

# COMSOL NEWS

THE MULTIPHYSICS SIMULATION MAGAZINE

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## Verify, Optimize, Revolutionize: Multiphysics Simulation Delivers Innovative Design Solutions

This year's issue of COMSOL News provides you with a front row seat to show how multiphysics simulation is advancing product development. Engineers and researchers strive to stay ahead of the game by employing innovative design solutions that result in reduced cost and increased revenues while providing safer and better products. But how do they do it?

You may have identified the familiar Boeing 787 Dreamliner featured on the cover. For this innovative jet airliner comprised of more than 50 percent carbon fiber reinforced plastic, engineers at Boeing used multiphysics simulation to investigate and verify thermal expansion in composite materials with expanded metal foil for lightning strike protection. Boston Scientific engineers are revolutionizing medical device design by gaining the knowledge required to control the underlying release mechanism of drug-eluting stents. Simulation provided vital optimization and design guidance to NASA engineers involved in the development of life support systems providing breathable air and drinkable water for astronauts.

These are just a few highlights of the many successes achieved by the engineers and researchers relying on the power and accuracy of multiphysics simulation. From lab-on-a-chip to building physics, to MEMS & robotics and containerless processing, there are plenty of exciting projects you can read about.

It's been an honor to work with the talented engineers, researchers, and designers featured in the articles and it is my pleasure to bring you this edition of COMSOL News, the multiphysics simulation magazine.

Enjoy your reading,



Valerio Marra

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"787-8 Flying Over Oregon Coast" from [www.boeingimages.com](http://www.boeingimages.com).

## COMSOL NEWS

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# She Created the Future.

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



Fluid-Screen (formerly Alpha-Screen) brings the functionality of a lab to a small portable device that fits in the palm of your hand and detects bacteria from blood and water in less than 30 minutes. Fluid-Screen uses a patented electric field and biosensor technology to rapidly collect and detect bacteria.

*"After being honored with the 2011 Create the Future Design Contest Grand Prize, the funding and publicity from the award was instrumental in helping us speed up the development of Fluid-Screen and make a working beta prototype," says Monika Weber, Founder and CEO of Integrated Microfluidic Devices.*

Fluid-Screen product test series will be launched in 2015 and enter the market in 2016.

## Now it's Your Turn.

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# Boeing Simulates Thermal Expansion in Composites with Expanded Metal Foil for Lightning Protection of Aircraft Structures

Modern aircraft such as the Boeing 787 Dreamliner are comprised of more than fifty percent carbon fiber composite requiring the addition of expanded metal foil for lightning strike protection. Researchers at Boeing are using simulation to verify that protective coatings on the metal foil will not fail due to thermal stress arising from a typical flight cycle.

BY JENNIFER A. SEGUI

The Boeing 787 Dreamliner is innovative in that it is comprised of more than fifty percent carbon fiber reinforced plastic (CFRP) due to the material's light weight and exceptional strength. Figure 1 shows the extensive use of composite materials throughout the aircraft. Although CFRP composites

inherently have many advantages, they cannot mitigate the potentially damaging electromagnetic effects from a lightning strike. To solve this problem, electrically conductive expanded metal foil (EMF) can be added to the composite structure layup to rapidly dissipate excessive current

and heat for lightning protection of CFRP in aircraft.

Engineers at Boeing Research and Technology (BR&T) are using multiphysics simulation and physical measurements to investigate the effect of the EMF design parameters on thermal stress and displacement



FIGURE 1. Advanced composites used throughout the Boeing 787 account for more than fifty percent of the aircraft body<sup>1</sup>.

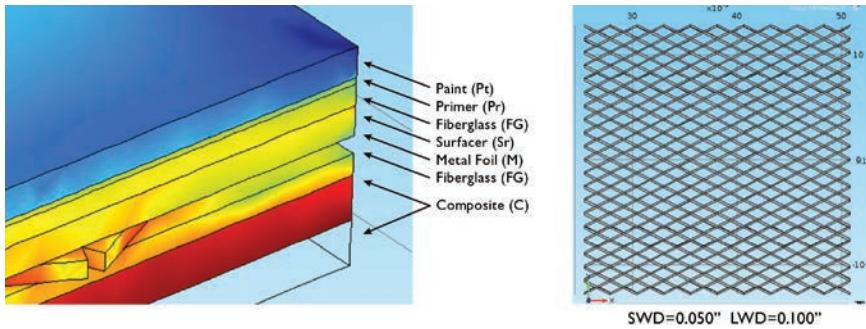


FIGURE 2. At left is the composite structure layout from the COMSOL model and, at right, the geometry of the expanded metal foil. SWD and LWD correspond to short way of the diamond and long way of the diamond. The mesh aspect ratio: SWD/LWD is one of the parameters varied in the simulations.

in each layer of the composite structure layout shown at left in Figure 2. Stress accumulates in the protective coating of the composite structure as a result of thermal cycling due to the typical ground-to-air flight cycle. Over time, the protective coating may crack providing an entrance for moisture and environmental species that can cause corrosion of the EMF, thereby reducing its electrical conductivity and ability to perform its protective function.

Contributing to the research effort at BR&T are project lead Jeffrey Morgan from Sealants and Electromagnetic Materials, Associate Technical Fellow Robert Greigor from Applied Physics leading the simulation, Dr. Patrice Ackerman from Sealants and Electromagnetic Materials leading the testing, and Technical Fellow Quynhgioa Le. Through their research, they aim to improve overall thermal stability in the composite structure and therefore reduce the risks and maintenance costs associated with damage to the protective coating.

### SIMULATING THERMAL EXPANSION IN AIRCRAFT COMPOSITES

In the surface protection scheme shown at left in Figure 2, each layer including the paint, primer, corrosion isolation layer, surfacer, EMF, and the underlying composite structure contribute to the buildup of mechanical stress in the protective coatings over time as they are subject to thermal cycling. The geometry in the figure is from the coefficient of thermal expansion (CTE) model developed by Greigor<sup>2,3</sup> and his

colleagues using COMSOL Multiphysics® in order to evaluate the thermal stress and displacement in each layer of a one-inch square sample of the composite structure layout.

The structure of the EMF layer is shown at right in Figure 2. In this study, the EMF height, width of the mesh wire, aspect ratio, metallic composition, and surface layout structure were varied to evaluate their impact on thermal performance throughout the entire structure. The metallic composition of the EMF was either aluminum or copper where an aluminum EMF requires additional fiberglass between the EMF and

the composite to prevent galvanic corrosion.

The material properties for each layer including the coefficient of thermal expansion, heat capacity, density, thermal conductivity, Young's modulus, and Poisson's ratio were added to the COMSOL model as custom-defined values and are summarized in Figure 3. The coefficient of thermal expansion of the paint layer is defined by a step function that represents the abrupt change in thermal expansion at the glass transition temperature of the material.

In the CTE model, the Thermal Stress multiphysics interface couples solid mechanics with heat transfer to simulate thermal expansion and solve for the displacement throughout the structure. The simulations were confined to heating of the composite structure layout as experienced upon descent in an aircraft where final and initial temperatures were defined in the model to represent the ground and altitude temperatures, respectively.

### IMPACT OF EMF ON STRESS AND DISPLACEMENT

The results of the COMSOL simulations were analyzed to quantitatively determine the stress and displacement in each layer upon heating and for

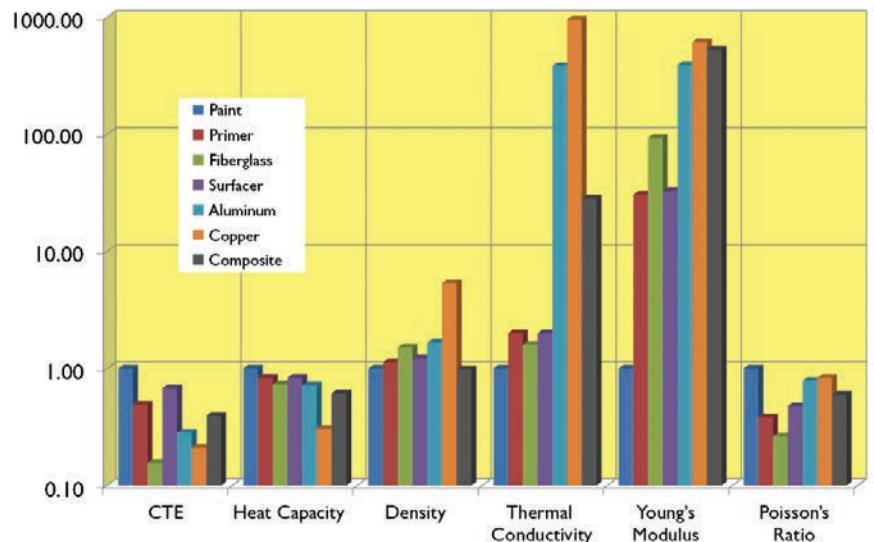
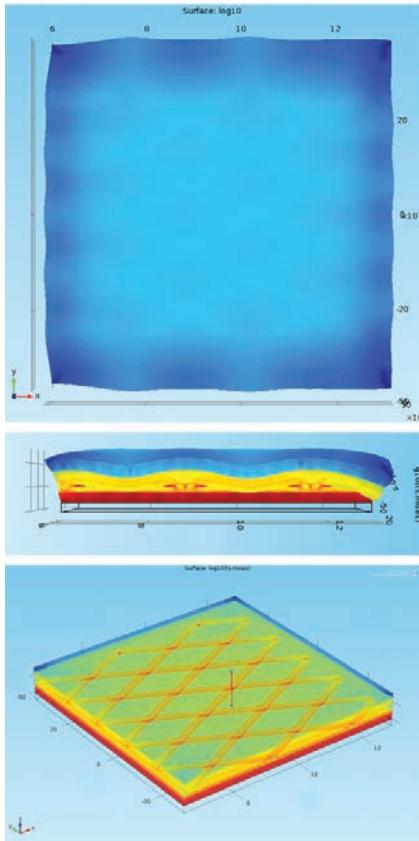


FIGURE 3. Ratio of each material parameter relative to the paint layer. The paint layer shows higher values of CTE, heat capacity, and Poisson's ratio indicating that it will undergo compressive stress and tensile strain upon heating and cooling.



**FIGURE 4.** Top, middle: top-down and cross-sectional views of the von Mises stress and displacement in a one-inch square sample of a composite structure layout. At bottom, transparency was used to show the high stress in the composite structure and EMF. Stress was evaluated along the vertical line extending through the depth of the sample.

varied properties of the expanded metal foil. An example of the simulation results is shown in Figure 4.

Through the paint layer at the top of Figure 4, it is possible to observe the displacement pattern of the underlying EMF. The magnified cross-sectional view clearly shows the variations in displacement above the mesh and voids in addition to the trend in stress reduction in the uppermost protective layers. Figure 5 shows the relative stress for each layer in surface protective schemes that incorporate either copper or aluminum EMF. The fiberglass corrosion isolation layer required by the aluminum EMF acts as a buffer, causing the stress to be lower in the aluminum than it is in the copper EMF.

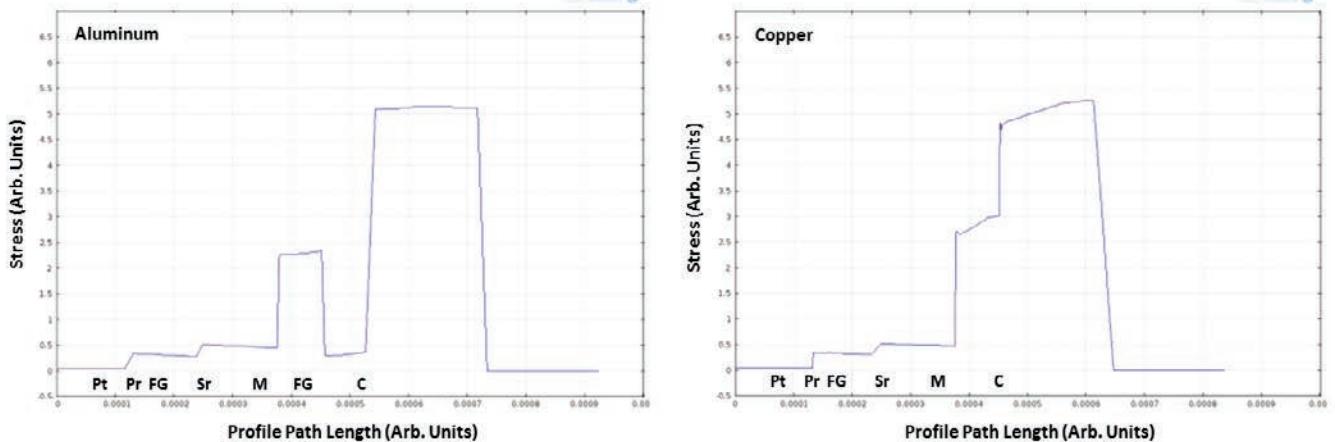
Despite the lower stress in the aluminum EMF, simulation results from the variation of the EMF design parameters reveal a consistent trend toward higher displacements in the surface protective scheme with the aluminum EMF when compared to copper. The larger displacements generally caused by the aluminum EMF can be attributed, in part, to the relatively higher CTE of aluminum.

Further analysis of the impact of the EMF design parameters was performed to confirm the effect of varying the height, width, and mesh aspect ratio on displacement in the protective layers. When varying the mesh aspect ratio, it was found that an increased ratio led to a modest decrease in displacement of about 2 percent for both copper and aluminum EMF, where higher ratio

“Increasing the mesh width or decreasing the aspect ratio are better strategies for increasing the current carrying capacity of the EMF for lightning strike protection.”

values correspond to a more open mesh structure. For any EMF design parameter, there is a trade-off between current carrying capacity, displacement, and weight. In the case of mesh aspect ratio, while choosing an open mesh structure can reduce displacement and weight, the current carrying capacity that is critical to the protective function of the EMF is reduced as well and needs to be taken into account.

Similarly with regard to the mesh width, varying the width by a factor of three led to a relatively minor increase in displacement of about 3 percent for both copper and aluminum EMF. However, varying the height of the EMF by a factor of four led to an increase in displacement of approximately 60 percent for both aluminum and copper. Figure 6 shows the relative values for displacement through each layer of the surface protection scheme for varied height of copper and aluminum EMF. Due to the lower impact on



**FIGURE 5.** Relative stress in arbitrary units was plotted through the depth of the composite structure layouts containing either aluminum (left) or copper EMF (right).

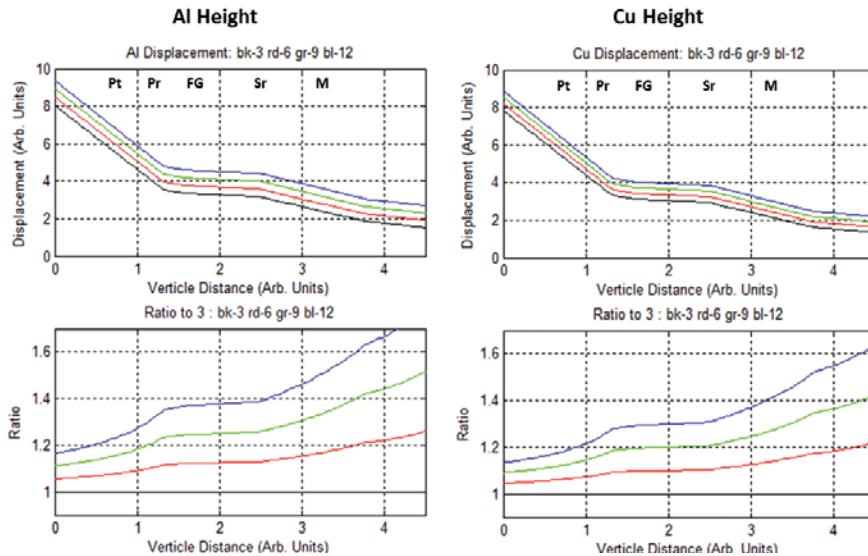


FIGURE 6. Effect of varying the EMF height on displacement in each layer of the surface protection scheme. The graphs at top show displacement in arbitrary units; at bottom, the ratio is the displacement calculated for each height normalized by the displacement for the smallest height.

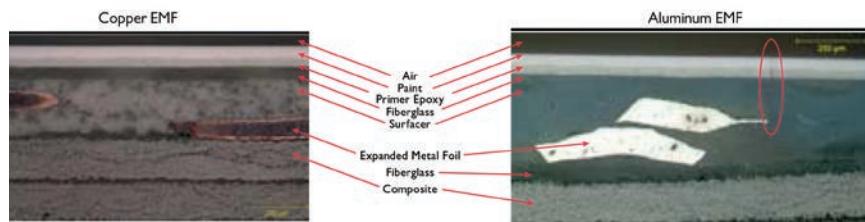


FIGURE 7. Photo micrographs of the composite structure layouts after exposure to moisture and thermal cycling. At left, the results for the copper EMF and at right, the aluminum.

displacement, increasing the mesh width or decreasing the aspect ratio are better strategies for increasing the current carrying capacity of the EMF for lightning strike protection.

### RELATING DISPLACEMENT WITH CRACK FORMATION

Greeger and his colleagues at BR&T qualitatively regard any projected increase in displacement as an increased risk for developing cracks in the protective layers since mechanical stress due to thermal cycling accumulates over time.

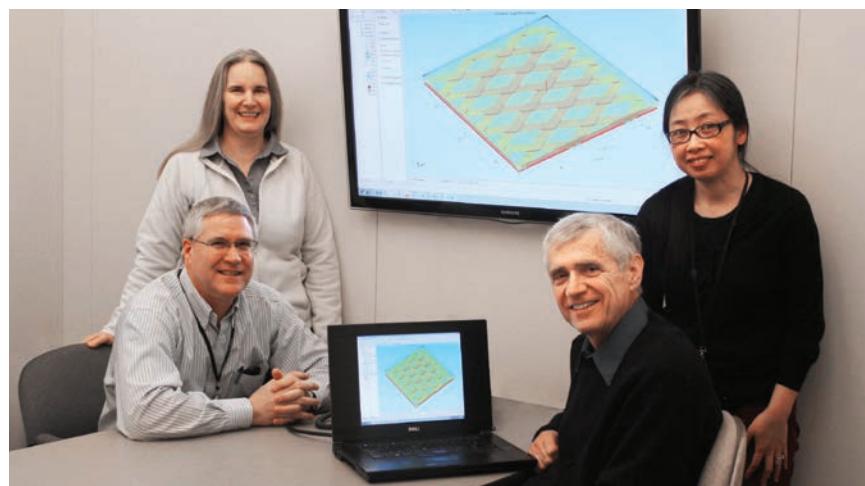
Experimental evidence supports this logic as shown in Figure 7 in photo micrograph cross-sections of surface protection schemes with aluminum and copper EMF after prolonged exposure to moisture and thermal cycling in an environmental test chamber. The layout with the copper EMF shows no cracks, whereas the aluminum EMF led to cracking in the primer, visible edge and surface cracks, and substantial cracking in mesh overlap regions.

Over the same temperature range, the experimental results correlate well with the results from the simulations that consistently show higher displacements in the protective layers for the aluminum EMF. Both simulation and experiment indicate that the copper EMF is a better choice for lightning strike protection of aircraft composite structures. Multiphysics simulation is therefore a reliable means to evaluate the relative impact of the EMF design parameters on stress and displacement to better understand and reduce the likelihood of crack formation. ■

### References

The information presented in this article is based on the following publicly available sources:

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- <sup>2</sup> J.D. Morgan, R.B. Greeger, P.K. Ackerman, Q.N. Le, *Thermal Simulation and Testing of Expanded Metal Foils Used for Lightning Protection of Composite Aircraft Structures*, *SAE Int. J. Aerospace* 6(2):371-377, 2013, doi:10.4271/2013-01-2132.
- <sup>3</sup> R.B. Greeger, J.D. Morgan, Q.N. Le, P.K. Ackerman, *Finite Element Modeling and Testing of Expanded Metal Foils Used for Lightning Protection of Composite Aircraft Structures*, Proceedings of 2013 ICOLSE Conference; Seattle, WA, September 18-20, 2013. 18-20, 2013.



Research team at Boeing Research and Technology, from left to right: Patrice Ackerman, Jeffrey Morgan, Robert Greeger, and Quynhgio Le.

# CONTINUOUS CASTING: OPTIMIZING BOTH MACHINE AND PROCESS WITH SIMULATION

As manufacturing processes become more sophisticated, the demand for bigger and better steel products increases. SMS Concast uses simulation to ensure their customers can bring steelmaking into new realms of size, quality, and complexity while simultaneously reducing energy consumption.

BY JENNIFER HAND

Halfway through the twentieth century, the steelmaking process was transformed when the batch process of ingot casting was replaced by continuous casting. With this technique, a constant stream of liquid steel is transformed into endless strands of glowing, solid metal (see Figures 1 and 2).



FIGURE 1. Discharge table of the continuous caster showing solidified strands being cut and discharged.

In ingot casting, the head of each ingot must be cropped after it is removed from the mold, producing waste metal. In continuous casting, however, this cropping must only be done at the very start and very end of each sequence during which several hundred tons of steel are cast, meaning far less waste material is produced. Additionally, the shape of the cast strands is far closer to the shape of the final rolled product. This

results in improved yield, superior quality, and better cost efficiency than previous methods. Not surprisingly, 95 percent of steel is made using continuous casting today.

SMS Concast has been a leader in this field for 60 years, designing and building technical equipment for steel melting, refining, and continuous casting. It has a worldwide market share of over 40 percent. "Continuous casting presents a huge number of variables that we need to analyze as we continue to improve the technology and advance the boundaries of what we know," explains Nicholas Grundy, Head of Metallurgy & Process Continuous Casting at SMS Concast. "We are constantly pushing the limits and the only way to understand something that we have never done before is to simulate it."

## SIMULATION ACROSS ALL REALMS

In continuous casting, molten, refined steel is typically brought to the caster in ladles of 30 to 350-ton capacity. The steel is teemed into a tundish that distributes the steel into one to eight strands. The first solid steel is formed in the open-ended, water-cooled copper molds and the formed strands are withdrawn out of the molds using driven rollers at speeds of 0.1 to 6 meters per minute, depending on section size (see Figure 2). After fully solidifying, the red-hot strands are cut into 3 to 15 meter-long pieces and left to cool.

The process of continuous casting produces a cast semifinished that is close in shape to the final product, greatly reducing the cost of further processing by rolling or forging. Depending on the shape of the mold, square profiles called billets can be cast for rolling into bars and wire for applications ranging from concrete reinforcement to piano wire. Larger, rectangular pieces called blooms can also be forged, for example to form a

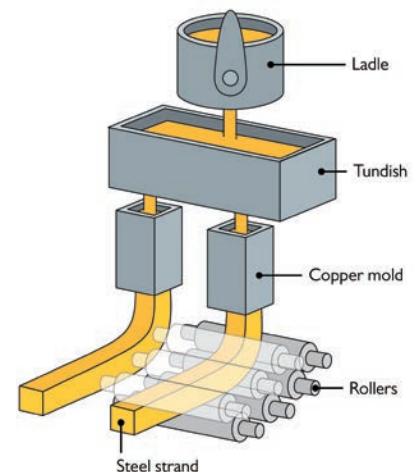


FIGURE 2. Continuous casting diagram. Liquid steel is brought to the caster in ladles. The tundish distributes the liquid steel to the copper molds and the formed strands are withdrawn out of the molds using driven rollers.

crankshaft or to be rolled into bars or rails. Slabs are rolled into sheet metal out of which everything from cars to oil tankers are produced.

SMS Concast uses simulation at every stage of the casting process: To analyze fluid flow in the tundish, primary solidification in the mold, solidification and mechanical deformation of the strand, and quenching or slow cooling of the cut blooms. "During solidification, we must minimize segregation of alloying elements towards the center of the strand, remove non-metallic inclusions, and improve the microstructure of the solidifying steel," describes Grundy.

