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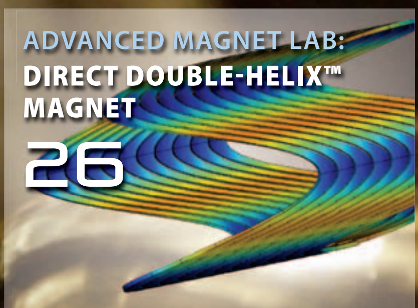
COMSOL NEWS

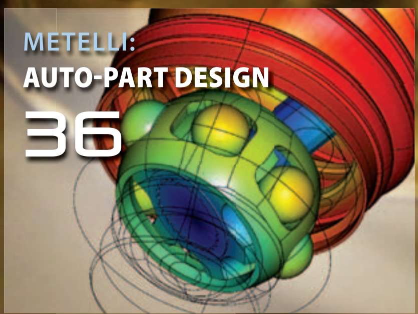
A TECHNICAL COMPUTING MAGAZINE

OSRAM SYLVANIA

Multiphysics Modeling in Discharge Lighting

COVER STORY PAGE 6





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The Multiphysics Community Has It All for You

The number of application examples from the COMSOL user community is soaring: We saw a record-breaking 350 papers presented at the annual user conferences. While we couldn't fit every paper into this magazine, you can access all 350 papers through the Multiphysics Community web site, **www.comsol.com/community**.

In this issue of *COMSOL News*, we collected presentations from the 2009 user conferences that we found most inspiring. Our favorite examples of simulation at work span the universe of engineering and science. They range from cooling super magnets in the CERN Large Hadron Collider to how NASA extracted water from the Moon, to more practical uses of modeling such as injection molding of medical implants and creating the perfect sound from line-array loudspeakers.

We hope that you enjoy this edition of *COMSOL News* and that you'll find these stories as much of an inspiration in your work as we have in ours.

To experience the multiphysics community first hand, we would like to invite you to the 2010 COMSOL Conferences. You will get a first look at the COMSOL API, attend over a dozen minicourses, and connect with fellow users. Learn more at **www.comsol.com/conference2010**.

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CEA	Golden Acoustics	NASA MSFC	U.S. Army
Continuum Blue	Kobelco Research Institute	OSRAM SYLVANIA	VTT

ON THE COVER

A corona discharge is used to study fundamental ignition processes in high-efficiency lamps.

PHOTO COURTESY OF DR. HELMAR ADLER, OSRAM SYLVANIA RESEARCH AND DEVELOPMENT.

COMSOL NEWS

We welcome your comments on COMSOL NEWS; contact us at news@comsol.com.


It's too expensive to develop new technologies in the real world.
Develop them in ours.

Analysis of Room Acoustics

JEFFREY CROMPTON, LUKE GRITTER, SERGEI YUSHANOV, KYLE KOPPENHOEFER, ALTASIM TECHNOLOGIES, COLUMBUS, OH & DOUG MAGYARI, GOLDEN ACOUSTICS, DETROIT, MI

COMSOL Multiphysics has been used to predict the acoustic response of rooms. The preferred acoustic response of recording studios, auditoriums, classrooms, theaters and conference halls are rooms that have an even energy response throughout the entire room and throughout the entire audio frequency range. This can be accomplished by using acoustic panels with complex surface structures (Figure 1) that scatter acoustic waves and diffuse sound level variability over the room volume and through the use of sound absorbing materials that prevent reflection from hard surfaces. Predictions developed using COMSOL Multiphysics have allowed the positions and designs of acoustic panels to be optimized, and the preferred materials for room construction to be identified without the need for continued iteration and experimental evaluations. Examples of the acoustic signatures of rooms at a frequency of 200 Hz with (Figure 2) and without (Figure 3) optimized acoustic treatments are shown. ■

Figure 1. Example of panel used to improve room acoustics.

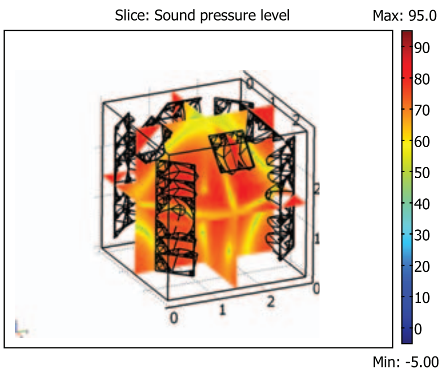


Figure 2. Acoustic signature of room containing optimized panel and material selection.

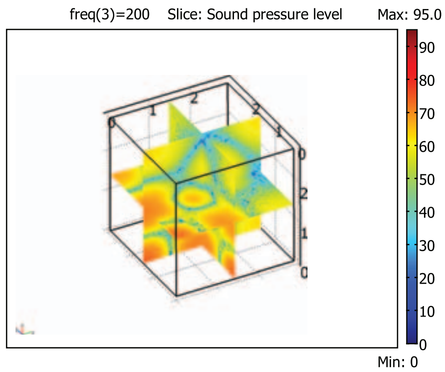


Figure 3. Acoustic signature of room not optimized for acoustic response.

Sonomagnetics Analysis

SERGEI YUSHANOV, LUKE GRITTER, KYLE KOPPENHOEFER, JEFFREY CROMPTON, ALTASIM TECHNOLOGIES, COLUMBUS, OH

Seawater is electrically conductive and consequently magnetic fields can be produced from the natural ebb and flow of ocean current. This magneto-hydrodynamic effect can be quantified by Maxwell's equations in a manner similar to that used in plasmas and electromagnetics. The magnetic fields and induced currents can develop naturally, or can be produced by an acoustic source imparting oscillations of the water mass through the Earth's ambient magnetic field. As the charged particles pass the flux lines, an induced electric field is developed together with an associated magnetic field; these currents and fields propagate mechanically with the acoustic wave.

