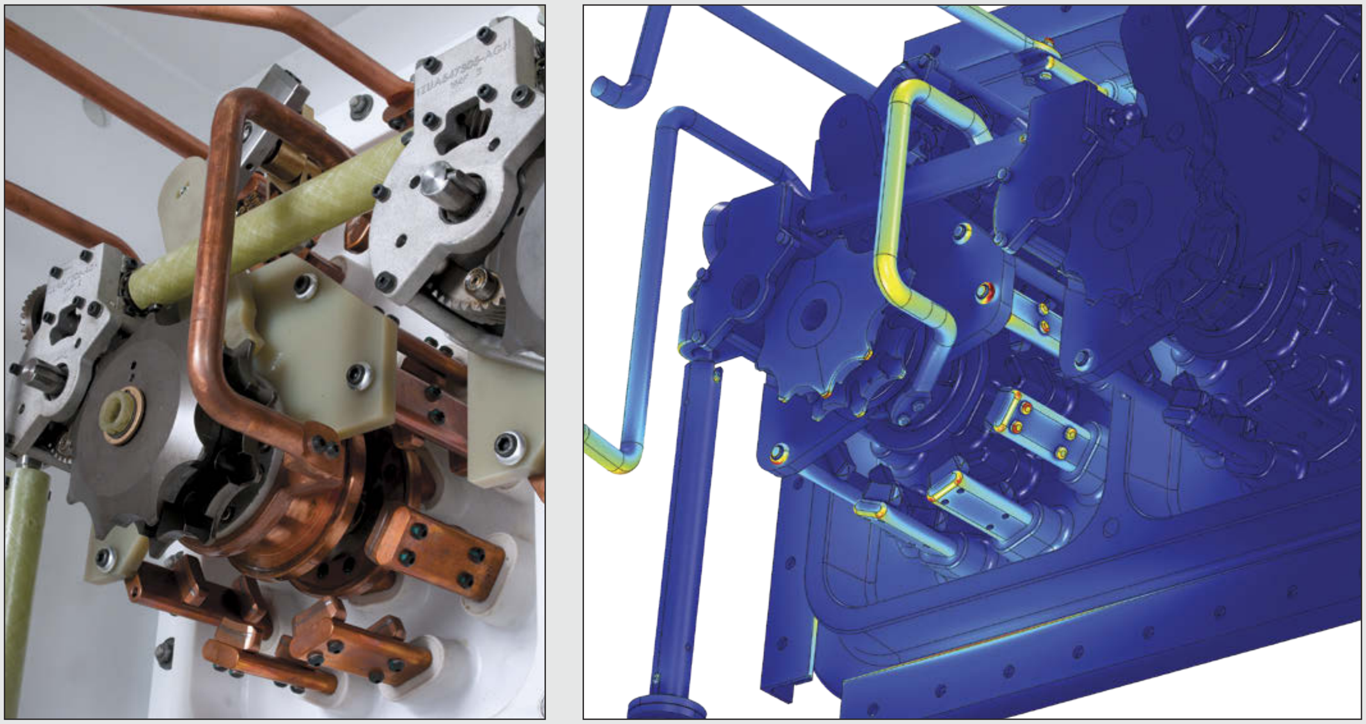
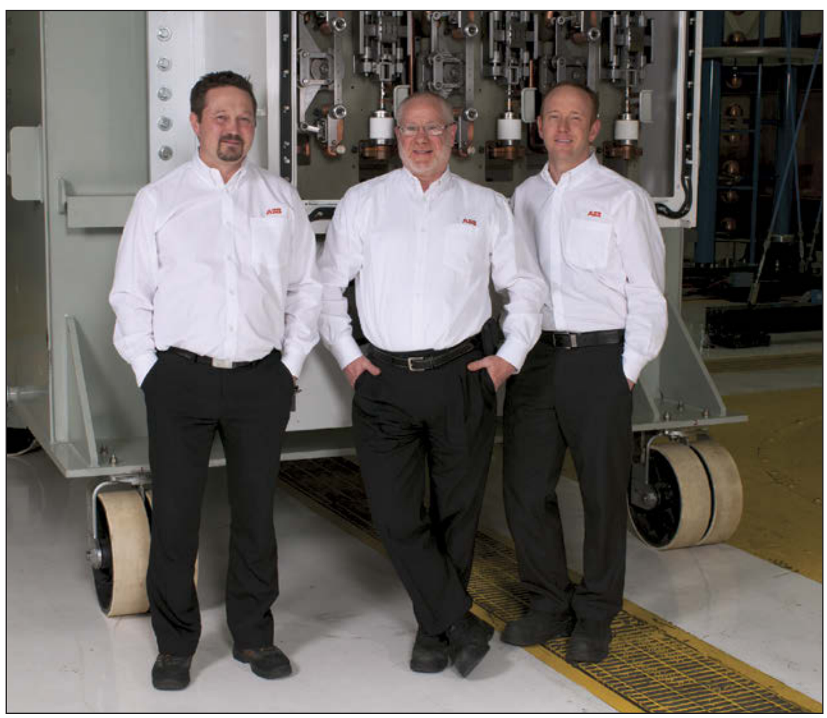


FIGURE 4: The photo above shows the selector assembly. The visualization shows a dielectric stress simulation of the selector mechanism when applying a voltage across two adjacent phases.

product safety and reliability. COMSOL is the common simulation platform linking Ludvika and Alamo design teams to enable the consistent application of these rules across the entire ABB LTC product portfolio. The geometry of the design is iterated until the results from COMSOL meet or exceed the ABB internal design rules. Dielectric testing is then performed in the high-voltage lab to determine the upper limit of the design's dielectric performance. This lets us compare the actual lightning impulse and 1-minute, 60-Hz high-voltage test results with the simulation. The correlation of this data assures us that COMSOL is providing results that are consistent with testing. This gives us confidence that we can rely on the COMSOL results for the predicted life of the product."

The Results

By using COMSOL simulation, the ABB research team was able to develop tap changers based on careful calculations of actual field conditions. The simulations let them optimize their designs so the equipment can economically and reliably perform 1 million operations over 30-plus years. ■



The type VRLTC tap changer design team. From left to right: Tommi Paananen, design engineer, David Geibel, engineering manager, and Bill Teising, development engineering supervisor. Design engineers not pictured: Mårten Almkvist, Jon Brasher, Josh Elder, Bob Elick, and Chris Whitten.

Multiphysics Simulation Helps Miele to Optimize Induction Stove Designs

Less than a decade ago, if you were to ask a master chef which type of cook stove he preferred, he would have answered gas, without question. Now, however, Miele has provided both professional chefs and at-home cooks with another, better option: the induction cook stove.

BY ALEXANDRA FOLEY

Induction cook stoves are known for their efficiency, with over 90% of the energy used going directly into heating the food being prepared. That is a tremendous amount when compared to gas or electric stoves, which in contrast demonstrate a mere 50% efficiency rate. If an induction cook stove could provide chefs with better precision and speed than a traditional stove, while still retaining optimal efficiency, the resulting cooktop would be a substantial breakthrough in the cooking appliance industry.

It was the mission of Miele, a world leader in domestic appliances and commercial machines, to create just such an induction stove. Researchers at mieletec FH Bielefeld, a joint research laboratory between Miele & Cie. KG and the University of Applied Sciences Bielefeld, Germany, used simulation and the multiphysics approach to improve, verify, and optimize their induction stove designs.

Using field-coupled simulation, Christian Schröder, co-founder and scientific director of mieletec, designed an optimized induction stove that lived up to Miele's motto of "immer besser." Translated from German, this means "forever better" and it drives the company to create long-lasting, functional, and great designs. "We're very happy with what mieletec has developed," says Holger Ernst, co-founder and scientific director of mieletec and head of the Innovations Department at Miele. "Mieletec was able to create an induction stove that's more precise than a gas stove, while still providing better energy efficiency."

FIGURE 1: The stovetop remains cool; in fact, the ice cubes are hardly melting, while the water inside the pot is boiling.

A Watched Pot Never Boils—Unless It's on an Induction Stove

A watched pot never boils. Whoever coined this phrase has probably never used an induction stove. Unlike gas or electric stoves, which can take ten to fifteen minutes to boil a pot of water, an induction stove can bring a cold pot of water to boiling in a matter of minutes. This is achieved using an entirely different heating technique than that of traditional stoves: induction heating.

An induction stove heats up a pot placed on the surface of the stove. While this sounds similar to the way in which a gas or electric stove functions, it's actually an entirely different process. Induction stoves heat the metal of the pot, not the stovetop (see Figure 1). "Instead of heating taking place on the stove," describes Schröder, "heating actually takes place inside the pot itself, leaving the stove cool to the touch." Traditional stoves heat the surface of the stove, which then heats the pot through conduction.

The working principle of an induction stove is based on the inductive heating effect. First, a pot is placed on copper coils located underneath the stovetop. When an alternating current (AC) is passed through the copper coils, it generates a magnetic field that induces currents inside the metal of the pot. These induced currents, called eddy currents, heat the pot by the Joule heating effect. The contents of the pot are then heated through conduction first and then convection.

Initially, induction stoves were designed using a trial and error process, where researchers relied on their experience for an initial estimation of what the frequency, coil size, and power output should be. The results were then altered until the best performance was seen, and this became the final design. However, this process can be very expensive and time consuming, and the engineer is left without enough information to know what is happening in the system, and whether the process has truly been optimized.

"Simulation allows you to extract data that you would never be able to get from an experiment," says Schröder. "With simulation, you can get a better idea about what's going on inside a coil or pot, so that you know what it is that you need to optimize."

Using COMSOL Multiphysics and CAD geometries from Miele, Schröder and his team of researchers from mieletec were able to find the optimal set of conditions for the stove's design. "Essentially, we were able to simulate the whole system, allowing us to improve upon the energy efficiency of the stove," says Schröder. The accuracy of their simulations allowed them to optimize their results within COMSOL Multiphysics, so that when the first prototypes were built, they already had a clear idea of how they would perform.

Design Challenges—When Pots are Singing and Moving on the Stove

The magnetic field induced by the coils creates a few interesting design challenges. "One of the biggest issues we faced is the noise that the pots emit when eddy currents are flowing through them," says Schröder. "The electrical current produces a high-pitched noise that is very difficult to get rid of. The only way to eliminate the noise is to adjust the frequency of the alternating current and geometry of the coil, so that the noise

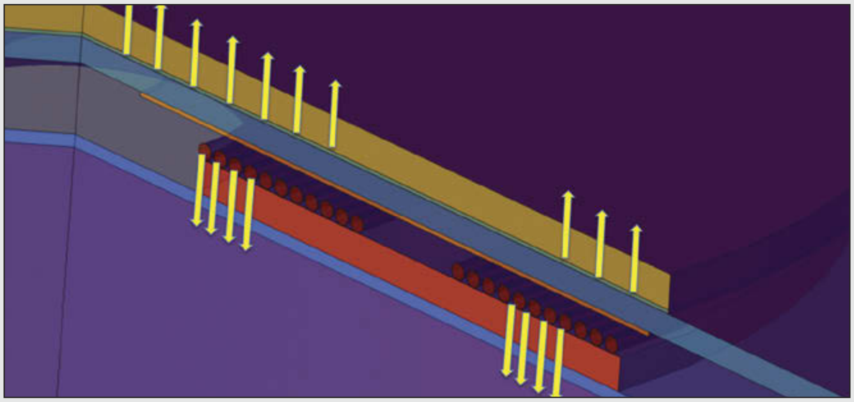


FIGURE 2: The simulated geometry consists of induction stove and pot. Several materials are taken into account (from bottom to top): aluminum (blue), ferrite (red), windings of the copper coil (brown), mica (orange), glass-ceramics (turquoise), metal pot (green and dark yellow). Lorentz forces acting on the induction stove-pot system are also shown (light yellow arrows).

FIGURE 3: Setup of a test campaign performed by staff scientists Werner Klose (left) and Mikhail Tolstykh (right). Because the stovetop has been removed, you can see the internal workings of the stove.

produced is at a higher pitch than what the human ear can pick up."

For example, in Germany the current from a household outlet is standardized at 220 V and 50 Hz. Utilizing an AC/AC converter, the frequency of the current in the coil can be increased until the noise produced by the pot is no longer audible. "Using simulation, we found the recipe for current frequency and coil design that produced the least amount of noise possible," comments Schröder. By increasing the frequency to 30 kHz, and optimizing the coil, mieletec built an induction stove that is almost silent to the human ear. Why almost silent? Because, even if the working frequency is not in the audible range, different noise generating phenomena, like magnetostriction (see Figure 2), can still occur at lower, audible frequencies.

> "We had to work with a natural convection heat transfer simulation where porous media flow was also involved, a truly multiphysics application."

The induction heating process was simulated using COMSOL Multiphysics in combination with the AC/DC Module and Heat Transfer Module. In order to obtain an accurate description of what happens in the stove and pot, heat transfer was solved simultaneously with electromagnetics and optimized to determine the best operating conditions. "At the moment, this is something that every manufacturer has to deal with," Schröder continues, "however, in the future, we hope to create an induction stove that really is silent."

Another challenge occurs because of the magnetic forces generated by the system. Since induction cookware is made of a paramagnetic metal, its interaction with the magnetic field results in an attraction force that can cause the pot to move around when placed on the stove top. This occurs because the eddy currents in the pot generate a magnetic field that interacts with the one generated by the coils. If the magnetic forces do not cancel each other out, the resulting net force will cause the pot to move across the stove.

"We needed to know the size to make the coils, what shape, and what materials to use," says Schröder, "It all boils down to material science." Using simulation, Schröder and his team (see Figure 3) were able to gain an understanding of how the properties of different materials affect their design with respect to thermal and electromagnetic performances. This enabled them to create a coil design that ensured the pot would stay put, while still providing the right amount of power for cooking.

Comparing Simulations with Prototypes

When it came to testing their prototypes, mieletec was impressed with the results that they found. "It was amazing," says Schröder. "We found that the results predicted by our simulations were in very good agreement with what the measurements on the prototypes displayed, which rarely happens with other software." Examples of these results can be seen in Figure 4 and Figure 5.

Because their simulations accurately demonstrated how the prototypes would

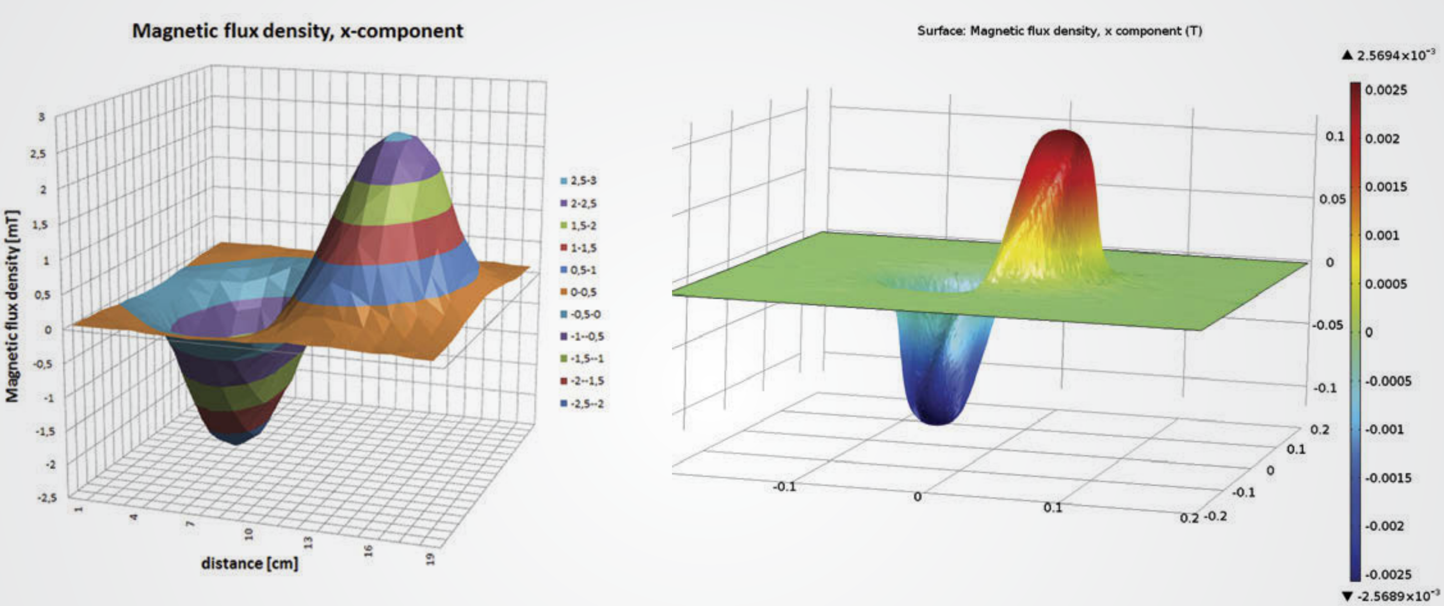


FIGURE 4: x-component of the magnetic flux density for a special coil design. There is a very good agreement between measurement (left) and simulation (right).

The scientific board of mieletec FH Bielefeld in front of a new convection oven design. **LEFT TO RIGHT:** Christian Schröder, Sonja Schöning and Holger Ernst.

perform, mieletec was able to save a lot of development time and reduce the number of experiments needed to finalize their designs by 80%.

In order to test that their induction stoves heat food homogenously, mieletec uses a pancake to assess heat distribution across the surface of the pan. "If the standard pancake comes out burnt in some places, and undercooked in others, then you know the stove isn't heating effectively," Schröder describes. "You want the pancake to be one smooth color and evenly cooked."Stiftung Warentest (www.test.de), a trusted German authority on consumer goods, ranked Miele stoves as the best in energy efficiency and more importantly, able to prepare a delicious, nicely browned pancake."

Simulation of Traditional Appliances

Mieletec is also working on additional kitchen appliances, such as convection ovens. In this application, a complete understanding of the materials and multiphysics interactions taking place were once again important when developing an optimized oven. In order to verify the optimized design, a test is performed in which a porous stone saturated with water is placed inside the oven. Over several days, the stone is passed through various heating cycles to evaluate the oven's heating rate and energy efficiency.

"We had to work with a natural convection heat transfer simulation where porous media flow was

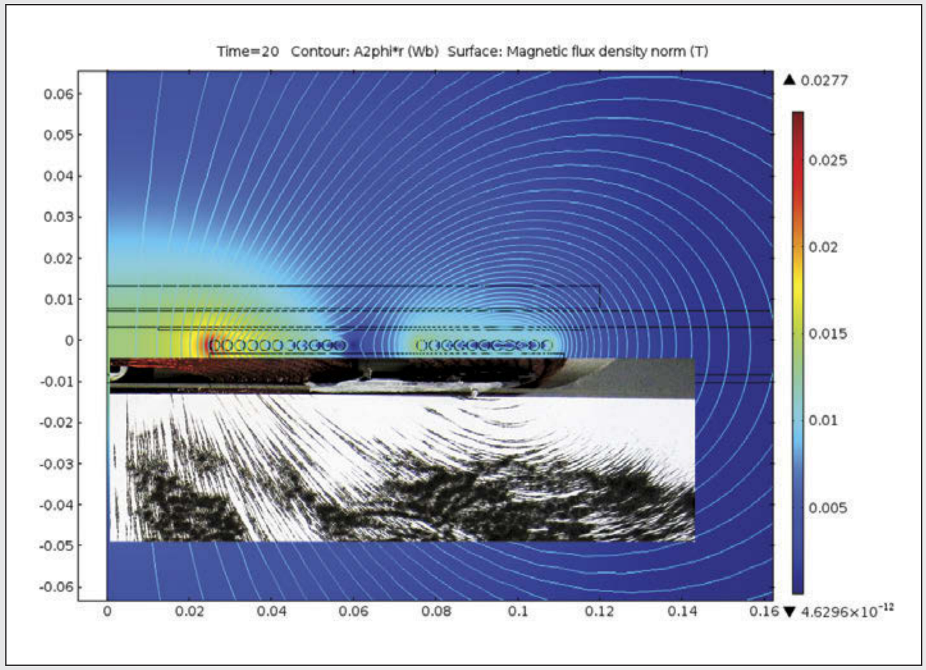


FIGURE 5: The comparison between COMSOL Multiphysics results (magnetic flux density norm) and experimental field lines shows that simulation is accurate and can be used to test other coil designs before building a prototype.

also involved, a truly multiphysics application," comments Schröder. "The simulation allowed us to measure the temperature of the stone at points in the experiment that were inaccessible to real sensors. Simulation allowed us to gain a better understanding of the design," he continues. "A test that in practice lasts for a few days took only a few hours to achieve when simulated. This resulted in important saving of time and resources. Not to mention the fact that our conventional ovens achieved the highest energy efficiency rating."

"A test that in practice lasts for a few days took only a few hours to achieve when simulated."

The Future of Domestic Appliances

Thanks to simulation, mieletec is delivering designs from which consumers are already benefitting in terms of improved energy efficiency and a better cooking experience. The next step is to reach a deeper understanding of the whole induction heating system by including complex multiphysics effects like magnetostriction and aging of materials. Additionally, mieletec is working on the next generation of induction stoves, known as multicoil induction stoves, which will allow a consumer to place their pots and pans anywhere on the stovetop, instead of inside predefined boundaries. The stove will automatically be able to sense the location of the pot, and adjust accordingly to produce optimal cooking conditions by turning on a certain set of coils.

These hot new designs in cooking appliances are revolutionizing the cooking industry, making safer and more energy efficient stoves available for at-home and professional chefs. "We're looking forward to seeing mieletec continue to deliver cutting-edge technologies using COMSOL Multiphysics to facilitate the design process," concludes Ernst. ■

Leopold Kostal GmbH, Dortmund, Germany

Switching Made Easy

Simulation of thermal, electromagnetic, and capacitive sensor performance plays a pivotal role in product development at KOSTAL, which supplies all of the world's leading automobile companies with interior switching modules.

BY JENNIFER HAND

"My nontechnical friends are astonished at the amount of technology in a seemingly simple product," says Matthias Richwin, senior manager for technology development and quality using simulation at KOSTAL. "They are equally intrigued by the fact that behind every switch in their cars, there is a multidisciplinary team of engineers." Richwin's friends are not unusual. There are drivers everywhere who turn on their headlights or windshield wipers with no awareness of the development effort behind a switch. Yet from freezing winter to sweltering summer, on dull rainy days and in bright sunshine, switches are expected to function consistently for the lifetime of a car.

FIGURE 1: A typical premium car line roof module with LED illumination.