"One way of achieving these improvements is by stirring the liquid steel," he says (see Figure 3). This is done using electromagnetic stirrers that generate strong rotating electromagnetic fields around the strands. This causes the liquid steel in the core of the strands to rotate. The field generated by the stirrers and the resulting flow pattern of the liquid steel is simulated using COMSOL Multiphysics®. Simulation is a crucial step in order to design the electromagnetic stirrers correctly and to achieve the best steel quality. Stirring is particularly important for highly-alloyed grades such as ball bearing steel, with high demands on cleanliness (with a minimal presence

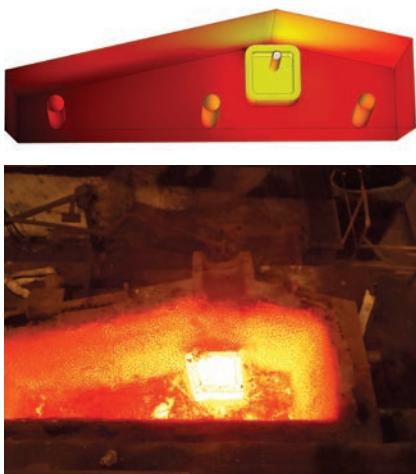


FIGURE 3. Model of a tundish using the CFD Module in COMSOL Multiphysics (top) and actual tundish during emptying of molten steel (bottom).

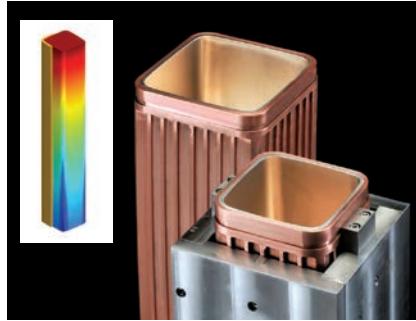


FIGURE 4. The water-cooled copper mold tube where the first solid steel shell forms is the heart of every continuous caster. Inset: Model of primary solidification and shell growth in the copper mold.

of non-metals), even composition (low segregation), and fine-grained microstructure.

"Essentially, most of the problems we face must be studied by combining various realms of physics such as electromagnetics, liquid or gas flow, mechanics and heat transfer. That's why we use COMSOL Multiphysics; we know of no other tool that links all these realms of physics into one single platform as seamlessly as COMSOL."

#### PREDICTING SOLIDIFICATION AND SHRINKAGE

One recent steelmaking trend is to roll strands of cast steel while they are still hot, rather than cooling them down and reheating them later in a reheating furnace. This is called hot charging, and avoids wasteful loss of thermal energy but demands an even more accurate understanding of how a strand solidifies. Grundy explains, "The copper mold is at the heart of each continuous caster. This is where the first solid steel skin is formed. A billet will only be faultless if the internal shape of the copper tube follows the shrinkage of the steel exactly, and a billet's surface must be faultless if it's to be hot-charged."

The SMS Concast team used their COMSOL model to understand the complex heat exchange processes taking place during the first solidification of the steel in the mold. The results guided the design of a new type of mold to cast billets with large rounded corners (see Figure 4). These corners stay warm after casting,

resulting in a more even surface temperature. This makes it possible to hot-charge the billets directly to the rolling mill, without leaving them to cool down and then heating them again in a reheating furnace fired with fossil fuels, as is the practice in a conventional steel plant.

The innovative mold design was successfully implemented at Tung Ho Steel in Taiwan in 2010, a steel plant that runs completely without a gas-fired reheating furnace, resulting in huge environmental and economic benefits. This reduces yearly emissions by 40,000 tons of CO<sub>2</sub>, about the same as the exhaust of 20,000 cars.

#### SIMULATE BUT ALSO VALIDATE

Grundy concludes, "Whenever possible, we like to validate our simulations with results from the real world or with physical models. For example, to validate our tundish flow simulation, one customer built a Plexiglas scaled water model and we



Nicholas Grundy displaying the simulation results of one of the CFD models of the continuous casting process.

found excellent agreement between the physical model and our flow simulations. As trust in our models grows, we gain the confidence to explore allowable designs." This approach clearly works well for the company; the world's widest beam blank (1150 x 490 x 130 mm) is already being cast on an SMS Concast caster in Germany, and the largest round section ever made (1000 mm in diameter) will go into production in a South Korean mill in 2015. ■

# SIMULATING THE RELEASE MECHANISM IN DRUG-ELUTING STENTS

Engineers at Boston Scientific are revolutionizing medical device designs. Their recent simulations of drug-eluting stents provide an understanding of the drug release mechanism by tying experimental findings to a computational model.

BY LEXI CARVER, COMSOL, INC.

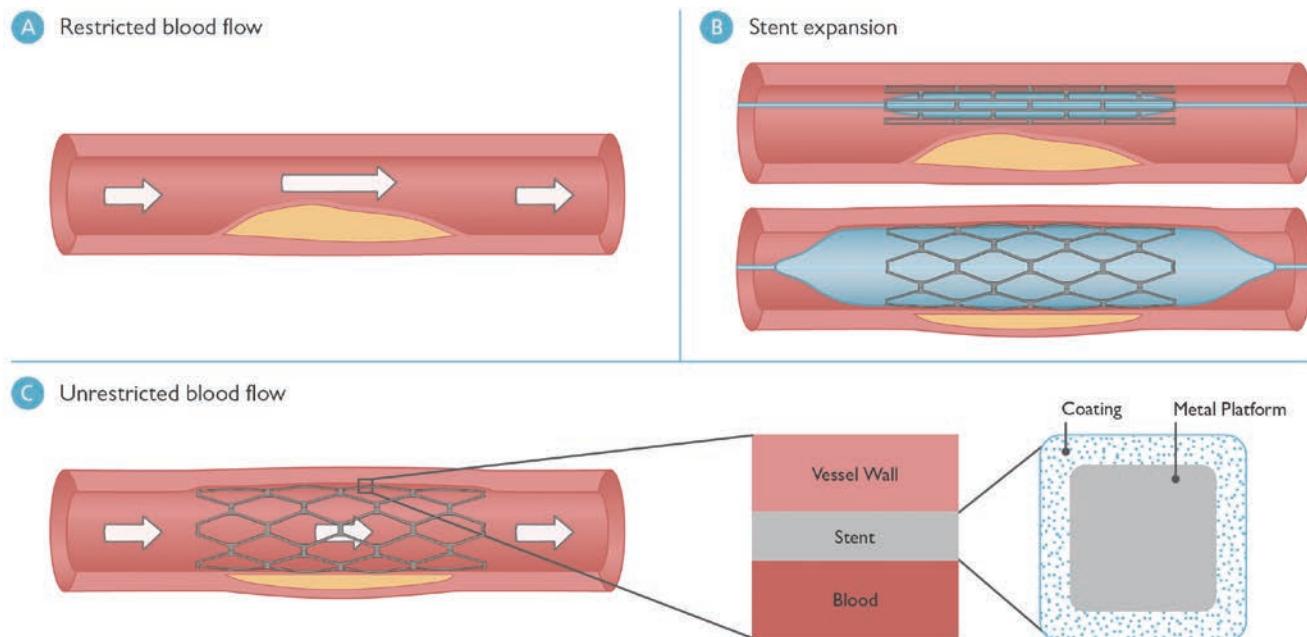
CONTRIBUTING AUTHORS: TRAVIS SCHAUER AND ISMAIL GULER, BOSTON SCIENTIFIC CORPORATION

Treating arteries in the heart that have been blocked by plaque is a common challenge for medical professionals. Known as stenosis, this condition restricts blood flow to the heart, resulting in symptoms such as shortness of breath and chest pain. It is sometimes resolved using stents, which are small, mesh-like tubular structures designed to treat blocked arteries. They are usually placed in the coronary artery and expanded with a balloon

catheter to keep the artery open, as depicted in Figure 1.

While stents are successful at holding arteries open, an artery can re-narrow because of excessive tissue growth over the stent. This is called restenosis and is the body's natural healing response, but it can actually impede recovery. Thus, drug-eluting stents were developed to deliver medicine — which acts to reduce cell proliferation and prevent the

unwanted growth — into the artery tissue. These contain a coating composed of medicine and a polymer matrix designed to provide a controlled delivery; each strand of the stent mesh is surrounded by this coating (see Figure 1C). Stent designs have improved dramatically in recent years in an effort to reduce restenosis rates, but much remains unknown regarding the release process.



**FIGURE 1.** A. Restricted blood flow in a vessel; B. Stent insertion and expansion; C. Normalized blood flow (left), arrangement inside a blood vessel (center), and cross-section of a stent strut (right).

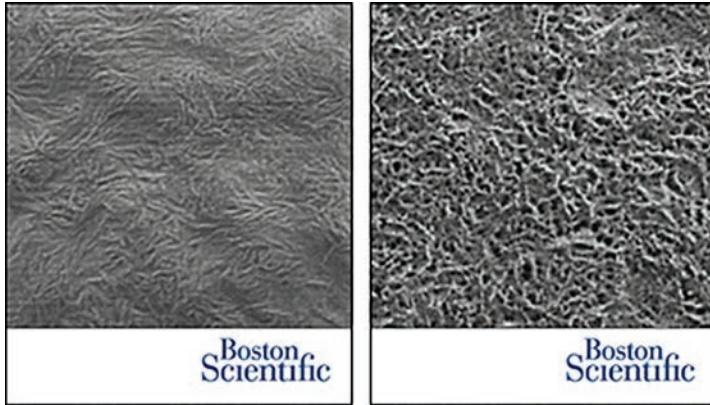


FIGURE 2. The coating microstructure prior to release (left) and the interconnected empty pores surrounded by the polymer matrix following the release from the coating (right).

**DRUG RELEASE BEHAVIOR**

Travis Schauer, Ismail Guler, and a team of other engineers at Boston Scientific, a company that develops devices and technologies to diagnose and treat a wide range of medical conditions, have sought to better understand the mechanism of medicine release with computer simulation. Using COMSOL Multiphysics®, they have modeled a stent coating to investigate the release profile (the rate at which the medicine diffuses out of the coating and into the vessel tissue) and the influencing factors. They used the Optimization Module in COMSOL to fit their simulation as closely as possible to experimental data curves. Schauer explained, “By gaining knowledge of the underlying mechanisms and

microstructure of the coating, we are able to understand the release process and tailor it to achieve a desired profile.” Ultimately, this may lead to a level of control over the release that has until now been impossible.

The stent coating that Schauer and Guler modeled is a microstructure with two phases: a medicine-rich, surface-connected phase and a phase with drug molecules encapsulated by a polymer. The development of this microstructure is affected by the solubility of the drug, the drug-to-polymer ratio, and the processing conditions during manufacturing. When the stent is inserted into an artery, the medicine-rich phase quickly dissolves and diffuses into the tissue, leaving behind interconnected cavities (pores) in the polymer coating, as depicted in Figure 2. Meanwhile, the molecules encapsulated by the polymer diffuse more slowly.

**MODELING MEDICINE DELIVERY**

Schauer and Guler idealized the complex geometry of the coating microstructure: in their model, the coating consists of a pattern of cylindrical pores filled with solid medicine surrounded by a polymer shell containing both the dissolved drug and solid drug encapsulated by the polymer. The molecules diffuse radially and axially, and the microstructure geometry only changes radially — at the boundary between shell and pore. Therefore, a two-dimensional axisymmetric model (see Figure 3) was sufficient.

Using COMSOL has allowed Schauer and Guler to easily customize their model. “We focused on understanding the transport phenomena at hand instead of spending time on cumbersome programming,” Schauer remarked. “We customized the underlying equations according to our needs directly through the user interface.” They performed simulations for two release profiles, in vitro and in vivo cases, seeking a description of the cumulative release of the medicine. “We wanted to understand why certain release profiles were observed,” said Guler and Schauer. “We compared experimental data to the release profiles generated in our simulations to confirm our findings.”

Schauer and Guler tracked both the dissolution of solid drug and the diffusion of dissolved drug. As it dissolves within the pores, the pores fill with liquid media from the surrounding tissue. The medicine has a different solubility limit in the liquid

“By gaining knowledge of the underlying mechanisms and microstructure of the coating, we are able to understand the release process and tailor it to achieve a desired profile.”

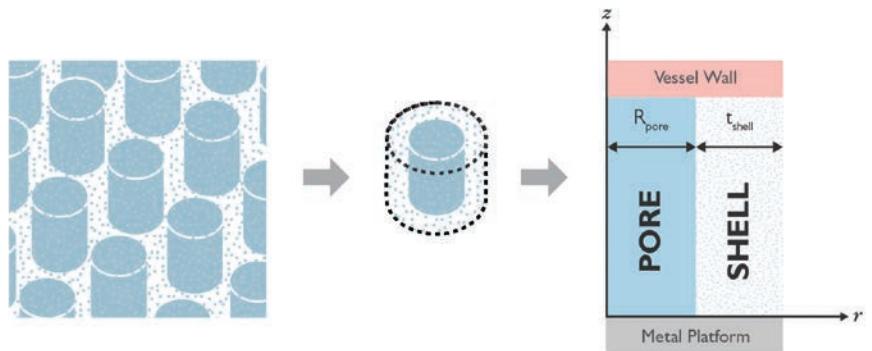


FIGURE 3. Idealized microstructure of the stent coating. A single pore-shell was modeled (center). The labels  $R_{pore}$  and  $t_{shell}$  (right) refer to the pore radius and the shell thickness.

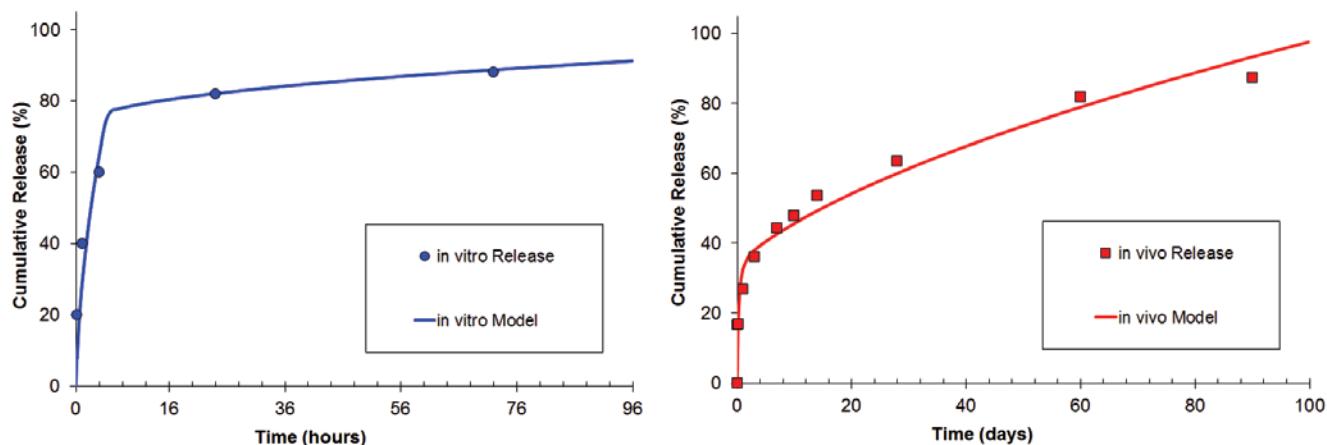


FIGURE 4. Simulation results alongside experimental results showing release curves for the in vitro and in vivo cases.

media than it does in the polymer, which results in a discontinuity in the dissolved medicine concentration at the interface between pore and shell. As Guler explained, “The appropriate interface conditions were easily implemented in COMSOL using a stiff-spring method, which ensured the continuity of the diffusive flux.” The customizable boundary conditions available in COMSOL Multiphysics allowed Schauer and Guler to easily add the necessary terms.

Certain model parameters had to be estimated because they were ‘effective’ values that could not be measured directly, such as the polymer shell

thickness. Another was the retardation coefficient that accounts for the twisted shape and constriction of the pores, steric effects, and other potential influences on the diffusion through the pores. These parameters were refined using the Optimization Module. Schauer and Guler made an initial guess for the shell thickness and retardation coefficient, based on experimental kinetic drug release (KDR) data. They compared the model’s predicted release profile to the KDR curves. Based on the results, the Optimization Module modified the shell thickness and retardation coefficient to obtain the best fit between the model results and

the experimental data. The release curves (see Figure 4) confirm that the medicine in the pores releases quickly, while the dispersed molecules in the shell diffuse slowly through the encapsulating polymer. The results in Figure 5 depict the faster dissolution and diffusion in the pore, compared to the shell.

#### FUTURE STENT STUDIES

Reducing restenosis rates is an ongoing goal for doctors and medical professionals that is greatly aided by drug-eluting stents. The modeling approach employed by Schauer and Guler offers valuable insight into one type of release mechanism. Although the simplified microstructure model does not capture all the details of the release curves, the pore-shell simulation showed good agreement, lending confidence to the appropriateness of their idealized model.

Researchers at the U.S. Food and Drug Administration (FDA) are developing even more comprehensive simulations, based on diffuse-interface theory, to examine the microstructure formation. These models aim to explain the relationship between processing, microstructure, and release behavior in controlled systems. Ultimately, simulation has the potential to give medical device designers more control over the delivery process, and improve treatment for patients with cardiovascular disease. ■

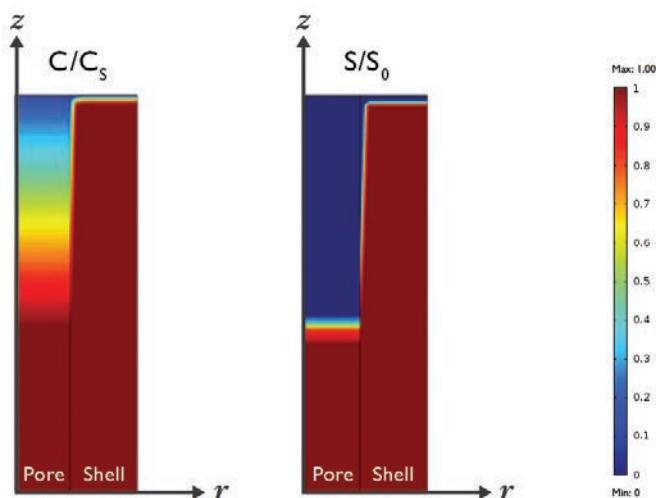


FIGURE 5. Predicted medicine concentration for the in vitro case at time = 2 hours;  $C/C_s$  = dissolved drug concentration/solubility limit (left),  $S/S_0$  = solid drug concentration/initial solid drug concentration (right).

# KEEPING COOL: SRON DEVELOPS THERMAL CALIBRATION SYSTEM FOR DEEP-SPACE TELESCOPE

Observing and analyzing regions in outer space where new stars and planets are born requires extremely sensitive detectors. Radiation and overheating can cause these detectors to fail. Using multiphysics simulation, a team at SRON is developing a calibration source for an imaging spectrometer that can operate with such vulnerable equipment.

BY LEXI CARVER

Heat management takes on a unique role in outer space, especially for cryogenic systems that demand extremely low temperatures in order to detect thermal radiation. This was a challenge faced by the engineering team at SRON Netherlands Institute for Space Research when designing the SpicA Far-InfraRed Instrument (SAFARI), an infrared camera that measures the complete far-infrared spectrum for each image pixel. SAFARI will fly aboard the Japanese Space Infrared Telescope for Cosmology and Astrophysics (SPICA).

SPICA will look deeper into space than any space telescope has before. Because SAFARI has ultrasensitive detectors, cooled to slightly above absolute zero, it can pick up weaker far-infrared radiation than previous space cameras. Precise on-ground and in-space calibration is crucial to the accuracy of the sensors and the success of the mission. To design and optimize these calibration systems, the team at SRON turned to a COMSOL Multiphysics® simulation as their guide.

## BEATING THE HEAT IN A TELESCOPE CALIBRATION SYSTEM

The calibration source for SAFARI contains a blackbody cavity or radiation source that provides radiation with a spectrum depending only on the source temperature, making it a very reliable and accurate calibrator. "However, SAFARI's detectors are so sensitive that the power produced by the source is approximately a million times too high and must be optically diluted using apertures and an integrating

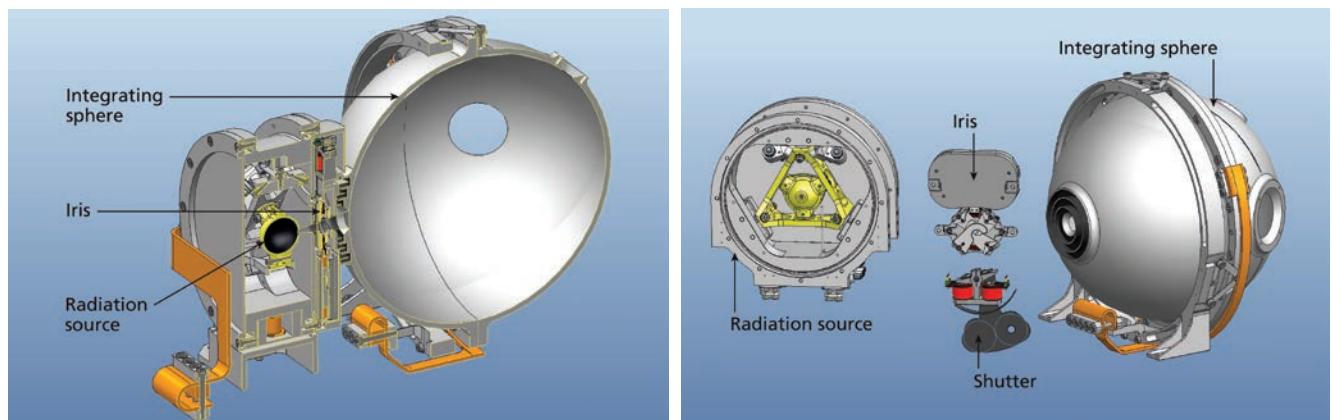
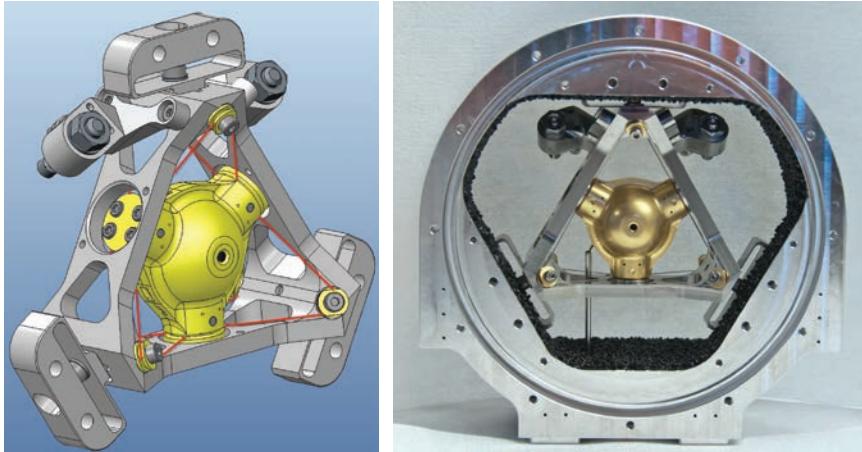


FIGURE 1. Left: Cross-section of the SAFARI calibration system. Right: Individual hardware components.



“COMSOL allowed us to quickly study different geometries that would otherwise be difficult to analyze.”

FIGURE 2. Left: CAD drawing of the radiation source with stainless steel suspension strings (highlighted in red). Right: Actual hardware.

sphere,” says Chris de Jonge, a design engineer at SRON. “After passing through the integrating sphere, radiation with the correct power and spectral distribution is then reimaged onto SAFARI’s detector arrays for calibration.” Between the radiation source and integrating sphere are a mechanical shutter and iris mechanism (see Figure 1). The shutter opens and closes the aperture to the radiation source, while the iris fine-tunes and modulates the output power.