The speed of sound is considered to be dependent on the depth, and the ocean is treated as a conducting medium.

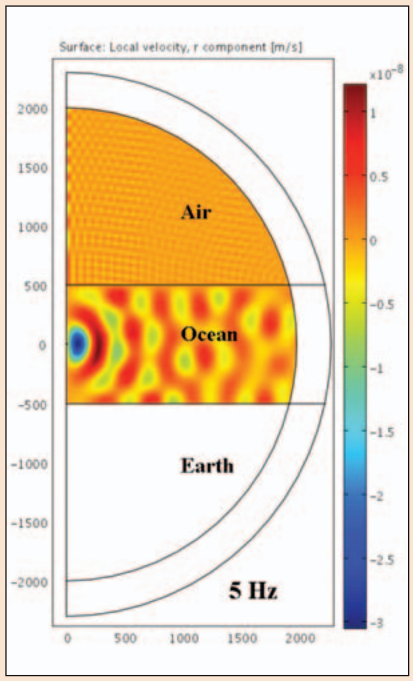


Figure 1. Radial component of acoustic velocity for source 500m below sea level.

Development of Mosquito Trap

JEFFREY CROMPTON, SERGEI YUSHANOV, KYLE KOPPENHOEFER, ALTASIM TECHNOLOGIES, COLUMBUS, OH & TOM KRUER, GIZMOTECH, EDGEWOOD, KY

Malaria causes the death of over 1 million people per year with a child under 5 dying every 30 seconds. Beyond the human toll, the economies of affected countries may lose billions of US dollars per year causing a downward spiral of poverty. To help prevent the spread of malaria AltaSim Technologies joined with Gizmotech to develop an effective and affordable mosquito trap for use in developing countries.

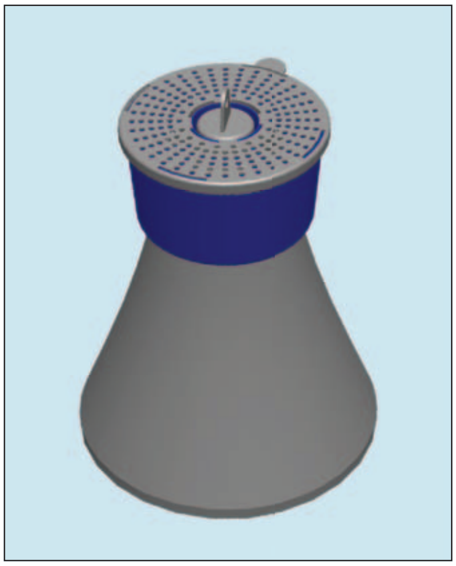


Figure 1. Passive solar mosquito trap.

The small cone-shaped trap combines inexpensive phase change wax and attractant derived from human sweat. During the day the wax absorbs solar energy; at night heat is released at the temperature of the human body causing evaporation of the attractant, thus mimicking the scent, moisture, and temperature profile of a sleeping human. Mosquitoes are attracted into the cone where they are trapped for disposal.

AltaSim Technologies used COMSOL Multiphysics® to analyze fluid flow and thermal distribution in the trap and subsequently optimize the temperature and flow velocities to trap mosquitoes. The analytical approach provided rapid verification of the technology and allowed optimization of the design prior to manufacture and use. ■

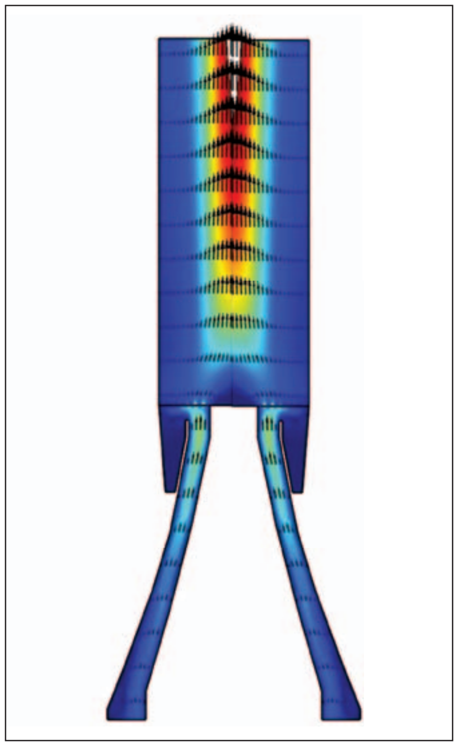
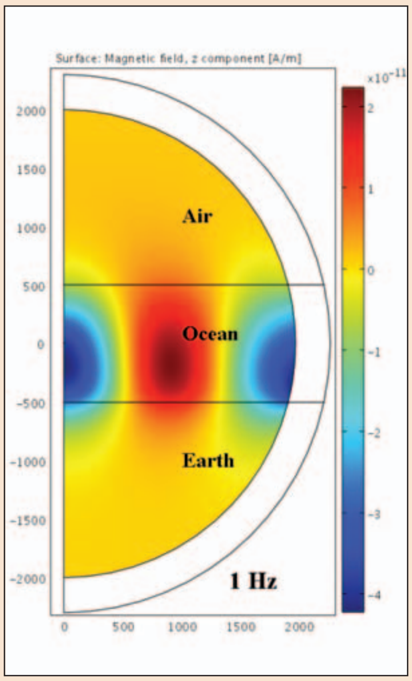


Figure 2. Flow through mosquito trap due to convection.