Six Decades of Electrical Switching

Considerations of style, safety, space saving, and user convenience have been the drivers for 60 years of innovation at the Automotive Electrical Systems division of KOSTAL Group. Since the early days when the company placed indicator switches by the steering wheel and created integrated-function pushbuttons, it has registered a wide range of patents. Core product areas include steering wheel column, center console, and roof module systems. Customers include BMW, Daimler, Ford, and the Volkswagen Group.

Richwin explains how simulation became an intrinsic part of the design process at KOSTAL: "We have some specialist tools, such as FEA software for mechanical design, but were increasingly in need of thermal simulation and anticipated a requirement for electromagnetic simulation, so I began to investigate the options. We selected COMSOL Multiphysics because it had by far the best user interface and offered integration with the CAD, electrical design, and manufacturing applications we use. In 2009, we began using the software for the thermal simulation of roof modules." Simulation is now so embedded in new product development at KOSTAL that it is simply considered a common design task and is considered to be key in three areas.

Lighting Efficiency Versus Heat Dissipation

The lighting inside today's cars is complex and highly integrated, and has moved far beyond the courtesy light that comes on when a door is opened. The roof module (see Figure 1) in a premium car is likely to house antitheft and satellite navigation systems as well as extras such as ambient lighting. "The industry has moved away from the classic bulb to LED displays," says Richwin. "Although LEDs are much more efficient because they require less

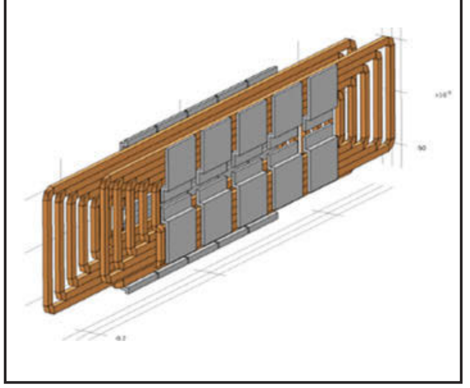


FIGURE 2: A numerically optimized coil pair for inductive charging, with a system efficiency of approximately 95% at 3 kW of electrical power.

power, 90 percent of the heat they dissipate goes into the printed circuit board (PCB) of the roof module. We tackle this particular challenge by using COMSOL Multiphysics to predict thermal behavior and optimize performance. Whereas we previously had to build and test, we can now easily predict performance and, for example, show a customer that a roof module will work at optimal brightness over the whole environmental range."

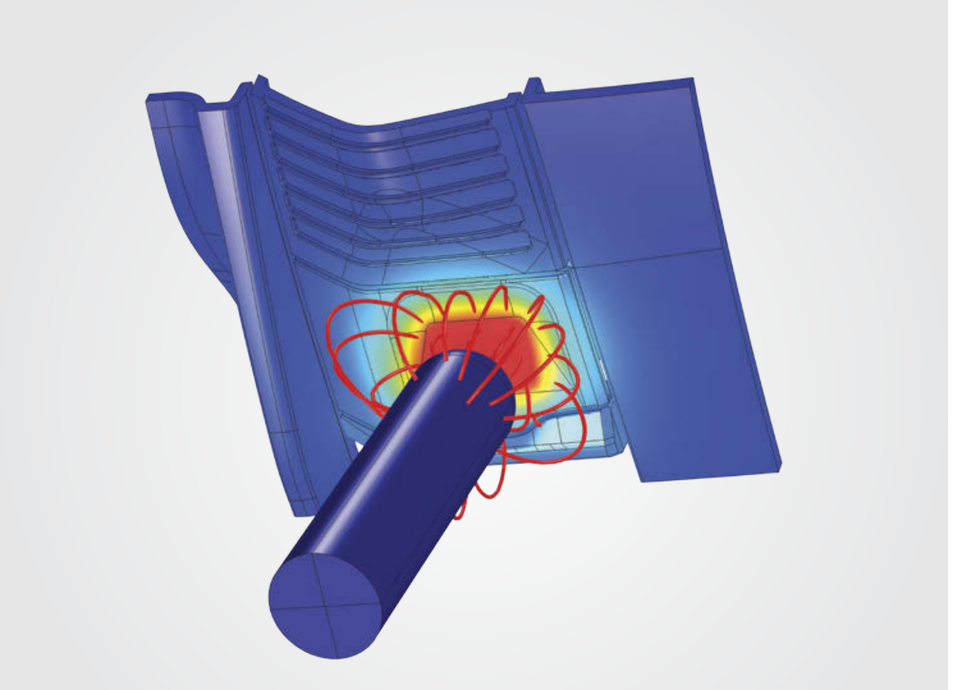


FIGURE 3. Modeling the electrostatic properties of a capacitive sensor system and a finger dummy.

Battery Charging That's Clean, Convenient, and Automatic

One of the disadvantages of an electric car is the need to charge it regularly, and as charging typically takes 6 to 7 hours, forgetting to do it one day may mean being stuck without transport the next. The team at KOSTAL therefore expanded on the electric toothbrush concept. Richwin explains: "The idea is to charge a car not by using a cable, but by moving it to a charging system. As with a toothbrush and its covered charging base, there are no contacts." This idea scores on every level — for security, safety, and comfort, the driver just parks the car in the same spot every day or night, with no need to even think about handling and plugging in a cable. "We worked on the basis that if a transformer is cut in two and the two halves are moved apart, it would still perform through inductive power transfer, albeit with less efficiency," comments Richwin. "Our task was to optimize the coil in each side so that the end product would be as effective as a cable-based system. We used COMSOL Multiphysics for the electromagnetic simulation (see Figure 2) of different options such as a ground plate partnered with a coil on the underside of the car, and a mounting on the wall partnered with a coil placed behind the number plate. It simply would not have been possible to develop this type of product without simulation."

Smartphone Expectations

Richwin cites another industry trend — minimizing the use of mechanical switches, as these are both complicated and vulnerable to fluid entry. At the same time, customers used to smartphones and tablets now expect similar touchpad-style sensors in a car. The transfer of this technology into cars is, however, not straightforward. Interaction with a smartphone is strongly visual; the user must look at a screen. In a car, though, there must be nothing that distracts the driver from driving, so user feedback has to be nonvisual. In addition,

FROM LEFT TO RIGHT: Daniel Klagges, Ingolf Münster, and Matthias Richwin.

the environment of a car is complex because its interior is densely packed with driver interface functions. Extremes of temperature, moisture, and dust according to location and climate pose further demands on components.

According to Richwin, capacitive sensors present various challenges: "We have to consider the potential for many different sizes of fingers and thumb pads, and the presence of additional material, such as a glove or hand cream. Then we have to decide on the level of sensitivity: whether we want proximity, whereby a finger has not yet touched a surface but is within a few centimeters; actual touch; or a combination, in which the sensor first detects the approach of a finger and then registers the touch."

The general aim is to make the sensor covering as thin as possible, which means that the team is looking for reliable and predictable performance from a plastic surface that is just 1 millimeter thick. Simulation is used to maximize sensitivity by optimizing the dimensions of the sensor, which lies on the PCB (see Figure 3). KOSTAL Group is also developing new surface materials; for example, pre-manufactured plastic foil on which the conductive structure could be printed to allow more flexibility and increase reliability.

Simulation Spurs Innovation

Richwin says, "The use of COMSOL Multiphysics enables us to check the feasibility of a technical concept very quickly, then optimize the quality, robustness, and cost of a product in development. We also save money by reducing the number of physical prototypes. However, it is in innovative areas such as inductive power transfer and capacitive sensor design that simulation becomes truly indispensible, because the alternatives are impossibly expensive or time-consuming." ■

Modeling The Electrochemistry of Blood Glucose Test Strips

Lifescan Scotland Ltd. uses multiphysics for product design and optimization.

BY GARY DAGASTINE

Self-monitoring of blood glucose levels is vital to effective diabetes control, and so every day, diabetics around the world share the same routine: They place a drop of their blood on a test strip and insert the strip into a meter to measure their glucose level.

But few of them probably stop to think that the humble little plastic test strip that makes self-monitoring possible is actually a highly engineered sensor. It must meet not only commercial goals for accuracy, ease of use, manufacturability, and cost, but increasingly stringent regulatory standards for medical products as well.

Lifescan Scotland Ltd. designs and manufactures blood glucose monitoring kits for the global market. Part of the Johnson & Johnson family of companies, Lifescan Scotland's research, development, and production facility in Inverness is regarded as a world center of excellence for those working in the field of diabetes.

The company's product range includes the popular OneTouch® brand of blood glucose monitoring systems and the specialized test strips that work with them, as well as diabetes management software, control solutions, and lancing devices (see Figure 1).

For about three years, Lifescan Scotland researchers have used COMSOL Multiphysics to characterize existing and new biosensor designs.

How a Complex Electrochemical Sensor Works

Lifescan Scotland's test strips comprise a plastic substrate, two carbon-based electrodes (called working and counter electrodes, respectively), a thin dry reagent layer, and a capillary volume where the blood is placed.

Conceptually, the blood mixes with and hydrates the dry reagent, producing an enzymatic reaction that generates a chemical product. The amount of this product is proportional to the amount of glucose in the blood.

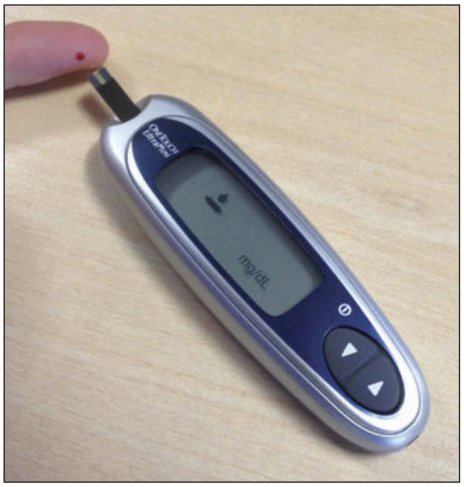


FIGURE 1: A test being performed with the OneTouch® strip and meter.

Then, when the strip is inserted into a meter, the battery-powered device polarizes the strip's working electrode. This sets in motion an oxidation process that generates a transient electrical signal, whose strength is proportional to the amount of the chemical product oxidized. The meter then applies an algorithm to convert the signal strength into a numerical value for the user.

Beyond Analytical Solutions

Historically, researchers at Lifescan Scotland relied upon analytical methods for product design. "We solved Partial Differential Equations (PDEs) using simplified assumptions of geometries, reagents, and boundary conditions," said Stephen Mackintosh, senior scientist. "Research Fellows Manuel Alvarez-Icaza, Steve Blythe, and Marco Cardosi built up many of these early modeling approaches. Our later work extended these models to include multiple chemical species, chemical interactions, and full electrochemistry."

However, although this approach does yield general solutions that encapsulate the main variables, it's not optimum in state-of-the-art product design because simplified assumptions ignore critical detailed chemical interactions.

"Our goals are to develop test strips that yield faster results, to reduce manufacturing costs, and to increase accuracy to meet ever-greater regulatory demands," Mackintosh said. "Finite and/or complex geometries are required to describe such systems, and in these cases, numerical models are more useful than analytical constructs.

"I began this progression by building more complex simulations using generic numerical PDE solvers. These could compute multiple species interactions very quickly, and worked well, but some electrochemistry components were still missing, and the underlying code was difficult to maintain," he said.

The underlying physics is complex, often incorporating Fick's laws of mass diffusion coupled with both Michaelis-Menten-based descriptions of enzyme-catalyzed chemical reaction kinetics, and Butler-Volmer expressions to understand concentration-dependent potential changes in addition to the battery-supplied potential of the meter.

Mass diffusion is a particularly important consideration. "There are many diffusing species in our simulations, with glucose just one example," Mackintosh said. "The tricky thing is, their diffusion coefficients may vary in subtle and complex ways depending on the specific properties of the blood sample (see Figure 2).

"Thus, we have to consider such things as the concentration of a generated product, the characteristic limiting rates of enzyme-substrate reactions, current density, concentration of oxidized species, and temperature. This would be impossible to do with precision using legacy analytical methods," he said.

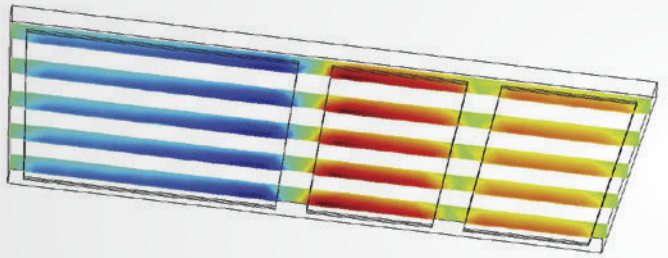


FIGURE 2: 3D slice plot, showing the concentration of a diffusing blood species in a simplified strip chamber, with both working and counter electrodes.

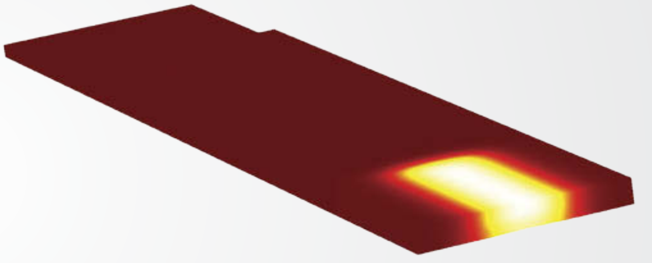


FIGURE 3: Study of the dissipation of heat from a drop of blood applied to a test strip (temperature distribution is shown).

Benefitting from the Multiphysics Approach

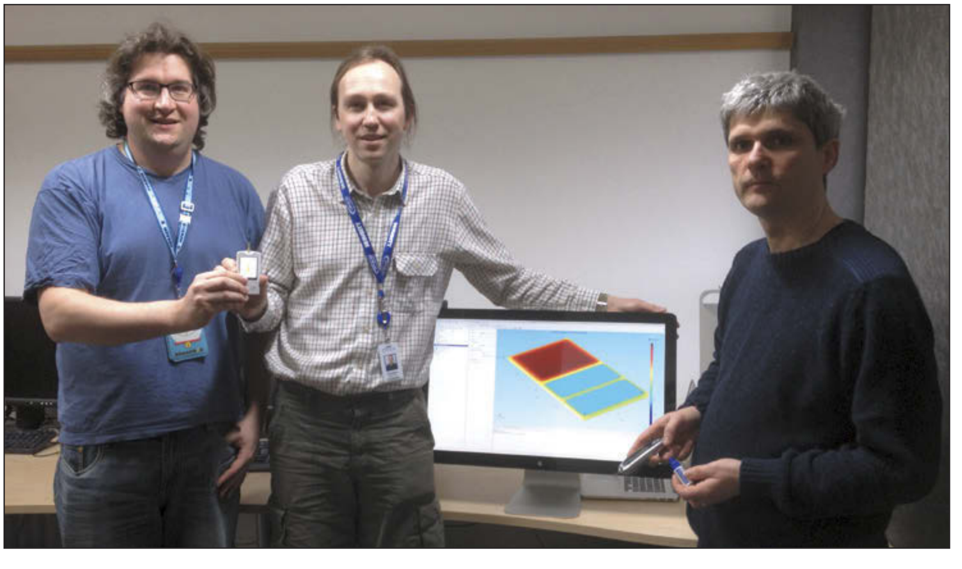
COMSOL Multiphysics has helped Mackintosh, a mathematician, develop powerful working models. "Other scientists in the R&D group provided valuable scientific background to these models, in particular Staff Scientist Jamie Rodgers, whose electrochemical expertise was invaluable," Mackintosh said.

COMSOL Multiphysics has several modules that extend its capabilities. The modules Mackintosh and the modeling and simulation team use most often are Heat Transfer to study temperature distribution (see Figure 3), and Batteries & Fuel Cells to facilitate development of detailed electrochemical reactions. These modules are then easily coupled to other capabilities included in COMSOL Multiphysics: Transport of Diluted Species to study mass diffusion, and PDE Interfaces to explore user-defined boundary conditions.

The team has automated mesh generation via the software's physics-controlled mesh setting, with extra refinement nodes added near each electrode-electrolyte boundary. Mackintosh said they also are considering use of the Microfluidics Module to extend their models to study such processes as the hydrophilic filling of the blood chamber from the applied blood drop.

Based on the success of this work, the use of COMSOL Multiphysics is being extended throughout the Inverness lab, and Senior Algorithm Engineer Adam Craggs is spearheading the required IT infrastructure. So that users without modeling experience can access these powerful tools, Craggs is implementing LiveLink™ *for* MATLAB® to create specialized graphical user interfaces (GUIs).

On the computing side, meanwhile, Craggs has taken advantage of COMSOL Client/Server mode to solve large problems more quickly by implementing a rack of Apple Mac Pro® computers to share the load of running the models.



Members of Lifescan Scotland's Research and Development group. From left are Adam Craggs, Senior Algorithm Engineer; Stephen Mackintosh, Senior Scientist; and Jamie Rodgers, Staff Scientist.

Developing Better Products

Mackintosh said COMSOL Multiphysics has aided with cost-effective optimization of device chemistry and geometry. Outputs such as the correlation between analyte concentration and current signal, at different time periods and with alternate layouts, along with the detailed concentration gradients the software has produced, have increased understanding of signal features and the impact of design changes, he said.

"We've used COMSOL Multiphysics to help develop and refine a range of blood glucose sensors that have enabled rapid model-based prototyping of alternative chamber geometries and/or reagent compositions," he said. "In fact, some of the output from our models is used to map the sensitivity of our products to manufacturing changes, an aid to future product development.

"Our simulation results are in good agreement with experimental work using existing systems and prototypes," Mackintosh said. "Of course, such models can never be used to make decisions on the safety or efficacy of medical devices released to the public, but they are a useful tool in the design and optimization of future products." ■

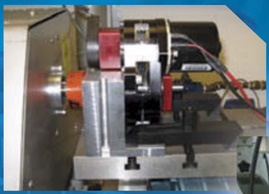
MATLAB is a registered trademark of The MathWorks, Inc.
Apple Mac Pro is a registered trademark of Apple

LAST CHANCE TO ENTER!
Entry deadline: July 1, 2013

It's Time

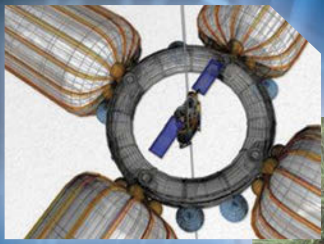
TRANSPORTATION & AUTOMOTIVE

MACHINERY & EQUIPMENT

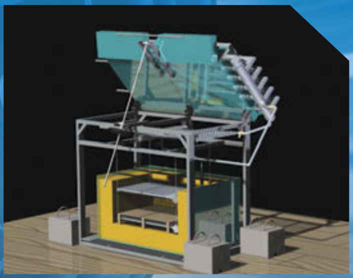


MEDICAL

AEROSPACE & DEFENSE



ELECTRONICS



SUSTAINABLE TECHNOLOGIES

Calling all design engineers. It's up to you.

Share your new product ideas with the world, the possibilities are endless!

• Generate new jobs • Improve health • Increase sustainability • Boost security
• Make transportation safer • Advance electronics • Accelerate productivity

SPONSORED BY

COMSOL

SAE International

TECH BRIEFS MEDIA GROUP
an SAE International Company

AEROSPACE & DEFENSE SPONSOR — TE connectivity AEROSPACE, DEFENSE & MARINE

TRANSPORTATION & AUTOMOTIVE SPONSOR — AVNET electronics marketing

ELECTRONICS SPONSOR — GORE

PRIZE SPONSORS — hp, Maplesoft

www.createthefuturecontest.com

to Create the Future

CONSUMER PRODUCTS

SAFETY & SECURITY

GRAND PRIZE: $20,000 — plus global recognition and publicity to business and industry leaders who can help bring your idea to market.

ACCEPTING INDIVIDUAL AND TEAM ENTRIES.

Get details at **www.createthefuturecontest.com**

CATEGORIES

- Aerospace & Defense
- Consumer Products
- Electronics
- Machinery & Equipment
- Medical
- Safety & Security
- Sustainable Technologies
- Transportation & Automotive

Create THE Future

DESIGN CONTEST 2013

University of Alberta, Edmonton, Alberta, Canada
Cross Cancer Institute, Edmonton, Alberta, Canada

MRI Tumor-Tracked Cancer Treatment

In a project that is truly breaking the boundaries of what was thought possible, a team from the Cross Cancer Institute in Canada is combining the superb quality of magnetic resonance imaging with the power of a linear particle accelerator to enable ultraprecise radiation therapy.

BY JENNIFER HAND

A rather unpalatable truth is that the targeting of radiation therapy for cancer involves significant uncertainty in accurately targeting tumors. On the other hand, magnetic resonance imaging (MRI) may be used to help by accurately identifying the location of a tumor in soft tissue, but it has to be carried out totally independently of radiation treatment delivered by a linear particle accelerator (Linac) because the two techniques conflict. MRI scanners need to receive extremely faint radio frequency (RF) signals from the patient to produce an image. The electrical needs of the Linac produce very large RF signals, however, that interfere with the process of collecting faint signals. On the other hand, electrons from the Linac need to be directed precisely onto a target to produce cancer-killing X-rays, but the stray magnetic fields from the MRI deflect the electrons, impairing the Linac's function.

If the two systems could be combined, they would form an ideal treatment system that could pinpoint any tumor at all times during treatment; in particular, tumors within the thorax or abdomen that move with breathing. This has until recent years been regarded as an impossible undertaking. Now, a team based at the Cross Cancer Institute in Edmonton, Canada, has proved that it is not.