Thermal management is vital: the system is held in a “super-dark” environment at 4.5 kelvins (K) to

decrease the background radiation from the equipment itself. Variation in the base temperature of the detectors, background radiation (affected by the orientation of the spacecraft), and power dissipated by the iris and shutter mechanisms can all disrupt calibration.

“The radiation source temperature can be set between 95 and 300 K to generate radiation — this creates a large temperature differential between the source and the 4.5 K environment, while available cooling power at these temperatures is limited to just tens of milliwatts,”

de Jonge explained. “To account for this, we needed to design a thermally insulating suspension system.” The SRON team needed a stiff suspension with a high resonance frequency that would prevent heat transfer from the source to the rest of the device while also protecting it from unwanted vibrations.

**DESIGNING A THERMALLY INSULATING SUSPENSION SYSTEM**

Using COMSOL simulations, de Jonge evaluated the heat load through the suspension and performed modal analyses on suspension concepts with different geometries and materials, seeking a tradeoff between mechanical stiffness and thermal load. “COMSOL allowed us to quickly

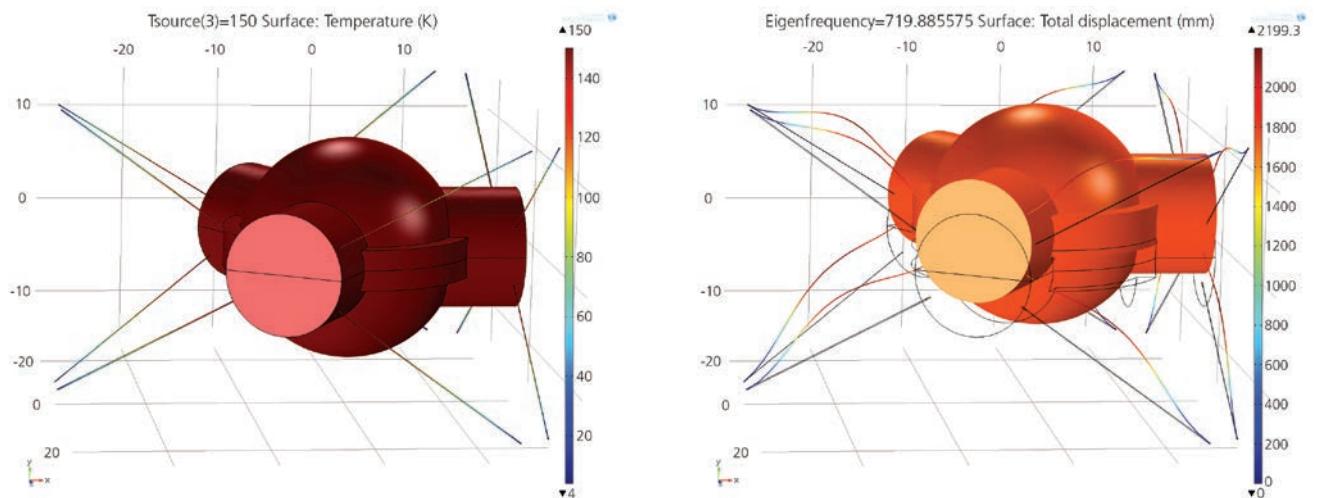


FIGURE 3. Left: Thermal model of the radiation source system with (1) stainless steel suspension strings, (2) the radiation source body, and (3) the interface between the suspension rig and the 4.5 K surrounding environment. Right: Modal analysis of the source, showing a resonant frequency of 720 Hz.

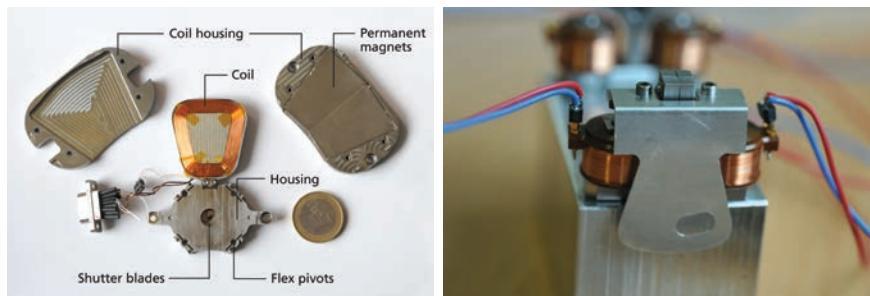
study different geometries that would otherwise be difficult to analyze,” de Jonge remarked. “Because of the large temperature gradient over the brackets and thermal properties that change very quickly as a function of temperature, temperature-dependent material properties had to be implemented. Ultimately, we chose the solution that had the best combination of mechanical stiffness and thermal insulation.” Based on the results, the team designed and optimized a configuration of thin (100  $\mu\text{m}$ ) stainless steel wires to hold the radiation source to a triangular frame (see Figure 2).

Because stainless steel has low thermal conductivity at cryogenic temperatures and the cross-section of the wires is very small, heat conduction through the wires was limited, which the simulation confirmed (see Figure 3). For a source temperature of 150 K, the experimental analysis showed 10.17 mW of conducted heat. The simulation results were in close agreement, accurate to within 0.01 mW. The design also had a resonant frequency of 720 Hz, high enough to ensure proper functioning of the radiation source.

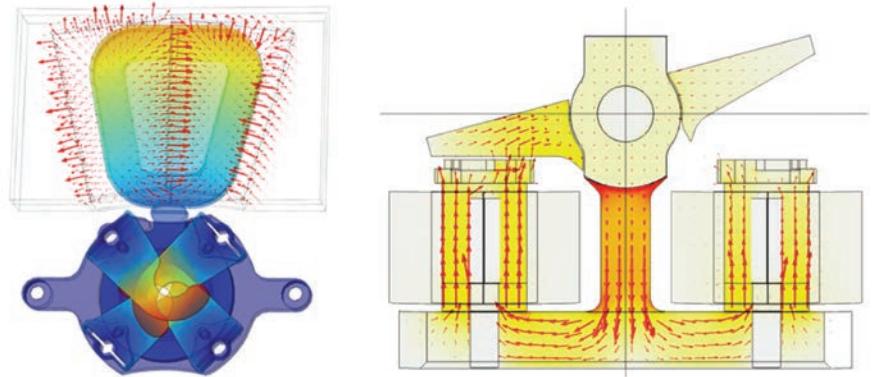
**OPTIMIZING THE IRIS AND SHUTTER FOR MAXIMUM EFFICIENCY**

Next, de Jonge optimized the coil-driven iris and shutter mechanisms (see Figure 4). The iris is driven by a voice-coil actuator and contains four stainless steel blades that rotate around frictionless bearings. The shutter is a magnetic latching device.

De Jonge used COMSOL to optimize the iris coil and housing



**FIGURE 4.** Left: Components of the iris assembly, including the coil, wiring, and housing. The edges of the blades (internal) are visible through the center of the aperture. Right: Shutter mechanism.



**FIGURE 5.** Left: Model of the iris mechanism showing the total displacement (surface plot) and magnetic flux density (arrows) of the blades and coil, respectively. Simulation was performed using the Multibody Dynamics Module and AC/DC Module. The geometry was imported using the COMSOL LiveLink™ for Creo™ Parametric. Right: Model of the shutter mechanism. Magnetic force was studied as a function of coil current and anchor angle.

geometry (his simulation results are shown in Figure 5), aiming to minimize the current and dissipated heat during actuation. By performing a parametric sweep over the main design parameters on the air gap and number of coil windings, the team developed an optimal coil design that has a low driving current of 38 mA and a dissipation of just 1.6 mW.

**SRON'S THERMALLY STABLE DEEP-SPACE SENSING SYSTEM IS ON THE WAY**

Because of SAFARI's sensitive detectors and the need for dissipative mechanisms in cryogenic systems, maintaining a controlled thermal environment is vital to the success of SPICA's mission. COMSOL allowed

de Jonge and the team at SRON to optimize their design for the best thermal, material, and structural conditions possible at extremely low temperatures. Their first tests of the SAFARI calibration source confirm the accuracy of the COMSOL simulations. SPICA is scheduled to launch into orbit in 2022, when SAFARI will help us unveil new mysteries of space beyond our solar system. ■



Chris de Jonge, Design Engineer at SRON, working on the SAFARI calibration system.

# Simulation Helps Improve Atmosphere Revitalization Systems for Manned Spacecraft

Life support systems for manned spacecraft must provide breathable air and drinkable water for the astronauts. Through the Atmosphere Revitalization Recovery and Environmental Monitoring project, engineers at NASA are developing atmosphere control devices for the safety of the onboard crew.

BY LEXI CARVER

Image courtesy of NASA

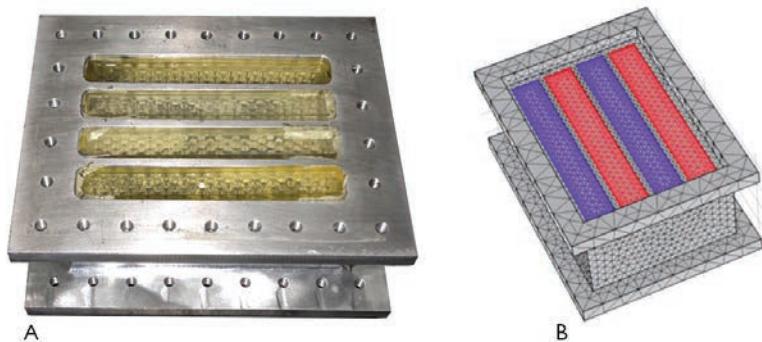


FIGURE 1. (A) Photograph of an IBD with four columns. (B) Meshed COMSOL model of the IBD. Purple regions indicate wet beds, red indicate dry.

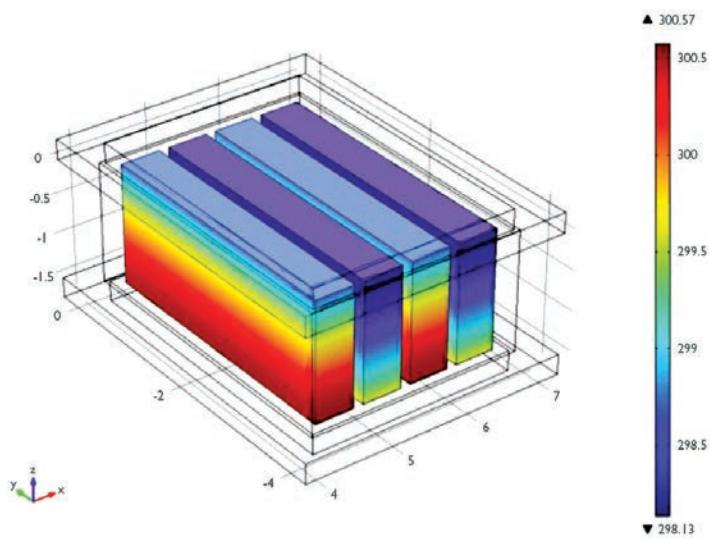


FIGURE 2. Simulation results showing temperature (K) in each bed. The first and third columns contain wet air flowing downward, the second and fourth dry air flowing upward.

The atmosphere in a manned spacecraft needs to be regularly revitalized in order to ensure the safety of the astronauts and the success of the space mission. For missions lasting a few months, this means air is continuously dehumidified, water collected for re-use, and carbon dioxide ( $\text{CO}_2$ ) ejected. One component of the onboard atmosphere control system is a water-saving device that Jim Knox, an aerospace engineer at NASA, is optimizing as part of the Atmosphere Revitalization Recovery and Environmental Monitoring (ARREM) project. He leads a team at the Marshall Space Flight Center (Huntsville, Alabama) that is aiming to make the assembly more cost-effective and efficient by reducing its power usage and maximizing the water saved; their goal is to save 80 to 90 percent of the water in the air. They hope to offer flight system developers at NASA an integrated approach to atmosphere revitalization and water collection that will ultimately increase the time and distance space missions can travel.

## SEPARATING WATER AND $\text{CO}_2$ THROUGH EFFICIENT ADSORPTION

Revitalizing the atmosphere inside a spacecraft requires separating water, removing  $\text{CO}_2$ , and returning the water to the air before it is condensed into liquid form. The water-saving system that the team developed (see Figure 1A) is called an Isothermal Bulk Desiccant (IBD). It consists of a chassis with enclosed channels called packed

beds, each of which is lined with silica gel pellets to promote water adsorption (a “dry” bed to draw water out) or desorption (a “wet” bed to return water to the air). Each pair of beds straddles an aluminum foam lattice used for transferring heat.

The water-saving process occurs in simultaneous half-cycles, with some air entering the dry beds while some leaves the wet beds. In a dry bed, water in the air is exothermally adsorbed onto the silica gel, drying the gas to save the water, before the air travels to a CO<sub>2</sub> removal system. The CO<sub>2</sub>-free air flows back to the wet bed. Meanwhile, the heat caused by adsorption in the dry bed is transferred to the wet bed via the aluminum lattice, causing water to desorb from the silica gel and return to the air. This heat transfer has the added benefit of lowering the temperature in the dry bed, allowing adsorption to continue longer. The water is pumped back into the cabin, and the CO<sub>2</sub> is expelled into space. After flowing out of the IBD, the cabin air will enter a heat exchanger and centrifugal separator that together condense and separate the liquid water, collecting it for re-use.

### SIMULATING GAS FLOW AND OPTIMIZING BED CONDITIONS

Using COMSOL Multiphysics®, Knox’s team modeled a four-column IBD to calculate the efficiency of the device (his model is shown in Figure 1B). The IBD geometry was created in Pro/ENGINEER®

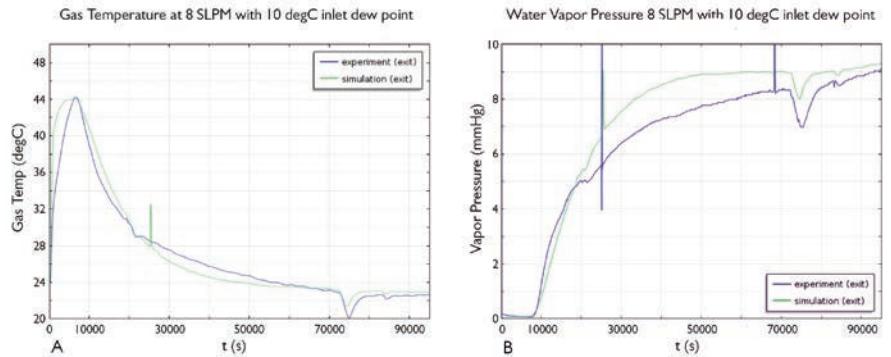


FIGURE 3. Simulation results for air at the exit showing (A) gas temperature, (B) water vapor pressure.

and imported using the LiveLink™ for Pro/ENGINEER®. “COMSOL let us perform this kind of multiphysics simulation on intricate geometries,” Knox remarked. “We needed to simulate porous media flow in the beds and heat transfer in multiple materials, input pressure boundaries, and find sorption rates.” They noted that dry beds gain heat as gas flows downward, due to the exothermic adsorption. Conversely, the wet beds lose heat as gas flows upward (see Figures 2 and 3).

One member of the team, Rob Coker, calculated the efficiency of the IBD using a breakthrough test where air was pumped through a dry bed. Initially, the air leaving the bed was completely dry; all the water vapor had adsorbed onto the silica gel. As more air flowed through, the water vapor concentration in the air at the exit increased; eventually, it had the same

humidity as the air entering since the silica gel pellets could hold no more water. Observing this process allowed the team to gather parameter values for the IBD model, and they compared the breakthrough and experimental results (see Figure 3). The capabilities of COMSOL let them track the water concentration, flow rates, and pressure with the boundary conditions for inflow, outflow, and wet and dry air changing for each half-cycle.

According to the simulation results, the IBD removed 85 percent of the water in the air and returned it to the atmosphere for collection. The model successfully predicted the efficiency of the IBD; from here they will be able to further refine the design for a thermally-linked bed.

### OFFERING NASA A RELIABLE APPROACH TO ATMOSPHERE REGULATION

The team’s COMSOL simulation provided invaluable optimization and design guidance for the water-saving assembly. They are increasing the IBD efficiency by minimizing power requirements and maximizing the water saved before CO<sub>2</sub> is ejected. This is one of many important parts of a revitalization system that they hope will extend the reach of space missions. They are also using COMSOL simulations to design new systems suited for longer missions, which enable the separation of oxygen from CO<sub>2</sub> and reduce the amount of O<sub>2</sub> that must be carried onboard. With these innovative designs and the powerful capabilities of simulation, we’ll soon have manned spacecraft traveling farther than ever before. ■



The atmosphere revitalization computer simulation team at the NASA MSFC. Left to right: Rob Coker, Carlos Gomez, Greg Schunk, and Jim Knox.

# Innovative Thermal Insulation Techniques Bring Vaccines to the Developing World

Intellectual Ventures' Global Good program has been hard at work creating new technology to bring vaccines to every corner of the world. The Passive Vaccine Storage Device uses just a single batch of ice and requires no external power to store medicine at cold temperatures for an entire month.

BY LAURA BOWEN

In many areas of the developing world, there is extremely limited access to electricity, and many places have never had any type of power infrastructure. This presents a huge challenge for aid workers and doctors. In the very recent past, vaccines that needed to be stored at cold, relatively constant temperatures could not be taken into the remote areas where they were needed most. As part of the Global Good program at Intellectual Ventures (IV), a team of innovators invented a thermos-like container called the Passive Vaccine Storage Device (PVSD)

that uses high performance insulation to completely change the way vaccines are stored in areas with little or no electricity (see Figure 1).

## MEETING STRICT SAFETY REQUIREMENTS

If not kept within the necessary temperature range at all times, vaccines can spoil and become unusable. Global Good's researchers were tasked with following the parameters dictated by the World Health Organization. To be delivered safely, the vaccines are required to

stay within a narrow window of 0° and 10°C.

The first prototype that the researchers designed was based on a cryogenic dewar, a device that relies on vacuum and multilayer insulation technology to store extremely cold liquids. Dewars that can normally hold liquid nitrogen or liquid oxygen for extended periods of time were only able to hold ice for a few days before it melted.

“Global Good’s researchers used experimentation along with thermal and vacuum system modeling with COMSOL Multiphysics in order to identify materials and designs that would allow the PVSD to maintain high vacuum levels at high temperatures.”



FIGURE 1. The Intellectual Ventures team and aid workers with the PVSDs designed to carry vaccines during a field study.

“COMSOL Multiphysics is great for reducing the amount of time spent on complex models ... having everything flow together in a seamless, easy-to-access way, where the multiphysics couplings are spelled out very clearly.”

Global Good’s researchers used experimentation along with thermal and vacuum system modeling with COMSOL Multiphysics® in order to identify materials and designs that would allow the PVSD to maintain high vacuum levels at high temperatures. Like a cryogenic dewar, the PVSD relies on multilayer insulation within a vacuum space to minimize heat transfer. The high quality vacuum virtually eliminates convective and gas conduction heat transfer, while the multilayer insulation dramatically cuts down on radiative heat transfer. The multilayer insulation, made of reflective, extremely thin sheets of aluminum and a low conductivity spacer, is similar to materials used in spacecraft.

#### SIMULATING VACCINE STORAGE IN EXTREME CONDITIONS

Researchers for Intellectual Ventures’ Global Good program used an environmental chamber to recreate conditions similar to the climate in Sub-Saharan Africa in order to rigorously test and understand the performance of their prototypes. However, building a quality prototype of a vacuum dewar is an involved effort, so to explore different design directions more efficiently before building prototypes, the team turned to COMSOL Multiphysics and its Heat Transfer Module and Molecular Flow Module, among others. Their challenges included optimizing the internal geometry for maximum cold storage time, maintaining higher vacuum capacity, and managing outgassing in the vacuum space. The minimization of outgassing is critical, as even moderate amounts of residual outgassing within the vacuum space over the life of the PVSD can cause the vacuum to lose its integrity, increasing heat transfer into the device.

The geometry of the device is optimized to maximize vaccine

hold time and to be as accessible as possible for health workers in the field. As a first line of defense against the elements, the outside of the device consists of a metal enclosure padded with protective rubber bumpers, while the inner part of the PVSD consists of a smaller shell connected at the very top to the outside with a cantilever neck (see Figure 2). Because of this design, conductive heat transfer can only happen at the connection point. In addition, a composite neck maintains the vacuum space so that there is no gas permeation from ambient air. According to David Gasperino, one of the engineers deploying COMSOL to support the PVSD design effort, “COMSOL Multiphysics is great for reducing the amount of time spent on complex models.” He went on to say that they especially appreciated “having everything flow together in a seamless, easy-to-access way, where the multiphysics couplings are spelled out very clearly.” The team found the breadth of modules available helpful for capturing the complex physics they needed to explore with their models.

#### IMPROVING STORAGE DEVICE DESIGN FOR FUTURE GENERATIONS

As a result of the experimental and theoretical work that went into the PVSD, the device is capable of making a significant impact on the vaccine cold chain in the developing world, allowing vaccines to travel into more remote regions and to be stored for longer periods of time without the need for power. Down the road, Intellectual Ventures will improve their storage device designs to keep vaccines cold for extended periods with even more efficiency. The team will continue working to create groundbreaking tools with the ability to save lives around the world. ■



FIGURE 2. Top: Thermal simulation of the PVSD shortly after loading; the process of melting ice blocks is modeled using the phase change feature in COMSOL Multiphysics. Bottom: The PVSD uses similar temperature control storage methods to a cryogenic dewar. With a single batch of ice, it can store vaccines for extended periods of time.

# BATTLING CORROSION IN NUCLEAR WASTE STORAGE FACILITIES

BY GARY DAGASTINE

Multiphysics simulations helped Sogin S.p.A. design a simple, energy-efficient dehumidification system to prevent corrosion in drums of radioactive waste.

Corrosion is a relentless and unforgiving enemy of metal, and the battle against it simply cannot be lost when steel drums full of nuclear waste are involved.

Such is the situation in Italy, where domestic nuclear power production has been halted, yet the need is ongoing to safely store low-level radioactive waste produced as a byproduct of power generation, research, medical, and industrial activities.

Sogin S.p.A. is the Italian state-owned company responsible for the decommissioning of Italy's nuclear sites and the management of radioactive waste.

## NUCLEAR WASTE STORAGE REQUIRES ACCURATE HUMIDITY CONTROL

One Sogin project is the ongoing renovation of a building at a former nuclear power plant located in the center of Italy. The goal is to meet Italian and international requirements for temporary storage of low-level radioactive waste until the waste can be delivered to the National Permanent Repository.