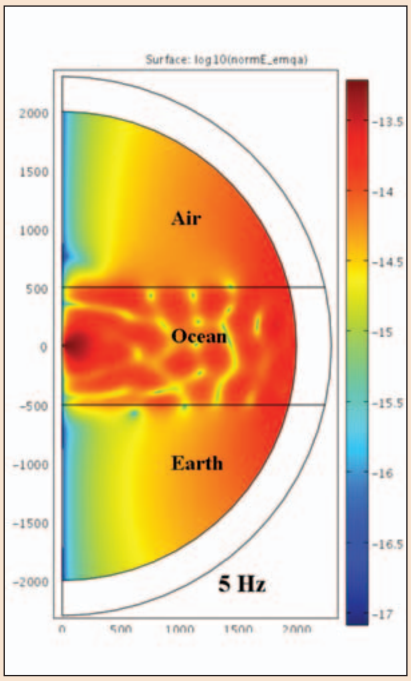
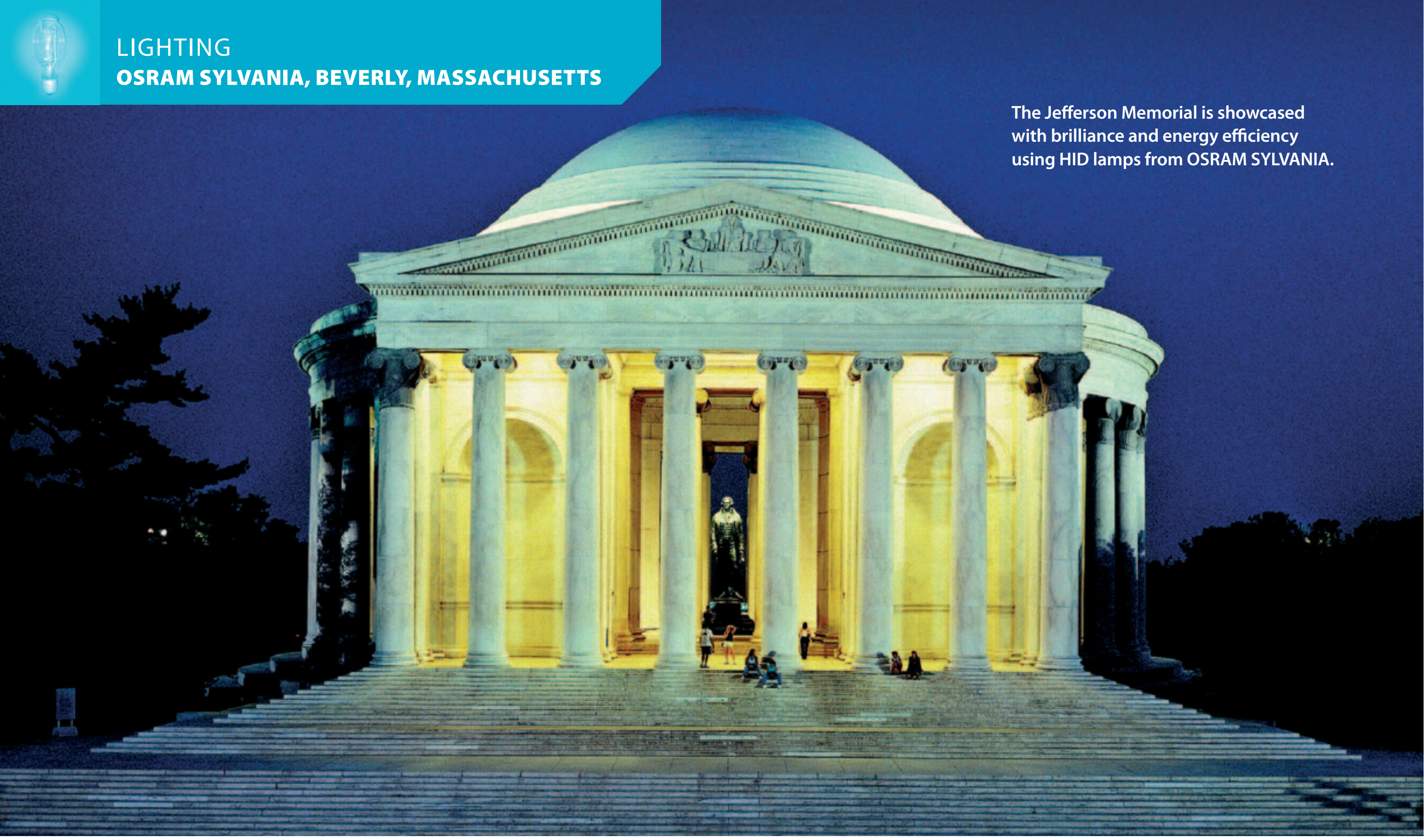


Figure 2. (left) Z component of magnetic field produced by 5Hz acoustic source 500m below ocean surface.

Figure 3. (right) Electric field produced by 5Hz acoustic source 500m below ocean surface.

This phenomenon has been studied by AltaSim Technologies to characterize the sonomagnetic field induced in the ocean by submerged acoustic sources over typical oceanographic scales. An acoustic source was placed 500m below sea level. This causes flow of charged material through the Earth's magnetic field. The speed of sound is considered to be dependent on the depth, and the ocean is treated as a conducting medium. The distribution of the radial component of the acoustic velocity at 5Hz is shown in Figure 1; the resulting magnetic and electric fields are shown in Figures 2 and 3. ■



The Jefferson Memorial is showcased with brilliance and energy efficiency using HID lamps from OSRAM SYLVANIA.