One Challenge After Another

Professor Gino Fallone of the University of Alberta, also in Edmonton, established a task force to attack the problem in 2005. Since then, he and his team have been knocking down barriers previously regarded as insurmountable. They achieved proof of concept in 2008 when they built a fully operational prototype designed for the head (see Figure 1). "It would be difficult to overstate the different engineering and physics issues within the Linac MR Project," Fallone says. "We have had to consider the design of the MRI

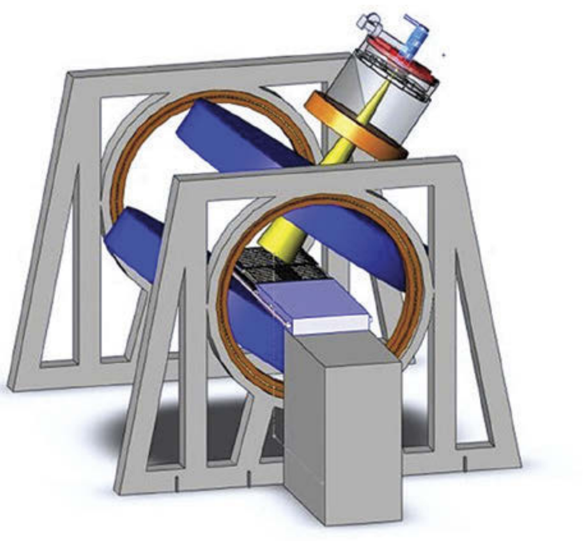
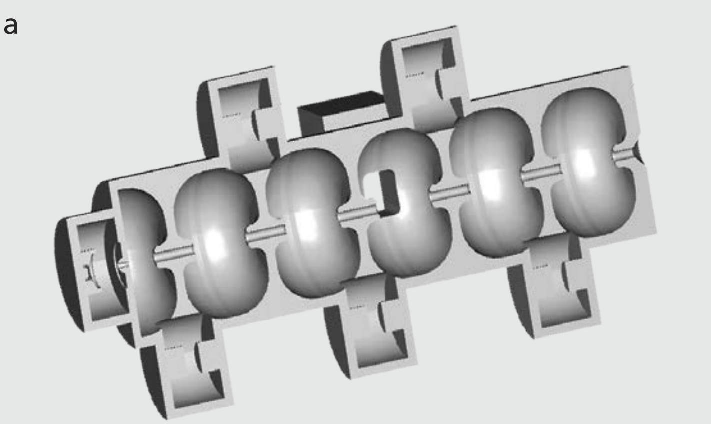


FIGURE 1: Configuration of the Linac MR system.



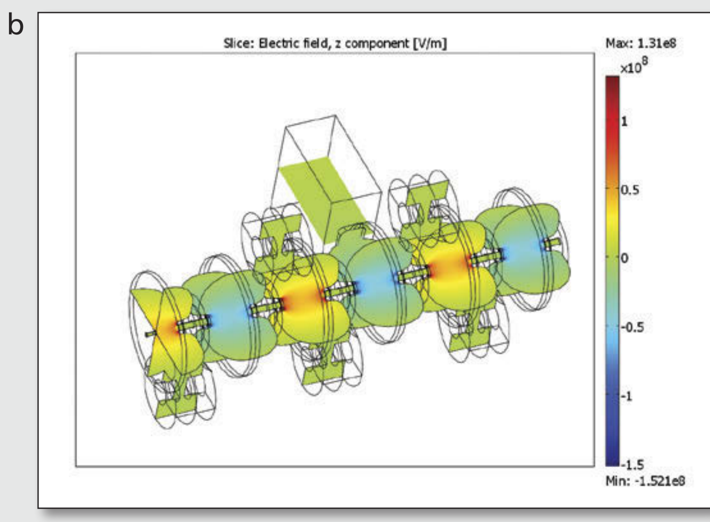


FIGURE 2: (a) Cutaway view and (b) electric field distribution of the short 10-MeV waveguide.

system, the Linac, the optimal combination of both, and the room in which the new installation would be housed."

Simulation plays a vital role in the progression towards clinical use of real-time, MRI-guided radiation, and team members have been using COMSOL Multiphysics since 2006.

"One of the earliest projects we did with a magnetostatic simulation was to establish a means of shielding the Linac from MRI's magnetic fields," says team member Stephen Steciw, an Associate Professor at the University of Alberta. "Having resolved that problem, we moved on to other issues such as simulating and optimizing the structure of the MRI scanner, which has to incorporate a hole for the beam of X-rays to pass through. We had previously investigated the impact on the image quality when a Linac rotates around an MRI. We therefore studied angle-specific field heterogeneities and different ways to circumvent these. We verified that designing the Linac and the scanner to move together as one whole system resolved this issue."

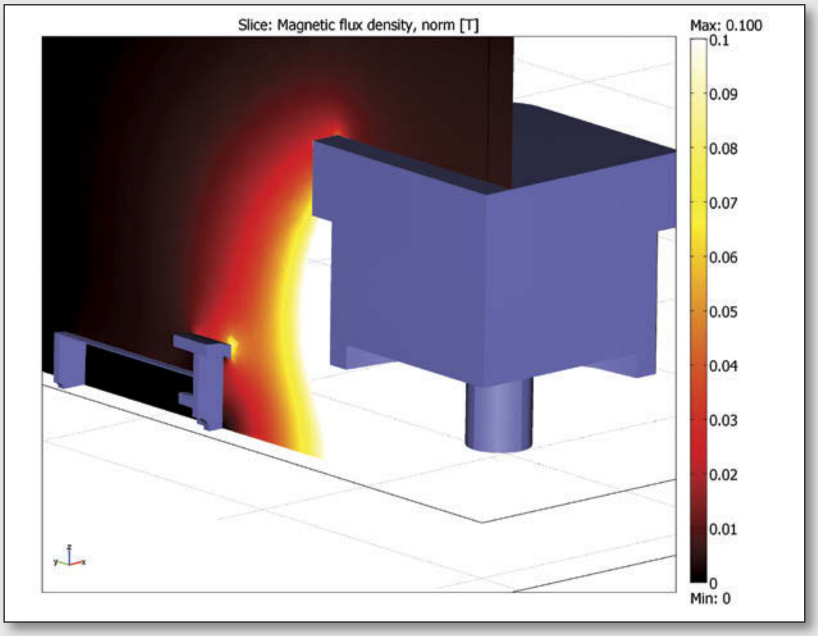


FIGURE 3: Passive shielding for a perpendicular Linac MR orientation (magnetic field lines perpendicular to electron trajectories).

Protecting the Linac

With regard to shielding the Linac, the initial aim was to shield down to 0.5 gauss, the magnitude of Earth's magnetic field. To accomplish this, the steel plate of the shielding wall was initially set at a thickness of 5 centimeters and a dimension of 200 cm by 200 cm. Joel St. Aubin, a former medical physics PhD graduate student who worked on the project, picks up the story. "Using COMSOL Multiphysics, we were able to verify the tolerances of the Linac to the magnetic field and reduce the shield to a radius of 30 cm with a thickness of 6 cm. The new shield was more than three times lighter than the original, much more practical from an engineering design point of view. This new shield also dramatically reduced the MRI's field inhomogeneities by more than three times, which is important for producing a distortion-free MRI image." In addition to the passive shielding of the Linac, the team also investigated active shielding, running an electromagnetic simulation of a counter magnetic field.

High Energy with a Short Waveguide

"We wanted the Linac MR to generate a 10-megaelectronvolt (MeV) electron beam," explains Steciw (see Figure 2). "Given current sizing options, that would have meant buying a waveguide that was actually capable of generating 22-MeV electrons and measured 150 cm — too much and too long for our needs. We estimated that we needed 70 cm in length, but by using COMSOL Multiphysics, we found out that we could take the waveguide right down to 30 cm. Now we are designing a new S-band waveguide. This reduction in length is of major importance because it means that the room we are constructing to take the Linac MR can be significantly smaller." COMSOL Multiphysics was also used to establish whether this special room needed to be magnetically shielded (see Figure 3). The results showed that it did, and further simulations determined the thickness of the special steel lining. The first whole-body Linac MR is being constructed inside this room and is expected to be in public use by 2016.

BACK ROW: Stephen Steciw, Joel St. Aubin, Gino Fallone. FRONT ROW: Devin Baillie, Dan Michael Santos.

Tight Targeting

The prototype is being used for fundamental research on the engineering of the system's critical component, and the team is now preparing the documentation required to seek government approval for a Linac MR to be used as an investigational device for humans in clinical trials. "COMSOL Multiphysics is an extremely practical and helpful tool that is enabling us in this important work," says Fallone. "Cancer patients currently have to undergo irradiation of the whole area around a tumor, and some internal organs are particularly difficult to treat because they are so difficult to see. The Linac MR is set to transform radiation therapy." ■

TRB, Decines, France

When It's Impossible to Take Actual Measurements, Multiphysics Provides the Answers

Extreme heat in a blast furnace makes it impossible to take measurements during certain parts of the process. At TRB we are using simulation along with actual outer temperatures in a blast furnace roof runner to find out how hot it gets inside.

BY SIMON CHIARTANO, TERRES RÉFRACTAIRES DU BOULONNAIS (TRB)

Blast furnaces, where molten metal reaches temperatures near 1500 °C, create an environment where every possible precaution must be taken to keep workers and production equipment safe. One potential hazard is when the molten metal first leaves a furnace through a taphole and travels through a runner where the slag is separated out (see Figure 1). If left totally exposed, the molten metal could splash and present great danger to operators and tools, or cause a halt in production.

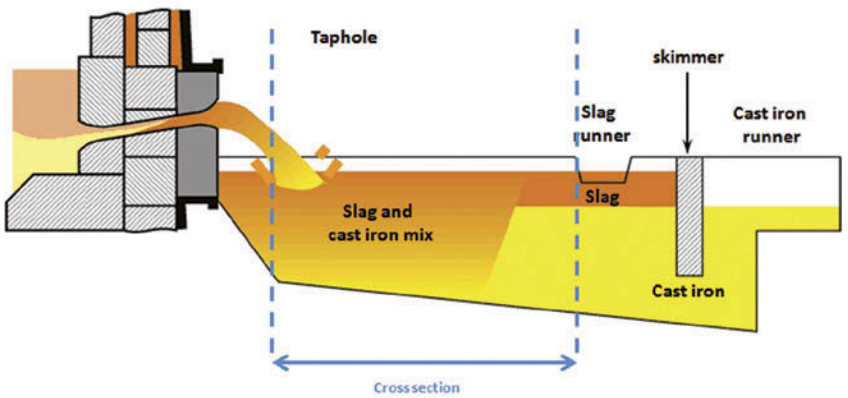


FIGURE 1: Molten metal exits a blast furnace (left) and travels through a runner where slag is separated from the cast iron (right). The cross-section being studied with COMSOL Multiphysics (see Figure 2) appears in the middle zone as indicated.

To contain splashes and provide protection, sections of the runner have a roof whose outer shell is made of cast iron with an inner lining made of concrete. This lining is necessary because, without it, splashing molten metal would quickly melt holes in the cast iron.

The concrete liner is subject to thermal shock as well as corrosion and erosion. A typical operating life for a roof runner is one month, after which time it must be relined. Given that a blast furnace can have two or three or even four taps, and we at TRB have hundreds of blast furnaces, it is clearly to our advantage to design them as economically as possible while maintaining overall safety.

Designing runners has traditionally been an inexact science because we cannot take accurate measurements of what is going on inside them. In the past we used trial and error methods to come up with the best type of concrete for liners and to determine the best thickness. If a liner got damaged too quickly, we simply tried a new combination. Much of these decisions are

"We can't place sensors inside because they would be exposed to extreme heat and splashing molten metal, which would destroy these expensive devices."

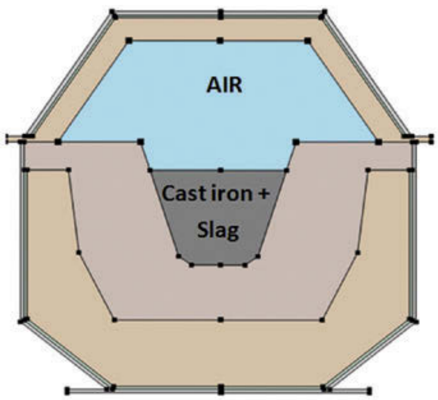


FIGURE 2: 2D geometry of a roof runner. The molten metal comes in contact with a concrete liner, and the outer shell is of cast iron.

based on the heat the liner is exposed to. However, until now we have had almost no idea of these temperatures. Are they 300 °C, 1000 °C? We just didn't know! We can't place sensors inside because they would be exposed to extreme heat and splashing molten metal, which would destroy these expensive devices. Instead, we turned to simulation with COMSOL Multiphysics and its Heat Transfer Module.

Pre-Heat the Oven

Under normal operating conditions, the molten metal doesn't enter a runner at room temperature. Thus, the first stage of our simulation was used to pre-heat the simulated runner based on a gas burner at 500 °C. This model also provides the cross-section 2D geometry we used for all further studies (see Figure 2). In the figure, note the two shades of brown, which correspond to two different types of concrete. One is in contact with molten metal and must resist the fluid, corrosion and thermal shocks. In this model, we only consider this inner layer of concrete. The second type of concrete never comes in contact with molten metal and serves as a mechanical frame. To study the pre-heating effects on the concrete, we set the simulation to only use conductive heat transfer, ignore air convection, and to assume a fixed temperature for the gas burner. The results now set the starting point for further investigations.

Is the Air Under the Roof Moving?

Following the pre-heating simulation just described, the next stage of the model studies the first time the molten metal in the blast furnace is tapped and sent through the runner. At this point we obtain the temperature of the air underneath the cover and see how it changes over time. For this, we modeled what happens when we tap the blast furnace and send molten metal through the runner for 75 minutes. Here we did couple the heat transfer by conduction in the solid components of the surface with the flow of the air due to natural convection. In the model it took us 300 seconds of simulated time for the walls in contact with the fluid to reach the same temperature of the metal (1500 °C). Once we reached this condition, conduction took place slowly through the layers, as shown in figure 3.

It is interesting to note that at roughly 500 seconds, the air profile is almost still (see Figure 4), a fact that plays an important role into the subsequent modeling steps. Specifically, we simplify some of those steps by not including the effects of moving

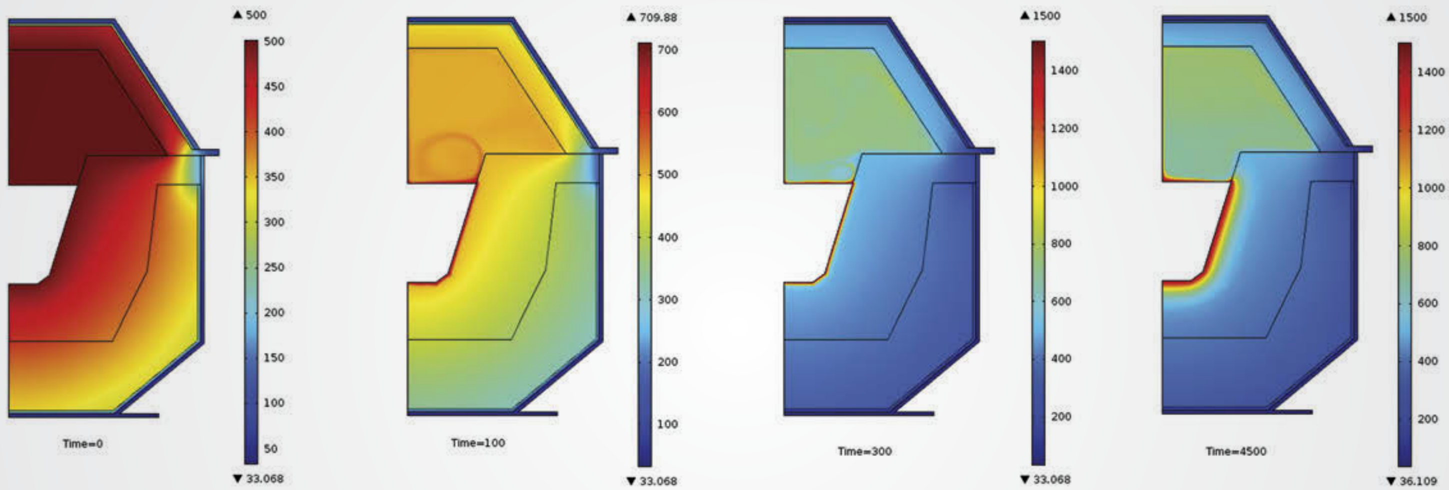


FIGURE 3: Simulation results show that after 300 seconds, the correct condition of 1500 °C is reached and heat transfer occurs mainly by conduction.

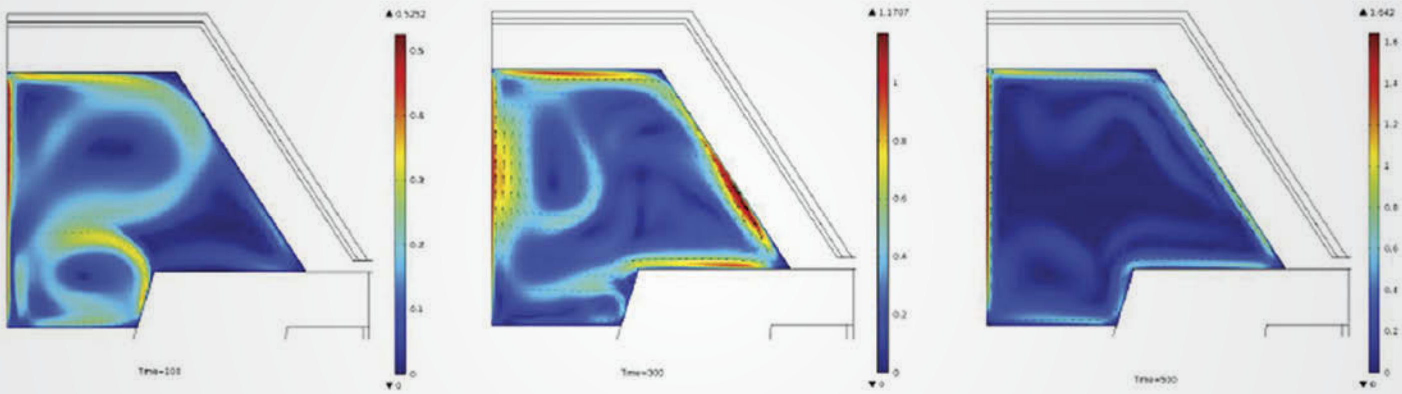


FIGURE 4: During the first tap, the simulation performed with COMSOL Multiphysics shows that after 500 seconds air under the roof runner is almost still.

air, which would not add significant information.

Simulating a 7-Day Heating Cycle

Studying the first tapping, however, does not allow time for the entire runner to heat up and thus does not provide results we can verify in practice, which was our ultimate goal. To approximate how an actual blast furnace operates, the next stage consists of having molten metal flow through the runner for 75 minutes, then having it remain empty for 75 minutes, and cycling through this for seven days of simulated time. As just mentioned, this stage does not include air convection; we set the temperature on the inner walls that are in contact with air to the temperature determined in the previous step.

However, there was one assumption we made thus far that could affect results, so we wanted to refine our model. Specifically, in the previous model we set the temperature of the air interface to the liner at a fixed value of 500 °C. However, when the metal stops flowing, the temperature of the bottom liner does not instantly drop from the 1500 °C of the metal to the 500 °C we had specified. We went to yet another simulation stage like the previous one with one big difference. When there is molten metal, we set the temperature at the fluid-liner interface to 1500 °C; when there is no metal, instead of setting it to 500 °C, we made it thermally insulated.

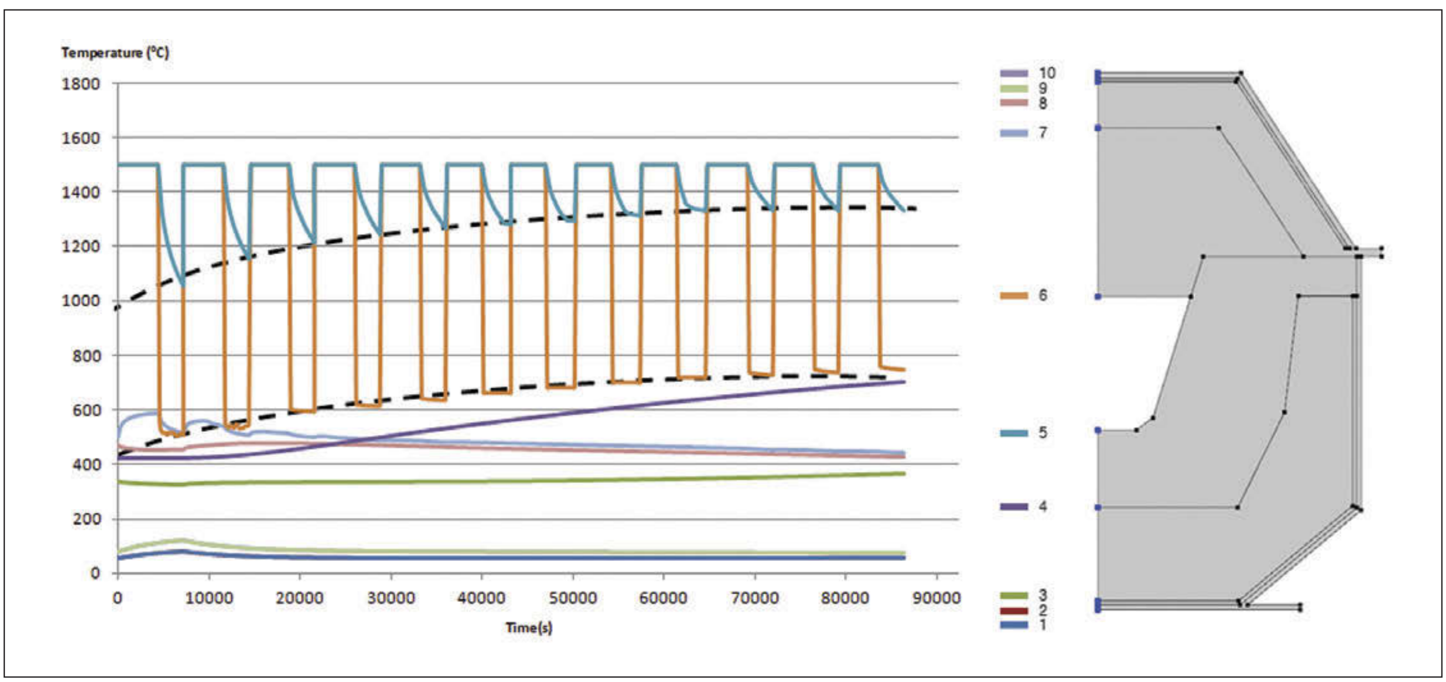


FIGURE 5: Results for 24 hours of simulated time. Trace 6 and 7 follow the temperature of the air at the interface with the molten metal and the top inner liner, respectively.

We then ran this model for 24 hours of simulated tapping and pauses. The results are shown in Figure 5.

Trace 6 follows the temperature of the air at the interface of the molten metal where it reaches (top dotted line) the set level of 1500 °C; without molten metal the temperature of the air alone drops off until it reaches roughly 750 °C (bottom dotted line). We can note that this temperature is much higher than the 500 °C from previous models. Trace 7 follows the temperature of the air where it comes in contact with the top inner liner, and that temperature starts to level off at roughly 430 °C after 24 hours.

Finally, we extended the study to a full week to see what temperature the outer cast iron shell would eventually reach. To make simulation time reasonable, we simplified this by setting the air temperature to the value found at the end of the previous stage; this is valid because Figure 5 shows that the interior air temperature has essentially stabilized. Similarly, we set the temperature at the fluid contact edges to the results in Figure 6. After another six days of tapping and breaks, we saw that the outer shell reaches a temperature of roughly 80 °C.