The temporary facility is an approximately 30 m x 15 m single-floor rectangular space divided into two rooms. The waste is stored in steel drums encased in concrete for radiological reasons. The drums have an external diameter of 0.8 meters, while the overpack is one meter in diameter. Relative humidity of 65

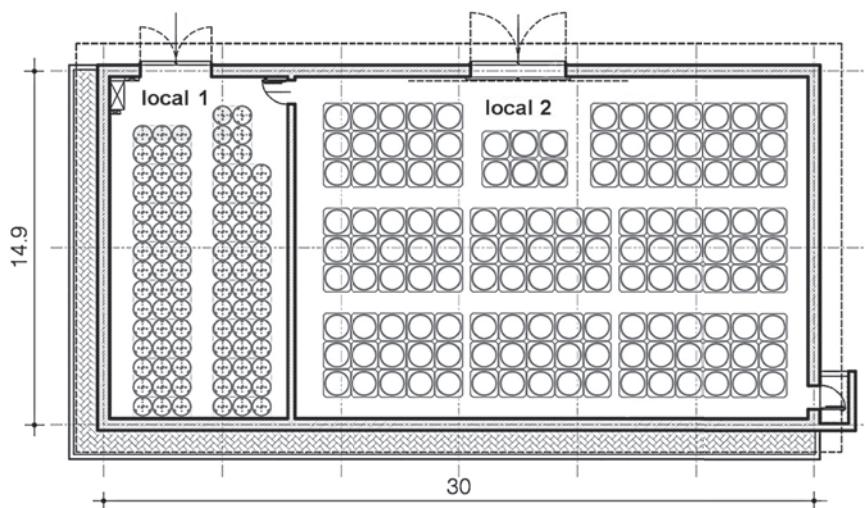
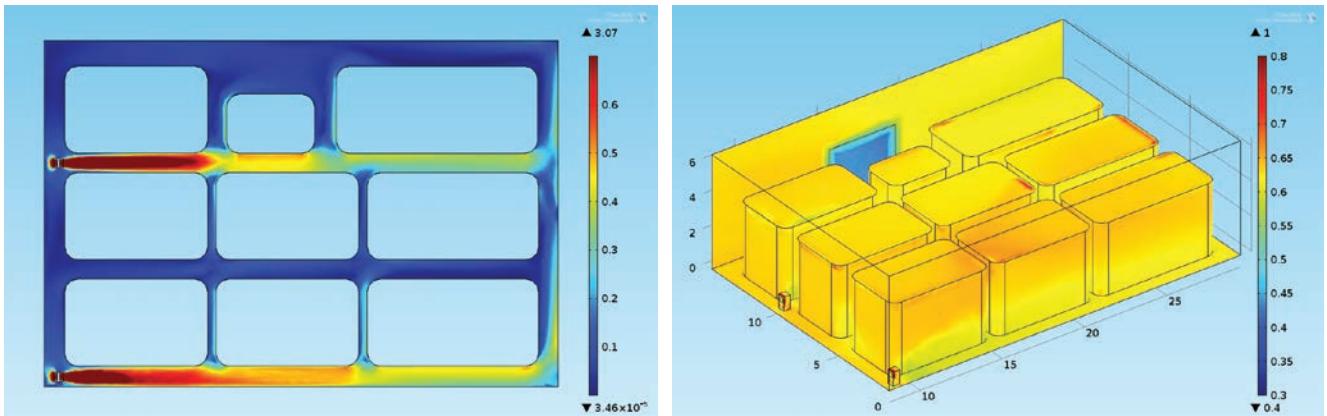


FIGURE 1. Floor plan for a space divided into two rooms and used as a temporary storage facility for low-level radioactive waste. The waste is stored in the rooms in non-stainless steel drums with a concrete overpack.

percent or lower must be maintained to prevent corrosion.

Gianluca Barbella is a Sogin structural engineer and Team Leader for the project. "The need to control air humidity is due to the non-stainless steel drums that are used. The concrete overpacks mean the drums aren't inspectable without first extracting them, which makes it difficult to constantly monitor the corrosion process. Also, the site is exposed to high levels of relative humidity. Therefore, humidity control is critical," he explains.

However, the cost of operating a heating, ventilating, and air-conditioning (HVAC) system to maintain optimum conditions over the anticipated 25-year life of the facility is substantial. In addition, because the facility can't be expanded, an HVAC system's space requirements would result in less space available for waste storage. Moreover, HVAC system downtime is inevitable because of both equipment malfunctions and scheduled maintenance.



**FIGURE 2.** For a room designed to store radioactive waste for up to 25 years, Italy's Sogin S.p.A. used COMSOL simulations to study air flow velocities in the room (left) and surface relative humidity throughout the room (right) that would result from various dehumidifier types and locations within the space. The results helped engineers design a dehumidification system that minimizes stagnant air, enables maximum operating efficiency, and optimizes relative humidity.

A potential alternative is to use industrial isothermal dehumidifiers instead, which are relatively small, mobile, require less maintenance, and have substantially lower operating costs. These units are based on the reverse Carnot thermal cycle: A fan draws air into the unit, where it passes over an evaporator and is cooled. Excess moisture from the air condenses into drops of water that fall into a tank. The air then passes through a condenser where it is warmed by several degrees. It is then recycled into the environment as drier, warmer air.

The Sogin project relied on numerical simulation to study the impacts of various sizes and configurations of two different industrial isothermal dehumidifiers. The analyses were carried out by Piergianni Geraldini, from the mechanical design department. The goals were to identify equipment requirements and also to determine optimum placement of the units in the rooms (see Figure 1).

#### SIMULATIONS HELPED DETERMINE OPTIMUM LAYOUT

The team first studied turbulent air flow in the room by performing stationary fluid-flow studies based on a single-phase incompressible k-epsilon turbulence model. Its purpose was

to reproduce the air velocity field in the storage area assuming the dehumidifiers were in use.

Then they used the results from those studies in time-dependent, fully-coupled simulations to study heat and moisture transfer within the room's atmosphere (see Figure 2). The overall results were used to develop an optimum layout for the dehumidifiers.

powerful capability to solve 3D heat and moisture transfer problems," says Piergianni. "COMSOL Multiphysics makes it easy to couple different physics, has an intuitive interface, and opens up the possibility of managing the entire modeling process within the same interface.

"The simulations helped us to design a layout based on the use

**"COMSOL Multiphysics makes it easy to couple different physics, has an intuitive interface, and opens up the possibility of managing the entire modeling process within the same interface."**

All simulations were conducted using COMSOL Multiphysics® and the Heat Transfer Module. "Without such a refined simulation tool, we would have had to model the dehumidification process using simplified approximations coupled with dehumidifier performance curves supplied by the units' manufacturers. But the simulations showed us that COMSOL has a

of two dehumidifiers that provides the same dehumidification capacity as other configurations, but they required four units," concludes Barbella. "The system we designed will limit stagnant air pockets, enable the units to operate at peak efficiency, and help us reduce the risk of drum corrosion once the facility is finalized and commissioned." ■

# Using Multiphysics Simulation to Prevent Building Damage

In extreme climates, moisture and temperature changes can damage building foundations. Vahanen Group is using multiphysics simulation to equip construction teams with assessments that help prevent frost damage and maintain safe building structures.

BY LEXI CARVER

Though they often go unnoticed, underground insulation and heating systems prevent critical damage to concrete building foundations, and keep occupants safe and warm indoors. Since concrete is porous, water and contaminants can enter the foundation. When the foundation or the soil underneath freezes, this can cause structural damage such as cracking. Some older buildings are protected from this by insulation, while others are protected by heated pipes that travel from the boiler to the building's indoor heating units.

Ongoing damage can lead to serious risks, such as the buckling or collapse of a building. To address the challenges of cold and moisture, Vahanen Group (Espoo, Finland), a company specializing in building services such as quality assessments and construction recommendations, analyzes the potential for frost damage in buildings being considered for renovation. Their work is especially vital in cases where renovations are necessary due to existing damage, for instance, where heating systems and pipes need to be replaced.

## WHAT'S THE BEST WAY TO INSULATE A BUILDING?

Pauli Sekki, building specialist at Vahanen, is using the simulation capabilities of COMSOL Multiphysics® to perform risk assessments — his goal is to discern whether certain renovations to foundations or heating systems would require adding external frost insulation. If added unnecessarily, this would waste valuable money, time, and work.

For one project, Sekki's COMSOL model (see Figure 1) includes the

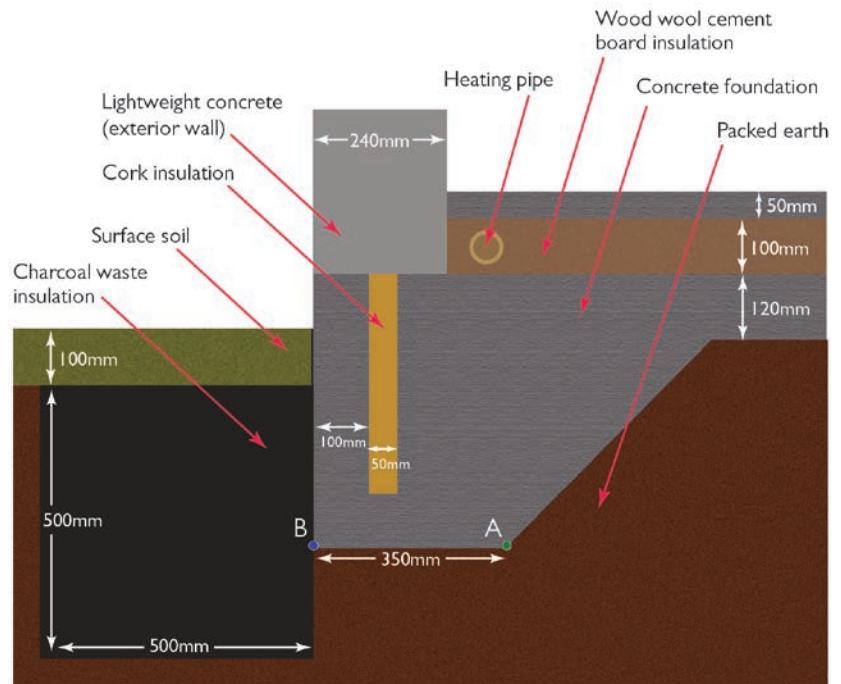


FIGURE 1. Schematic of the building model geometry. The heating pipe runs from the boiler to the indoor heating units, and keeps the foundation warm at the same time.

foundation, levels of loose soil and packed earth, several types of insulation, lightweight concrete walls, and a pipe from a heating system passing underneath a building near the wall and foundation.

First Sekki simulated temperature changes based on local climate data for Helsinki, Finland. Government frost table data provides annual total freezing degree hours (FDH), a quantity representing the number of degrees that the daily mean temperature is below 0°C. (For example, for a day with an average temperature of -5°C, the FDH is 5

degrees x 24 hours = 120.) An annual total sums the FDH from each day in a year (the annual freezing index), typically about 14,000 FDH for Helsinki.

From the existing data, Sekki generated a “critical freezing” quantity to account for abnormally cold winters that occur, on average, every fifty years (with about 40,000 FDH). Given the importance of building strength and longevity, any renovations would have to withstand not only a typical winter climate, but also these rarer, harsher conditions. “Design and construction teams turn to Vahanen to verify that their

renovation plans are safe, will last, and are the best use of the available materials and resources," Sekki explained. "And we turn to COMSOL for that information."

In this example, he needed to determine whether renovations including the complete removal of a damaged heating pipe would endanger the building. Was the existing insulation sufficient? To answer this question, he modeled heat transfer in the pipe, the insulation, and the foundation. "Tools in COMSOL Multiphysics are very easy to use for this kind of complex model," he commented. "The almost unlimited possibilities for setting boundary conditions were a huge advantage."

### PREDICTING THE POTENTIAL FOR FROST DAMAGE

Sekki used his simulation to predict temperatures at the two lowest corners of the concrete foundation (points A and B in Figure 1). He

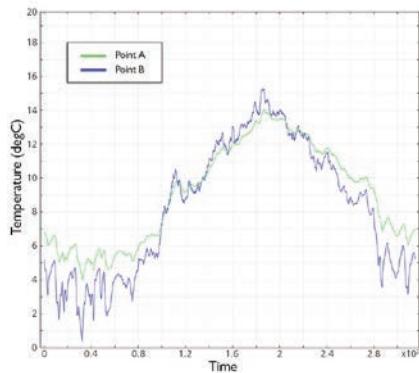


FIGURE 2. Simulation results showing temperatures over a typical year (14,000 FDH) for the renovated building with EPS insulation added.

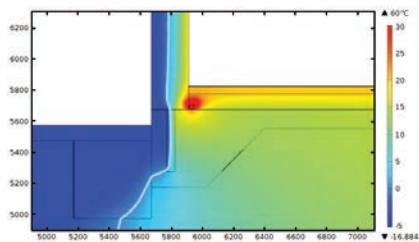


FIGURE 3. Temperature distribution for the unrenovated building for extreme winter conditions (40,000 FDH) occurring every 50 years.

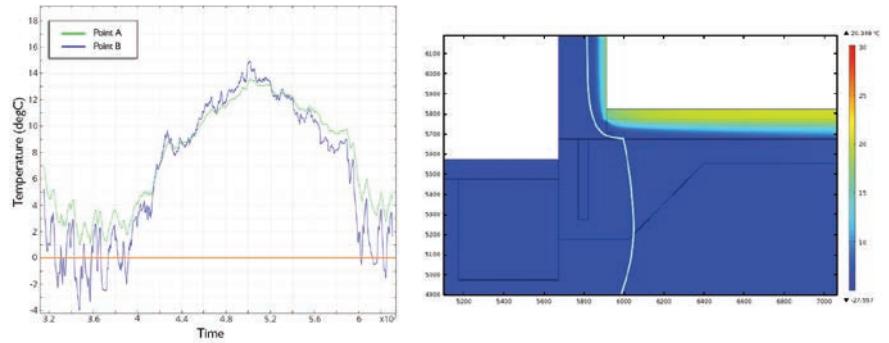


FIGURE 4. Temperature results (40,000 FDH case) for the building after renovations and additional EPS insulation. The orange line (line graph) and vertical contour (surface plot) indicate 0°C.

investigated three cases: the original structure, the structure after heating system renovations (where heat transfer from a pipe would no longer occur), and the structure after renovations that additionally replaced damaged wood wool cement board (WWCB) with expanded polystyrene (EPS) insulation.

For a typical year in Helsinki, the ground stayed warm enough to prevent damages to the building in its original state as well as after heating system renovations. However, after the WWCB insulation was replaced with EPS, the ground near the foundation dipped to 0.5°C (see Figure 2), low enough to be a concern. "The new EPS-insulated structure would have been at risk for frost damage," Sekki said. "Thankfully, multiphysics simulations are helping us avoid that."

### KEEPING STRUCTURES STRONG FOR THE WORST WINTERS

After simulating the building during a longer winter, he found that only the foundation of the original structure stayed safely above freezing temperatures (see Figure 3).

The ground around the foundation of the renovated structure with WWCB dipped to -2°C in the simulation. The foundation of the renovated structure with the replacement-EPS insulation dipped even farther, to -4°C. This meant removing the heating pipe would risk serious damage to the building foundation (see Figure 4). It would be necessary to install additional insulation at the same time.

### PRESERVING STRUCTURAL INTEGRITY THROUGH SOUND RECOMMENDATIONS

Sekki is using his findings to ensure safe building renovations in climates like Helsinki. Using simulation, he is able to assess the heating needs of structures with complicated geometries, and can test different insulation materials and thicknesses to make sure the techniques he recommends are safe and sufficient. To further their aims of providing strong support to construction teams, Vahanen is also using COMSOL to model transient heat and moisture transport, and indoor air flow. "Thanks to simulation, we can make good recommendations to our customers," Sekki remarked, "and prevent changes that would ultimately cause structural damage." ■



Pauli Sekki, building physics specialist for Vahanen Group.

# OPTIMIZING HEMATOLOGY ANALYSIS: WHEN PHYSICAL PROTOTYPES FAIL, SIMULATION PROVIDES THE ANSWERS

In order to take measurements that are inaccessible using just physical prototyping, HORIBA Medical turned to simulation to optimize and improve their line of leading hematology analysis equipment.

BY ALEXANDRA FOLEY

Laboratory tests, such as hematology analysis, influence up to 70 percent of critical decisions including hospital admittance, discharge, and treatment. The accuracy of these

tests, therefore, is of the utmost importance to the bottom line — curing a patient's ailment or saving a life. At HORIBA Medical, a worldwide supplier of medical diagnostic

equipment, simulation software plays an important role in the research and development process, helping to ensure that these tests are as accurate and encompassing as possible.

At the center of HORIBA Medical's cutting-edge hematology analysis equipment is a well-known approach to blood analysis that uses a combination of optical measurement and electrical impedance to analyze a sample. The impedance measurement device utilizes a micro aperture-electrode system through which blood passes (see Figure 1). Electrical impedance is then used to count the number of cells and measure the size and distribution of erythrocytes (red blood cells), platelets, and leukocytes (white blood cells). After impedance measurement, a laser and optical detector are used to sort the different types of leukocytes.

Considerations for the production of HORIBA Medical's line of hematology and clinical chemistry equipment include speed, accuracy, size, and ease of use for their customers. "Today, in vitro diagnostics specialists have to design systems that are capable of carrying out increasingly complex tests, while simultaneously making results easier to interpret," describes Damien Isèbe, Scientific Computing Engineer at HORIBA Medical. "Numerical simulation allows us to design devices that meet these goals." HORIBA places numerical simulation at the center of its research activities and

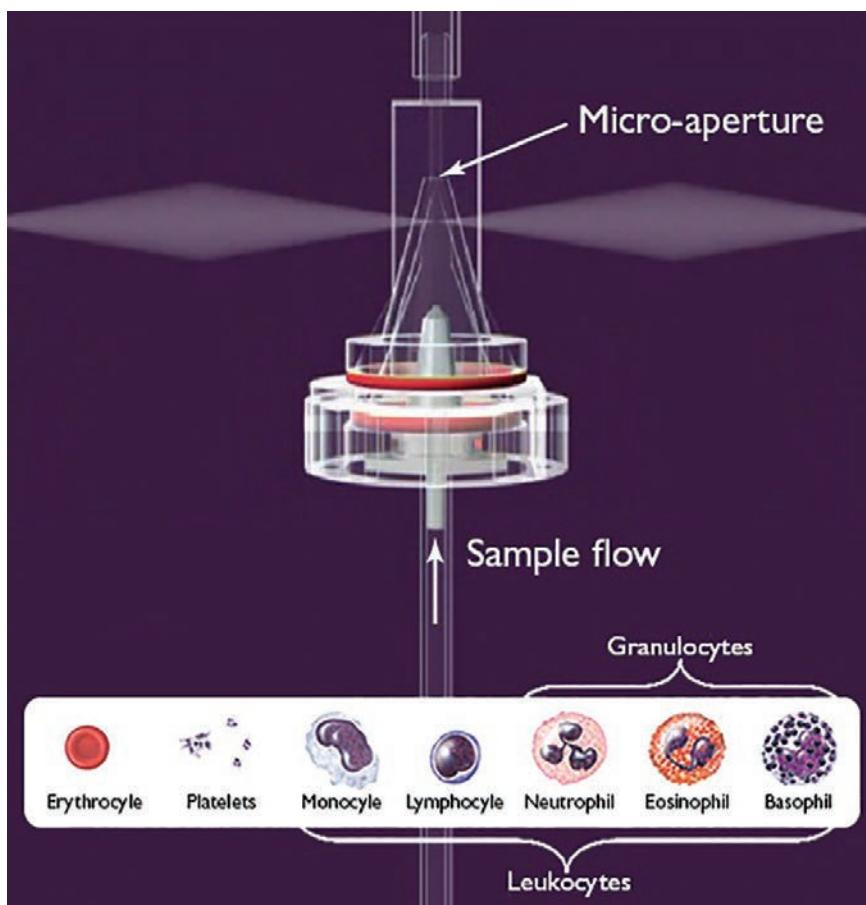


FIGURE 1. Diagram of the aperture-electrode system present in the ABX Pentra Series Analyzers.

10 percent of its revenues are invested directly in research and development activities.

### SIMULATION OF THE MICRO APERTURE-ELECTRODE SYSTEM

Isèbe uses COMSOL Multiphysics® to improve the electrical impedance system in the Pentra Series (see Figure 2), one of HORIBA Medical's most advanced hematology analyzers. The fully-automatic process begins with the placement of a blood sample in an analysis chamber, where it travels through a hydraulic channel and is then diluted with reagents. After dilution, the sample is sent into a counting and measurement chamber that consists of a micro-aperture flanked by a pair of electrodes (see Figure 3).

The electrodes generate a strong electric field inside the counting chamber, and as the particles within the blood sample pass through



FIGURE 2. The ABX Pentra 60C+ (left) and Pentra 80 XLR (right), two hematology analyzers of the Pentra Series, use an aperture-electrode system for counting and sizing blood particles by impedance measurement.

corresponding to a larger molecule (see Figure 3).

"Inside the counting chamber there are a lot of complex physical processes: high fluid velocity, pressure drop through the aperture, heat transfer, intense electric field, and also a risk of pollution due to mechanical

into the software environment.

"Importing the CAD model of the measurement chamber allowed us to extract the computational domain," he explains. "In this case, if we want to compute fluid flow in the system, the simulation software automatically creates the fluid domain directly from the CAD model." Once the aperture-electrode system geometry (see Figure 4) was imported into COMSOL, analysis and optimizations could then be performed using the actual geometry of the device being manufactured.

"Due to advancements in computational analysis and supercomputing capabilities, numerical simulation has become the third pillar of science, next to theory and experimentation."

the micro-aperture, the electrical impedance of the medium induces a change in voltage between the two electrodes. This voltage difference is then used to count the number of particles and determine the particle's size, with a greater voltage difference

design issues," describes Isèbe. "We use COMSOL to develop a better understanding of how these physics interact within the device." One of the key advantages that Isèbe found with COMSOL Multiphysics was the ability to import CAD models directly

### COMPLICATIONS AFFECTING ACCURATE MEASUREMENT

The main goal of Isèbe's work was to optimize the impedance measurement system by analyzing and controlling for factors that can negatively influence the accuracy of the device. This includes the particle trajectory through the aperture as well as its orientation, both factors that affect the measured difference in voltage.

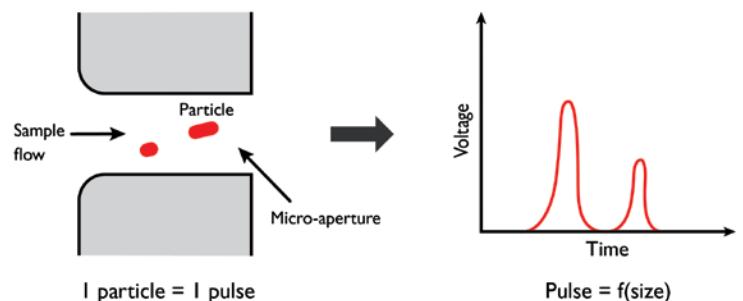
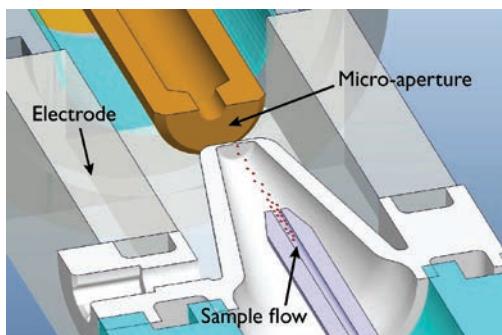


FIGURE 3. Principle of impedance measurement.

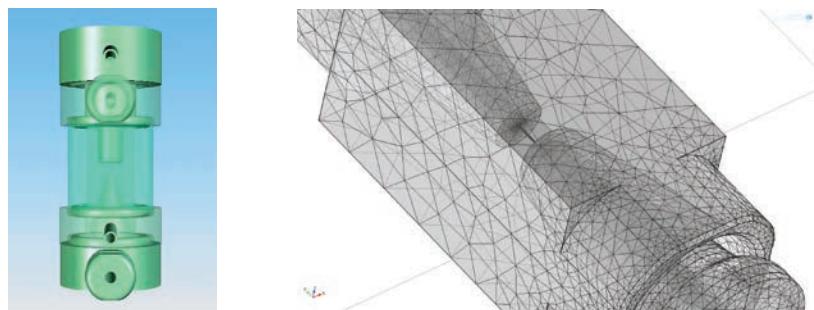


FIGURE 4. CAD model of the micro aperture-electrode system, which was imported into COMSOL Multiphysics using the CAD Import Module.