Multiphysics Modeling in Discharge Lighting

BY THOMAS D. DREEBEN, OSRAM SYLVANIA

Modeling is being used extensively to reduce the amount of energy consumed by lighting. Worldwide, the energy consumption of lighting is approximately 2800 TWh, 20% of the global supply of electricity. At a conservative 10 cents per kWh, the cost of this energy is $280 billion per year. For the light-sources industry, gross annual income is approximately $25 billion, one order of magnitude smaller than the cost of energy used for lighting. As we pursue reduced energy consumption in all of our light-source technologies, we expect to offer global energy savings that repeatedly offsets the full cost of operating our industry.

High-Intensity Discharge Lamps

Research and development of high-intensity discharge (HID) lamps is a key component of this effort. An HID lamp works by driving alternating current between two electrodes to establish an arc discharge through a gas. The gas is enclosed in a hermetically-sealed arc tube made of quartz or ceramic. A 175-W mercury-filled HID lamp is shown in Figure 1. Most of the light from a running HID lamp is emitted from the arc, which typically reaches temperatures of 5000-6000 K. HID lamps are commonly used to supply light in expansive spaces both indoor and outdoor, where they offer advantages in space efficiency and energy efficiency.

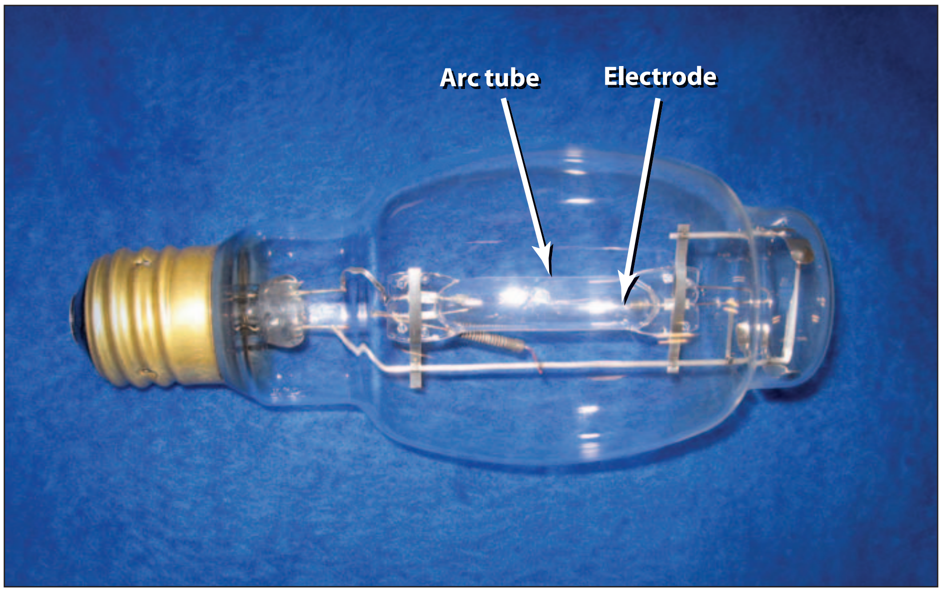
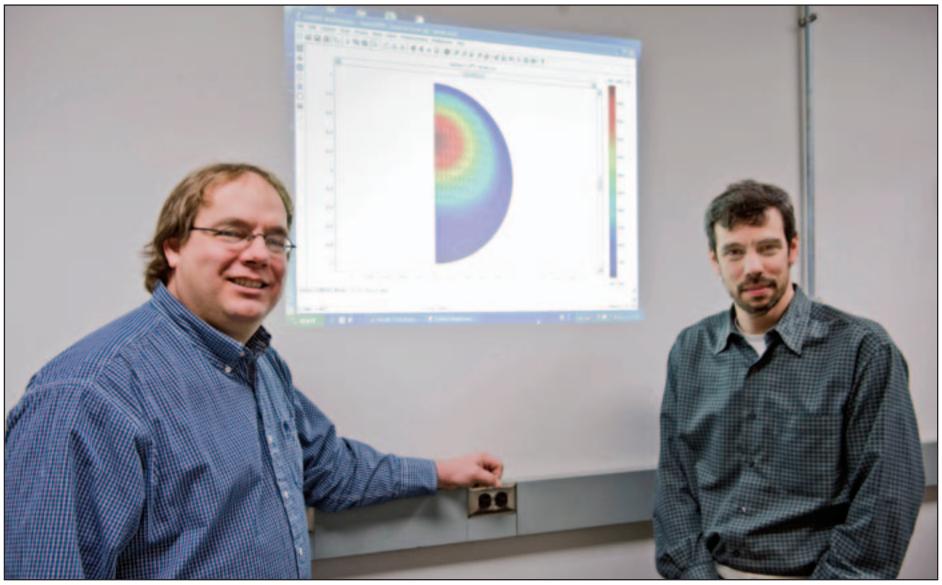


Figure 1. An HID lamp, with the arc tube and one of the two electrodes labeled.



Jo Olsen (left) and Thomas Dreeben, with OSRAM SYLVANIA (Beverly, MA) showcase their simulation results from their acoustic arc straightening study.

> "Modeling is necessary because many of the key mechanisms are beyond the reach of experimental measurement techniques."

Acoustic waves are generated in an HID lamp through systematic modulation of the current that powers the lamp at frequencies that correspond to standing sound waves. Although acoustic phenomena are known to cause unwanted effects in some circumstances[1], proper application of acoustics has been shown to enable a 50% increase in lamp efficiency over current HID technology[2]. If such an improvement could penetrate the US market, a simple estimate offers potential energy savings of 50 TWH per year, equivalent to the total energy that was generated by wind power in the US in 2008.