> “Thanks to simulation, we reached an accurate calculation within 10 degrees.”

Verify Our Simulation to Optimize the Roof Runner

To verify the model, we took thermal imaging photos of an actual roof runner (see Figure 6). We found that its temperature, 76 °C, was in reasonably good agreement with the model. Next, we opened up a roof runner and used imaging techniques to measure the temperature of the liner (see Figure 7). We realize that when you open the cover, the temperature inside will rapidly drop, so the actual temperature inside during operation will be higher. In Figure 7, the hottest temperature is 300 °C, which gives us reasonable confidence that our simulated temperature of 430 °C (Trace 7 of Figure 5) is sufficiently accurate for our immediate purposes since we estimate a temperature drop of around 100 degrees. We had no idea whatsoever what this temperature was going to be and now, thanks to simulation, we reached an accurate calculation within 10 °C. The simulation has given us considerable understanding of what is going on inside the roof runner.

We were surprised when we found the temperature inside the cover is between 400 °C and 500 °C; we had expected it to be much higher. Until now, our concrete liners have been very thick, but thanks to simulation we have learned that we have likely overengineered them. Although we haven’t factored in the roof wear mechanism, simulation provided us with great insights: we know now that we can reduce the thickness of concrete on roof runners. Besides saving the cost of raw materials in future roof runners by making the liner thinner, if they are lighter they will also be easier to maneuver, which will improve production rates. ■

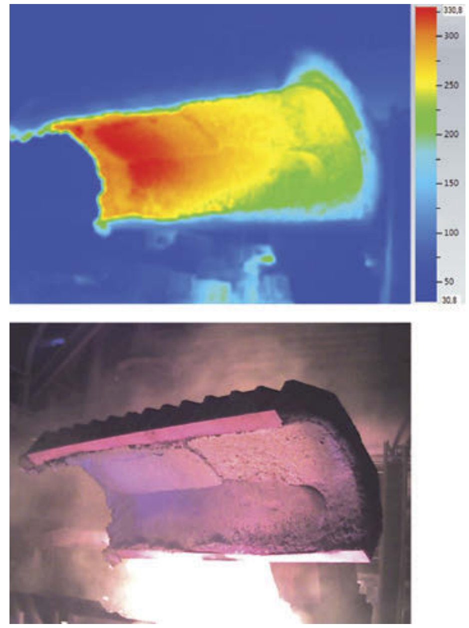


FIGURE 7: Thermogram of the inside of a roof runner (top) and a standard photograph from the same angle (bottom).

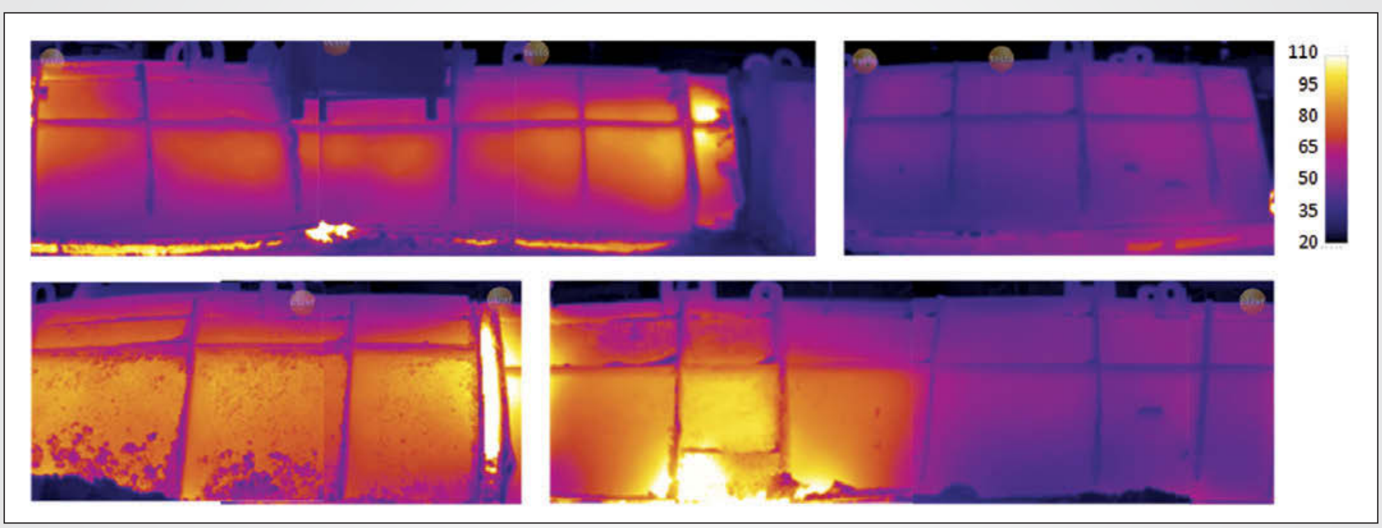


FIGURE 6: Thermogram of an actual roof runner.

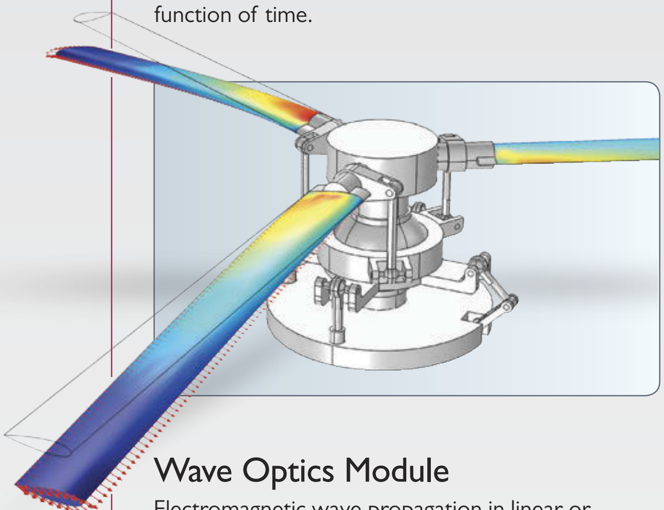
Breakthrough analys
COMSOL Multiphysic

Five new add-on modules open new frontiers in multip

New Modules

Multibody Dynamics Module

Dynamics of assemblies of rigid and flexible bodies connected with joints. Multibody dynamics analyses can be time-dependent, stationary, frequency-domain, or eigenfrequency. Joints can be assigned applied forces and moments as well as prescribed motion as a function of time.



COMSOL Mu

ELECTRICAL
- AC/DC Module
- RF Module
- Wave Optics Module (New)
- MEMS Module
- Plasma Module
- Semiconductor Module (New)

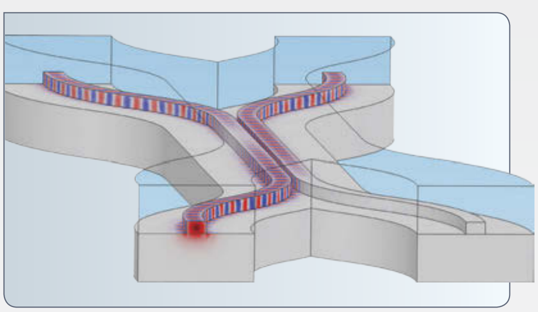
MECHANICAL
- Heat Transfer Module
- Structural Mechanics Module
- Nonlinear Structural Materials Module
- Geomechanics Module
- Fatigue Module
- Multibody Dynamics Module (New)
- Acoustics Module

FLUID
- CFD Module
- Microfluidics Module
- Subsurface Flow Module
- Pipe Flow Module
- Molecular Flow Module (New)

CHEMICAL
- Chemical Engineerin
- Batter Fuel Cells
- Electrode Mod
- Corro Mod
- Electroch Mod

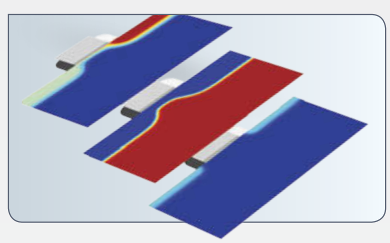
Wave Optics Module

Electromagnetic wave propagation in linear or nonlinear optical media. The groundbreaking Beam Envelope Method enables 3D simulation of elongated optical devices with greater accuracy.



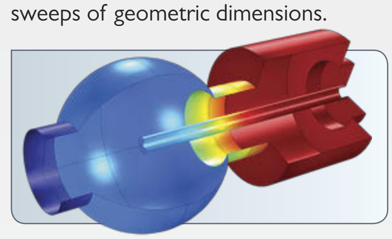
Semiconductor Module

Detailed analysis of semiconductor device operation at the fundamental physics level with electron-hole transport of PN junctions, transistors, and diodes.



Molecular Flow Module

Accurate modeling of low pressure gas flows in complex CAD geometries of vacuum systems. Free molecular flow simulations based on the angular coefficient method with fast parametric sweeps of geometric dimensions.



© Copyright 2013. COMSOL® COMSOL Multiphysics®, Capture the Concept®, COMSOL Desktop™, and LiveLink™ are either registered trademarks or trademarks of COMSOL AB. All other trademarks are the property of their respective owners, and COMSOL AB and its subsidiaries and products are not affiliated with, endorsed by, sponsored by, or supported by those trademark owners. For a list of such trademark owners, see www.comsol.com/tm.

sis tools expand the
cs® simulation platform

hysics simulation. For details visit www.comsol.com/4.3b.

ultiphysics®

Reaction
g Module

ies &
Module

position
ule

sion
ule

New
emistry
ule

MULTIPURPOSE

Optimization Module

Material Library

Particle Tracing Module

INTERFACING

LiveLink™ *for* MATLAB®

LiveLink™ *for* Excel®

CAD Import Module

ECAD Import Module

LiveLink™ *for* SolidWorks®

LiveLink™ *for* SpaceClaim®

LiveLink™ *for* Inventor®

LiveLink™ *for* AutoCAD®

LiveLink™ *for* Creo™ Parametric

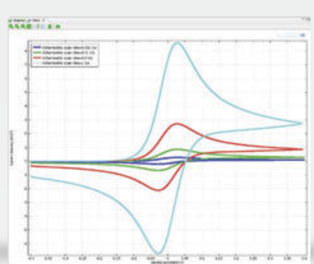
LiveLink™ *for* Pro/ENGINEER®

LiveLink™ *for* Solid Edge®

File Import *for* CATIA® V5

Electrochemistry Module

For the modeling of electrolysis, electroanalysis & electro-dialysis applications as well as electrochemical sensors & the electrochemistry of biomedical devices.



New in COMSOL Version 4.3b

COMSOL Multiphysics

Productivity enhancements throughout the simulation workflow such as:

- 2D Model Work Planes from the Cross Section of 3D Geometries
- Coordinate Systems for Curvilinear Shapes
- Increased Automation for Swept Meshing

CFD Module

- Frozen Rotor Feature for Rotating Machinery in CFD Applications
- SST Turbulence Model and a New CFD Solver
- Thin Screens for CFD Applications

Heat Transfer Module

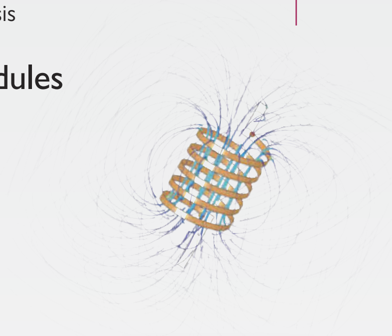
- Multi-Wavelength Surface-to-Surface Heat Radiation
- Heat Transfer with Phase Change
- Thermal Contact

Structural Mechanics Module

- Bolt Pre-tension
- Beam Cross-Section Analysis

AC/DC and RF Modules

- New Magnetics Solver
- Electrical Contact dependent on Mechanical Pressure
- Periodic Structures for Electromagnetic Waves



COMSOL

Tessera Technologies, San Jose, CA, USA

Silent Air Cooling: A New Approach to Thermal Management

A multi-disciplinary team at Tessera Technologies has leveraged simulation to develop a completely new system for cooling Ultrabooks.

BY JENNIFER HAND

For Tolstoy on the train, debates at the dinner table and browsing in bed, thin and light tablets have become an essential tool for entertainment, clarification and communication. Serious data handling, however, calls for the power of a bigger device and when tablet users, accustomed to silent running, turn on a notebook, or an even thinner Ultrabook™, the first thing they notice is…noise.

A fundamental requirement for optimal performance, removing heat from electronic devices is an unavoidable necessity and for portable computers this has, up to now, been achieved by a small mechanical fan. The trend towards 'thin' Ultrabooks means that a typical fan unit is now squeezed into a height of less than 10 mm. With a couple of millimeters allowance top and bottom for air gaps and casing, the actual fan blade measures only a few millimeters and that is pushing the limit of effectiveness. Although some of the latest fans can operate in cavities of less than 5 mm, performance is markedly diminished because smaller blades move less air with each revolution and thus have to turn faster, creating even more noise. The truth is that engineers have nearly exhausted the potential for improving fan technology just as the consumer threshold for noise tolerance has fallen even further.

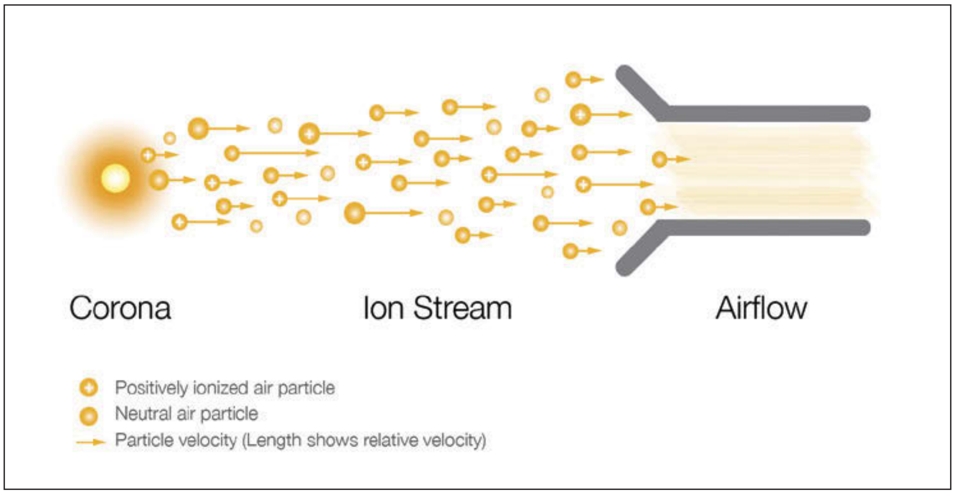


FIGURE 1: Working principle of Silent Air Cooling™.

As a University of Washington student in 2001, Nels Jewell-Larsen recognized the need for research in this area and began a development program. Developing a silent replacement for rotary fans has been the core of his work since then. For the past five years he has been Senior Program Manager heading up a specialist development effort within Tessera Technologies Inc. where Ken Honer is the division lead. "We've put together the best team in the world," says Jewell-Larsen. "We called on experts in areas such as material science, mechanical and electrical design, thermal management, and high-volume manufacturing. We have been able to turn my original idea into a real-life product that is leaps and bounds beyond the early university lab prototypes where it started." As a result, Tessera Technologies

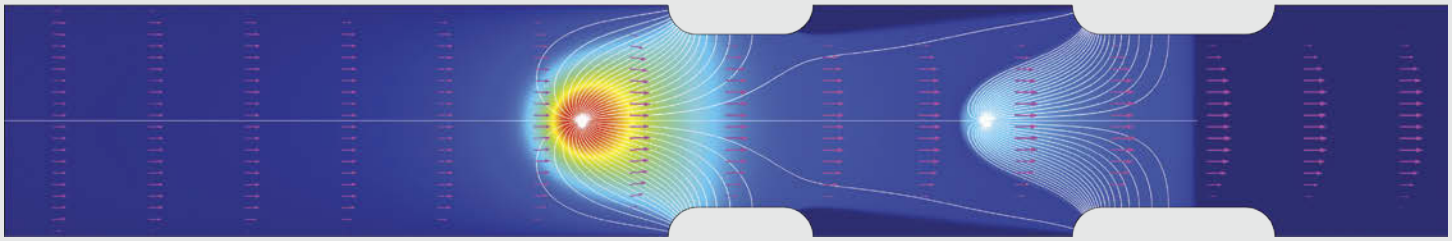


FIGURE 2: Multiphysics plot of a two stage Silent Air Cooling air mover. Space charge density as a surface map (red color indicates higher space charge density) with space charge flux lines shown by white lines. Air velocity displayed as arrows, with arrow length linearly scaled to velocity.

FIGURE 3: Silent Air Cooling's size compared to a pencil.

has just launched a new product based on this breakthrough technology called Tessera® Silent Air Cooling™.

Rotating Blades Not Required

"Probably the first thing to note is that Silent Air Cooling is not a fan, since it does not use a rotating blade to move air," says Jewell-Larsen. "It uses an electric field and charged air to create airflow, a totally different concept. Electronics cooling has never been done this way before." The technology relies on an electric field that charges and pushes nitrogen molecules in ambient air; these collide with other molecules in the air, transferring momentum and producing a continuous stream of laminar airflow. It involves the application of a voltage between two electrodes, generating a very high electric field near one of them that creates positively charged nitrogen ions. The ions created are pushed towards the second electrode generating a constant pressure source (see Figure 1). "Because the electric field does not change with time there are no pressure waves, so there is virtually no sound." In addition to being noise-free, Silent Air Cooling (SAC) fits in a very thin cavity, 4 mm and below, since it doesn't need rotating fan blades and doesn't need an air plenum above or below it.

"Simulation has been at the core of our product development because the team needed to take in account electrostatics, charge generation and transport, fluid dynamics and heat transfer (see Figure 2). We are in a niche field and there was no dedicated simulation software for this when we started, so we looked at several offers," comments Jewell-Larsen. "We even considered a custom-made software at one point. We then began using COMSOL Multiphysics because of its in-built flexibility."

Gustavo Joseph, Head Thermal Engineer, expands on this. "Many software packages can easily simulate the movement of fluid or electrostatic forces independently. What is very difficult to simulate is the generation of ions, their transport in an electric field and the force generated on air molecules resulting in the needed cooling flow. COMSOL Multiphysics is the only commercial off-the-shelf (COTS) available software that would allow us to build all our own equations and couple them into the already available fluid dynamics and electrostatics capabilities."

Joseph and Jewell-Larsen used COMSOL Multiphysics to design the core engine of the new technology, termed 'the blower' by the team. "As the main objective was to maximize pressure and airflow for cooling, we simulated different geometry and materials to optimize these parameters. After we designed the key aspects of the blower in COMSOL Multiphysics we ported that over to a CAD software to design the rest of the system."

> "Simulation has been at the core of our product development because the team needed to take in account electrostatics, charge generation and transport, fluid dynamics and heat transfer."

The end result is a reliable, compact unit that operates at less than 15 dBA, which is below the average threshold for hearing (see Figure 3). Additional features include a self-cleaning system and, as there are no bearings, the system is easy to maintain. Tessera has over 140 patents in this area and initiated pre-production manufacturing late in 2012. The target market includes suppliers of portable computer devices and Tessera has been working with companies wishing to license the technology.

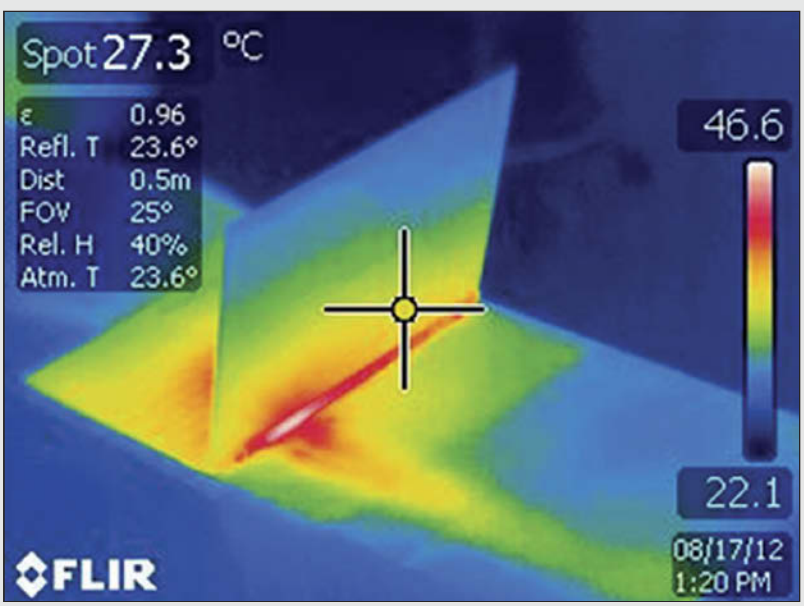


FIGURE 4: Thermogram of an Ultrabook being cooled by a Silent Air Cooling air mover.

Silent and Powerful

"Tablets are both portable and silent. Ultrabooks are powerful, capable, and thin, but noisy. There has not, so far, been a device that combines power with complete portability and silence. Now there is," concludes Jewell-Larsen. "We have demonstrated that the technology works in Ultrabooks (see Figure 4) and our objective is to have this technology in as many devices as possible, with designers free to build form factors that are thinner and thinner. This technology is going to have a really positive impact for users." ■

Ultrabook is a trademark of Intel Corporation in the U.S. and/or other countries.
Silent Air Cooling is a trademark of Tessera Technologies, Inc. in the U.S.

Analysis of Spiral Resonator Filters

Improved performance coupled with reduced size requires the development of novel filter designs for use in advanced wireless systems.

BY SERGEI P. YUSHANOV, JEFFREY S. CROMPTON, AND KYLE C. KOPPENHOEFER, ALTASIM TECHNOLOGIES

Increasing demand for more advanced wireless systems necessitates the introduction of novel designs that are capable of simultaneously fulfilling multiple operating and performance criteria. The implementation of high data rate transmission systems has required the development of innovative designs for microwave filters that must fit within a reduced volume to allow integration of multiple filters in more compact wireless systems. Additionally, the filter's specific passband frequencies and quality factors must be achieved within the system's geometrical and topological constraints. Spiral resonator filters offer one option for significantly reduced size compared to conventional ring resonators. An array of spiral resonators can be directly fabricated on a printed circuit board and because of their characteristic response, they can be designed to occupy minimal volume.

To characterize the operation of these devices, a mathematical construct named the scattering matrix (*S*-matrix) is used that describes how the RF signal interacts with the device. The signal may reflect, exit other ports and dissipate via heat or electromagnetic radiation; the *S*-matrix represents each of these signal paths. The order of this matrix is $n \times n$ with n equaling the number of ports in the system; thus, S_{ij} represents the scattering for the j input port and the i output port such that S_{11} specifies the ratio of signal reflected from port 1 for an input on port 1, and S_{21} specifies the response at port 2 due to a signal at port 1.