For example, when a particle passes close to the edges of the aperture where the electric field exhibits high gradients (see trajectory T2 in Figure 5), the particle is exposed to higher electric fields than one that passes through the center of the aperture (see trajectory T1 in Figure 5). Such a phenomenon is known as edge effect. Due to this effect, the resulting electrical pulse is distorted and computation of the particle's size results in overestimation.

This is further complicated by the particle's orientation through the aperture. The electric field distribution changes depending on a particle that passes horizontally or vertically through the aperture, again

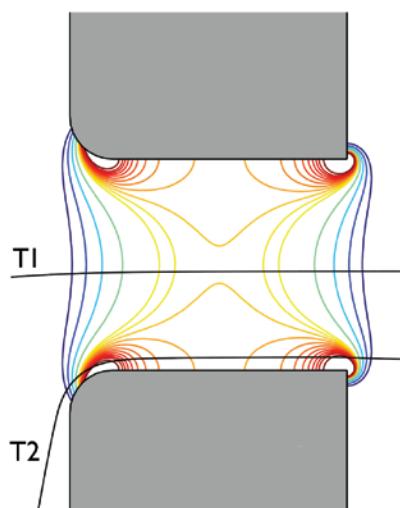


FIGURE 5. Electric field contour plot inside the electrode-aperture. Two possible particle trajectories, T1 and T2, are shown.

resulting in an overestimation of the particle's size (see Figure 6).

### A REAL IMPROVEMENT FOR DIAGNOSTIC EFFICIENCY

Isèbe used simulation techniques to develop a way to account for varying particle trajectories and

“Simulation allows us to improve processes that are inaccessible with just physical prototypes.”

orientations. “Since this is a very small system, it's very difficult to take any measurements experimentally,” describes Isèbe. “Simulation allows us to improve processes that are inaccessible with just physical prototypes.”

Historically, counting and sizing of biological particles in an aperture-electrode system have been completed with the assumption that a sample is evenly distributed within the micro-aperture. The mean particle size was then determined statistically to compensate for errors due to particle trajectory and orientation. This compensation ignores the electrical pulses generated by the particles that pass close to the edge, but in practice it is difficult to differentiate the altered pulses from the normal ones due to the high speed of counting.

In order to improve the accuracy of the device, Isèbe developed numerical models to prove that hydrodynamic focusing could be used to reduce analysis error (see Figures 7 and 8). “Hydrodynamic focusing uses sheath flow to control the sample rate inside the aperture and to direct

the sample flow along the central axis of the aperture,” says Isèbe. “The simulations of this system use a multiphysics approach that models the electrical pulses resulting from the impedance variation combined with particle fluid flow analysis.”

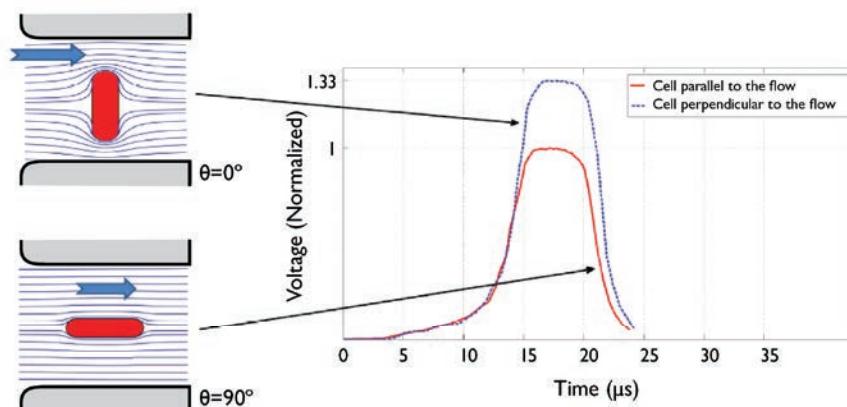


FIGURE 6. Effect of particle orientation on the electric field distribution within the electrode-aperture system and the resulting difference in voltage.

Isèbe ran simulations to analyze how hydrodynamic focusing improves impedance measurement, and to determine the optimal configuration of the device. “Using these models, we can precisely compute the velocity field within the device and analyze the acceleration phase at the entrance of the micro-aperture. We can then use this information to determine which designs produce the most accurate results.” The simulation results demonstrated that hydrodynamic focusing greatly improves the accuracy of particle measurement (see Figure 8, top).

Next, these analyses were compared to the experimental results. “When we compared the simulation and experimental results for the two cases, we estimated that the hydrofocusing device is about twice as accurate as the non-hydrofocusing one,” explains Isèbe referring to Figure 8, bottom.

#### SIMULATION JUSTIFIES TECHNOLOGICAL INNOVATION

The design and optimization of this system of electrical impedance measurement for hematology analysis was truly a multiphysics application, involving the coupling of mechanical, fluid, chemical, and electrical analyses. The resulting devices, the ABX Pentra Series, are among the most accurate

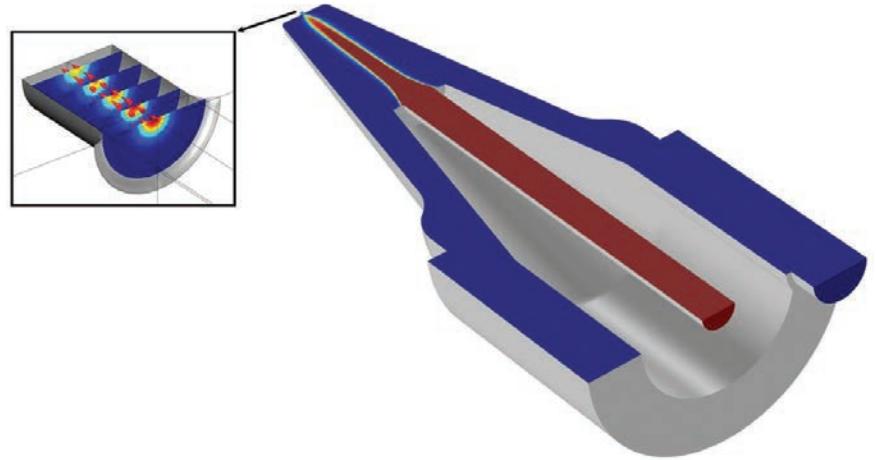


FIGURE 7. Hydrodynamic focusing simulation, showing how sheath flow is used to direct the sample along the central axis of the electrode aperture (sample flow in red and sheath flow in blue).

fully-automatic analyzers on the market today. “Using simulation, I was able to justify the implementation of this technique for hematology analysis into the diagnostic equipment at HORIBA,” says Isèbe. Currently, Isèbe is working on improvements to the particle fluid flow analysis, and plans for future research include 3D processing and the deformability of particles under hydrodynamic

stresses. “Due to advancements in computational analysis and supercomputing capabilities, numerical simulation has become the third pillar of science, next to theory and experimentation,” says Isèbe. “Simulation is now a critical tool for research and development at HORIBA Medical, and it’s a key resource used for decision-making in technological innovation.” ■

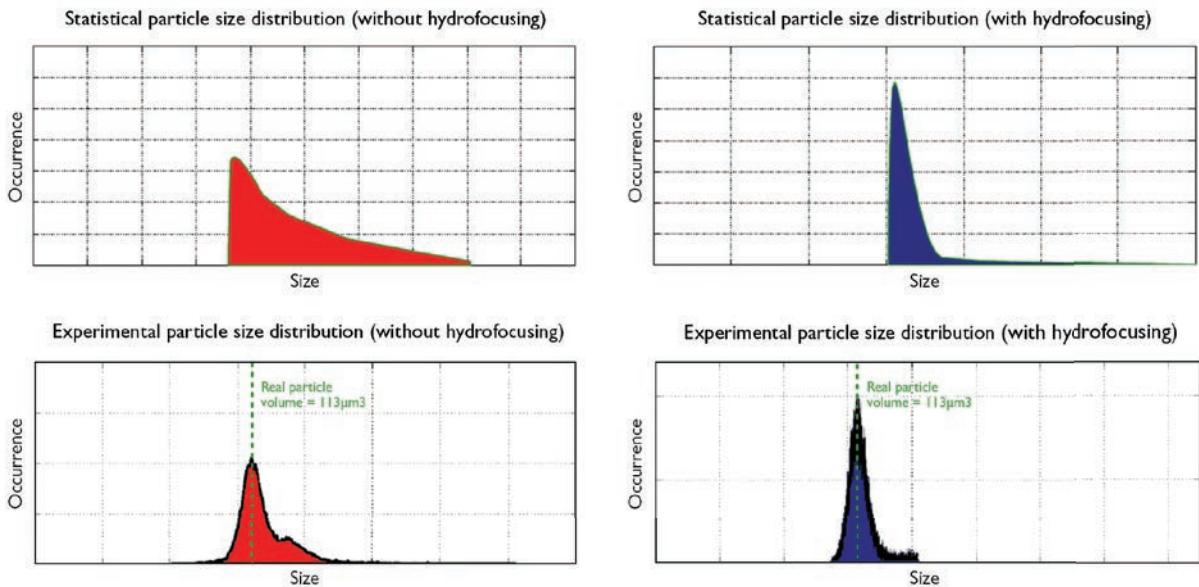


FIGURE 8. Top: Simulation results of the static particle size distribution without hydrofocusing (left) and with hydrofocusing (right). Bottom: Experimental validation without hydrofocusing (left) and with hydrofocusing (right).

# Optimizing Built-in Tire Pressure Monitoring Sensors

Miniature sensors that regulate automobile performance are designed in a very particular way to operate properly while housed directly on moving automobile tires. They need to have the sensitivity to pick up measurements while in motion and the durability to withstand the elements.

BY LAURA BOWEN

Tire pressure is the unsung hero of automobile performance. When inflated to the proper pressure, tires are the exact shape that the designers intended. As air pressure decreases, the tires need more energy to move. Drivers can easily forget to maintain their tire pressure in the day-to-day routine of moving from one place to another. Punctures can take place and go completely unnoticed. That is why having an onboard sensor that alerts the driver when it's time to add more air makes all the difference. Creating these sensors requires careful consideration of all the fine details, and simulation provides the tools for finding just the right design.

## TIRE PRESSURE SENSORS SHAPE DRIVING EXPERIENCE

One consequence of low tire pressure is a significant reduction in fuel economy. Additionally, vehicles running on low tires can add tons of greenhouse gases to the atmosphere over time. Low tire pressure can also make it hard for the vehicle to stop, or cause the car to slip on wet surfaces. Automakers are generally required to attach pressure monitoring sensors to wheels that inform drivers if a tire falls below the intended pressure, and Schrader Electronics is currently the global market leader in tire pressure monitoring technology.

Schrader Electronics manufactures 45 million sensors annually and provides sensors to leading automotive companies including GM, Ford, and Mercedes. For a sensor to

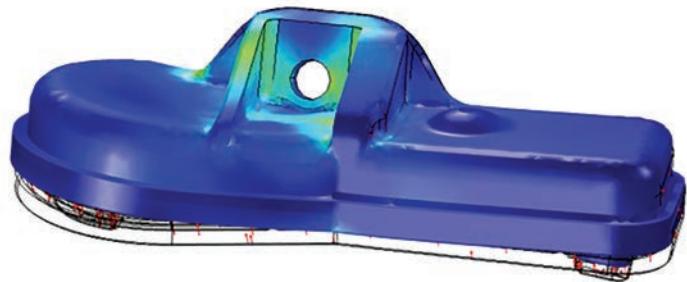
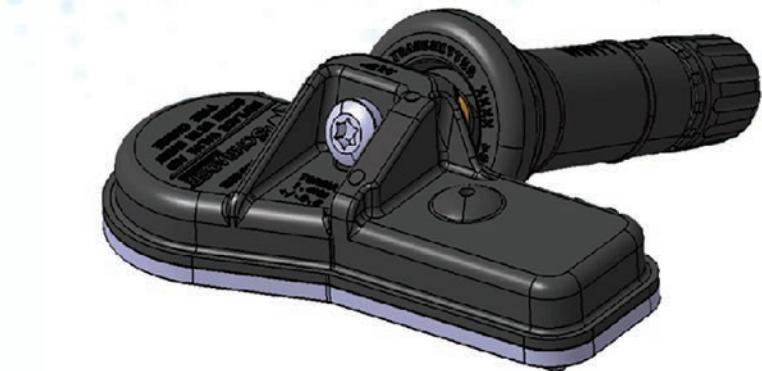


FIGURE 1. Top: A Hi-Speed Snap-In Tire Pressure Monitoring Sensor (TPMS) used to monitor tire pressure and send measurement info. Bottom: 10x amplification of stress and deformation on the transmitter housing as a result of centrifugal loading produced by the wheel's rotation.

survive road conditions throughout the life of a vehicle, reliability and durability are key. Consideration is given to shock, vibration, pressure, humidity, temperature, and various dynamic forces when designing for the necessary functions, geometry,

and materials. Christabel Evans, an engineer with the Schrader Electronics mechanical design team, has been using finite element analysis (FEA) and multiphysics simulation to build successful, efficient tire sensors for all kinds of vehicles.

“COMSOL is user-friendly and it is fast to learn — the engineers picked it up right away.”

#### DESIGNING BETTER SENSORS WITH FEA

The Hi-Speed Snap-In Tire Pressure Monitoring Sensor, shown in Figure 1, is a frequently-used product at Schrader that mounts directly on the wheel assembly and measures tire pressure — even when the car is in motion. When the tire pressure decreases too much, a warning goes off, alerting the driver that it is time to stop and re-inflate the tire.

Schrader Electronics has been creating sensors for almost 20 years, but Christabel Evans and her colleagues wanted a more efficient approach for product design and testing. They simulated their designs using FEA and iterated the process — this allowed them to minimize experimental cost and to evaluate design performance during development. Schrader Electronics found that the existing FEA software options were expensive if they wanted to deploy it to their entire team. They turned to using the Structural Mechanics Module and the CAD Import Module of COMSOL Multiphysics®. They started with a series of tests, comparing standardized samples with simulations to validate the software and build confidence in the results.

#### IMPROVING SENSITIVITY AND DURABILITY WITH BETTER SIMULATION TOOLS

Over time, the researchers began incorporating more natural parameters into their simulations, from dynamic loads such as centrifugal force, to environmental stresses such as temperature change, to static factors such as pressure and crush load. The



FIGURE 2. A spin test simulated on the collar of the device shows stress induced by the centrifugal force concentrated at the bolt locations.

Hi-Speed Snap-In TPMS consists of a transmitter made up of a circuit housed in an enclosure and attached to a valve stem with a cap. The valve stem connects to the tire rim and allows air to pass through. On the Hi-Speed TPMS, the valve geometry includes a rib that helps retain the assembly in the rim hole.

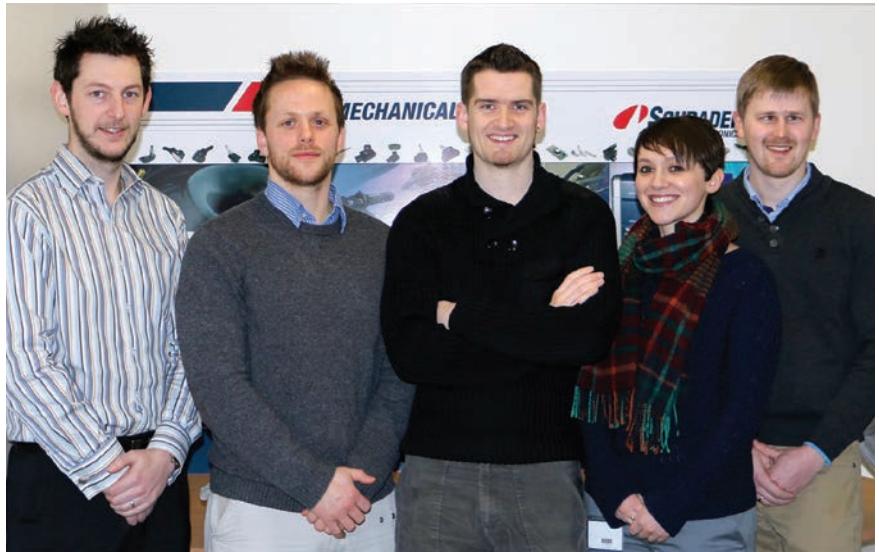
In Figure 1, Schrader Electronics measured the stress on the enclosure from outside forces like tire fitment, shock, or vibration from the road

conditions, and the deformation that occurs when the device is loaded under these conditions. Figure 2 shows a component designed for a spin test machine that rotates the part at high speed. This component was analyzed to verify that the material choice would be able to handle the required loads.

By analyzing several models simultaneously, Evans and her team were able to find the one that works best and improve upon their design. They focused on testing different geometries, materials, and load scenarios.

The researchers at Schrader were able to learn COMSOL Multiphysics software much faster than similar simulation packages, and deployment through the organization was easier because of flexible licensing options. According to Evans, “COMSOL is user-friendly and it is fast to learn — the engineers picked it up right away.”

At the moment, Schrader plans to spend most of their focus on design and growth, with some emphasis on failure analysis, but they hope to improve their development-focused approach with the aid of simulation tools. They are working hard to improve driver comfort, environmental impact, and road safety with each new design. ■



COMSOL is used by many engineers across multiple teams within the Mechanical Engineering Department at Schrader Electronics. From left to right: Andrew Herron, Sam Guist, Adam Wright, Christabel Evans, and Russell McKee.

# Researching a New Fuel for the HFIR: Advancements at ORNL Require Multiphysics Simulation to Support Safety and Reliability

Research into the conversion of the High Flux Isotope Reactor to low-enriched uranium fuel to meet requirements established by the Global Threat Reduction Initiative is ongoing at Oak Ridge National Laboratory. Researchers have turned to multiphysics simulations to evaluate the safety and performance of the new fuel and reactor core design.

BY ALEXANDRA FOLEY

In simple terms, when a beam of neutrons is aimed at a sample, some neutrons pass through the material, while others scatter away at an angle, similar to balls colliding in a game of pool. The final deflection patterns and energies of the neutrons can then be interpreted, allowing scientists to gain information about the fundamental properties of studied matter. This enables neutron-scattering scientists to determine the atomic and magnetic structures of materials and ultimately to achieve a deeper understanding of the world around us.

The High Flux Isotope Reactor or HFIR (pronounced High-FIR) at the Oak Ridge National Laboratory (ORNL) includes a neutron scattering facility that is used by over 500 researchers from around the world each year. The HFIR is a multi-purpose research reactor that also provides stable and radio isotopes to customers in academia, industry, and the medical field. In addition, the HFIR offers unique irradiation experiment facilities and neutron-activation analysis capabilities. The high power production of the HFIR (85 MW) likewise produces a high flux of neutrons to the targets, thereby providing one of the highest steady-state neutron fluxes of any research reactor in the world (see Figure 1).

The HFIR was designed to use highly enriched uranium (93 percent U-235 or HEU), which is similar to a weapons-grade uranium. However, in response to the increasing awareness of the risks caused by the proliferation of nuclear materials, the Global Threat Reduction Initiative has called for the conversion of research reactors using HEU fuel to low-enriched uranium (LEU) fuel.

While many of the world's nuclear reactors have already been converted, a few high-performance

neutron scattering initiatives, isotope production, irradiation experiments, and neutron activation analyses.

“Successful conversion of the HFIR will preserve reactor performance, minimize negative effects on operation efficiency, and help to ensure safety,” says Franklin Curtis, PhD graduate student at ORNL. “We have found that COMSOL is a superior tool for achieving these goals because of its multiphysics capabilities, its use of the finite-element method, and the ability to input user-defined equations.”

“We have found that COMSOL is a superior tool for achieving these goals because of its multiphysics capabilities.”

HEU reactors still remain. Among these is the HFIR, which, due to its unique fuel and core design (see Figure 2) as well as the high power density of the reactor, presents a complex and challenging task for fuel conversion. Researchers at ORNL are using COMSOL Multiphysics® simulation software to explore the impact that the fuel change will have on the HFIR's performance and on

## A PROPOSED LEU FUEL FOR THE HFIR

ORNL researchers involved in the project have developed alternative fuel designs that use a uranium-235 enrichment of 19.75 percent instead of the current 93 percent. In order to accommodate the changes in nuclear characteristics, density, and thermal properties of the LEU fuel, the HFIR core fuel meat — the fissile material located in the fuel plates — must be

redesigned (see Figures 2 and 3). The new design will retain the existing overall geometrical characteristics of the current HFIR core external to the fuel meat.

Additionally, preliminary studies have found that in order to maintain the same neutron flux, the HFIR will have to operate at 100 MW instead of 85 MW, presenting greater demands on the thermal margin of the reactor. "Because we are working with a nuclear reactor, safety is of the utmost importance to us, and we need to know that our models are accurate and reliable," says James D. Freels, a senior research staff engineer at ORNL. "Our models must undergo a rigorous validation process and ultimately must be reviewed and accepted by our Department of Energy regulator in order to continue with the conversion."

Researchers at ORNL are conducting validation studies of the COMSOL code to prove its accuracy. As Curtis describes, "My project at ORNL has been to establish a fluid-structure interaction (FSI) simulation technique that is validated against current safety basis calculations for the HEU fuel and that will allow for the evaluation and safety analysis of the designs using the LEU fuel, while still allowing the reactor to retain the required coolant flow rate."



FIGURE 1. Technicians replace a fuel element of the HFIR at ORNL. The HFIR has operated since 1966 (over 452 fuel cycles) and is currently the only operating nuclear reactor at ORNL. *Image courtesy of the Oak Ridge National Laboratory, U.S. Dept. of Energy.*

### FSI MODELING OF FUEL PLATE DEFLECTIONS

One of the main components of the HFIR is the fuel plates, which control the distribution of velocity and temperature at which coolant enters and flows through the reactor core. These fuel plates can slightly oscillate and deform in response to

changes in velocity and temperature due to reactor operation. One of the most important studies conducted on plate-type research nuclear reactors is to determine the maximum flow rate possible before the deflections interfere with the reactor's performance and safety. "If the deflections are large enough," says Curtis, "It can cause the fuel plates to reduce flow area or even touch one another, altering flow within the channels and disrupting the rate at which coolant flow enters the core."

Representative tests using flow geometries similar to the HFIR can offer insight into fuel plate deflections and be used for code validation. The Advanced Neutron Source Reactor (ANSR), a proposed reactor at ORNL that has since been canceled, had a similar design to that of the HFIR and underwent extensive experimental testing, providing valuable results to validate the COMSOL code<sup>1</sup>.