Modeling for Lighting Research

In an engineering setting, modeling is often used as a time and cost-saving measure: By providing equivalent information to experiments, models can be used to reduce the number of prototypes that need to be built. In a research setting such as ours, the needs are somewhat different: The primary role of modeling is to help build the knowledge base. To that end we use modeling and experimental work in complementary roles: Experiments expose critical aspects of the problem that models cannot reach, and models expose critical aspects of the problem that experiments cannot reach. Where the two methods provide overlapping information, comparisons are made to build credibility and clarify the limits of the model's application. Because we often use the model to provide information for which the experimental evidence is indirect, there is a stronger burden on the model to get the physics right.

We use COMSOL® primarily for the flexibility that it offers. Because of the exploratory nature of our modeling, we routinely "user-define" the full set of governing equations and parameterize every coefficient and dimension. This requires considerable mathematical freedom, much more than the "user-defined functions" that most packages normally offer. The general and weak forms in COMSOL's PDE mode, together with

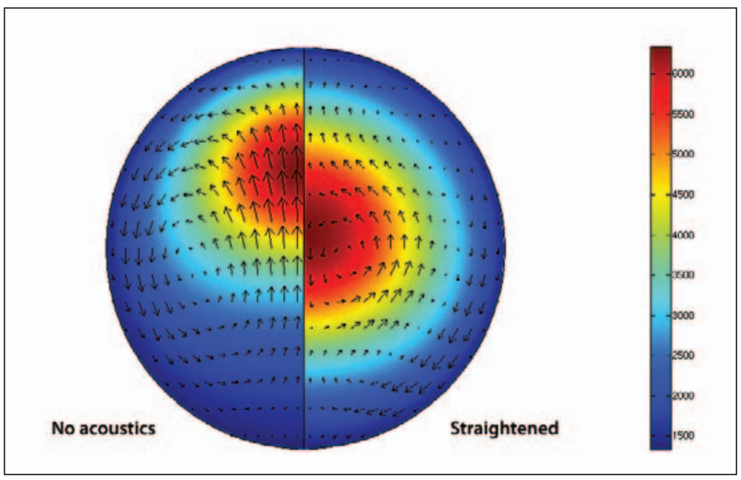


Figure 2[3]. Comparison of a bowed arc with an acoustically straightened arc. Temperature (K) is shown in the color map and vectors represent streaming velocity. The arc is the region of temperature greater than 5000 K.

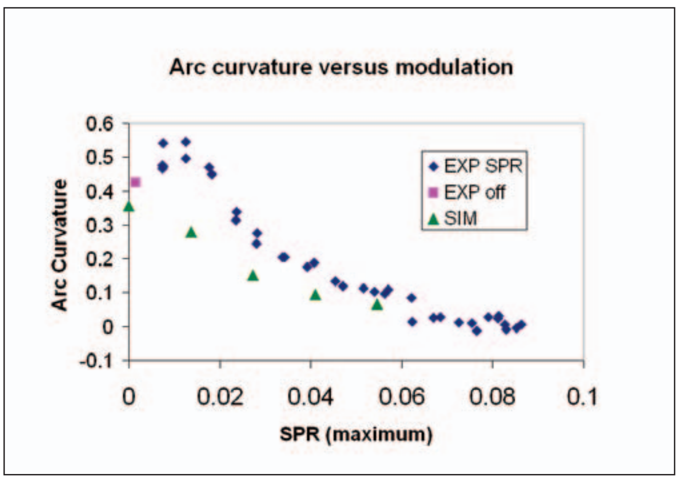


Figure 3[3]. Arc curvature versus spectral power ratio (SPR), a measure of the amplitude of acoustic excitation. Curvature is normalized by the arc-tube inner radius.

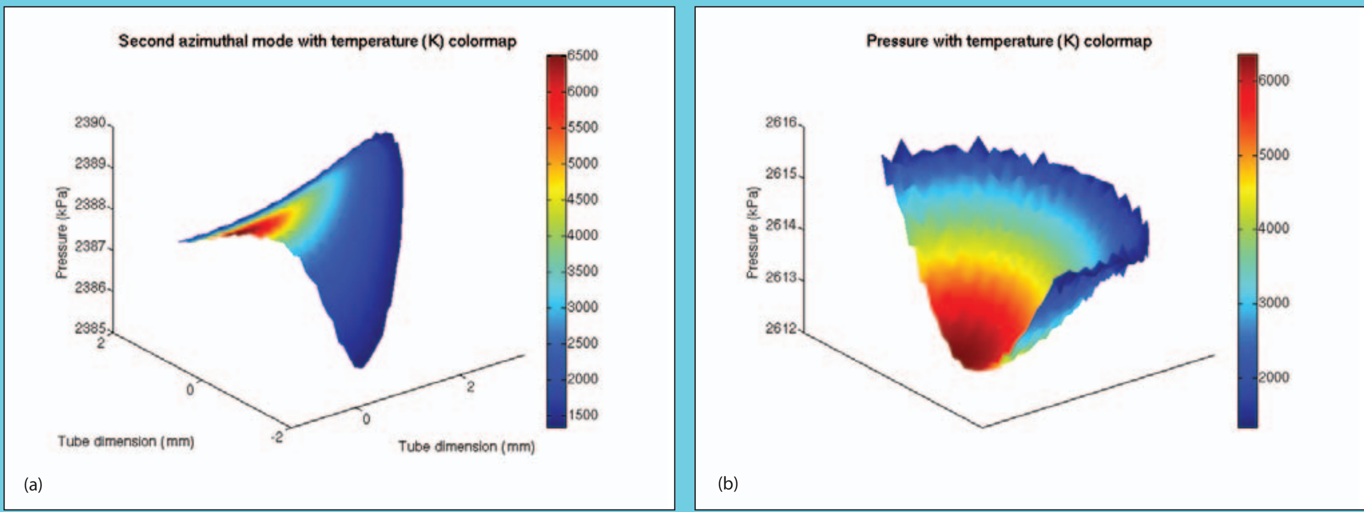


Figure 4[3]. Pressure modes that are needed for arc straightening. The second azimuthal mode (a) initially causes streaming flows that lower the arc from its bowed position. The first radial mode (b) causes streaming flow that holds the arc close to the center.

scripting through the MATLAB® interface, give us the flexibility that we need to grow our modeling into new areas of research.