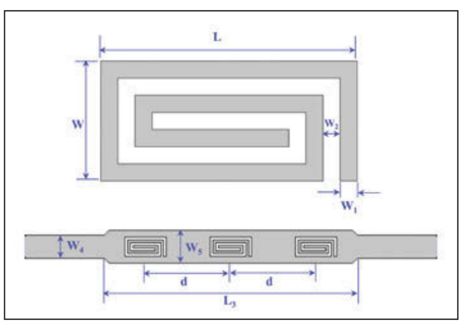


FIGURE 1: Microstrip filter based on rectangular type spiral resonators etched on the center line of the microstrip.

Spiral Resonator Simulation

A compact microstrip filter (see Figure 1) using spiral resonators was designed to produce a resonant frequency of 7.2 GHz (Lim *et al.*)

A model was set up using COMSOL Multiphysics (see Figure 2), in which the microstrip line is represented as a perfect electric conductor (PEC) surface on a dielectric substrate, with another PEC surface on the bottom of this substrate acting as a ground plane. Two lumped ports are modeled as small rectangular faces that bridge the gap between the PEC faces of the ground plane and the microstrip line at each port. A small air domain bounded by a scattering boundary (SBC) surface is added to avoid back reflection of radiated fields and reduce the size of the modeling domain. The model includes the dielectric substrate defined as a volume with the relative permittivity of the dielectric.

The experimental and simulation results for and over a range of frequencies of interest are shown in Figure 3, where S_{11} specifies the ratio of signal reflected from

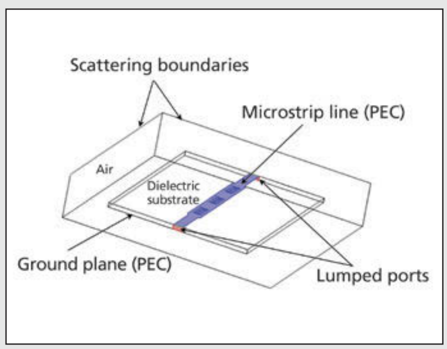


FIGURE 2: Model of the bandstop resonator filter. Some exterior faces are removed for visualization.

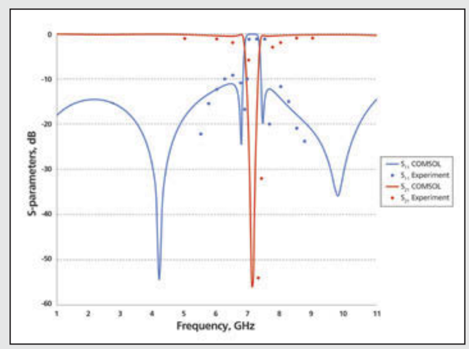


FIGURE 3: Frequency response of the bandstop spiral resonator filter comparing experimental measurement (Lim *et al.*) with COMSOL simulation.

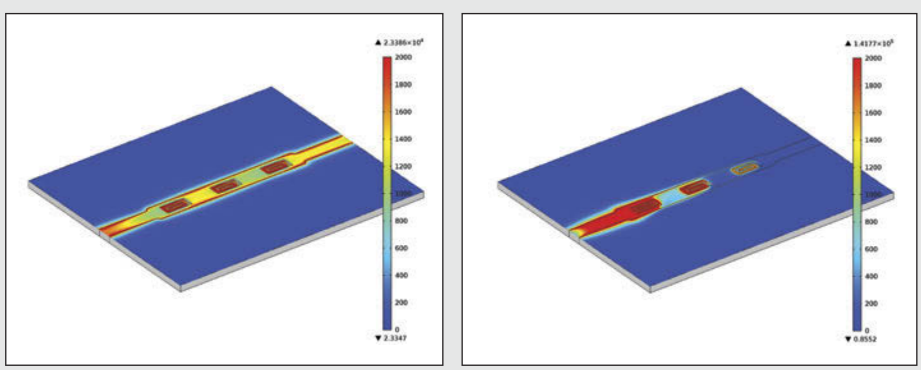


FIGURE 4: Electric field (left) and at (right) resonant frequency.

port 1 for an input on port 1, while S_{21} specifies the response at port 2 due to a signal at port 1.

The simulation results agree well with experimental data for the transmitted and reflected signals and demonstrate rejection of frequencies outside the required frequency cutoff. The resonant frequency is 7.2 GHz and the bandwidth of the stopband is 0.5 GHz (7.1-7.6 GHz) with the reference level of $|S_{21}|$ = -10 dB. A deep rejection band (S_{21} > -50 dB) is obtained at the resonant frequency with a steep cutoff; a flat passband (S_{21}< 1.2 dB) is observed, suggesting the proposed spiral filter design has low insertion losses thus limiting its effect on transmitted signal when integrated into a circuit.

The data can also be visualized by the electric field distribution below and at the resonant frequency. (see Figure 4) Below the resonant frequency a high level of signal is transmitted through the device; at the resonant frequency of 7.2 GHz a high level of signal is attenuated, thus demonstrating the degree of signal selectivity developed by the filter design.

Fractal Spiral Resonator Band-Stop Filter

A fractal spiral resonator developed by Palandöken & Henke is shown in Figure 5.

The filter is composed of two unit cells of electrically small artificial magnetic metamaterials formed with the direct connection of two concentric Hilbert fractal curves. Operation is based on the excitation of two electrically coupled fractal spiral resonators through direct connection with the feeding line. Simulation results for the transmission (S_{21}) and reflection (S_{11}) losses are shown in Figure 6; the selectivity of the filter is 100 dB/GHz with a 3 dB reference insertion loss.

The electric field distribution developed by the fractal spiral resonator is shown in Figure 7; below the resonant frequency, signal passes through the filter; at resonance the signal is highly attenuated with an extremely low level of signal transmitted.

Conclusions

The performance of a spiral resonator filter has been analyzed using COMSOL Multiphysics and shown to demonstrate agreement with experimental data. A compact microstrip based spiral resonator filter with a resonant frequency of 7.2 GHz shows low insertion losses with a high level of performance and sharp cutoff over the specified frequency range. Analysis of a fractal spiral resonator consisting of two unit cells of magnetic metamaterials operating at a resonant frequency of ~1.3 GHz also shows a high level of selectivity at 100 dB/GHz. Analyses of this type can be extended to assess the performance of other filter designs prior to fabrication and integration into operating circuits. ■

REFERENCES

Ho Lim, Jong-Hyuk Lee, Sang-Ho Lim, Dong-Hoon Shin, and Noh-Hoon Myung, Proceedings of Asia-Pacific Microwave Conference 2007.

M. Palandöken, H. Henke, "Applied Electromagnetics Conference", p. 1–4, 2009.

The team at AltaSim Technologies.

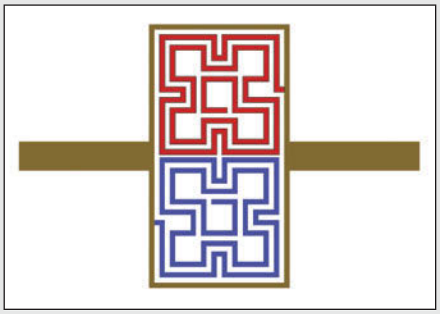


FIGURE 5: Geometry of metamaterials fractal spiral resonator: two fractal resonators are connected anti-symmetrically along the feeding line.

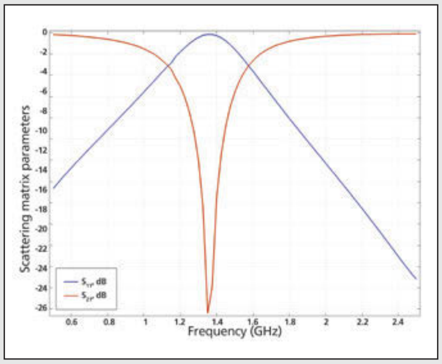


FIGURE 6: Reflection and transmission parameters of the fractal spiral resonator.

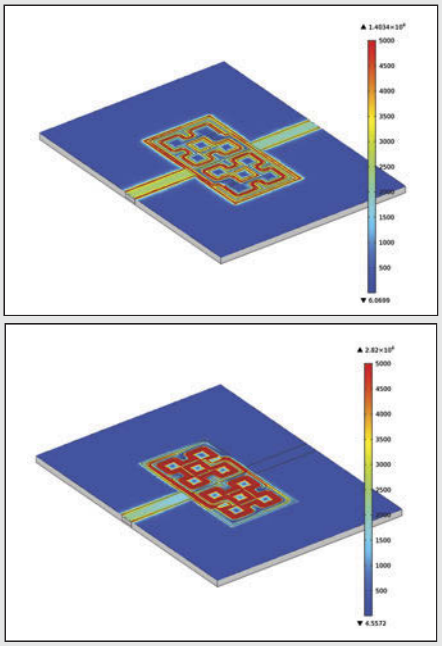


FIGURE 7: Electric field at a frequency below the resonant frequency (top) and at the resonant frequency (bottom).

Magnets Improve Quality of High-Power Laser Beam Welding

Researchers are looking at the effects of stationary magnetic fields on laser beam welding quality. Simulation helps them find the best choice of magnets.

BY MARCEL BACHMANN, VJACESLAV AVILOV, ANDREY GUMENYUK AND MICHAEL RETHMEIER,
BAM FEDERAL INSTITUTE FOR MATERIALS RESEARCH AND TESTING

Photo courtesy of BAM

Welding is one of the most critical operations for the construction of reliable metal structures in everything from ships to reactor vessels. When welds fail, often the entire structure fails, and expectations on weld quality have never been higher. Any process that uses a localized heat source, such as welding, is likely to result in some distortion. The welding process of very thick metal components is not inherently stable and is barely controllable without external forces.

> "This welding process is extremely complex and, thanks to COMSOL Multiphysics, we managed to achieve accurate results."

Creating the Keyhole

In high-power laser beam welding, a small amount of metal in the region of the highest laser intensity vaporizes. This penetration welding creates a vertical cavity in the workpiece that is known as a keyhole. In this process, the laser beam not only melts the metal, but also produces vapor. The dissipating vapor exerts pressure on the molten metal and partially displaces it. The material, meanwhile, continues to melt. The result is a deep, narrow, vapor-filled hole, or keyhole, which is surrounded by molten metal. As the laser beam advances along the weld joint, the keyhole moves with it through the workpiece. The molten metal flows around the keyhole and solidifies in its trail. This produces a deep, narrow weld with a uniform internal structure.

Well-known issues in deep-penetration welding of aluminum are the highly dynamic behavior of the melt due to its low viscosity. Combined with high heat conductivity, the resulting weld pool is very wide. The weld surface becomes unstable with the result being spattering and the ejection of droplets from the weld metal that results in underfills, undercuts, craters, blowholes or blowouts — all of which can have a detrimental effect on the weld's mechanical properties. If material is missing, there is often the need for post-treatment with arc welding to fill in the missing material or make the weld more visually appealing,

Marcel Bachmann is a researcher at the BAM German Federal Institute for Materials Research and Testing in Berlin. Here he is standing in front of a laser beam welding machine.

which is an indicator of surface quality. In addition, a smooth weld surface becomes very important in places such as the food industry where rough surfaces could harbor bacteria populations.

One side effect of an uncontrolled welding process is droplets that accelerate from the weld bead. These droplets make the process "dirty" and lead to a lack of material after the weld has cooled down. Second, the Marangoni effect leads to a non-uniform weld, which can be a reason for stresses and/or distortion of the workpiece. Part of the weld pool is moving under surface tension and electromagnetic forces, thus inducing a non-uniform distribution of the material and different solidification rates in different parts of the weld pool. Once the bead solidifies, it is likely constituted by different materials because of non-uniform distribution and cooling times.

Decelerating the Melt

Is it possible to counteract such effects? Under a grant from the German Research Foundation, BAM is investigating various methods to control and reduce them. In this particular case, we are applying a stationary magnetic field to the laser welding process. With the help of COMSOL Multiphysics, we have determined the distribution of the magnetic field required to improve the uniformity of the weld.

In particular, we wanted to reduce the effects of the Marangoni effect. At the surface, there is a very high temperature at the point where the laser beam impacts the metal, and the temperature drops off rapidly with distance away from the weld. The resulting high temperature gradients cause a flow of metal directed from the middle of the weld pool towards the outer boundary due to the temperature-dependant surface tension (the Marangoni effect). Our goal is to have a perfect weld, which means that we need to suppress this flow so the energy goes into the depth of the pool rather than spreading out on the surface.

Consider that a perfect weld would have side walls that are parallel, with solidification taking place at all depths at the same time. An actual weld without the application of external forces has more of a wine glass shape (Figure 1a), with a strong curvature of the solidification front. This leads to heavy stresses in the workpiece and relatively large distortions after it cools. However, when a static magnetic field is applied perpendicular to the welding direction, the weld takes on a more homogeneous shape that starts to resemble a V (Figure 1 b-d), which is closer to the desired form.

This ability to change the weld shape is due to the Hartmann effect. Specifically, for an electrically conducting liquid such as a molten metal, a magnetic field induces electric currents that create a Lorentz force field with a component directed against the original melt flow direction.

To model this effect, we simulated in 3D heat transfer, fluid dynamics, and electromagnetics, and for this I used the CFD Module and the AC/DC Module. First, we model the electromagnetic field to calculate the Lorentz forces; these results are then used as a volume force to calculate the velocity and pressure of the turbulent flow in the weld pool. This allows us to solve for the heat transfer where the velocity field is taken from the previous turbulent flow simulation. Temperature, of course, influences the material properties, so we go back and recalculate the Lorentz forces, which also depend on the velocity of the flow. This looping continued until the simulation reached the desired accuracy to a steady state solution where the solution is self-consistent, i.e. satisfies all the physics involved.

To verify the model, we took actual welds done with and without magnets, cut them, and polished the macrosections. Then

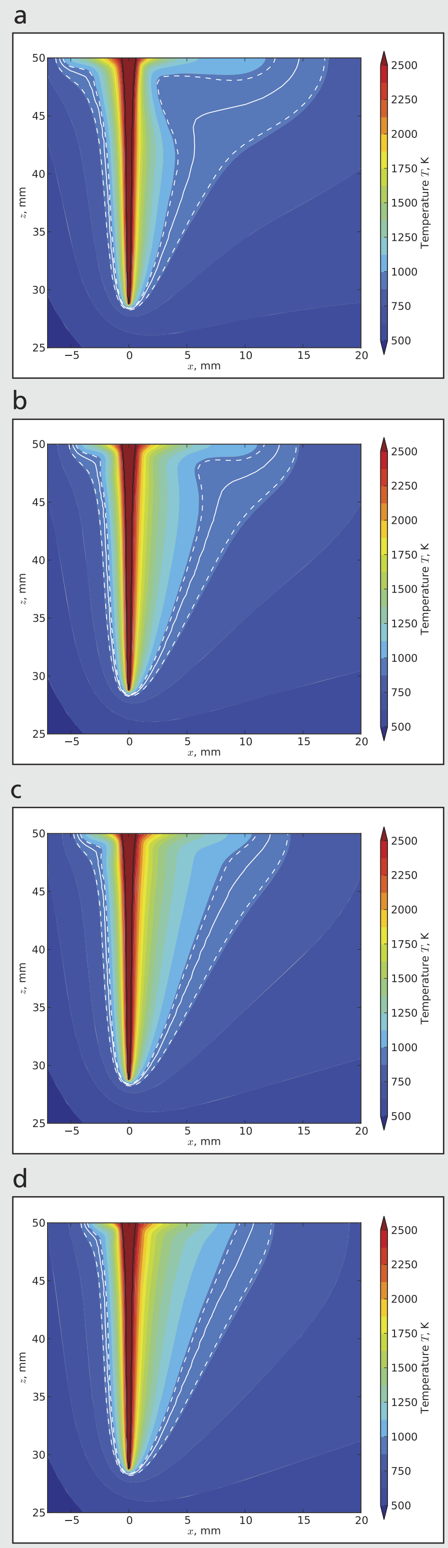


FIGURE 1: A plot of temperature in the symmetry section of a weld shows that without any magnetic field applied (a), the weld takes on a wine glass shape. With the addition of a magnetic field (b = 0.50 T, c = 1 T and d = 2 T), the shape starts to take on the form of a V.

we superimposed the simulation results, which show good agreement (Figure 3). This welding process is extremely complex and, thanks to COMSOL Multiphysics, we managed to achieve accurate results.

In my opinion, COMSOL's advantage is the combination of easy handling, very comfortable geometry building and meshing, and the ability of using pre-defined multiphysics modules — yet nevertheless, having the option for manual tuning and case-dependent modification. These include, for instance, temperature-dependent material properties coming from experimental data points or analytical expressions, using source terms for the velocity modeling in the solid phase, inclusion of gravity effects, and inclusion of latent heat of fusion. All of these can easily be taken into account for the calculation.

We were also pleased with the software's ability to make easily available quantities originated from all the physics. For instance, it took us just one click to let the fluid flow physics know that the volume force acting in the weld pool was the Lorentz forces. This is just an example that can be extended to all the current and future multiphysics coupling that we may need.

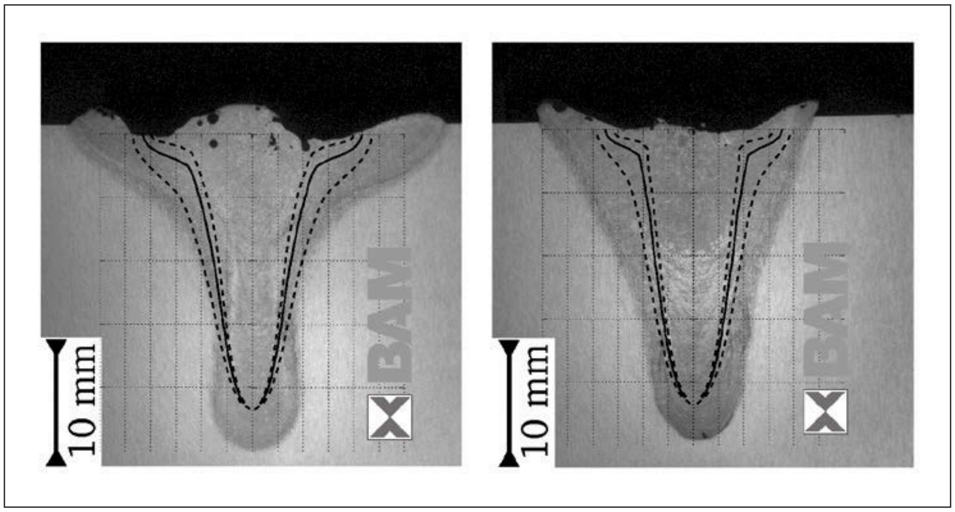


FIGURE 2: A photo of actual welds with COMSOL Multiphysics results superimposed on them achieved with a welding velocity of 0.5 m/min at a laser power of 16 kW. The left image shows a weld without any applied magnetic field and the resulting wineglass shape. The right image shows the case with B = 0.5 T and how the weld has more of a V shape with straight sides as opposed to the wineglass shape on the left.

Thanks to the COMSOL Multiphysics simulation, we have identified the underlying effects and now understand how to counteract them. The next step is to learn how to put this knowledge into practice at a large scale. We have identified which magnetic fields improve the quality of this welding process, and we will be performing further experiments to redefine the whole welding process. ■

Free Hands-on Multiphysics Simulation Workshop

Attend a free modeling workshop for a live demonstration of COMSOL Multiphysics. The philosphy of our workshops is for you to *learn-by-doing*. The goal is to teach you the skills needed to build simulations in COMSOL Multiphysics. Join us for this unique hands-on experience.

All attendees will receive a 2-week trial of COMSOL Multiphysics.

Find a workshop near you at www.comsol.com/workshops

COMSOL

Learn more & request
a FREE TRIAL at
spaceclaim.com/comsol

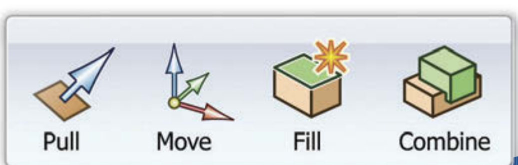
CAD Slowing You Down?

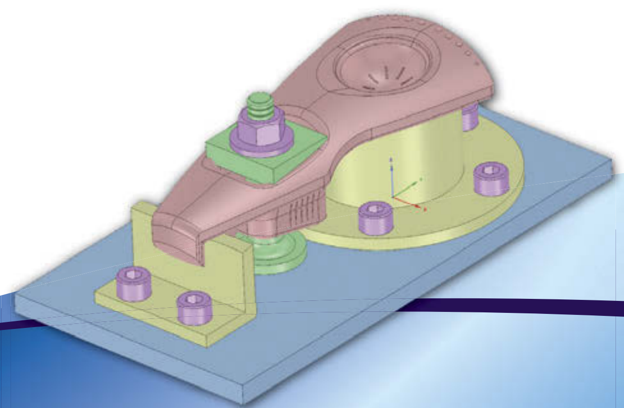
Do CAD problems slow you down
when preparing models for CAE analysis?

With SpaceClaim Engineer, you can focus
on the analysis rather than preparing the model.

SpaceClaim solves common CAD problems:

>> Open native CAD models from all major traditional CAD systems
>> Repair poor geometry quickly and easily
>> Optimize CAD models for input to all major CAE systems
>> Prepare CAD models yourself for meshing and analysis
>> Work confidently in 3D without the complexities of traditional CAD
>> Support and enable simulation-driven design initiatives





SpaceClaim Engineer:
Powerful yet easy-to-use 3D for all engineers.

Toll Free: 800-636-6004 +1-978-482-2148 info@spaceclaim.com

© Copyright 2012 SpaceClaim Corporation. SpaceClaim is a registered trademark of SpaceClaim Corporation. All other names mentioned herein are either trademarks or registered trademarks of their respective owners.

SPACECLAIM CORPORATION

Visit Us Online at www.spaceclaim.com

Altran, Pisa, Italy

Picking the Pattern for a Stealth Antenna

A frequency selective surface that acts as an RF filter and helps reduce the radar cross section of antennas consists of a pattern of geometrical objects. There are literally thousands of possibilities, and testing each one physically would take enormous amounts of time. With simulation, though, we can find promising candidates in just minutes.

BY FRANCESCA DE VITA, SIMONE DI MARCO, FABIO COSTA AND PAOLO TURCHI, ALTRAN ITALY

For roughly 30 years, the Altran Group has been a global leader in innovation and high-tech engineering and consulting, providing services covering every stage of project development, from strategic planning through to manufacturing, to key players in the aerospace, automotive, energy, railway, finance, healthcare and telecom sectors.