The ANSR was designed to have fuel plates with a similar involute shape to the HFIR and with cooling flow velocities of about 25 m/s. One test of the ANSR involved experiments to determine the deflection characteristics of the fuel plates. "The involute fuel plates of the HFIR and ANSR have different fuel meat designs than those of other, simpler curved-plate research reactors in the U.S.," says Curtis. "The overall shape maintains a constant coolant channel

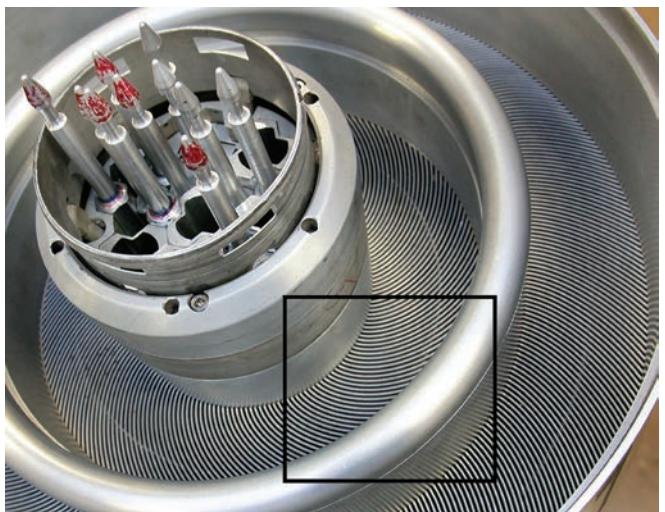
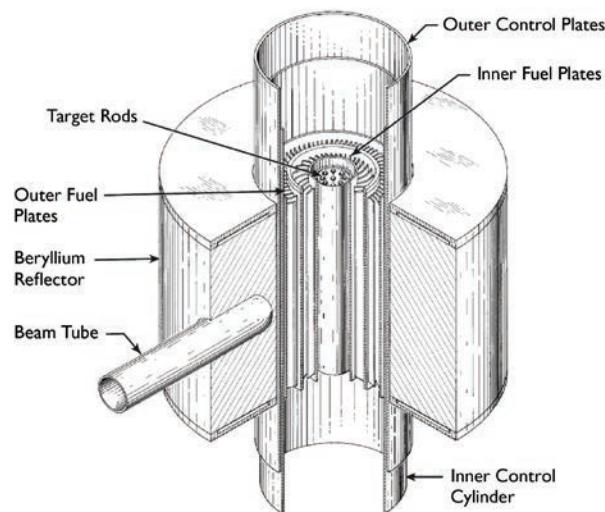
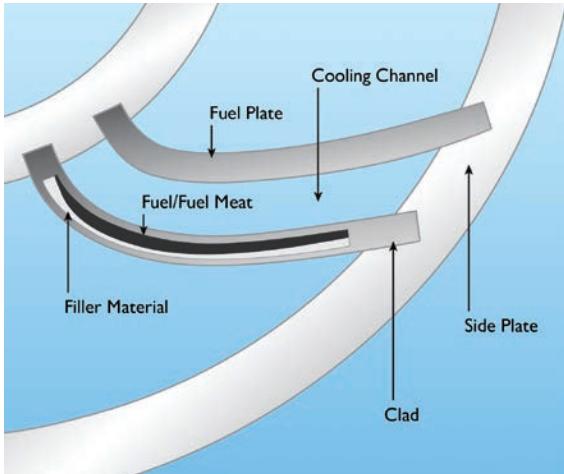
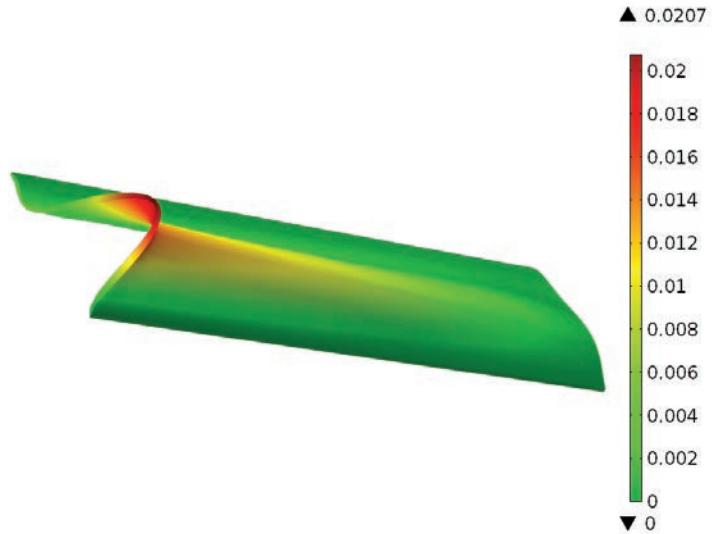


FIGURE 2. Left: A simplified schematic of the current HFIR core. The core of the reactor consists of a series of concentric annular regions divided into inner fuel plates and outer fuel plates. Right: The black box represents the leading edge of the fuel plate that was analyzed in fluid-structure analysis at ORNL. *Images courtesy of the Oak Ridge National Laboratory, U.S. Dept. of Energy.*



**FIGURE 3.** The three regions that make up the current HFIR HEU fuel plate — the fuel (or fuel meat), filler material, and clad. The coolant channel surrounds the fuel plate. The LEU conversion process will change the internal fuel meat. *This image is not to scale and is not an official ORNL figure. It is a reproduction of the design concept of the HFIR core created by COMSOL.*



**FIGURE 4.** Leading edge deflection of the involute fuel plate. Eigenfrequency analyses predicts the “S” shape deflection of the involute fuel plate of the ANSR and HFIR.

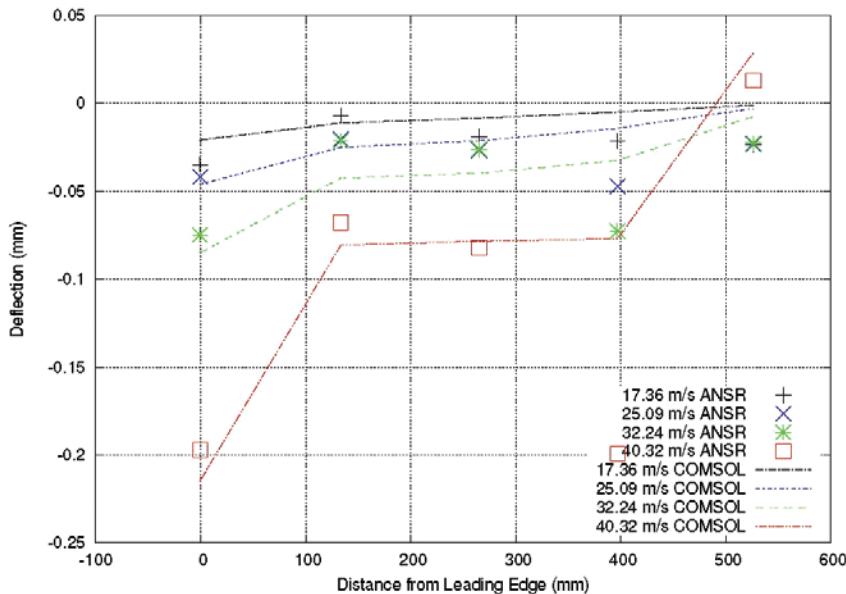
thickness in the core. However, because of their unique shape, the HFIR requires that special attention be paid to the new fuel and core design in order to allow the reactor to maintain the needed flux of neutrons.”

To understand the mechanical FSI taking place within the COMSOL model, a single-plate, two-channel model was developed. The initial analyses first examined flat plates, and the increased complexity of the

involute shape of the fuel plates was later analyzed. The resulting model accurately predicted the FSI and resulting deformations of the ANSR fuel plate experiments along the plate’s length (see Figure 4).

Current FSI simulations include a turbulent CFD analysis of the coolant channels and the fluid-structure deflections of the fuel plates. Previous attempts to solve the FSI problem at ORNL used a weakly coupled approach where the fluid domain was solved first and then the information was used in the structural analysis. “However, this approach was met with an unstable solution and limited success,” says Curtis. “In our current analysis, we instead use the fully-coupled study available in COMSOL Multiphysics and have found that this improved both the stability and accuracy of the ANSR model.” Using this fully-coupled approach, Curtis found that simulations at different flow rates showed excellent agreement with the experimental results (see Figure 5).

Currently, a model of the inner fuel plates of the HFIR using LEU fuel is being developed based off of the analysis techniques used for the ANSR model (see Figure 6). “We’re



**FIGURE 5.** Experimental results of the fuel plate deflection of the ANSR flow tests compared against simulation results for different fluid flow rates.

very happy with the preliminary results that we've obtained from this model," says Curtis. "Over the next few months, we'll continue to improve upon this model to contribute toward a safety basis case for ultimate fuel conversion." The model will later be combined with other COMSOL models being developed at ORNL that couple multidimensional conduction of heat along the plate, thermal-structure deflections of the fuel plate, and other physics such as fuel defects, corrosion, and flow blockages.

**VERIFICATION AND VALIDATION IS KEY**

When designing something as complex as a nuclear reactor, engineers must take every precaution in order to ensure the safety of the design. This requires extensive validation of the simulations being created, as well as the verification of the code itself. "Other simulations of past experiments at ORNL have validated the thermal, structural, and turbulence modeling capabilities of

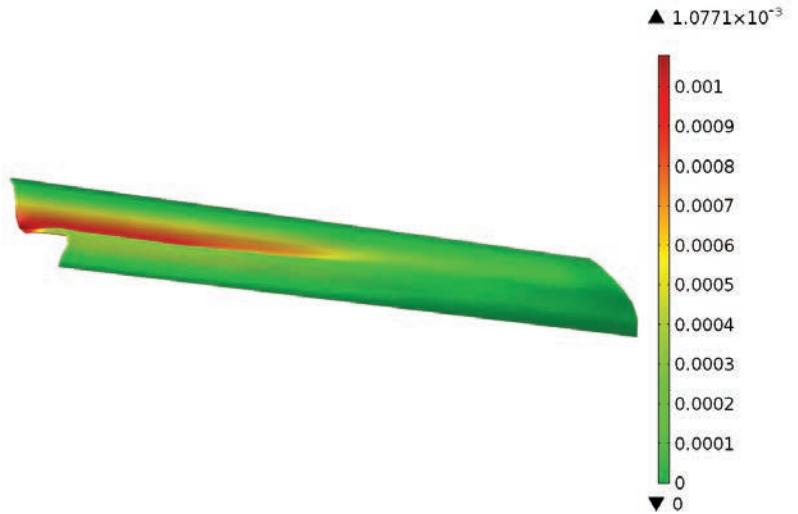


FIGURE 6. Deflection of the leading edge of a HFIR fuel plate.

COMSOL Multiphysics," says Curtis. "Our recent studies have verified the FSI tools of COMSOL, which will allow us to design and optimize the new HFIR core with confidence." ■

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# Gaining Insight into Piezoelectric Materials for Acoustic Streaming

Numerical simulations are helping researchers understand the interplay between surface acoustic waves and microfluidic flow.

BY GARY DAGASTINE

Microfluidic devices are key to many applications such as lab-on-a-chip sensors for medical diagnostics and low-cost flow sensors, but their small size makes effective pumping and fluid mixing challenging.

The mechanical behavior of fluid in geometries a few hundred microns and smaller can differ significantly from behavior at the macroscale. This is because at small scales the ratio of a fluid's surface area to its volume is much larger, and factors such as surface tension, heat transfer, and viscosity play more prominent roles.

Researchers at the SUNY College of Nanoscale Science and Engineering (CNSE) in Albany, NY are exploring the use of surface acoustic waves (SAWs) to induce fluid streaming as a possibility for fluid actuation. Because sound travels at different velocities in substrates and fluids, dispersion results in the wave being launched into the liquid at an angle. The attenuation of this pressure wave causes acoustic streaming (see page 35, at bottom, for more details).

In order to effectively design such devices, an understanding of the acoustic properties of the piezoelectric material used to generate SAWs is a critical first step. In this respect, numerical simulation can be a very powerful tool for helping determine, for example, the effects of various electrode metals and geometries on acoustic wave propagation. The insight gained can be used to inform design decisions.

Graham Potter, a graduate researcher at CNSE, is studying the use of a variety of piezoelectric materials for applications utilizing acoustic streaming. CNSE is part of a unique university-industry partnership with SEMATECH, a worldwide semiconductor

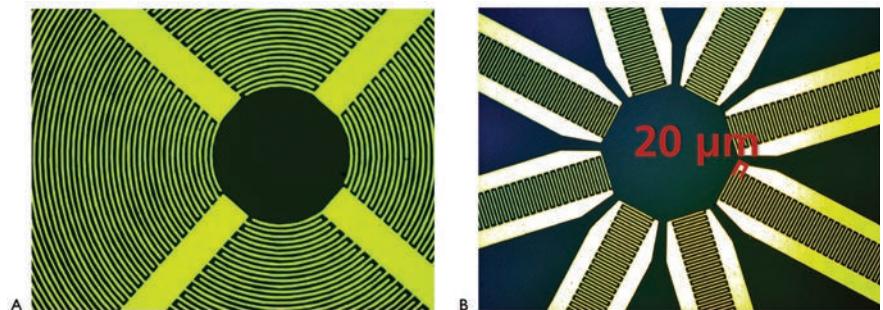


FIGURE 1. A) Optical image of interdigitated transducers or IDTs in a circular pattern on lithium niobate, used to launch surface waves toward a focal point. B) A series of linear IDTs in a two-port configuration. These devices can be used to test the acoustic streaming effect at select orientations over the surface, as well as for experimental validation of simulation results. The 20  $\mu\text{m}$  segment corresponds to the size of the modeled region.

industry research consortium aimed at addressing critical challenges in advanced technology manufacturing.

Potter works in Professor James Castracane's laboratory at CNSE; his team designs devices built with piezoelectric substrates such as 128° Y-cut lithium niobate ( $\text{LiNbO}_3$ ). "The angle of the cut is determined with reference to the crystallographic axes. This particular orientation has traditionally been used in band-pass filters due to the existence of a Rayleigh wave, a type of SAW, with strong electromechanical coupling propagating in a single direction along the wafer surface," he explained.

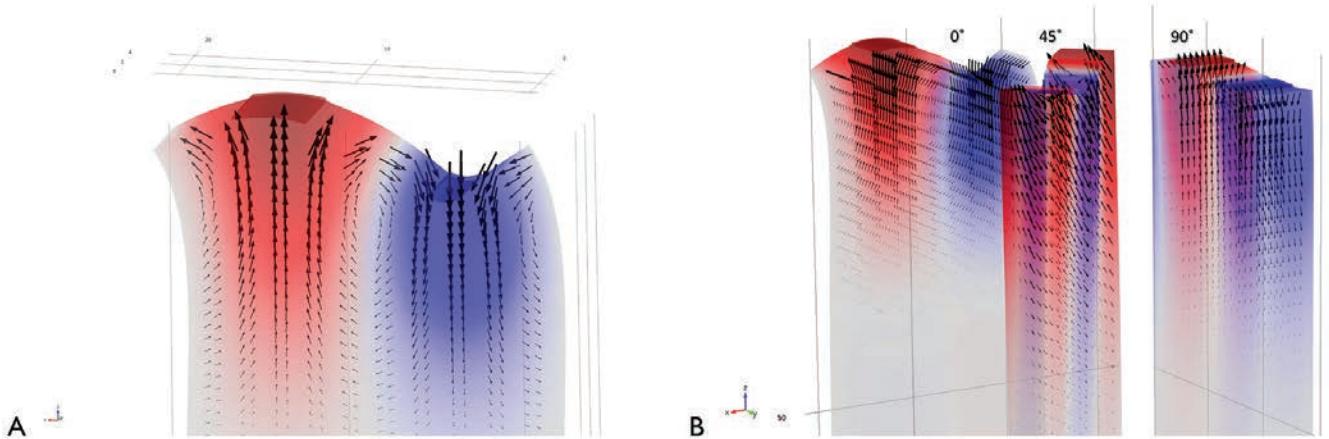
"For this reason, many acoustic streaming studies using this material have been limited to linear devices oriented in one direction. We are interested in building circular or focusing device architectures (see Figure 1A). For this reason, and due to the anisotropy of the crystal, we needed to better understand the propagation characteristics of

waves over the entire surface," Potter continued.

In his setup, arrays of gold electrodes, known as interdigitated transducers or IDTs, are fabricated on a piezoelectric substrate. Alternating current is applied to the electrodes causing the surface to harmonically vibrate due to the inverse piezoelectric effect, generating a SAW. "By varying the orientation of these test devices over the surface (Figure 1B), the resonant frequency and acoustic streaming response can be determined as a function of propagation direction," Potter explained.

## STRONG AGREEMENT BETWEEN SIMULATION AND EXPERIMENT

Simulations were conducted at multiple material orientations using COMSOL Multiphysics® (see Figure 2) and validated against devices fabricated at CNSE. "We observed close agreement between our simulations and the experimental measurements (see Figure 3). This has encouraged the



**FIGURE 2.** A) The vertical displacement and displacement field lines at resonance, obtained from the simulations. For this orientation (0° rotation relative to the crystal X-axis) a Rayleigh wave is observed, with the hallmark displacement in the sagittal plane confined within a few wavelengths of the surface. B) Superimposed images of material displacements for simulations conducted at multiple orientations (0-90 degrees relative to the crystal X-axis), corresponding to orientations of fabricated devices.

further use of COMSOL Multiphysics in our design process and has really accelerated our understanding of the problem,” said Potter.

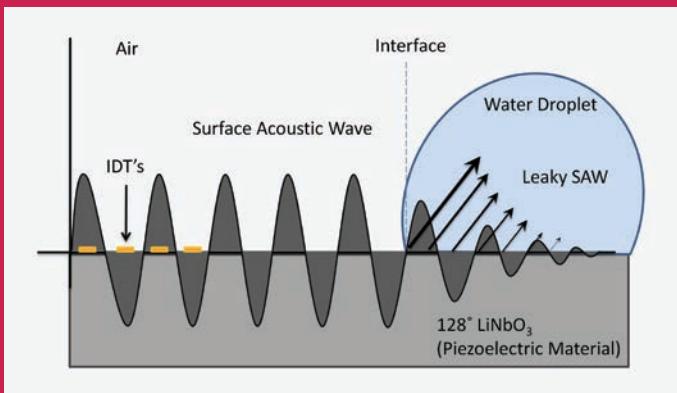
“For instance, we wanted to confirm that surface waves with greater vertical displacements would have higher streaming velocities. In fact, we were able to correlate the result from simulations to the experimentally measured streaming velocities,” he said. “Pieces of information like this are helping to shed light on aspects of the problem and are ultimately leading to tangible design choices.”

Potter has used the Piezoelectric Devices interface in COMSOL Multiphysics for frequency domain analysis in this

particular study. From his simulations he was able to determine the resonant frequency and phase velocity of the SAWs, important design considerations in optimizing their device geometry for acoustic streaming. “Our group is interested in optimizing the streaming effect through a variety of means, and because this work is multidisciplinary by nature, the multiphysics capabilities of COMSOL are very helpful,” he said. “We plan to continue using COMSOL in our research so we can investigate the effects of multiple parameters on our device performance simultaneously, helping to reduce the amount of time we spend prototyping.” ■

Rotation from X-Direction (°)	Experimental Resonance (MHz)	Simulated Resonance (MHz)	Relative Error (%)
0	192.25	190.5	.9
15	187.75	188.2	.24
30	*damaged	182.5	N/A
45	178.75	176.8	1.1
60	174.25	176.0	1.0
75	177.0	177.2	.1
90	178.75	178.7	.03

**FIGURE 3.** Comparison of simulated and experimentally-determined device responses at select orientations. The experimental resonance is determined by measuring insertion loss for devices (Figure 1B) via a network analyzer. The simulated resonance is determined from peaks in admittance, obtained from frequency domain simulations.



## HOW ACOUSTIC STREAMING WORKS

A surface acoustic wave (SAW) can be launched by patterning interdigitated transducers (IDTs) onto the surface of a piezoelectric material. The Rayleigh surface wave will propagate in air with little attenuation; however, upon contacting liquid the wave will begin to “leak” into the fluid. At this point it is referred to as a leaky SAW.

The angle at which it enters the liquid is determined by the SAW’s velocity relative to the speed of sound in the liquid. The attenuation of this pressure wave over a long enough time scale results in fluid flow. The process is known as acoustic streaming, first experimentally observed for the case of standing wave modes by Faraday in 1831.

# SIMULATION-LED STRATEGY FOR CORROSION PREVENTION

Costing billions of dollars annually, corrosion is everyone's problem. Fundamental research in corrosion science at the Naval Research Laboratory will enable scientists to design materials that inherently prevent corrosion.

BY JENNIFER A. SEGUI

Corrosion is a complex multiphysics problem that is currently under investigation by Siddiq Qidwai, a mechanical engineer, and his colleagues at the Naval Research Laboratory (NRL) in Washington, D.C. "In the long run, the success of our research will result in microstructure-corrosion correlations that will enable material designers to include or preclude certain features in the development of new corrosion-resistant materials," explains Qidwai.

A 2011 National Academy of Sciences report from the National Research Council in the U.S. states that a "lack of fundamental knowledge about corrosion and its application to practice is directly reflected in the high societal cost of corrosion." Based on figures reported in December 2010, as much as 600

billion dollars, that is 2 to 4 percent of the U.S. gross national product, were spent to repair or prevent corrosion damage.

The transportation industry including sea, air, and ground transport is particularly affected by corrosion where maintenance costs to preserve passenger safety and vehicle longevity are extremely high. "For the Navy specifically, corrosion is the number one maintenance problem," says Qidwai.

## SMALL GRAINS WITH BIG IMPACT

Pitting corrosion occurs in a metal when electrochemical reactions and mass transport in an adjacent

electrolyte solution result in localized loss of material, as shown in Figure 1. "The pit keeps growing and eventually the material or component will fail under load," says Qidwai, emphasizing the effect that corrosion can have on the strength or integrity of a material.

Qidwai and his colleagues have come up with an innovative and comprehensive approach to better understand pitting corrosion. "We are modeling the growth of corrosion pits in metals in a seawater environment," he explains. "The microstructure of the metal has not been the focus of attention in previous work and consequently the challenges associated with irregular growth

"Our goal is to perform fully-coupled multiphysics modeling of pit growth under the application of mechanical forces to quantify the overall effect on structural integrity."

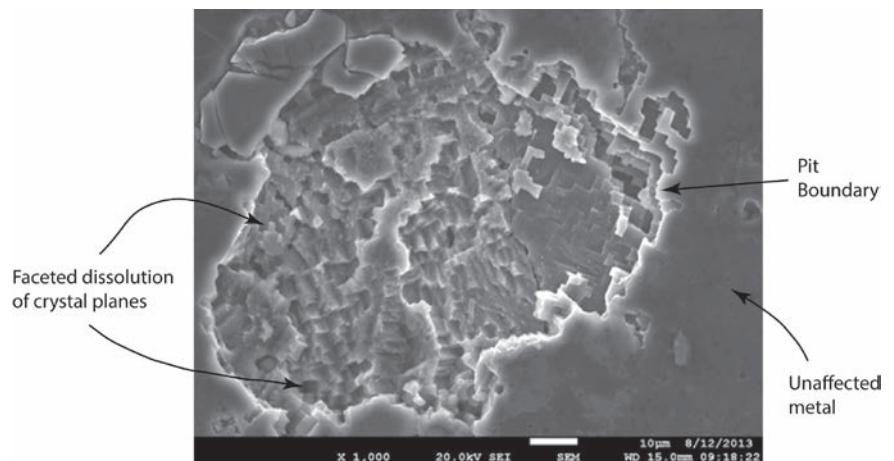


FIGURE 1. Example of pitting corrosion (top-down view) in an aluminum alloy clearly demonstrates the characteristic localized loss of material. The formation of pits can reduce the strength of a material. Image courtesy of C. Feng and S. Policastro, NRL.

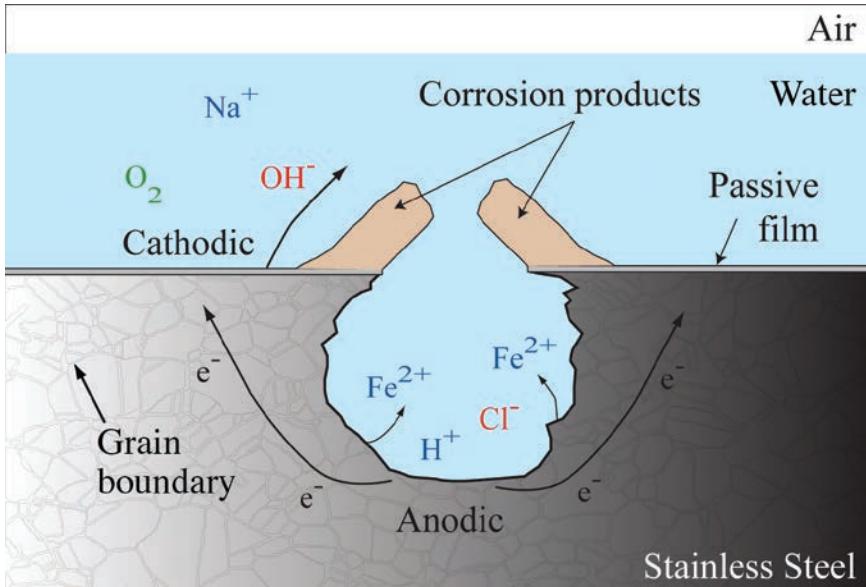


FIGURE 2. Corrosion in metals, such as stainless steel, is the result of electrochemical reactions and mass transport in an electrolyte solution. An irregular corrosion front develops due to the material microstructure.

due to microstructure have not been considered. Our goal is to perform fully-coupled multiphysics modeling of pit growth under the application of mechanical forces to quantify the overall effect on structural integrity with material microstructure taken into account."