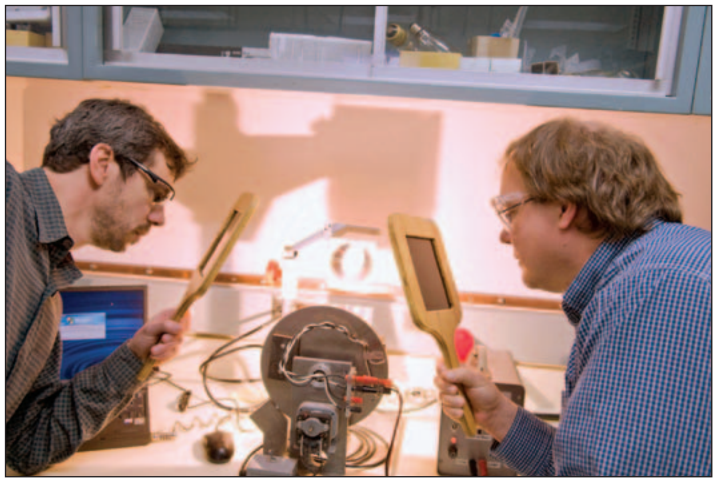
Model Description[3]

Modeling of acoustics and its effect on HID lamp performance involves capturing the physics on two separate time scales. On the smaller scale of 10^{-5} sec, compressible unsteady flow simulates instantaneous sound-wave propagation. On the longer time scale of 10^{-2} sec, "streaming" flows are resolved, where streaming refers to flow that is time-averaged over the acoustic scale[4]. This flow results from the convective terms in the governing equations and is responsible for all acoustic effects on HID-lamp performance. To capture the full physics on both time scales, the model formulation includes governing equations that conserve mass, momentum in two or three directions, energy, and electric current, all in a fully coupled, compressible, and unsteady formulation.

Arc Straightening in HID Lamps

One of the key capabilities of acoustics is straightening a bowed arc in an HID lamp. Arc bowing occurs in a horizontally-running lamp, where strong temperature and density gradients exist between the arc and the wall, and buoyancy forces act to move the arc up against the top wall. Simulated arc bowing and acoustic straightening is shown in an arc-tube cross section that is perpendicular to the arc in Figure 2.

Model output of the arc's vertical location is compared with experimental results in Figure 3.



Inspecting the arc of the HID lamp.

The benefit of reproducing arc straightening on the computer is that we obtain access to detailed information about the structure of the sound waves that are needed to bring about arc straightening. Arc straightening occurs as a result of two different modes of pressure, the second azimuthal and the first radial, shown in Figure 4.

Through techniques such as arc straightening, acoustic excitation enables us to greatly enhance the efficiency of HID lamps, and save energy on a global scale. Modeling enables us to estimate and visualize the important aspects of acoustic enhancement in HID lamps that we need to understand, predict, and control. Modeling is necessary because many of the key mechanisms are beyond the reach of experimental measurement techniques. COMSOL gives us the mathematical flexibility that is needed to represent acoustics in HID lamps. ■

References

[1] R. Schafer and H. P. Stormberg, Investigations on the fundamental longitudinal acoustic resonance of high pressure discharge lamps, *J. Appl. Phys.*, **53** (5), p. 3476-3480, 1982.

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[3] J. Olsen and T. D. Dreeben, "Experimental and Simulated Straightening of Metal Halide Arcs Using Power Modulation", *IEEE Transactions, submitted*.

[4] Lord Rayleigh, On the Circulation of Air observed in Kundt's Tubes, and on some Allied Acoustical Problems, *Transactions of the Royal Society of London*, **175** (1), 1883.

Microwaving Moondust with COMSOL

Cryogenic trapped water is just under the surface of lunar soil at the Moon's poles. Microwave energy can be used to efficiently extract this water from permafrost. COMSOL permits calculation of the extraction process.

BY CATHLEEN LAMBERTSON

"Water and other compounds found on the Moon represent potential resources that could sustain future lunar exploration."

In 1999, NASA's Lunar Prospector revealed concentrated hydrogen signatures detected in permanently shadowed craters at the lunar poles. While scientists have long speculated about the source of vast quantities of hydrogen at the poles, recent discoveries made by NASA's Lunar CRater Observing and Sensing Satellite (LCROSS) are shedding new light on the question of water on the Moon. Preliminary data from LCROSS indicates that the mission successfully uncovered water during the Oct. 9, 2009 impacts into the permanently shadowed region of Cabeus crater near the Moon's south pole. These findings could have far-reaching implications as space exploration is being expanded past low-Earth orbit.