Antenna as the Weak Point

Our team works mainly in the aerospace and defense industry, and we have developed projects related to studies of antenna placement as well as radar cross section prediction and control. One of them is addressing one of the largest leaps in defense technology developed in recent years — stealth airplanes and ships that avoid radar detection. They generally do so by combining several technologies including the shape of the target's surfaces to reflect energy away from the source and the use of radar-absorbent materials. However, if a ship's or aircraft's antenna is to operate properly it cannot be completely covered up — and that makes it one of the remaining components with a large radar cross section (RCS) and it can essentially destroy the overall system's invisibility to radar.

The RCS depends on the polarization and frequency of the incident wave. When an electromagnetic wave is incident on a target, electric currents are induced in the target and a secondary radiation from that target produces a scattered wave. The scattered field is partially reflected straight back to the source of the incident wave, and this is the principle upon which radar is based. The peak reflected wave is related to the standard antenna gain and its peak effective surface area. In this case there is an ironic twist: antenna designers normally look to maximize antenna gain, but to lower the RCS they must do the opposite of what they normally do, specifically reduce the gain.

One way around this problem is to employ a frequency selective surface (FSS). It consists of a pattern of shaped holes or surfaces on a substrate and essentially creates a bandpass filter. In the intended frequency range, for instance where radio operators are transmitting or receiving,

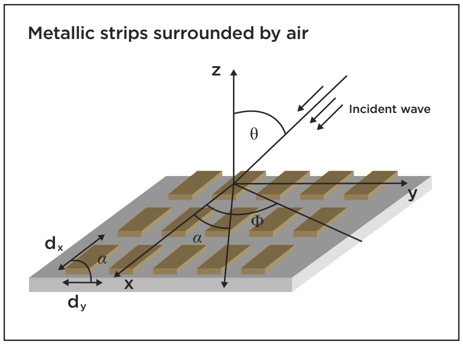


FIGURE 1: An example of a frequency selective surface (FSS) made up of a series of metallic strips.

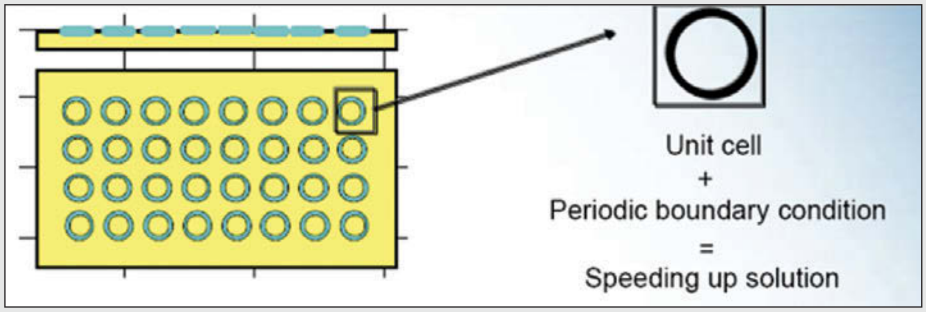


FIGURE 2: PBC functionality from COMSOL significantly speeds up the solution to our FSS study by simulating only a unit cell.

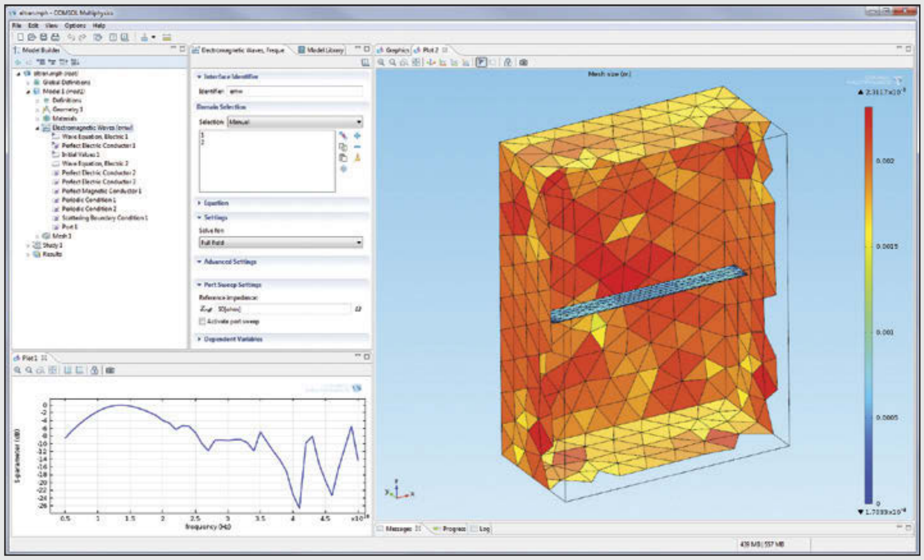


FIGURE 3: A simple example FSS based on a metallic strip array, with its meshed geometry (right), and frequency response curve (lower left). The latter shows the S11 parameter in dB and is at a scale of 10^{10} with a resonance at about 40 GHz. The dip corresponds to maximum transmitted power.

the antenna acts as normal; at other frequencies, the FSS absorbs rather than scatters incident radiation. Antennas are generally housed in a protective enclosure called a radome; for aircraft, often located at the nose. If that enclosure is made of such a FSS, its RCS is significantly reduced at all but the operating frequencies.

Geometric Patterns as a Filter

Frequency selective surfaces are usually constructed from periodically arranged metallic patterns of an arbitrary geometry. They have openings similar to patches within a metallic screen (see Figure 1). The performance of a FSS is linked to its shape, thickness, choice of substrate and the phasing between individual elements. We have focused on the physical configurations and the resonant frequencies for certain bandwidths. And COMSOL Multiphysics has been an invaluable tool in these studies.

As shown in Figure 1, a FSS consists of a series of geometrical objects. The FSS can be electrically large in terms of wavelength with very many instances of the object, which would make simulating the entire surface extremely cumbersome and expensive in terms of compute power and time. Luckily, COMSOL Multiphysics has a very convenient answer to this problem in the Periodic Boundary Condition (PBC) feature. It allows the simulation of a single cell unit and thus a less time-consuming process (see Figure 2). This feature provides for continuity of the electric and magnetic fields so we get equivalent results as if we had simulated an entire array of objects.

> “The ability to try any number of shapes highlights the capacity of the software to help us be efficient in finding a good solution.”

We were very impressed with the time and memory savings possible with a PBC while keeping the level of accuracy we needed to study the behavior of a given geometry. For a simple structure without a dielectric substrate, we estimate it cuts simulation time by a factor of 100; for a very large electrical structure, this could even be 1,000 times or more.

Figure 3 (upper left) shows an example FSS made of simple metallic strips surrounded by air. The simulation mesh was created for one of the metallic strips, and you can see from the frequency plot (bottom right) that it has a passband in the region of 40 GHz.

To validate our simulation, we first analyzed a case already dealt with in the literature and replicated the known results in COMSOL Multiphysics with the aim of tuning the simulation procedure. In a second step, we took this same validated simulation and modeled other

Altran's simulation team, from left to right: Fabio Costa, Simone Di Marco, Francesca De Vita and Paolo Turchi.

types of FSS while changing geometries and materials and evaluating the impact of these changes on FSS performance.

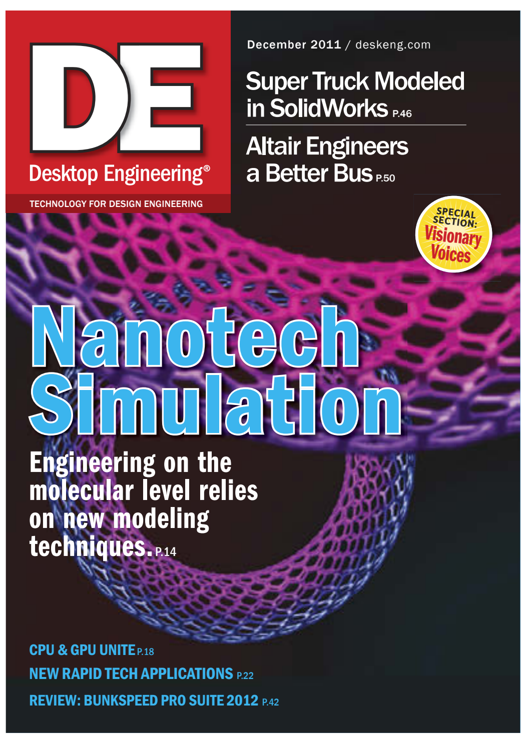
We have used the software to investigate the frequency responses of a variety of simple shapes and sizes and how they are distributed on a surface. It is also possible to make the design more complicated by using two structures with complementary behavior. In this way we can, for example, create a design with multiple resonant frequencies. The ability to try any number of shapes highlights the capacity of the software to help us be efficient in finding a good solution. The alternative would be actually fabricating various shapes for the FSS and physically testing them, which would involve far more time and expense. With modeling, in a few minutes we can determine if a pattern is worth pursuing in detail.

We are now starting to expand our model to include the effects of the dielectric substrate. In addition, we hope to soon start working with optimization algorithms to help in cases where we face constraints such as maximum unit cell size. ■

FREE SUBSCRIPTION!

If you do simulation-driven design, you need to sign up today at:

www.deskeng.com/subscribe



Multiphysics Simulations Help Track Underground Fluid Movements

Multiphysics simulations are helping geophysicists at the Colorado School of Mines develop a way to track underground fluid flows and to better map and understand subsurface formations and dynamics. One potential application: tracking the fracking fluids used in unconventional natural gas and oil extraction.

BY GARY DAGASTINE

Geophysicists characterize underground formations and events by detecting and analyzing acoustic waves that propagate to the Earth's surface from seismic activity. These waves arise from earth movements caused by natural events such as earthquakes, from underground explosions deliberately set to explore geological features, and from the hydraulic fracturing, or fracking, of tight formations with the goal of increasing permeability.

Although acoustic waves can travel long distances, they have major limitations in providing details about formation properties. They can't be used to directly identify and track the liquids flowing through them, called pore water. Innovative research at the Colorado School of Mines, however, suggests that electromagnetic disturbances that can occur in association with seismic events might provide this missing information.

Electromagnetic waves don't propagate as far as acoustic waves, but theoretical models and laboratory experiments conducted with the aid of numerical multiphysics simulations show they can identify and track pore water. The evolving technique, based on work pioneered by Russian and Japanese researchers, opens the door to the complementary use of acoustic and electromagnetic analyses to create a more comprehensive view of the underground world than we now have.

Such a seismoelectric capability would enable better monitoring of shallow earthquakes along tectonic faults and active volcanoes. It also would lead to better tools for the safe development of unconventional energy resources via fracking, and for more effective secondary/enhanced oil recovery in previously worked oil reservoirs.

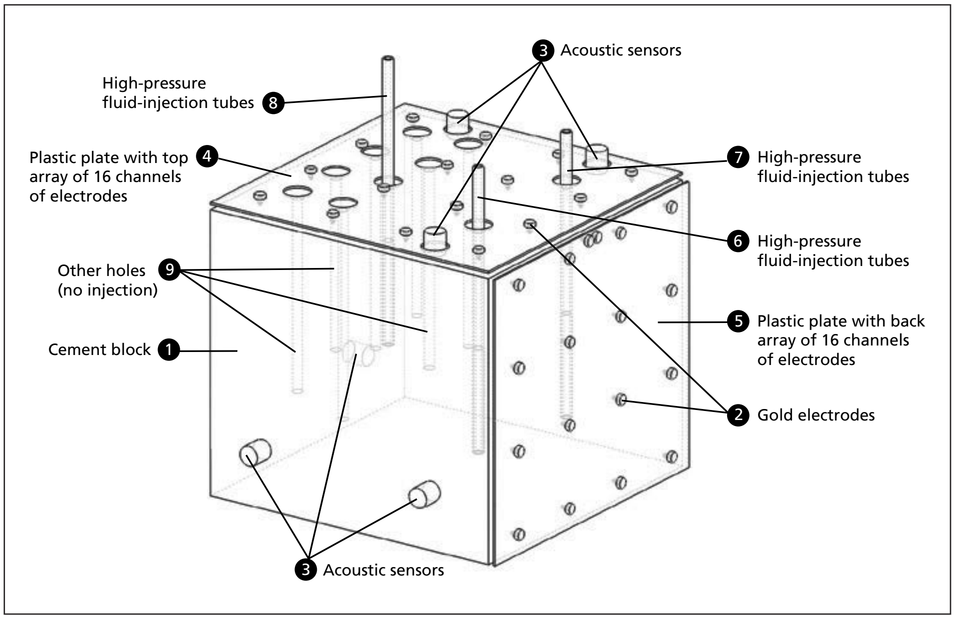


FIGURE 1: Illustration of the cement block used in hydraulic fracturing experiments. (1) Cement block, (2) Gold electrodes, (3) Acoustic sensors, (4) Plastic plate with top array of 16 channels of electrodes, (5) Plastic plate with back array of 16 channels of electrodes, (6-8) High-pressure fluid-injection tubes, (9) Other holes (no injection).

Fracking is a particularly critical and timely issue because of the growing use of the technique, in which fluid is injected into the ground at high pressure to fracture low-permeability shale formations to extract the gas and oil in them. It is vital to know where fracking fluid is going so that the fracking process can be optimized, and to avoid contamination of shallow aquifers.

Geoelectric Signals

Subsurface electromagnetic disturbances stem from the net deficiency of electrical charges on the surfaces of minerals. This deficiency is compensated for by excess charges in the pore water. The flow of the pore water with these excess charges is responsible for an electrical current density (on the order of few milliamperes per square meter).

Because the current varies according to the kinds of formations the water passes through, the hope is that useful inferences can be made based on these electrical signals, which could be detected by a network of electrodes placed on the ground surface and/or in boreholes.

"This method is analogous to electroencephalography — EEG. In EEG, electrical signals are generated at the synapses between the neurons and recorded on the scalp. EEG has been a key method to understand how the brain is working," said André Revil, a leading researcher in this evolving branch of geophysics. "If you put electrodes on your head, you can monitor the electrical activity in areas of interest within your brain, and make informed inferences. We are trying to do the very same thing underground."

Revil is associate professor of geophysics at the Colorado School of Mines, one of the world's leading colleges of mineral engineering, and also a faculty member with the Centre National de la Recherche Scientifique (CNRS) in France. His team for this work includes students Harry Mahardika, who has done a great deal of forward modeling and some inverse modeling with multiphysics software; Allan Haas, who has been the lead experimental investigator; and Marios Karaoulis, research associate, who has co-supervised their work along with Revil.

The team is part of the Colorado college's Unconventional Natural Gas Institute (UNGI). UNGI serves as a focal point to facilitate and promote research and development in all areas of unconventional natural gas, encompassing coal bed methane, tight gas sands, shale gas, and gas hydrates. UNGI combines the resources of seven academic departments and 11 research centers and consortia, forming a critical mass of expertise in the fast-growing field.

Forward and Inverse Modeling

"We found that fracking releases both seismic and electromagnetic energy, and so we developed theories about what the electrical activity associated with these events should look like," Revil said. "To do this, we used COMSOL Multiphysics to simulate fracking events and to produce synthetic seismograms and electrograms, and we coupled MATLAB® and COMSOL to conduct many iterations of forward and inverse modeling thanks to the LiveLink *for* MATLAB®.

"COMSOL saved us a great deal of time because all of the necessary underlying physics, such as hydromechanical equations, is very well defined in the software and we didn't have to spend time calculating it."

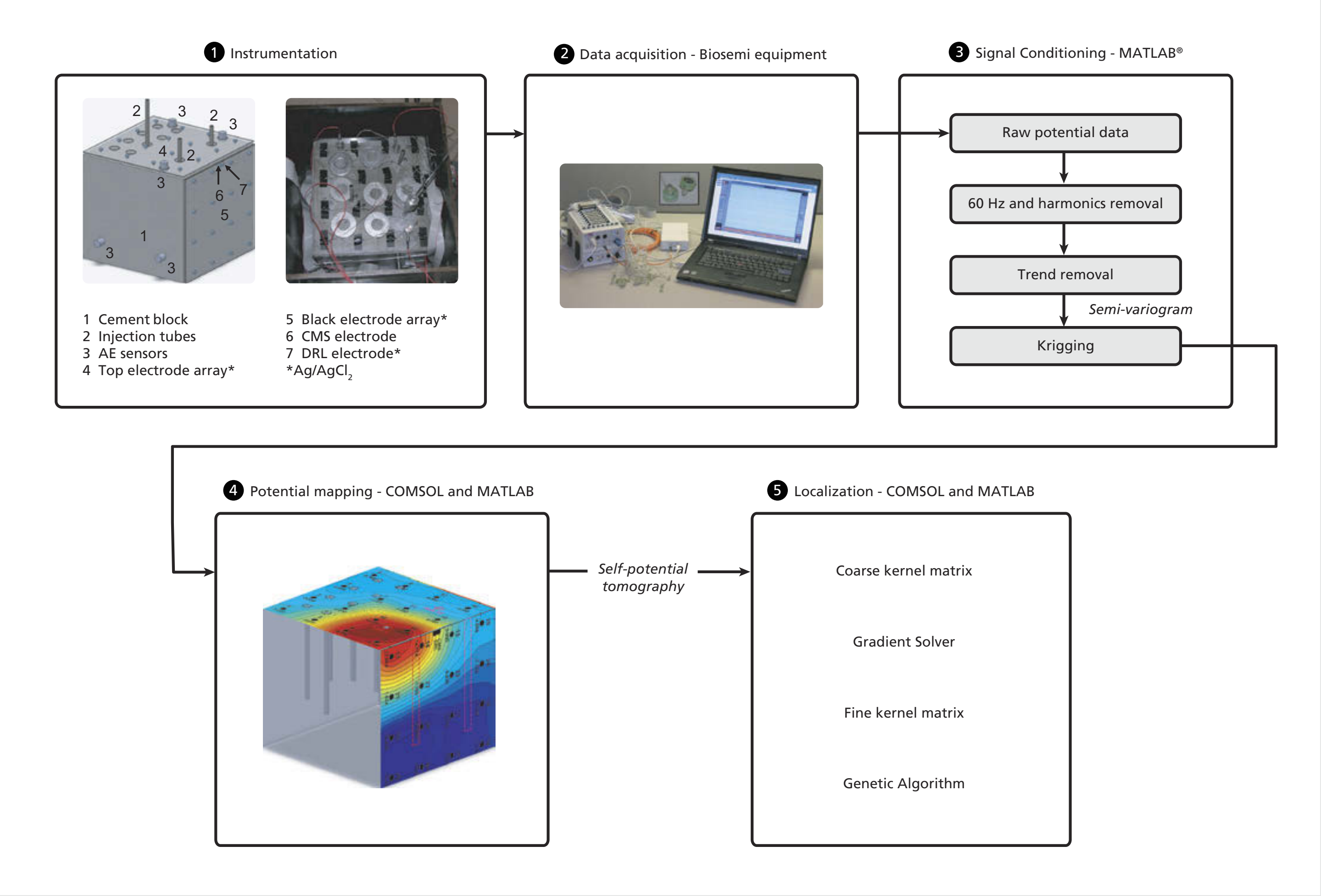


FIGURE 2: Flow chart for the processing of the electrical data. (1) Instrumentation of the porous cement block, (2) Data acquisition system, (3) Signal conditioning of the raw data, (4) Mapping the voltage response using ordinary kriging (geostatistical inferences), (5) Localization of the causative sources in the block.

MATLAB is a registered trademark of The MathWorks, Inc.

The forward modeling generated synthetic seismograms and electrograms corresponding to simulated fracking events, while the inverse modeling did the opposite: the inverted simulations calculated all of the possible parameters of the fracking events from the synthetic sensor data. The differences between the forward and inverted results narrowed with repeated adjustments and iterations until a match was obtained.

The next step was to determine how well all of this corresponded to reality. The team designed a laboratory experiment in which they would repeatedly hydraulically fracture a porous cement cube by pumping in saline water under high pressure. The purpose was to see if electric signals could be passively recorded and then inverted to pinpoint the positions of actual fluid leakages over time. They drilled several 10-mm-diameter holes, or "wells," at varying depths in the 30.5 × 30.5 × 27.5 cm cube (see Figure 1).

Various ways to seal the well bores were tested, and stainless steel tubing with a 9.5 mm outside diameter was placed into the holes to simulate well casing. The cube was instrumented with 32 nonpolarizing silver/silver chloride electrodes for voltage measurement, 16 each on the top and one side of the block, plus six acoustic emission sensors mounted on three sides (see Figure 2).

Experiments Validated the Simulations

During the tests, electrical signals were detected that corresponded to fluid leaks along the well seal (see Figure 3), as were bursts of acoustic emissions and fluid pressure changes.

"We used a two-step process to invert the electrical data to pinpoint the position of these leaks," Revil said. "First, we applied a deterministic least-square algorithm to retrieve the source current density at a given point in the block at a given time. Then, we used a genetic algorithm, or probability sampling, to refine the position of the source current density.

"The results of the inversion were in excellent agreement with the location of the wells in question, and also with the acoustic emissions in the vicinity of the wells," he said. "This showed us definitively that passively recorded electric signals can be used to monitor fluid flow along wells during leakages. It also suggests they might be able to monitor fluid flow in numerous other applications that involve hydromechanical disturbances."

The Next Step: Field Trials

The next step is to develop field trials to investigate this technique further, from a few meters to several kilometers in scale.