The irregular corrosion growth due to the metal microstructure is shown schematically in Figure 2 and arises because of the unique size and shape of each individual grain. Each grain can also have a particular crystallographic orientation that can affect the corrosion rate or front movement locally. Secondary phases, precipitates, and twin boundaries are additional features of a metal that can affect the initiation and growth of corrosion pits.

#### CORROSION SIMULATIONS WITH METAL MICROSTRUCTURE

"A complete description of pit growth," explains Qidwai, "requires the coupling of electrochemical and mass transport equations for multiple ionic species and constitutive descriptions of reaction rates and species diffusion in the electrolyte, while tracking the metal-electrolyte interface or corrosion front whose

movement depends upon the history of the solution." Figure 2 depicts the complex corrosion mechanism simulated by Qidwai in COMSOL Multiphysics® and Figure 3 shows the corresponding model geometry used to evaluate pit growth in metals.

"In developing a complex model, our strategy is to start with simpler numerical studies. Currently in our simulations we solve the electrochemical and mass transport equations

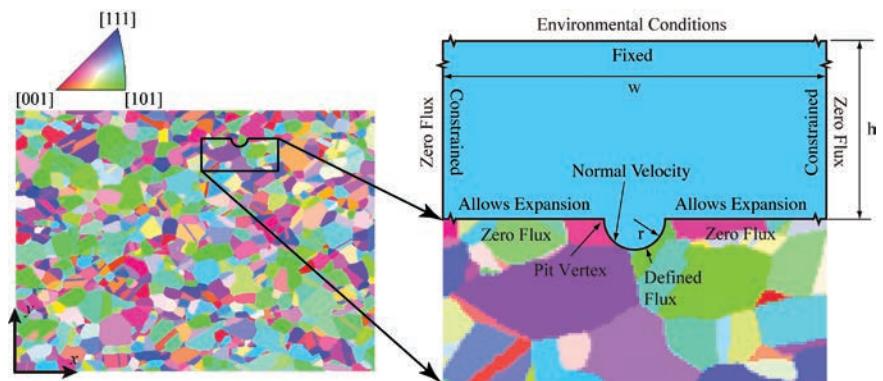
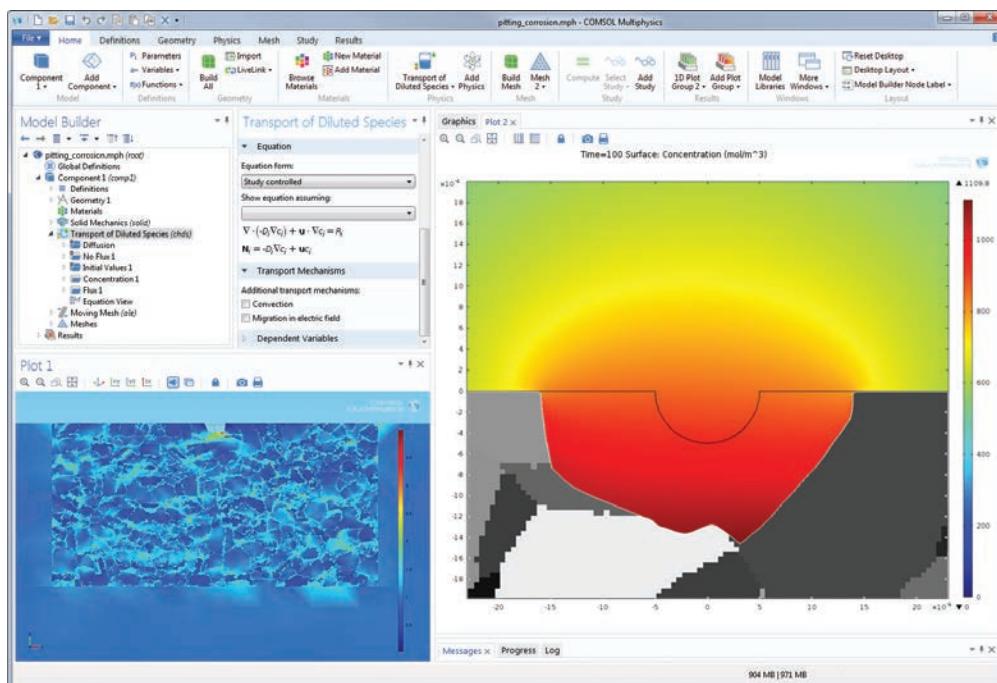


FIGURE 3. At right, the model geometry implemented in COMSOL Multiphysics to evaluate pit growth in metals. The reconstructed metal microstructure, at left, was determined using orientation imaging microscopy at NRL. The colored legend corresponds to the crystallographic orientation of each grain.

"You can use COMSOL Multiphysics with the Corrosion Module to solve this problem. All the work that previously seemed so difficult, now is so easy because you have the module doing a lot of the work for you."

separately. In future work, we will create a fully-coupled electrochemical mass transport model of corrosion." To create their models, they have used the transport of diluted species physics for mass transport, the Laplace and Poisson's equations for the electric potential, and the moving mesh (ALE) technology for the corrosion front. "You can use COMSOL Multiphysics with the Corrosion Module to solve this problem," says Qidwai. "All the work that previously seemed so difficult, now is so easy because you have the module doing a lot of the work for you."



**FIGURE 4.** Screenshot of the COMSOL environment. Plot 1 shows the von Mises stress in the metal with regions of higher stress surrounding the pit. Plot 2 demonstrates pit growth with an irregular corrosion front and shows the distribution of average metal concentration in the electrolyte.

Incorporating the microstructure into a multiphysics model of pitting corrosion is a formidable challenge tackled initially at NRL through the use of orientation imaging microscopy (OIM) to acquire 3D images of the metal microstructure. An OIM-based reconstructed image of steel is shown in Figure 3.

An integrated method was used to incorporate the microstructure of 316 steel into a multiphysics model of pitting corrosion implemented in the COMSOL environment. "At every location along the corrosion front, we have to determine the crystal orientation to calculate the corresponding pitting potential, which in turn determines the corrosion rate and movement of the front," says Qidwai. The pitting potential is determined in MATLAB® for a particular crystallographic orientation and ultimately used by the COMSOL model to calculate the corrosion rate and advance the corrosion front. "LiveLink™ for MATLAB® has been an essential feature for us in order to include the effect of the metal microstructure." The properties of 316 steel were custom-

defined in the model. Simulation results in the COMSOL environment, presented in Figure 4, demonstrate localized loss of material due to pitting.

In developing their multiphysics model of pitting corrosion, Qidwai found that "COMSOL is so versatile that it will give you a solution even for very complex applications. This is where experimental validation is the key." Insight gained from their simulations has already provided the



From left to right: Siddiq Qidwai (NRL), Virginia DeGiorgi (NRL), and Nithyanand Kota (Leidos Corp.) are researching the fundamental mechanism of corrosion in metals.

impetus for the development of a novel experimental method to evaluate corrosion at the micron scale. The results from the experiments will be used to validate the model and establish the relationship between microstructure, pit shape, and growth.

#### THE FUTURE OF CORROSION PREVENTION

As the model is validated and further evolves, it will also include fully-coupled structural mechanics analyses to elucidate the impact of pit growth in a metal on its strength and reliability. At present, a decoupled structural analysis of microstructural steel has been successfully implemented as shown in Figure 4. Qidwai and his team at NRL are also actively developing methods to quantify the relationship between microstructure, pit growth, and mechanical performance. "Establishing this relationship is our ultimate goal and will enable material designers to create materials that better resist and even prevent corrosion, therefore reducing the exorbitant cost and inconvenience shared by everyone." ■

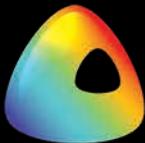
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# Patterning Cells with the Flip of a Switch for Bioengineering Applications

Simulation aids researchers in understanding how unevenly-shaped cells rapidly form patterns under an applied electric field. This method, dielectrophoresis, is currently under development at Clemson University and Tokyo Electron for layer-by-layer material assembly.

BY JENNIFER A. SEGUI

Significant growth in biofabrication research over the past decade has been accompanied by the development of innovative patterning methods to manipulate molecules or groups of cells to create, for example, organized constructs and reactive biological systems. These engineered biomaterials can be used for a wide range of applications, including early stage drug development and testing.

Dielectrophoresis (DEP) has emerged recently as a promising method for patterning cells and for nanoscale assembly of materials for electronics, energy, and medical applications. "DEP is particularly attractive for cell or material patterning because it provides a precise and efficient technique for layer-by-layer assembly that is suitable for industry-scale mass production," explains Guigen Zhang, Professor of

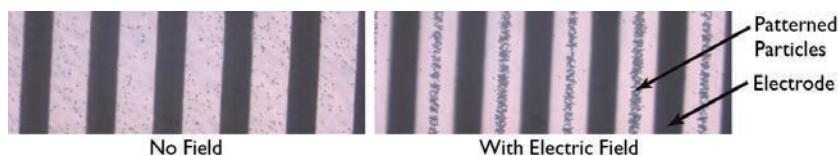


FIGURE 1. Under an applied electric field, the disordered sample of particles at left assembles into organized lines between pairs of electrodes that alternate between positive and ground potential.

Bioengineering at Clemson University where he leads the Biosensors and Bioengineering Laboratory. "In DEP, a non-uniform electric field applied across a single layer of dielectric particles can be used to pattern the entire sample in mere seconds, at the flip of a switch" (see Figure 1).

Zhang is working in collaboration with researchers Jozef Brcka, Jacques Faguet, and Eric Lee from Tokyo Electron U.S. Holdings, Inc. to better

understand the fundamental principles behind DEP and optimize its use for patterning<sup>1-3</sup>. Their investigation entails using multiphysics simulation in combination with experiment to verify new theories and equations governing the DEP force. Drawing from the investigation of DEP for complex biological systems could also produce novel bio-inspired methods for enhancing the capabilities of tools for the semiconductor industry.

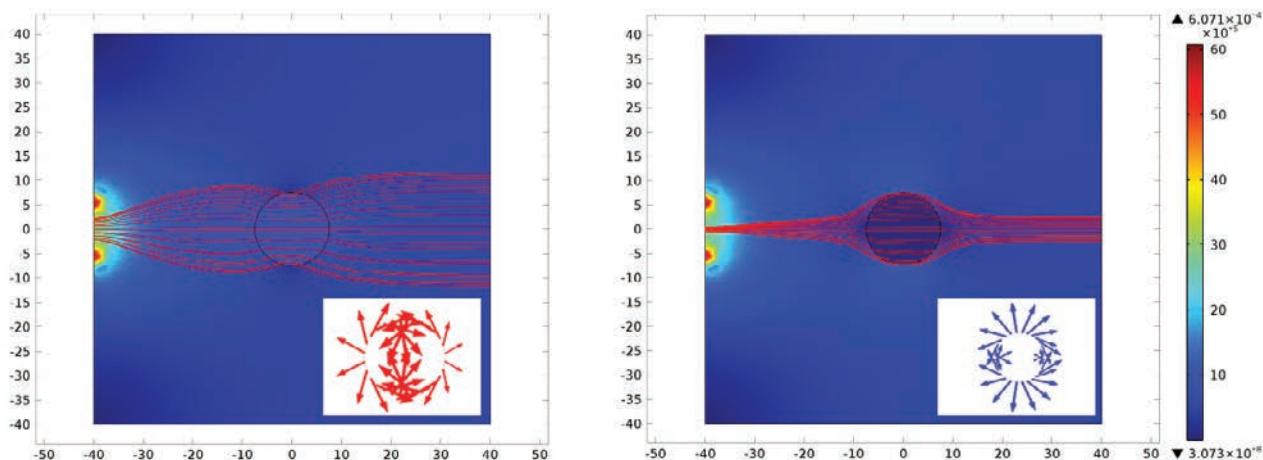
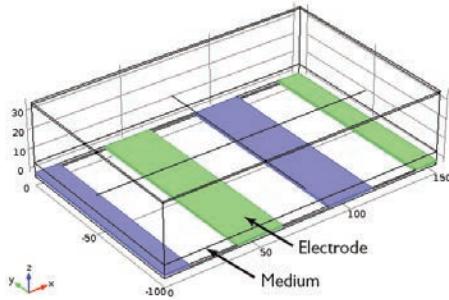
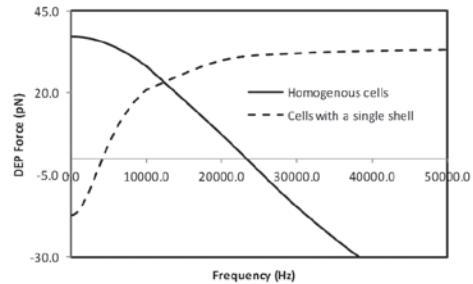


FIGURE 2. Simulation results from COMSOL Multiphysics® demonstrate surface polarization for a model of a particle suspended in a medium and subject to a non-uniform electric field. At left: Positive DEP occurs when the particle is more polarizable than the suspension medium creating a net DEP force that points left, in the direction of increasing field strength. At right: Negative DEP occurs when the particle is less polarizable than the suspension medium, causing the particle to move toward the right in the direction of decreasing electric field strength.



**FIGURE 3.** The model geometry is shown with the parallel electrodes biased with alternating potential and ground in the simulations.



**FIGURE 4.** Plot of the frequency-dependent DEP force experienced by a cell when it is modeled as a homogenous body or as a nonhomogeneous body with a single shell.

### MECHANISM OF DEP

In DEP, either non-uniform AC or DC electric fields are applied to dielectric particles or cells in media causing them to become polarized. The relative polarizability of the particle and media ultimately determines the dipole orientation and, consequently, the direction of movement along the field lines (see Figure 2).

Zhang and his colleagues have identified several discrepancies or limitations of the existing DEP theory to accurately explain observed behavior such as cell rotation, particle alignment, and electric field distortion. Their research aims to address these limitations and elucidate the impact of the observed behavior on pattern formation.

### SIMULATING THE DEP FORCE FOR CELLS

Several 2D and 3D models have been developed by the Clemson-Tokyo Electron collaboration using the Electrostatics interface, Moving mesh interface (ALE), and the equation-based modeling capabilities in COMSOL Multiphysics®. Each model investigates the variables affecting the DEP force experienced by

particles leading to the observed rotation and alignment behavior.

In the 3D models, the electrode setup consists of equidistant rectangular strips of gold coated with insulating aluminum oxide where alternating electrodes are positively biased and grounded (see Figure 3). Particles or cells are suspended in deionized water or other media in the models.

To illustrate the limitations in existing DEP applications, shell models that take into account the nonhomogeneous properties of cells were used to calculate the complex permittivity and then the DEP force in the simulations. Additionally, in some studies, the formation of an electric double layer and the particle size were taken into account when calculating the conductivity of the particle.

For example, the magnitude of the simulated DEP force determined using a single-shell model, which takes into account the nonhomogeneous properties of the cell membrane, appropriately shows a trend that is actually the opposite of the original theory (see Figure 4). Zhang notes that, “with

COMSOL, simulation is no longer a black box approach, thus enabling us to better understand the factors affecting DEP.”

Although single-shell models for cells provide a more accurate prediction, to incorporate the nonhomogeneity in other cellular components including the nucleus, Zhang and colleagues developed a volumetric approach to account for electric field distortion and to quantify the DEP forces and torques experienced by cells<sup>3</sup>. “Simulation results based on the new approach successfully confirm experimental observations that cells could rotate due to the noncircular shape of the cell body and off-centered nuclei,” reports Zhang.

By developing and validating comprehensive multiphysics models that incorporate a multitude of factors, their work provides a wealth of information and a better understanding of how DEP can be used with great selectivity to pattern cells and other materials. Zhang believes that their “efforts will someday help realize many potential capabilities of DEP for important bioengineering applications including bioprinting, biofabrication, and biosensing for advancing drug screening and discovery, tissue engineering, and regenerative medicine.” ■

### References

Refer to the following online resources from the Proceedings of the COMSOL Conference 2013, accessible at [www.comsol.com/papers-presentations](http://www.comsol.com/papers-presentations):

- <sup>1</sup> V. Pandian, et. al. *Some Commonly Neglected Issues Which Affect DEP Applications*.
- <sup>2</sup> Y. Zhao, et. al. *Effect of Electric Field Distortion on Particle-Particle Interaction Under DEP*.
- <sup>3</sup> Y. Zhao, et. al. *Elucidating the Mechanism Governing the Cell Rotation Behavior Under DEP*.



At left, from left to right: Johnie Hodge, Sam Bearden, Guigen Zhang, Yu Zhao, and Vandana Pandian from Clemson University. At right, also from left to right: Jozef Brcka, Eric Lee, and Jacques Faguet from the Technology Development Center at Tokyo Electron U.S. Holdings, Inc.

# Scattering of Electromagnetic Waves by Particles

Particles can be characterized by the unique scattering patterns produced by their interaction with electromagnetic waves. Optical scattering measurements cover a broad range of applications such as meteorology, particle sizing, biomedical, and metamaterials.

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

As electromagnetic waves propagate through matter they interact with particles or inhomogeneities that perturb the local electron distribution. This variation produces periodic charge separation within the particle, causing oscillation of the induced local dipole moment. This periodic acceleration acts as a source of electromagnetic radiation, thus causing scattering.

## PARTICLE SIZE MATTERS

Scattering of electromagnetic waves by particles can be illustrated by two theoretical frameworks: Rayleigh scattering that is applicable to small, dielectric, non-absorbing spherical particles, and Mie scattering that provides a general solution to scattering that is independent of particle size. Mie scattering theory converges to the limit of geometric optics at large particle sizes. Consequently, Mie scattering theory can be used to describe most scattering by spherical particles, including Rayleigh scattering, but due to the complexity of implementation, Rayleigh scattering theory is often preferred.

The Rayleigh scattering model breaks down when the particle size becomes larger than approximately 10 percent of the wavelength of the incident radiation, at which point Mie theory must be applied. The Mie solution is obtained by analytically solving Maxwell's equations for the scattering of electromagnetic radiation by spherical particles; it is modeled in terms of infinite series rather than a simple mathematical expression.

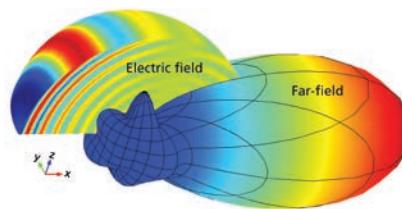


FIGURE 1. Electric field due to Mie scattering of the incident wave in the x-direction showing enhanced scattering in the forward direction.

Mie scattering differs from Rayleigh scattering in several respects: it is mostly independent of wavelength and is larger in the forward direction than in the reverse direction (see Figure 1). The greater the particle size, the more light is scattered forward. In addition to the many atmospheric effects of light scattering, applications of Mie scattering include environmental models such as dust particles in the atmosphere and oil droplets in water, as well as medical technology used to measure cell nuclei in biological systems or the collagen fibers in body tissue.

## MIE SCATTERING

Implementation of analytical solutions for Mie scattering by a particle or object is complex and requires solving Maxwell's equations to represent the incident, scattered, and internal fields. These take the form of infinite series expansion of vector spherical harmonics, allowing the cross sections, efficiency factors, and distributions of intensity to be predicted. Further, the

influence of particle geometry, the angle of incidence of the wave, and the particle material properties can be investigated.

In electromagnetic wave scattering problems, the total wave decomposes into the incident and scattered wave components. Important physical quantities can be obtained from the scattered fields. One of these is the cross section, which can be defined as the net rate at which electromagnetic energy crosses the surface of an imaginary sphere centered at the particle, divided by the incident irradiation ( $P_{inc}$ ). To quantify the rate of the electromagnetic energy absorbed ( $W_{abs}$ ) and scattered ( $W_{sca}$ ) by the particle, the absorption ( $\sigma_{abs}$ ), scattering ( $\sigma_{sca}$ ), and extinction ( $\sigma_{ext}$ ) cross sections are defined as:

$$\sigma_{abs} = \frac{W_{abs}}{P_{inc}}, \quad \sigma_{sca} = \frac{W_{sca}}{P_{inc}}, \quad \sigma_{ext} = \sigma_{abs} + \sigma_{sca}$$

The total absorbed energy is derived by integrating the energy loss over the volume of the particle. The scattered energy is derived by integrating the Poynting vector over an imaginary sphere around the particle.

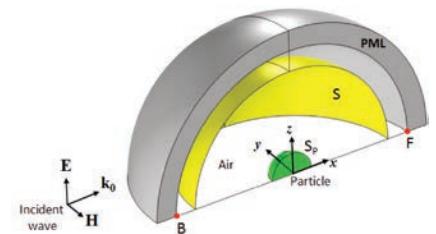


FIGURE 2. Model geometry for Mie scattering by a spherical particle.

**COMPUTATIONAL ELECTROMAGNETICS**

A computational model of Mie scattering was developed using COMSOL Multiphysics® and its RF Module. It solves for the scattering off of a dielectric, magnetic, or metal spherical particle with radius  $\alpha$ . The model geometry is shown in Figure 2.

The air domain is truncated by a perfectly matched layer (PML) inserted

to limit the extent of the model to a manageable region of interest. The solution inside the domain is not affected by the presence of the PML, which lets the solution behave as if the domain was of infinite extent. This layer absorbs all outgoing wave energy without any impedance mismatch that could cause spurious reflections at the boundary. The PML is useful in maintaining the solution at the desired

level of accuracy and optimizing usage of computational resources. COMSOL also supports far-field calculations, which are done on the inner boundary of the PML domain where the near field is integrated. The surface  $S$  is used to calculate total scattered energy. An incident plane wave travels in the positive  $x$ -direction (see Figure 2), with the electric field polarized along the  $z$ -axis. Perfect magnetic conductor (PMC) and perfect electric conductor (PEC) boundary conditions are used on the  $x$ - $z$  and  $x$ - $y$  symmetry planes, respectively. The plane wave incident on the sphere is defined by its amplitude, wave vector in the air, and circular frequency. COMSOL conveniently provides all the necessary

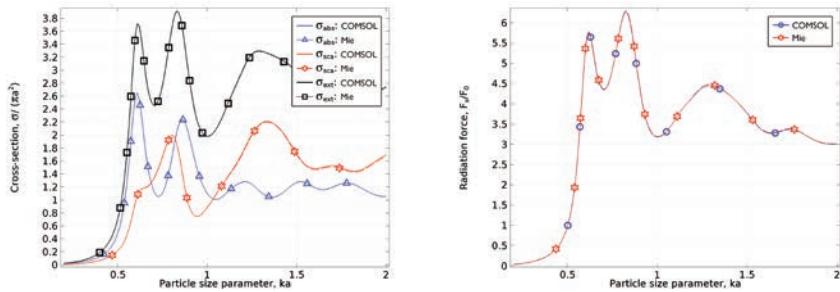


FIGURE 3. Cross-section parameters and radiation force for a dielectric particle with refractive index  $n = 5 - 0.4j$  and relative permeability  $\mu = 1$ .