The Importance of Moon Water

Water and other compounds found on the Moon represent potential resources that could sustain future lunar exploration. According to Dr. Edwin Ethridge, a Materials Scientist in the Materials & Processes Laboratory at NASA Marshall Space Flight Center (Huntsville, AL), *in-situ* resources are very important since they do not have to be launched out of Earth's gravitational well. "It is very expensive to get mass into space. The weight of a payload that goes into space is only a very small fraction of the total rocket weight on the launch pad," he said. For example, it costs around $50,000 per pound to launch anything to the Moon. The cost of getting the payload into orbit

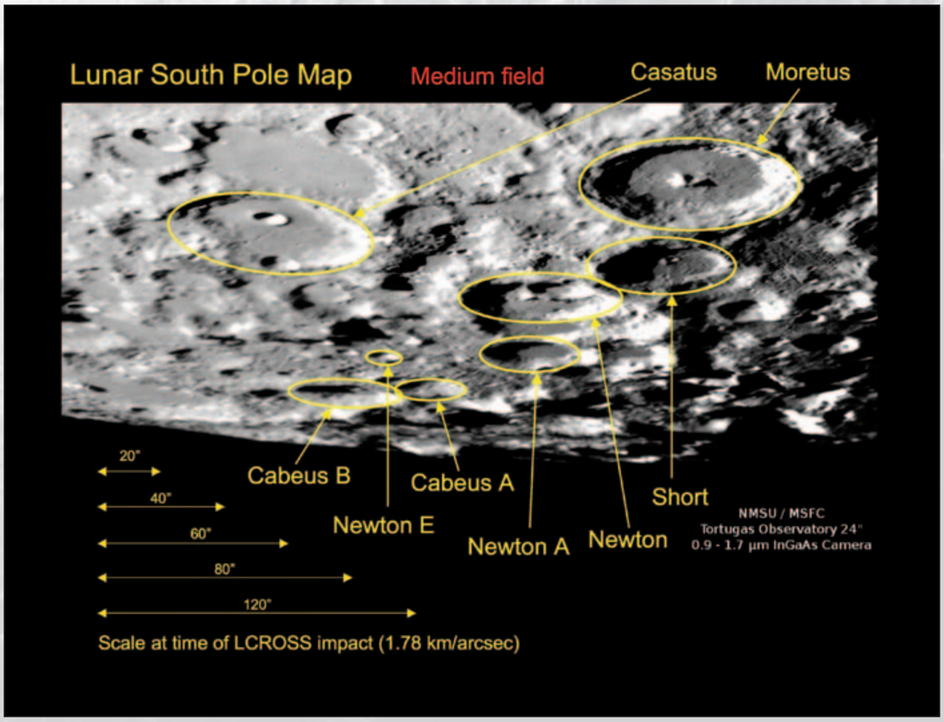


Figure 1. Labeled composite image of the South Pole taken by New Mexico State University/Marshall Space Flight Center, using the Tortugas 24" telescope. (Credit: NMSU/MSFC)

"Since the temperature varies with time as the soil heats, temperature-dependent soil dielectric properties can be incorporated into the model along with temperature-dependent thermal conductivity of the soil. Whatever the properties of the lunar soil might be, we can simply put them into COMSOL and do a calculation."

is the total cost of the rocket, rocket hardware, engines, and propellant. And since water is one of the resources that will have to be resupplied to a manned lunar outpost, water would be part of the total cost of the payload taken to the Moon.

While water and oxygen can be recycled on a manned lunar outpost, no process is 100% efficient. Dr. Ethridge cited estimates indicating that one ton of water and one ton of oxygen per year would be required for the early stages of a manned outpost. This fact alone makes it necessary that a water extraction process will be developed for use at an outpost. And once the water is extracted, oxygen can be obtained from the water by electrolysis. "We are looking at the process of extracting the water from the soil. Water is water. Run it through a purification system and you could drink it. We will extract water [and then] electrolysis can be used to split the water into hydrogen and oxygen."

The Extraction Process

As a principal investigator examining the Use of Microwaves for the Extraction of Volatiles From Lunar Soil, Dr. Ethridge asserts that microwave processing to extract water has unique advantages over other processes. "Because of the high vacuum, the thermal conductivity of lunar soil is very low. The Apollo astronauts measured the thermal conductivity and it is comparable to aerogel, a super thermal insulator." Additionally, microwave energy is advantageous because it heats from the inside out. This means that the excavation of lunar soil could be unnecessary, thereby minimizing Moon dust and the negative aspect of perhaps having to strip-mine the Moon. Simply put, using microwaves could greatly reduce the complexity, additional infrastructure, resources, and power requirements of other processes. This is why Dr. Ethridge is currently developing microwave extraction technology for operation on the Moon.

The basic components of the microwave extraction system include a microwave source, waveguides to deliver the energy to the soil, and a cold trap to capture the water vapor (Figure 2). First, the microwave energy penetrates and heats the soil and, since ice is relatively transparent to microwave energy, heat is transferred from the soil particles to the water ice condensed onto the surface of the soil. On the Moon, water ice transforms directly to water vapor by sublimation. Once in the cold trap, the water vapor will transform back to ice. In addition to the system components, a power source and a rover to transport the extraction system will be necessary.