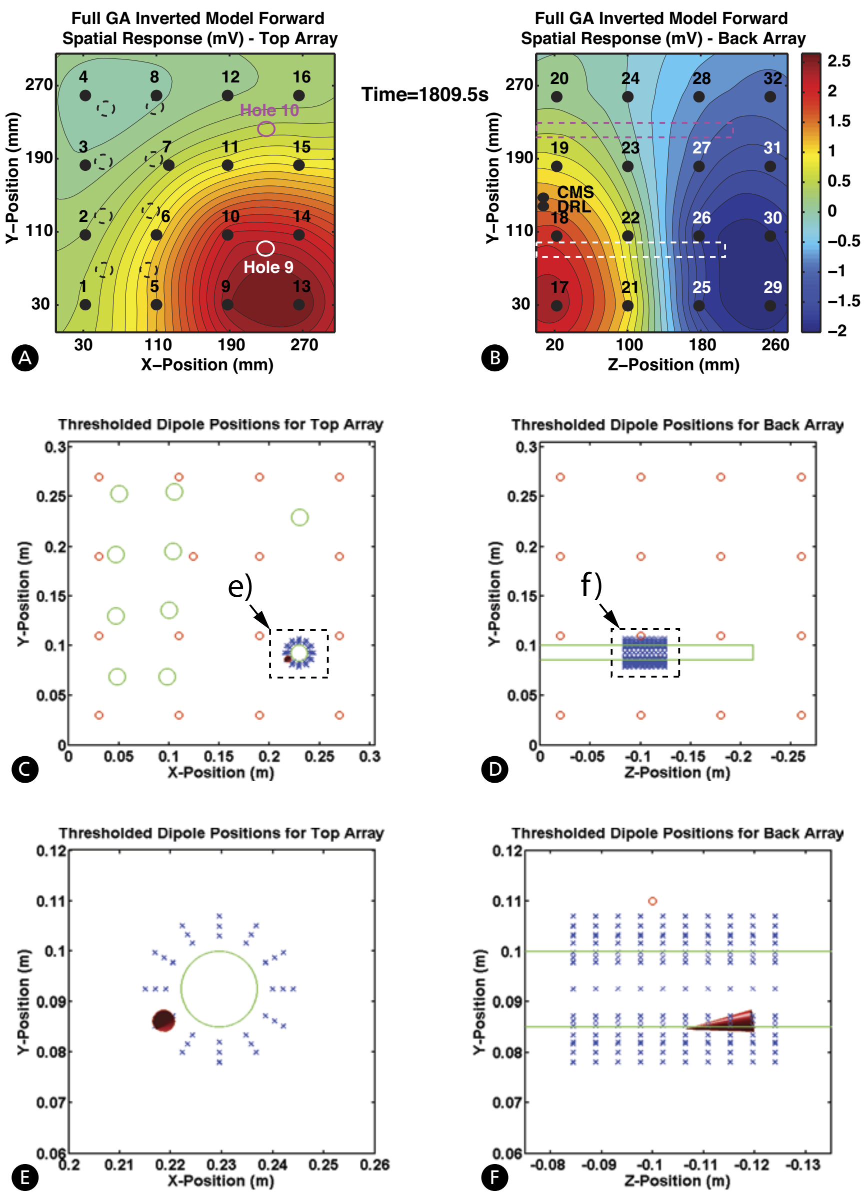


FIGURE 3: Forward-modeled voltage distribution of a dipole for one event (a and b), Spatial location of the dipole within the concrete block (c and d), Close-up of the dipole location (e and f), showing an off-vertical orientation of the dipole moment.

If all goes well, long-sought solutions to important problems may be at hand, such as development of aquifer monitoring and safety systems; better ways to assess the integrity of old, plugged, and abandoned wells; and perhaps even the ability to characterize fractured rock systems via the movement of the fluids within them.

The ultimate goal, said Revil, is to combine the electric data with pressure and acoustic data for a fully integrated analytical capability.

"That level of data fusion has never been done before," he said. "It is a tremendously exciting time to be working in this area." ■

Veryst Engineering, Needham Heights, MA, USA
Massachusetts General Hospital, Boston, MA, USA

Modeling Inertial Focusing in Straight and Curved Microfluidic Channels

Researchers from Massachusetts General Hospital and Veryst are using multiphysics analysis to investigate the microfluidic process of inertial focusing.

BY JOSEPH MARTEL AND MEHMET TONER OF BIOMEMS RESOURCE CENTER, MASSACHUSETTS GENERAL HOSPITAL, AND NAGI ELABBASI, DAVID QUINN, AND JORGEN BERGSTROM, VERYST ENGINEERING

In many medical procedures and tests it is necessary to isolate cells of interest for further analysis. Microfluidics has revolutionized the way in which these tests are conducted. One of the most promising microfluidic techniques to separate and concentrate cells of interest is called inertial focusing. Originally discovered in the 1960s, the phenomenon of inertial focusing found new utility in microfluidics, and in particular biomedical device design, recently playing a key role in a device enabling the ability to detect cancer from a blood sample. The phenomenon is characterized by suspended particles in a flow spontaneously migrating across streamlines to equilibrium positions within a channel cross-section, where they continue to flow in an ordered formation. By changing the geometry of the channel it is possible to control the equilibrium positions of particles of different sizes.

This phenomenon occurs when the particle Reynolds number, ReP, is approximately equal to 1 and is due to the balance of two forces; a shear gradient lift force directed towards the walls of the channel and a wall-interaction force directed away from each wall. The balance of these two forces determines the equilibrium position (see Figure 1). In a straight channel with a rectangular cross-section this leads to a pair of equilibria centered on the long faces of the channel as shown in Figure 2A. The addition of curvature to the channel changes the resulting force on the particles thus altering the equilibrium positions. A secondary transverse flow occurs across the channel due to the momentum of the faster moving fluid in the center of the channel, which induces a drag force on the particles and thus adjusts their equilibrium positions, as depicted in Figure 2B. The strength of this secondary flow depends on the curvature of the channel and is characterized by the non-dimensional Dean number, De. The equilibrium positions for a particle in curved channel flows are consequently a function of the channel dimensions, particle size, particle and channel Reynolds numbers, and Dean number.

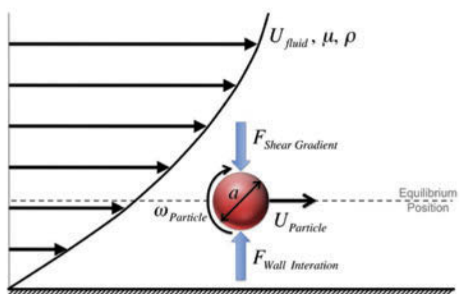


FIGURE 1: Basic forces acting on a particle in a microchannel.

The CFD Model

We developed CFD models in COMSOL Multiphysics to predict the equilibrium locations of the particles and their variation with flow and geometry parameters. To simplify the model and reduce solution time the analysis was divided into two steps. In the first step, we solve a CFD problem that does not include the particle. This gives the standard Hagen-Poiseuille flow solution for straight channels and the Dean flow solution for curved channels. We then map this solution to the inlet boundary of a second CFD model with the particle represented as a void in the CFD domain, with appropriate moving wall conditions to account for the translation and rotation of the particle. Both CFD models were parameterized to facilitate the investigation of the effect of flow and geometry parameters.

The reaction forces and moments on the particle are calculated from the CFD solution and are used to update the particle's translational and rotational velocity components. To accomplish this, we set up global ordinary differential equations (ODEs) specifying the equilibrium of the particle in terms of its linear and angular velocities.

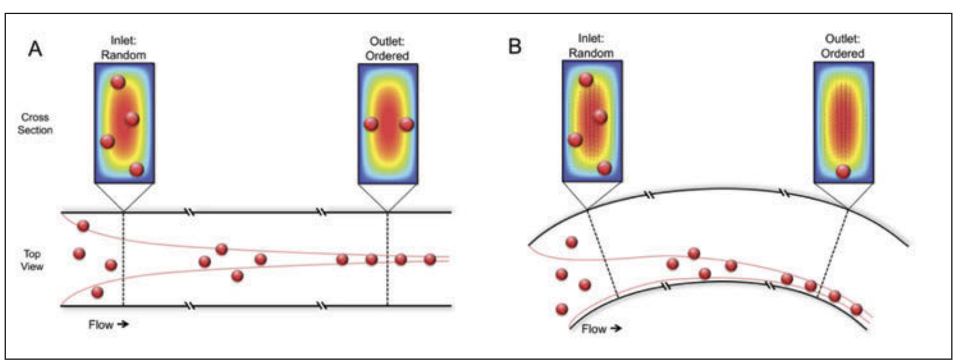


FIGURE 2: Effect of inertial focusing in straight (A) and curved (B) channels. Particles are randomly introduced but become ordered due to inertial focusing, as shown in the cross-section images.

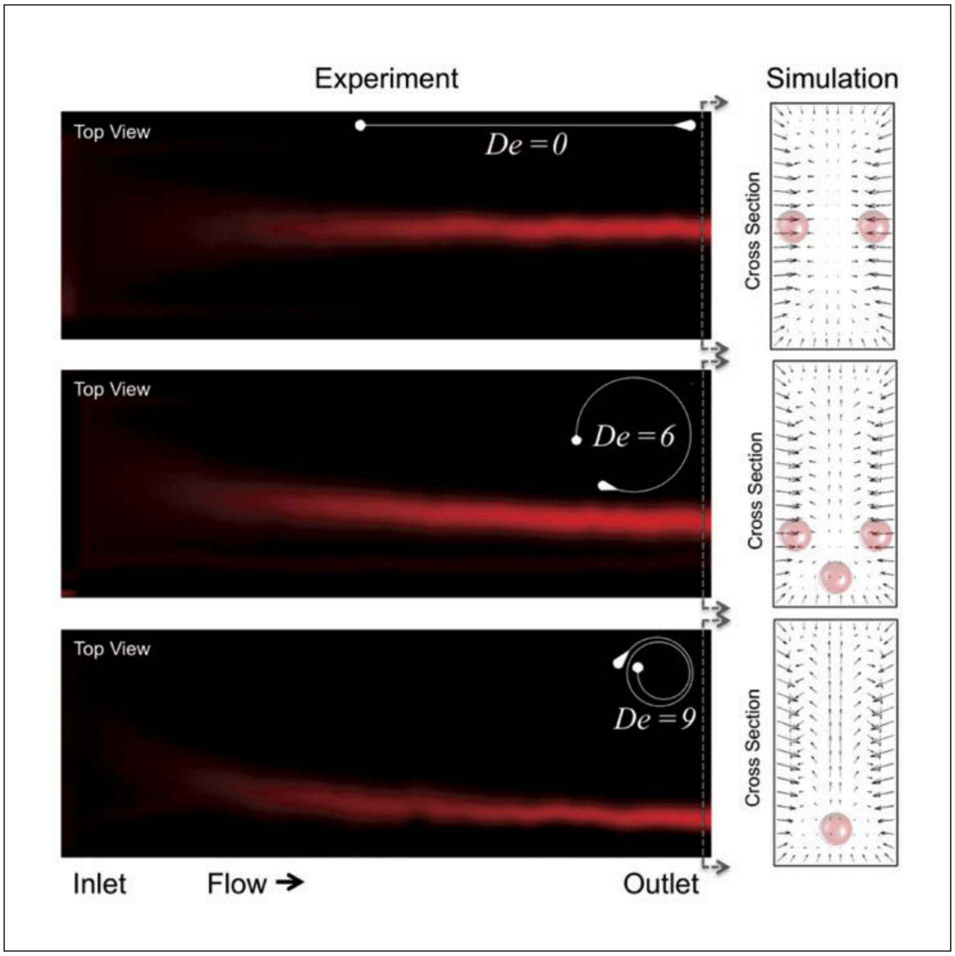


FIGURE 3: Experimental fluorescent microscope images (left) of the longitudinal section of the microchannels showing the distribution of particles along the channel. The cross-section plots (right) show the simulated resultant forces on the particles. The simulated equilibrium positions are marked by the particles and they closely match the experimental results. The data is shown for the same Reynolds number in three microfluidic devices of different curvatures. The curvature of the device is indicated in the inset seen in the upper right corner of the fluorescent images.

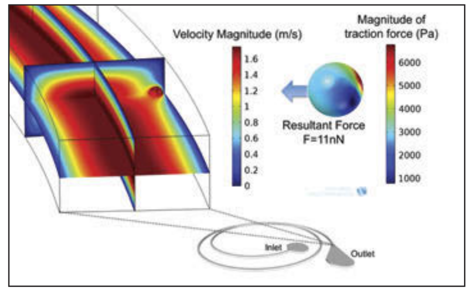


FIGURE 4: Velocity profiles (left) and surface tractions (right) on a particle at a specific non-equilibrium position.

COMSOL Multiphysics solves these global equations simultaneously with the fluid dynamics equations, which significantly speeds up the solution process. Solution time is also improved via the COMSOL Multiphysics unique capability to automatically evaluate the coupling terms between the fluid variables and the global variables in the Jacobian matrix.

After finding the rotational and translational velocities of the particle that are in equilibrium with the surrounding fluid, the transverse inertial lift forces are calculated. We can then add the effect of the Dean flow, assuming Stokes drag on a particle and the Dean flow velocities obtained in the first model.

It is important to recognize that the solution approach described here is required in order to predict inertial focusing since standard particle tracing is not applicable. In a straight channel, for example, standard particle tracing will predict that a neutrally buoyant particle inserted at a specific location in the channel cross-section will remain at that location. There are no general analytical equations relating the forces and moments that govern inertial focusing to the fluid flow conditions obtained in the absence of the particle. We are, however, developing expressions for the forces and moments acting on particles based on the above CFD solution. We can then use the COMSOL Multiphysics particle tracing capabilities to predict particle motion, including rotation, and inertial focusing by applying the developed expressions as user-defined force and moment equations.

Validation and Results

The model was first validated against the established solution for straight channel flow in a 50 µm square cross-section channel. In this case, the equilibrium particle positions are known to be centered on each face of the square and 10 µm away from the walls for a 10 µm diameter particle at a channel Reynolds number of 20.

We then compared the CFD model predictions to experimental measurements for both straight and curved channels that are 50 µm tall, 100 µm wide and 4 cm long. Figure 3 shows experimental and simulation results for a channel Reynolds number of 100 and three Dean numbers: 0, 6 and 9 (the channel is straight when the Dean number is zero). For each case, we show the particle distribution along the channel length collected using fluorescent streak microscopy and the force field calculated for that cross-section with the equilibrium positions (net force = 0) highlighted. The simulation results are in good agreement with experimental measurements for all three cases, and illustrate the dependence of the equilibrium positions on the channel curvature. Figure 4 shows the velocity in the channel and surface tractions on the particle for one channel/particle configuration where the force is dominated by the wall-particle interaction.

The ability to rapidly iterate through design changes in COMSOL Multiphysics and build a comprehensive theory for the operation of such devices will save experimental time as well as guide the design and optimization of our life-saving diagnostic devices. ■

Sonar Dome Vibration Analysis

Scientists at INSEAN, The Italian Ship Model Basin, have developed a way to calculate the effects of turbulent boundary layer flow on a bulbous bow housing sonar system with an easy-to-use simulation model to reduce self-noise.

BY JENNIFER HAND

A bulbous bow, the protruding bulb that sits below the waterline at the front of a vessel, has become a standard design feature in large ships. It significantly reduces wave resistance when traveling long distances at a speed near to maximum capacity, resulting in more stability and fuel efficiency.

In recent years there has been a move towards utilizing the bulbous bow to house different types of sonar system but there are questions about the extent to which structural vibration interferes with the functioning of the transducer array inside such a sonar dome. In particular, the pressure fluctuation that arises from the turbulent boundary layer (TBL), a thin layer of fluid where gradient of velocity and the resulting shear stress magnitudes are much higher than in the laminar case, is thought to be one of the major causes of self-noise for on-board sensors. A team from INSEAN therefore set out to investigate.

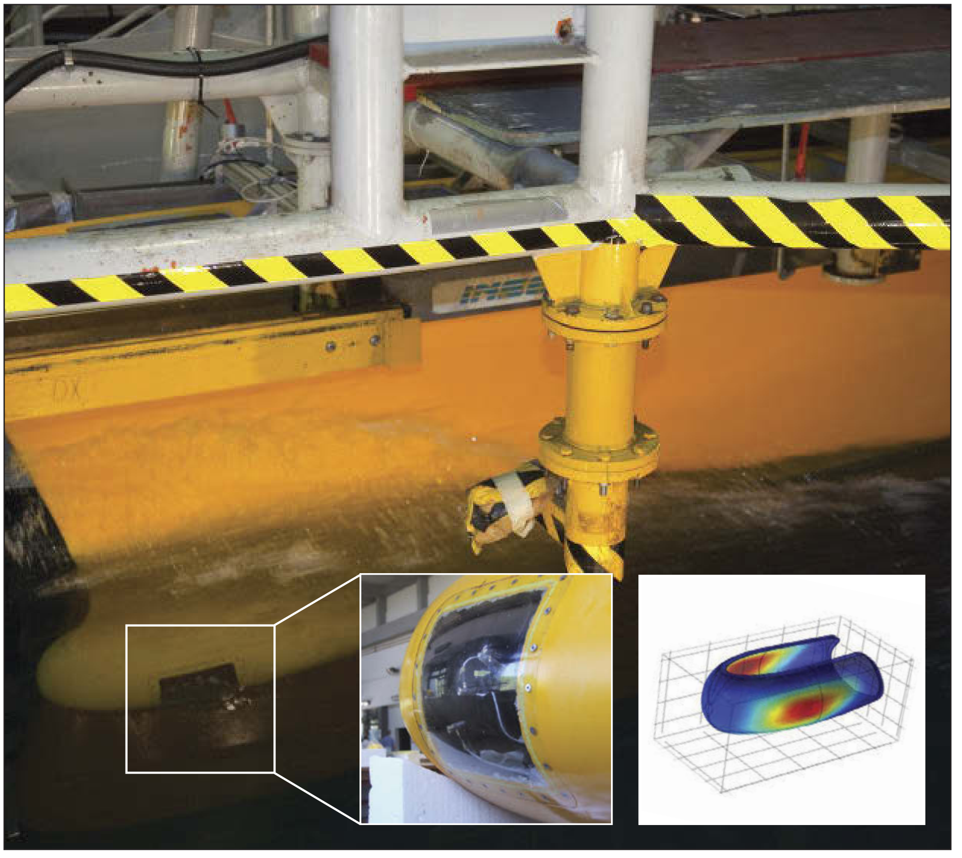


FIGURE 1: Experimental campaign on a 1:8 scaled model of the bulbous bow. A section of the bulbous bow has been substituted with a transparent material on which accelerometers have been placed (bottom middle). The simulation shows the system's structural response (bottom right).

Testing a Scale Model

Francesca Magionesi, a researcher at INSEAN, explains: "Most existing research on wall pressure fluctuation has been done using simple geometries and ideal flow conditions that do not take into account the free flow of water over a complex curvature. So our first aim was to understand the frequency spectra of wall pressure fluctuations induced by the turbulent boundary layer acting on a bulbous bow."

This was done by building a large-scale model bulbous bow that was rigid and conducting an experiment to characterize wall pressure fluctuations within one of the two towing tanks at INSEAN. "This was tricky not only because of the effects of structural curvature and fluid loads but also because we had to capture the higher frequency component of pressure fluctuations using miniaturized pressure transducers," reports Magionesi. Despite this, the team managed to measure wall pressure fluctuations at different locations along the bulbous bow and model these loads in terms of auto and cross spectral densities.

In a second experiment the researchers substituted a section of the bulbous bow with an elastic linear material (a transparent polymethyl methacrylate, PMMA, thermoplastic) and obtained its structural response (see Figure 1).

The team then turned to simulation to replicate the results of the physical testing.

"To evaluate the dynamical response of an elastic structure to the turbulent boundary layer load it would normally be necessary to use direct numerical simulation of the fluid flow coupled with a structural code," explains Magionesi. "But the high Reynolds number typical of a real naval application makes this approach impossible because of the tremendous computational time and

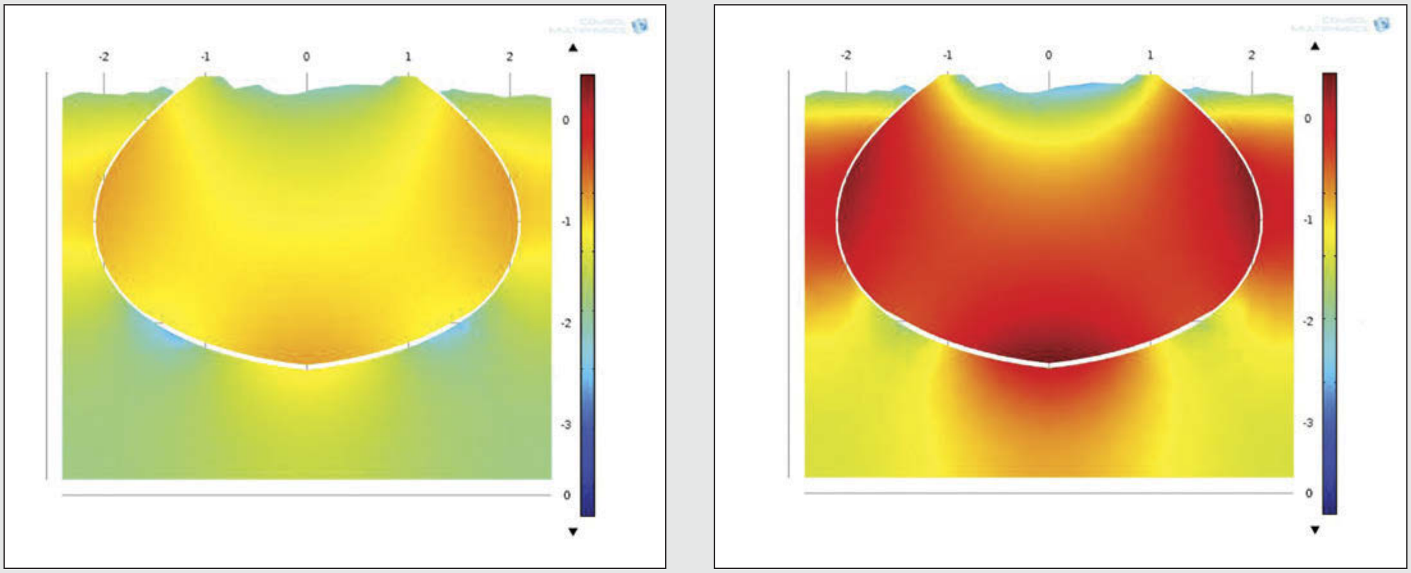


FIGURE 2: Sound pressure level at a cross section of the 3D bulbous bow simulation for a cruise velocity of 15 knots (left) and 30 knots (right).

memory requirement. We therefore developed a simplified expression of the fluid load, based on a weak coupling between fluid and structure, which assumes that structural vibration would not affect fluid excitation, and a simplified fluid load expression. In this way we validated the experimental-numerical procedure at scale model level."

> "In order to predict the noise and vibration caused by the flow of water interacting with the structure of the bow, we tested at different velocities using the structural, fluid and acoustic domains."

Simulating at Full Size

The next stage was to create a full-scale model within COMSOL Multiphysics, which would take into account the complexity of the composite material used for the bulbous bow. The results of an in-house program, a code that solves the Reynolds Averaged Navier-Stokes (RANS) equations, allowed the team to rescale the wall pressure fluctuations measured on the small model and obtain full-scale excitation data at relatively low computational cost. These data were used as input for COMSOL Multiphysics and inserted as a pressure load in the numerical model (see Figure 2).