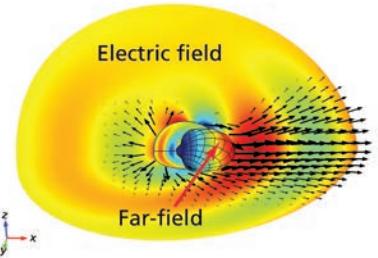


FIGURE 6. Distribution of the  $z$ -component of the electric field due to scattering of the incident electromagnetic wave by a particle of  $0.1\mu\text{m}$  radius. The arrows show the time-averaged power flow of the relative fields at a frequency of 950 THz.

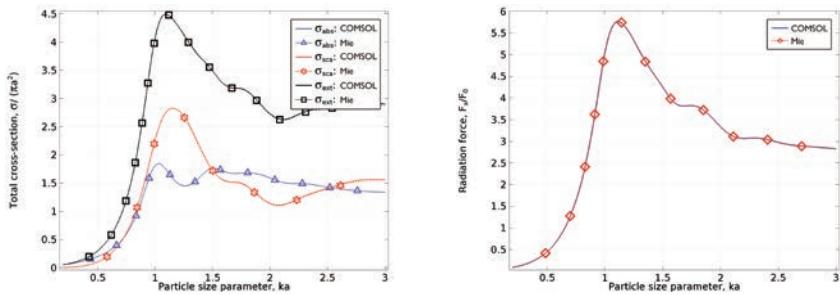


FIGURE 4. Cross-section parameters and radiation force for a magnetic particle with relative permittivity  $\epsilon = 1$  and relative permeability  $\mu = 8 - 2j$ .

functionality to calculate scattering integrals. Scattering characteristics for the three types of particles considered are shown in Figures 3, 4, and 5. The results of the computational analysis show good agreement with available experimental results<sup>1</sup>.

Simulation of Mie scattering problems enables visualization of the effects of small particles on an incident electromagnetic wave (see Figure 6) to allow better understanding of the interactions. ■

**References**

<sup>1</sup>Mätzler, C., *MATLAB Functions for Mie Scattering and Absorption, Version 2*, IAP Research Report, (Bern: Institut für angewandte Physik, Universität, 2001), No. 2002-11.

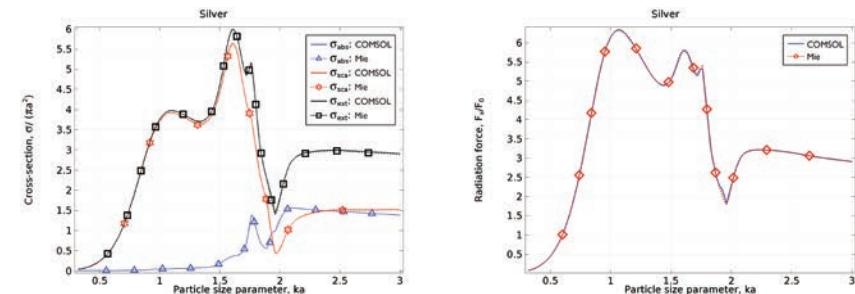


FIGURE 5. Cross-section parameters and radiation force for a silver particle with dielectric constants.

# FLOATING ON SOUND WAVES WITH ACOUSTIC LEVITATION

Sound is a formidable power. Under the right conditions, it can manipulate and change the state of matter. The pharmaceutical industry is turning to acoustic levitation to address the ever-present need for high-quality medicine delivery systems, especially as technology for treating patients expands and becomes more customized.

BY LAURA BOWEN

At Argonne National Laboratory, part of the United States Department of Energy, Kamlesh Suthar and Chris Benmore are hard at work implementing acoustic technology to transform the manufacturing of pharmaceuticals. The team is turning to multiphysics simulation to improve their acoustic levitator—a device that generates sound waves to lift and manipulate matter.

## ACOUSTICALLY MANUFACTURED PHARMACEUTICALS

By mixing chemicals while they spin and float in the air, Argonne is working to facilitate more

efficient production and delivery of pharmaceutical products. In a controlled environment, the levitator provides a containerless and contaminant-free space for creating high-purity amorphous chemicals. According to the team at Argonne, “Many amorphous drugs are mixed with a polymer to help keep them stable for a long time.” At the midpoint of each node of the standing waves in Suthar’s acoustic levitator, molecules gather into droplets and form small spheres (see Figure 1). The droplets float a few millimeters apart and gently rotate, suspended, between two small piezoelectric transducers.



FIGURE 1. The acoustic levitator creates standing sound waves that allow droplets of liquid to levitate. The levitator is made of two transducers, each coated with a thin layer of foam to control the wave pattern.

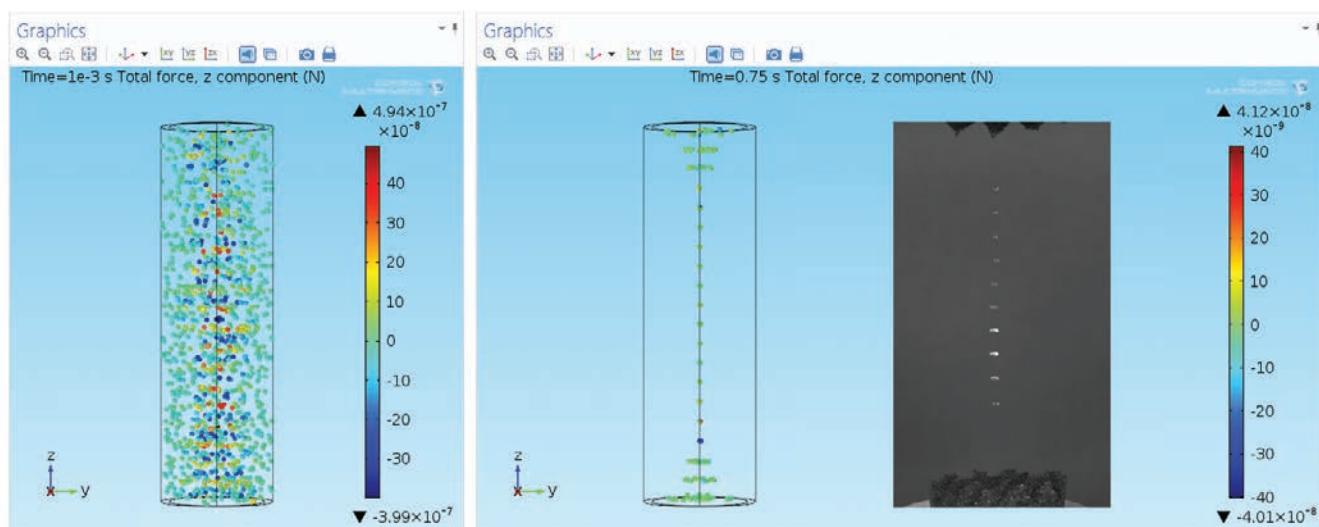


FIGURE 2. The initial distribution of the particles at  $t=0.001$  (left). Particles gather into droplets at  $t=0.75$  and photograph of physical particle distribution (right).

A magnitude and frequency slightly above the audible range, 160 dB and 22 KHz, generates standing acoustic waves with pockets of high-pressure zones. The transducers convert electrical energy into acoustic pressure. The method set in place by Suthar and Benmore is a powerful technique for developing medicine. It is easier for human bodies to absorb and process amorphous chemicals because they are more soluble and bioavailable than when in crystalline form.

### THE LIFTING POWER OF ACOUSTOPHORETIC FORCE

Designing the geometry just right to control the movement of the particles was crucial to the function of the levitator. In this experiment, several counterbalancing forces work together to create a phenomenon that allows the particles to float in a controlled way (see Figure 2). The acoustophoretic force, particle-particle interaction, drag, gravity, and surface tension of the droplets need to be taken into account. Specific patterns of Gaussian profile foam made of polystyrene were designed to remove any unwanted acoustic waves generated by the transducers and act as a filter along the edge of each one, creating a well-defined standing wave that reflects evenly, with little interference.

These parameters cause the particles to arrange vertically, then rapidly form into droplets. The droplets stay in the desired vertical position because they are constantly moving horizontally.

### HOW ACOUSTIC SIMULATION STACKS UP AGAINST EXPERIMENTS

The team created a COMSOL Multiphysics® simulation to verify their synchrotron-based x-ray experiments at APS, the Advanced Photon Source, a facility that holds the brightest storage ring-generated x-ray beams in the western hemisphere. They used the Acoustics Module and Particle Tracing Module, add-ons to COMSOL. They first considered the frequency and material properties of the piezoelectric transducers and any thermal effects that might impact the levitator. They then used a trial-and-error method to

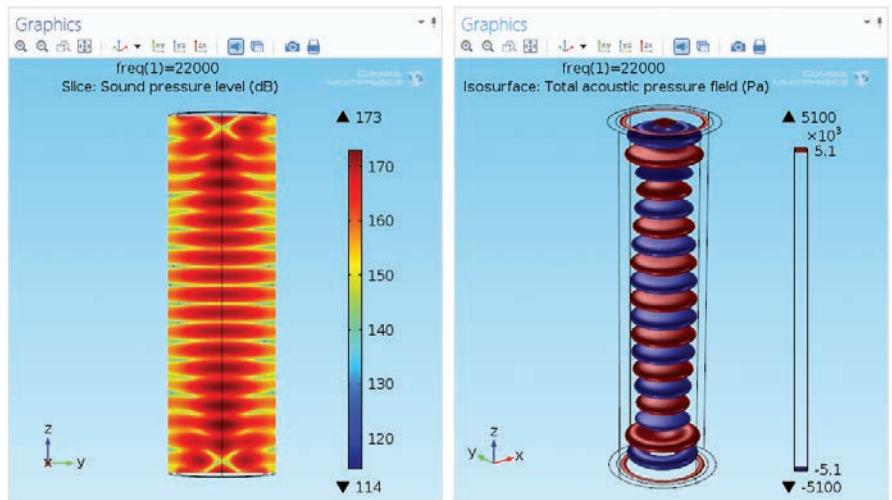


FIGURE 3. Regular sound pressure level generated due to a standing pressure wave at 22 KHz frequency (left) and pressure pockets with alternative pressure value (right).

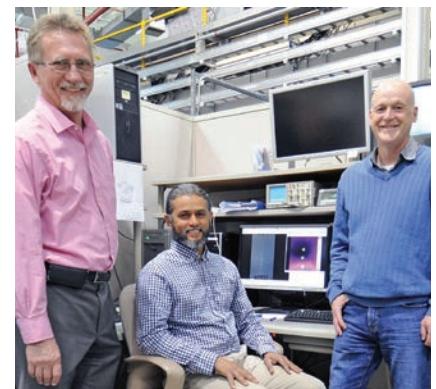
find a foam geometry that allowed them to control how individual droplets would form. In addition, they considered how changes to the viscosity and surface tension can affect their shape. The interference creates droplet structures that Suthar mapped with a fluid structure interaction (FSI) simulation. He considered all of the relevant effects using the CFD Module and level set method, a numerical way to keep track of interfaces between different media during the simulation. Using the level set method to control the shape of the droplets at various shifts in acoustic modes helped Suthar to achieve a spherical shape and control the way the droplets interacted.

When the researchers ran the experiment to verify their design, they discovered that the results of the simulation were consistent with the behavior of the droplets in the high-speed photographs that they took at APS. The simulation results showing the acoustic field distribution (see Figure 3) were also similar to the experimental results.

As Suthar explains, “With the constructive interference of pressure waves, we get a standing pressure wave with positive and negative pressure pockets. Within these pockets, the sound reaches roughly the level of water droplet levitation. So if you sprinkle water mist, the

droplets are pushed to the center and levitate due to the balancing forces involved.”

The researchers at Argonne solidified their design with the help of multiphysics simulation. As the scientists continue to hone the designs of their acoustic levitators, the possibilities for innovation are infinite. Pharmaceutical developers will be able to control the concentration, droplet size, and amount of each chemical in medicine. The discoveries that Argonne is making have wide applications in the global medical community. This is especially true where new resources and machinery could mean truly life-changing advances for patients. ■



The Argonne team, from left to right: Patric Den Hartog, Kamlesh Suthar, and Chris Benmore.

# Actuation Technique for Miniature Robots Developed using Multiphysics Simulation

Researchers at the French Atomic Energy and Alternative Energies Commission are making miniature robotic manipulators easier to build and operate. They hope to offer a less expensive actuator than those currently used in surgical devices; one day, it may revolutionize the methods seen on the operating table.

BY LEXI CARVER

Minimally invasive surgery depends on small, flexible tools with reliable actuation and consistent performance. Robotic devices have entered the operating room as assistants to procedures requiring hours of standing on the part of the surgeon. But many robotic surgery devices are expensive, bulky, and exhausting to operate. Christine Rotinat, researcher at the Systems and Technologies Integration Laboratory of the French Atomic Energy and Alternative Energies Commission (CEA LIST, Gif-sur-Yvette, France), has sought to create an alternative.

## IMPROVING SURGEON EXPERIENCE THROUGH PHASE-CHANGE ACTUATION

Rotinat's goal was to provide surgeons affordable, versatile robotic tools that

would reduce their pain following long procedures. The device would need to be inexpensive, miniaturized, produce high forces with relatively large displacements, exhibit reasonable electrical consumption, and follow medical guidelines. For instance, high voltages are unsafe, and magnetic fields cannot be present around equipment such as MRI machines.

Rotinat investigated miniature phase-change actuators, which create movement and force from the volume expansion that occurs when a material shifts from the solid to the liquid state. She needed a material with a high expansion rate and stress tolerance, and a phase change occurring at a temperature between the patient's body temperature and the authorized limit. Rotinat examined a microactuator created by

Goldschmidtböing et al. that relies on paraffin, a wax hydrocarbon that expands 10-20 percent by volume when heated from a solid to a liquid. It was combined with carbon black particles, creating a conductive composite that would support Joule heating when an electric current passed through.

Goldschmidtböing's microactuator contains a chamber filled with conductive paraffin at a 2 percent carbon black concentration, covered by a silicon membrane and a metal sealing chip for applying a current, separated by an electrically insulating layer (see Figure 1). The paraffin expansion causes the silicon membrane to deflect outward, driving the movement of the actuator.

Rotinat and her team evaluated the mechanical behavior and control aspects of this composite in the CEA

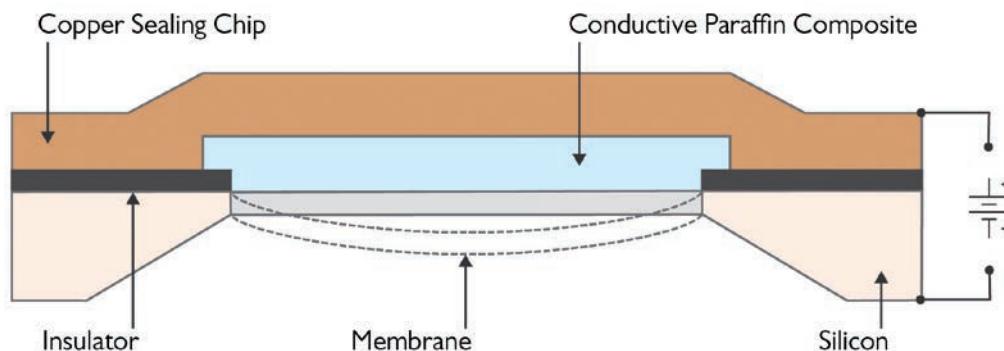


FIGURE 1. Schematic principle of a phase-change microactuator based on Goldschmidtböing et al.

“We can easily parameterize and change the actuator height, the membrane thickness, and the wax composite model.”

LIST miniature actuator (see Figure 2), while her colleague Panagiotis Lazarou built a predictive model in COMSOL Multiphysics® to optimize its design. To simulate the composite behavior in the device, Rotinat and Lazarou calibrated their model based on the study of Goldschmidtböing’s microactuator.

**PREDICTING ACTUATOR BEHAVIOUR USING MULTIPHYSICS SIMULATION**

Lazarou’s simulation incorporated geometric, thermal, mechanical, and electrical parameters. “COMSOL enabled straightforward coupling of the physics involved,” he explained. “This is a multiphysics problem with nonlinear electrical conductivity; density and specific heat capacity; and a changing viscosity, all of which affect the deflection.” COMSOL allowed him to investigate exactly how each parameter influenced the displacement.

“We use COMSOL as a prediction tool,” Lazarou remarked. “We can easily parameterize and change the actuator height, the membrane

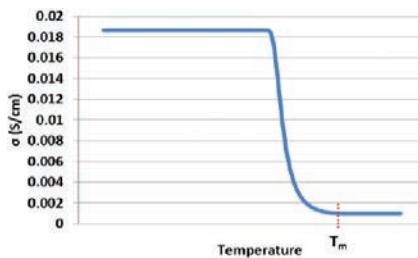


FIGURE 2. Approximation of the nonlinear electrical conductivity changing with temperature. Here, the melting temperature T<sub>m</sub> is approximately 42.8°C.

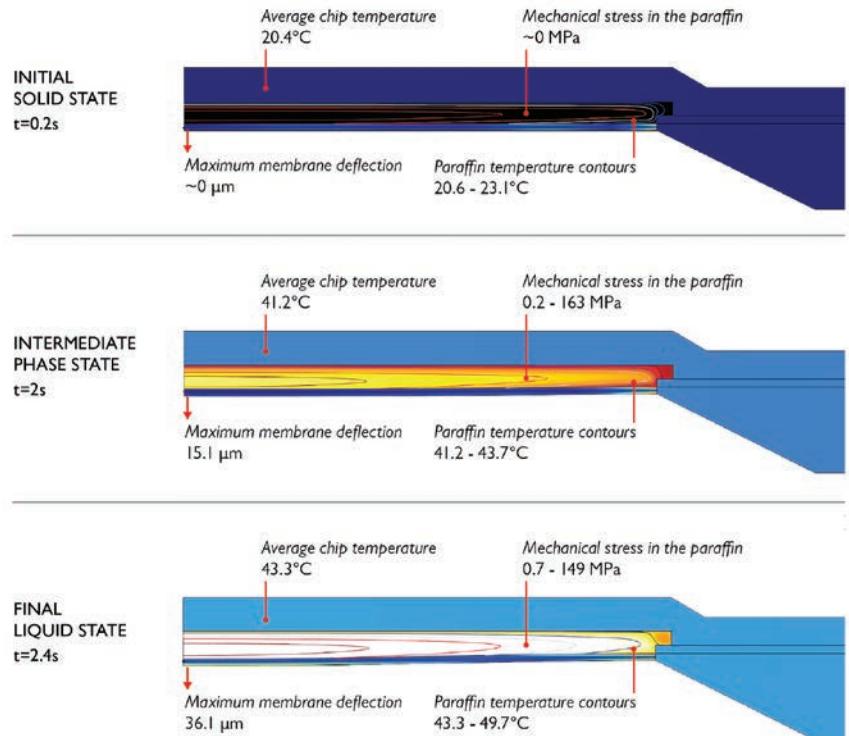


FIGURE 3. Validation model with results showing temperature ranges for the chip and paraffin, stress in the paraffin, and the deflection of the membrane.

thickness, and the wax composite model. Moreover, resistivity increases as temperature rises, since the carbon particles spread apart when the paraffin expands.” Lazarou approximated this behavior by modeling the electrical conductivity distribution (see Figure 2).

The deflection of the simulated membrane (see Figure 3) was very close to the deflection exhibited by Goldschmidtböing et al., reflecting the accuracy of the model and the conductivity approximation. This allowed Rotinat and Lazarou to adapt the model and optimize the CEA LIST miniature actuator design.

**THE NEW FACE OF ROBOTIC SURGICAL TOOLS**

Lazarou successfully built a realistic multiphysics model of a phase-change actuator, simulating mechanical behavior and control aspects. He is applying his simulation to the design and optimization of the CEA LIST integrated miniature actuator, to produce the high loads

and range of movement he and Rotinat envisioned. It will have low electrical consumption, meet medical requirements, and will lessen costs and the burden on surgeons. The prototype — which is to be completed in 2014 — will be thoroughly tested before being integrated into a robotic surgical tool. We’ll soon see an affordable, easy-to-use surgical robot in the operating room. ■



Panagiotis Lazarou and Christine Rotinat working on a microactuator simulation.

# From Concept to Market: Simulation Narrows the Odds in Product Innovation

BY CHRIS BROWN, SHARP LABORATORIES OF EUROPE

In today's electronics industry, innovation is essential for growth, while a short time from idea to market is the key to realizing maximum value. The argument that huge gains are possible by improving decision-making processes at an early stage of R&D—known for good reason as the “fuzzy front end”—is undoubtedly sound. In my experience, however, it is the quality of an idea and, crucially, the quality of the evidence supporting that idea that can really make the difference. Even the best processes cannot produce decisive outcomes when dealing with potentially ground-breaking technologies backed up by scant evidence. A quick, cost-effective way of narrowing the odds is needed.

Sharp Laboratories of Europe (SLE) in Oxford, UK is part of a global network of Sharp R&D sites responsible for delivering new technologies to the corporation. Our role is not only to support the continuous improvement of Sharp's current product portfolio, but to secure the future success of

nature of our work brings with it an increased complexity, as our researchers must understand how all the parts fit together and the complicated relationships that exist at the boundary between two physical systems.

Fortunately, as the complexity of the problems we face in the lab has increased, advances in computer modeling provide a helping hand in the form of powerful finite element simulation tools such as COMSOL Multiphysics®. For us, a key advantage of COMSOL is that it enables virtual experiments to be carried out that cross the boundaries of different physical mechanisms and that would be difficult, time-consuming, and costly to try out in the real world.

One example of where COMSOL has been a valuable tool is in our project to develop a lab-on-a-chip device for medical diagnostic applications. The project leverages Sharp's LCD manufacturing expertise and is based on a technology, known

“Fortunately, as the complexity of the problems we face in the lab has increased, advances in computer modeling provide a helping hand in the form of powerful finite element simulation tools such as COMSOL Multiphysics.”

Sharp in the longer term through more radical innovation to create entirely new product lineups.

A distinct change in the lab since I joined SLE almost 15 years ago is the move to a more multidisciplinary way of working. There has been a shift in focus to systems or products as a whole, such as health systems and energy systems. The multidisciplinary

as digital microfluidics, that enables precise control and manipulation of sub-millimeter-scale fluid droplets on top of an electronic sensor array. A key challenge in the development of the device lay in designing the fluid input ports to allow biological fluids and test reagents to flow onto the array under electronic control. Critically, the multiphysics capability of COMSOL



**CHRIS BROWN** is manager of the Health & Medical Devices group at Sharp Laboratories of Europe. He holds B.A. and M.Eng. degrees in Electrical and

Information Sciences from Cambridge University. After spending 10 years developing display technology for Sharp, including three years in Japan, he now leads a multidisciplinary research initiative combining electronics and biology to create new devices for the healthcare market. He is glad to still find the time to work with COMSOL.

enabled us to model interactions between the solid-liquid interface, electric field distribution, and fluid flow simultaneously. The result was an initial design for a fluid input structure that provided a more accurate starting point for experimental work when compared with simple hand calculations. The consequent reduction in the number of physical design iterations helped us reduce the R&D prototyping time and cost, and will help bring the device to market more quickly than could otherwise have been achieved.

As electronics continue to proliferate into yet more facets of modern life, the boundaries between what were once distinct scientific and engineering disciplines will become ever more blurred. In research organizations such as SLE, where scientists and engineers are faced with increasingly complex problems and where speed of development is increasingly vital, COMSOL Multiphysics is well placed to become a truly indispensable tool. Those of us working in the fuzziness appreciate the guiding hand it provides. ■