"Livelink™ *for* Pro/ENGINEER® enabled us to bring CAD data for the different parts of the bulbous bow into COMSOL Multiphysics," explains Magionesi. "Because this data had not been developed for finite element analysis we had to improve the quality in certain places, particularly with regard to the different thicknesses of the bow wall. We really appreciated the flexibility to carry out these small changes directly within COMSOL Multiphysics. Another reason we like the software is the capacity to analyze any number of physics in one unified package. In order to predict the noise and vibration caused by the flow of water interacting with the structure of the bow, we tested at different velocities using the structural, fluid and acoustic domains. That was really important because it gave us the opportunity to insert governing equations directly."

The team later used COMSOL Multiphysics LiveLink™ *for* MATLAB® to move their homemade code over to MATLAB®.

An Easy-to-Use Tool for Complex Systems

According to Magionesi the most important achievement is an easy-to-use tool with which to evaluate the noise and vibration level induced by turbulent boundary layer load at full scale, i.e. with a high Reynolds number. "Yet we only had to perform the experiment with a small model scale that captured turbulent boundary layer excitation," she reflects.

"We also used COMSOL Multiphysics to ascertain the parametric qualities of materials. By varying the characteristics of these, we extended the scope of our tool beyond sonar sensors to the design of the bulbous bow itself so that we could address drag as well as vibration levels. Our research led us to create a multi–disciplinary tool for achieving global optimization of the bulbous bow sonar system at the design stage. Our aim now is to integrate this tool with other aspects of analysis and make it available for others to use." ■

MATLAB is a registered trademark of The MathWorks, Inc.
Pro/ENGINEER is a registered trademark of PTC Inc. or its subsidiaries in the U.S. and in other countries.

Highly Accurate Li-ion Battery Simulation

Due to the many physics involved and strong dependence on temperature, batteries are intrinsically nonlinear. A COMSOL Multiphysics simulation changes that equation, simplifies battery modeling, and brings these nonlinear aspects to light.

BY MIKAEL CUGNET, FRENCH ATOMIC AND ALTERNATIVE ENERGY COMMISSION (CEA)

Whether in cell phones, hybrid/electric vehicles, or airplanes, batteries have become virtually indispensable to modern life. Traditional means of evaluating battery performance with advanced chemistries such as lithium-ion don't provide sufficient information to allow researchers to better optimize them. Thus they are turning to simulation software to get a deeper understanding of what is going on inside the cells, information they can use in the design of batteries that are more reliable and safe.

EIS and ECM Methods Used Primarily Until Now

In vehicles, battery management systems (BMSs) are designed to protect the battery, predict vehicle range, and update the range prediction depending on driving conditions. These BMSs use circuit models often derived from electrochemical impedance spectroscopy (EIS), a widely used technique to characterize batteries. With readings from an EIS system, it is possible to construct an electronic component model (ECM) that consists of resistances and capacitors connected both in series and in parallel (see Figure 1, right). With the results from an ECM study (see Figure 1, left) you can, for instance, determine a battery's internal resistance, which in turn dictates how much energy it can deliver — is it good enough to propel a vehicle, enough to light up an emergency exit sign, or enough to power a cell phone? Some people attempt to get additional information from used batteries, but it is understandably difficult to do an accurate study on a burned-out battery.

With an ECM, you get component values that mix the contributions of various phenomena occurring in the cell. However, there is a gap between the meaning of the electrical components in the equivalent circuit models and the physical equations characterizing the batteries. In our case, an ECM does not provide any information about important cell properties like the electrode active material resistance, the reaction rate, the specific capacitance, and the diffusion coefficient. We can get this information from a multiphysics model.

Realistic Multiphysics Simulation

Rather than work with an equivalent circuit model, we at INES decided to create a physics-based model of a $LiFePO_4$/Li half cell. Its output is likewise a plot of impedance vs. frequency so we could compare its results to those of EIS measurements for verification. This model, though, gives us a great deal more information that we can use in the design of batteries that are more reliable and safe.

Because I am very familiar with the equations governing battery behavior, I built my own model from scratch in COMSOL Multiphysics to give me full control of all parameters and even deeper understanding from the simulation.

The physical battery model is a half cell in the shape of a button battery (see Figure 2). I need to study the half cell rather than a conventional battery in order to separate the electrodes and get a more precise evaluation of their physical properties; if I were to work with a complete cell, I would get a mix of all the phenomena occurring in each electrode without knowing to which electrode I should attribute the resulting parameter values.

The corresponding simulation actually consists of two coupled 1D models (see Figure 3). The first model represents the macroscopic level. It is made up of two domains: the working electrode, plus the separator between the iron-phosphate electrode and the lithium foil, which also serves as the counter-electrode (see Figure 3, left). The second model represents the microscopic level, which has only one domain. It models a spherical particle of iron phosphate, which is the main component of the working electrode's active material (see Figure 3, right).

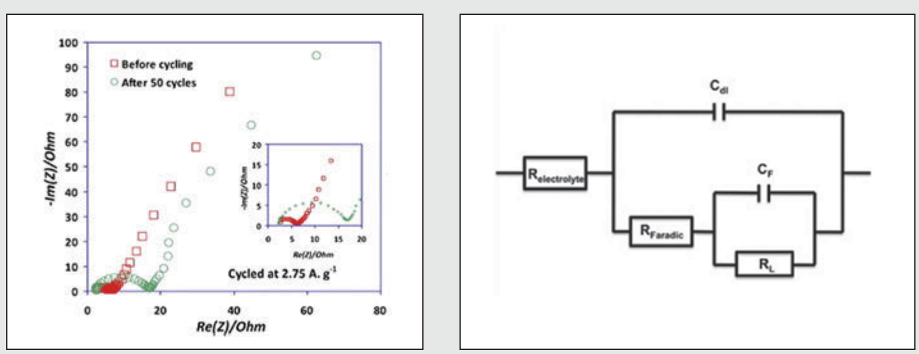


FIGURE 1: Using Electrochemical Impedance Spectroscopy (EIS), battery impedance is measured at a range of frequencies in the milliHertz to kiloHertz range. From this impedance plot (left), it is possible to construct an equivalent circuit model (right).

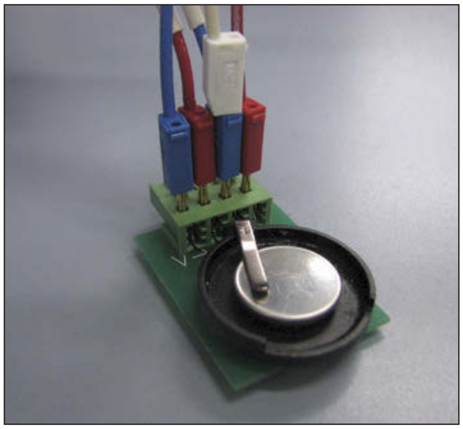


FIGURE 2: Half cell used as the basis for modeling and for verification.

Everything Done with PDEs Entered Through the GUI

Both models were created exclusively with partial differential equations (PDEs). The macroscopic model uses equations for the conservation of current for the electronically conducting solid phase, the conservation of current for the ionically conducting liquid phase, and the material balance on the salt $LiPF_6$ dissolved in the liquid phase. These three equations then couple into the microscopic model equation, which is Fick's Law characterizing solid-state diffusion of the reduced-lithium species in the particle.

All the model equations are time-dependent, so it is not possible to derive the impedances for the plot directly from the equations. Doing so would require that you assume they are linear, which I didn't want to do because they are in fact nonlinear and non-stationary. Next, I wanted to simulate how the system physically behaves when you stimulate it with sine waves of various frequencies. Thus it is necessary to run the model at each sinusoidal-excitation frequency and read the results. I measure 6 points per decade from 10 mHz to 200 kHz, and the total simulation run takes 15 minutes. To run the model for each frequency we saved the model as an M-file readable by MATLAB®. We then ran LiveLink™ *for* MATLAB® to process the results to get the full impedance spectrum of the half-cell.

The inputs to the model are the cell's state of charge, set to 100%; the magnitude of the sinusoidal excitation voltage (7.1 mV centered around the cell's equilibrium potential of 3.490V); and the frequency of the excitation (from 10 mHz to 200 kHz). The model outputs are the cell current in response to the excitation voltage, the potentials in the electronically conducting solid phase and ionically conducting liquid phase, and the concentration of lithium ions in the solid phase (with the microscopic model) and the liquid phase (with the macroscopic model).

The Importance of the Electric Double Layer

One feature of COMSOL Multiphysics that proved essential was the electrical double layer (EDL). In all Li-ion battery models in the literature, the current density localized at the interface between the particle surface and the liquid includes only the Butler-Volmer equation for electrode kinetics. Despite the use of this equation, the semicircle at the left of Figure 4 characterizing charge transfer does not appear because such models cannot predict it. This happens because all the PDEs in the model behave like a pure resistance at frequencies higher than 10 Hz. However, things change when you add the EDL because you add a capacitive component in addition to the reaction rate equation. This somewhat corresponds to a capacitor connected in parallel to a resistance. Since I wanted to accurately mimic what happens in my half cell, I added this component in the PDEs in order to take EDL into account.

Figure 4 shows the optimized values of some key parameters I was able to identify at specific frequencies. First, I did a sensitivity analysis of my model for those specific frequencies, which means I investigated the impact of the variation of my model parameter values on the impedance. Then I found out that for each frequency I had to adjust a specific parameter in order to get a good match with my experimental data. Finally, to get those optimized values, I wrote a MATLAB® program using an optimization function coming from the Optimization Toolbox coupled with my simulation from COMSOL Multiphysics. It is important to get those optimized values because they provide information on the value of critical cell properties, such as the active material resistance, reaction rate, EDL capacitance and diffusivity of ions.

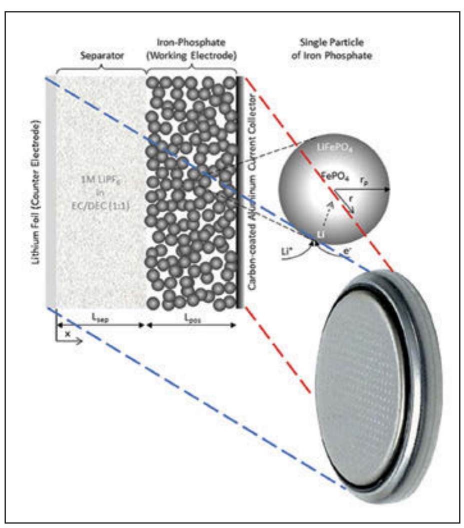


FIGURE 3: Modeling of the half cell at macroscopic (left) and microscopic (right) level.

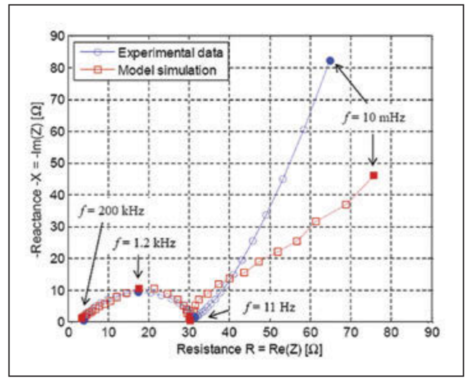


FIGURE 4: EDL allowed for a perfect agreement between simulation results at high frequencies.

Taking the Next Step Towards a Better Understanding of Batteries

Our simulation results are useful for obtaining some critical physical values. Specifically, at this stage I can clearly see that the active material used in my electrode indeed has poor electronic conductivity. I can also see that the capacitive behavior of the cell is far from being negligible at frequencies higher than 10 Hz. This means that the EDL must be taken into account if you want to model the cell behavior during pulse operation or specific usage profiles. In terms of resistance, the weakest part has been identified as the charge transfer resistance resulting from the reaction rate.

In the impedance spectrum, you might notice that the curves at low frequencies (right side) deviate somewhat. This shows what happens because the active material particle scale is not well described in our approach. We do not yet know what is responsible for this effect — perhaps a missing phenomenon somewhere in the model, or some parameter values must be adjusted. This is the focus of our current work. ■

MATLAB is a registered trademark of The MathWorks, Inc.

Understanding the Origin of Uncertainty in Thermometer Calibration

Researchers are using simulation to improve calibration of temperature sensors.

BY JENNIFER HAND

Thermometers have widespread application ranging from their role in measuring temperature in common consumer goods to integration in sophisticated medical and industrial technology or processes. Like any measurement device, they must be calibrated with the International Temperature Scale of 1990 (ITS-90).

The Calibration Process

ITS-90 is based on fixed points at which a pure metal changes its phase by melting or freezing. During the phase change process heat is either absorbed or released by the metal without changing its temperature. At a fixed-point, a thermometer immersed in it observes a temperature plateau that can be used as a practical reference.

Jonathan Pearce, who leads contact thermometry at the UK's National Physical Laboratory, explains: "The ITS-90 is disseminated to users with the standard platinum resistance thermometer. This is a very sensitive device capable of measuring temperatures with a precision of the order of a microkelvin."

The platinum resistance thermometer calibrates using a fixed-point cell. This is typically a graphite crucible, which is a container with a well running through its center for insertion of the thermometer (see Figure 1). In the container is a material of very high purity, typically 99.9999%. The central well allows a thermometer to be inserted so that the sensing element at its bottom is completely immersed in the fixed-point metal. The container is then placed in a furnace to allow controlled melting and freezing of the metal.

FIGURE 1: Cross-section of a typical fixed-point cell showing the graphite container, the metal ingot, and the central well for insertion of the thermometer.

Despite the high performance device, the uncertainty of temperature during calibration can still be in the order of 1 millikelvin. To better understand the microscopic behaviour, Pearce, working with Surrey University student Matthew Large, turned to COMSOL Multiphysics.

Simulating Morphological Instability

Freezing or solidification is much less well-behaved than melting. For example, some areas will solidify before others thus influencing the freezing temperature.

The simulation utilizing the phase-field method implemented in COMSOL Multiphysics provided the researches with fascinating insights: under certain conditions the liquid-solid interface is not planar at all; as freezing progresses, ripples become apparent at the interface. These become cells that begin to protrude outwards (see Figure 2) with their tips being at a significantly lower temperature than their roots. "This positive feedback loop is very interesting," says Pearce. "Although such an effect was predicted by Mullins and Sekerka in the 1960s, this is the first time we have observed its manifestation in this context. Our main objective was to simulate freezing behavior by investigating the effect of furnace settings on the process and identifying what the actual sensor used was measuring. The working model we ended up with is a very powerful means of understanding the influence of heat and mass flow on the evolution of the liquid-solid interface."

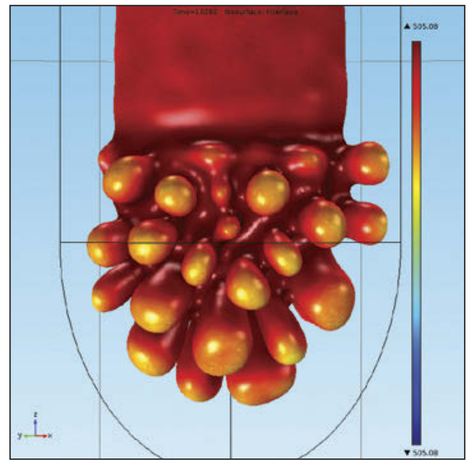


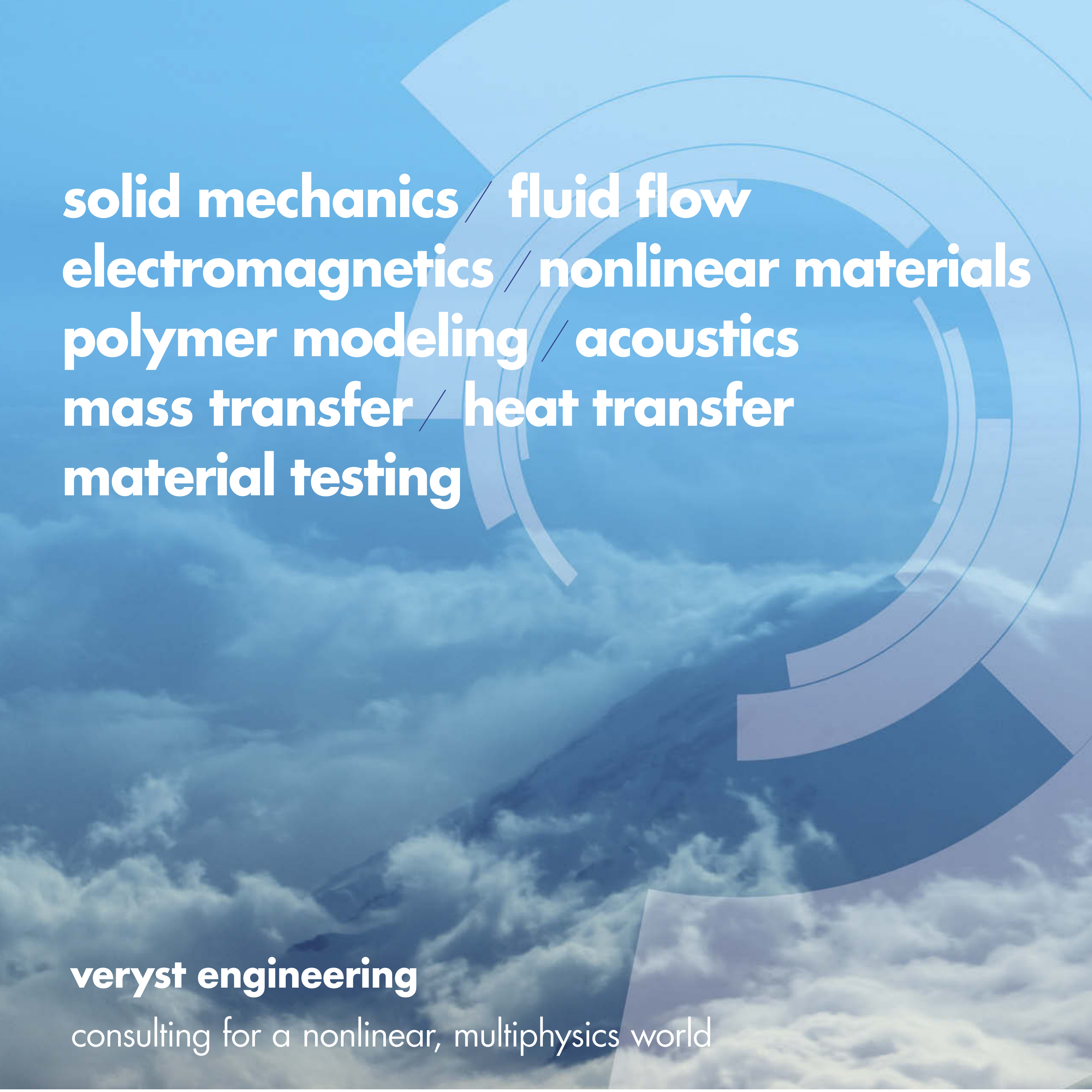
FIGURE 2: Morphological instability at the liquid-solid interface.

"The working model we ended up with is a very powerful means of understanding the influence of heat and mass flow on the evolution of the liquid-solid interface."

Through simulation, it is possible to identify specific behavior in a system that is difficult to observe experimentally and yet contributes to the overall uncertainty in a measurement. The information gained through simulation can be applied to a thoughtful re-design of the device ultimately improving measurement precision. ■

More Information

http://www.npl.co.uk/temperature-humidity/



Experienced COMSOL Multiphysics Consulting team using engineering fundamentals and modeling to solve complex industrial problems:
Biomedical / Consumer Products / Energy / Manufacturing / Transportation

Veryst Engineering, LLC / contact@veryst.com / 781-433-0433

COMSOL certified consultant

GUEST EDITORIAL

Engineering Analysis: From Slide Rules to Apps

BY JAMES D. FREELS, OAK RIDGE NATIONAL LABORATORY

As an undergraduate student, I completed one of the very last slide-rule courses. A few years later, a key event steered me toward computer simulation as a career goal. A senior-level laboratory experiment in our nuclear engineering department required us to alter a FORTRAN computer program that was provided to simulate a reactivity-induced power excursion of a research nuclear reactor. At that time, our computing environment consisted of punched-card readers interfaced to an IBM mainframe computer. In the final analysis, we "tweaked" certain reactivity coefficients and decay constants to try to match the output from our experiment, which was enabled as a set of data points from a strip chart recorder. Even at that time, and using what are now considered crude computational tools, I recognized that simulation was perhaps the greatest value offered by a computer.

During my full-time graduate school years, computer terminals evolved, and punch cards became scarce. After acoustic couplers, dial-up modems, and the passage of several years, the desktop personal computer replaced the terminal, but we still interfaced to the larger computers from our desktops. We were amazed as each stage of the computer evolution was made available to the practicing simulation engineering analyst. Indeed, I can well remember hallway discussions during which the statement was often made that "someday we will be able to solve time-dependent, Navier-Stokes equations in 3D right on our desktop computers."

In case you're not aware, that someday is now.

In the last several years, during this, the later portion of my engineering career, I have been fortunate enough to become an enthusiast of COMSOL Multiphysics. I often need to correct some of my colleagues when they describe COMSOL as a computational fluid dynamics or CFD resource. That oversimplification is far from accurate. In the past, I have described COMSOL as a "finite-element toolbox for engineering analysis." Perhaps a more appropriate short description of COMSOL would be a "high-level programming interface for multiphysics simulation." Even these broad definitions do not begin to encompass all the possible methods and applications COMSOL is capable of.

I have certainly had an advantage in using and appreciating COMSOL because my graduate work involved using finite-element methods with CFD simulations. Further, over the years I have been fortunate to be teamed with many enthusiasts in the field of engineering analysis. Indeed, some of us dreamed of building a code system similar to COMSOL, though we came up short of our goals. The old adage, "If you can't beat 'em, join 'em," certainly rings true with me, and with great enthusiasm. What I particularly enjoy now is helping others use COMSOL, young and old alike. In particular, younger engineering analysts have readily accepted this new technology.

Therefore, the announcement at the most recent COMSOL Conference of the future release of low-cost, problem-specific physics builder "apps" should be a winner.

As slide rules are now a collector's item and pocket calculators are as common as any off-the-shelf commodity, perhaps the COMSOL app will also be a resource available to many practicing engineering analysts in the near future. ■

"What I particularly enjoy now is helping others use COMSOL, young and old alike."

JAMES D. FREELS is a senior research staff member with Oak Ridge National Laboratory's Neutron Science Directorate, in the Research Reactors Division, working with the High Flux Isotope Reactor. He holds B.S. (1977) and M.S. (1979) degrees in nuclear engineering, and a Ph.D. (1992) in engineering science and mechanics, all from the University of Tennessee, Knoxville. His primary professional interests are computer simulation, computational fluid dynamics, heat transfer, and systems transient analysis. In addition to his activities with COMSOL and finite-element analysis, he has a strong interest and experience base in the Linux operating system and related installed software.