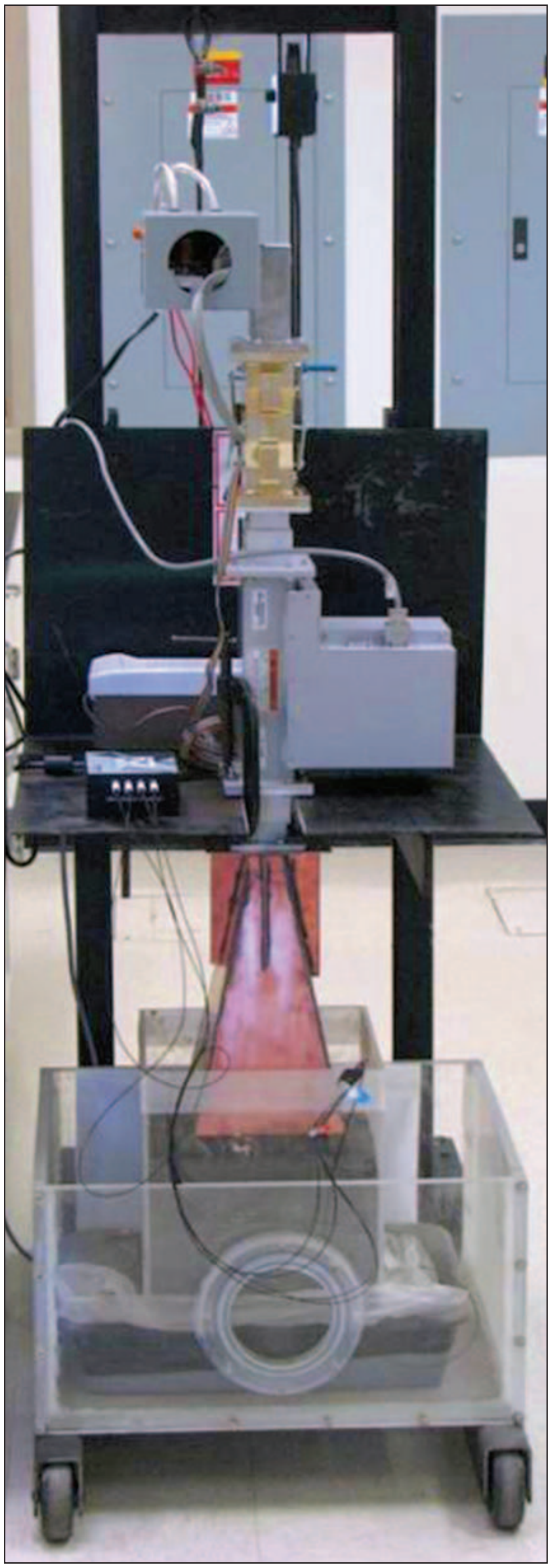


Figure 2. Demonstration hardware to test the beaming of microwave energy down into lunar soil simulant (in the box) with the microwave hardware mounted on a mobile platform. Initial test of the coupling of microwave energy into the simulant.

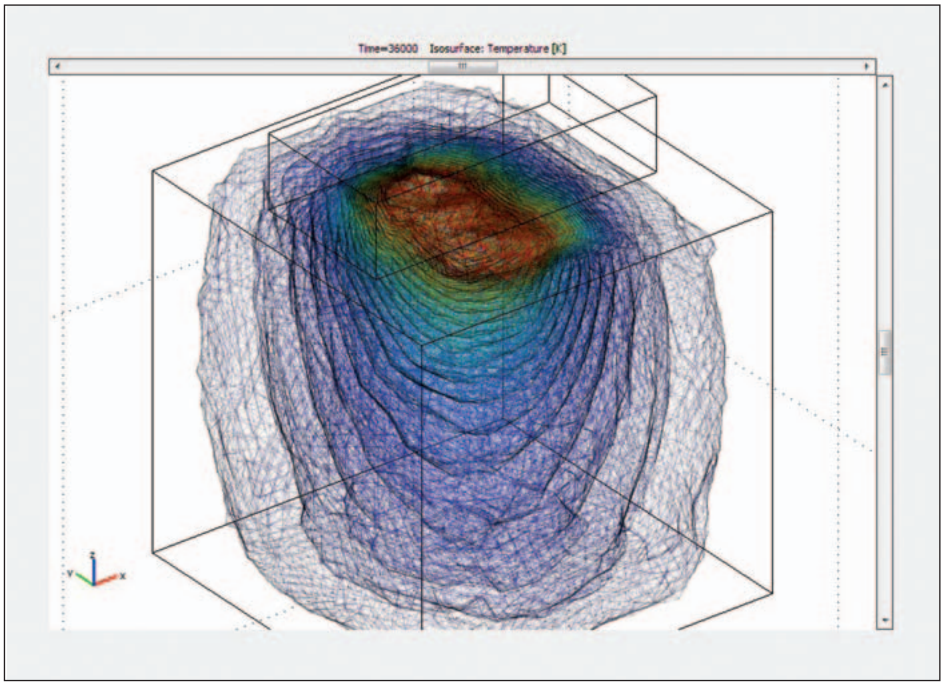


Figure 3. Transient solution of the penetration of microwave energy (0.5 GHz) into lunar soil simulant with heating of the soil. Colors represent constant temperature isotherms. The AVI movie shows the progressive heating of the soil over a period of 10 hours. Watch the movie at http://science.nasa.gov/science-news/science-at-nasa/2009/07oct_microwave/

Simulating the Moon

Since the microwave processing parameters and hardware requirements for water extraction is a complex multiphysics problem, Dr. Ethridge employed simulation to address the challenges. "When I wrote the proposal for the microwave extraction of water, the COMSOL calculations were part of the originally proposed work."

COMSOL is being used to calculate the microwave penetration into and heating of simulated lunar soil. The properties of the simulant are approximated by complex electric permittivity and magnetic permeability measured in the lab. "Calculations can be performed on different geometries, for a range of microwave frequencies and different power levels, for the simulated lunar soil," said Dr. Ethridge. "Since the temperature varies with time as the soil heats, temperature-dependent soil dielectric properties can be incorporated into the model along with temperature-dependent thermal conductivity of the soil. Whatever the properties of the lunar soil might be, we can simply put them into COMSOL and do a calculation."

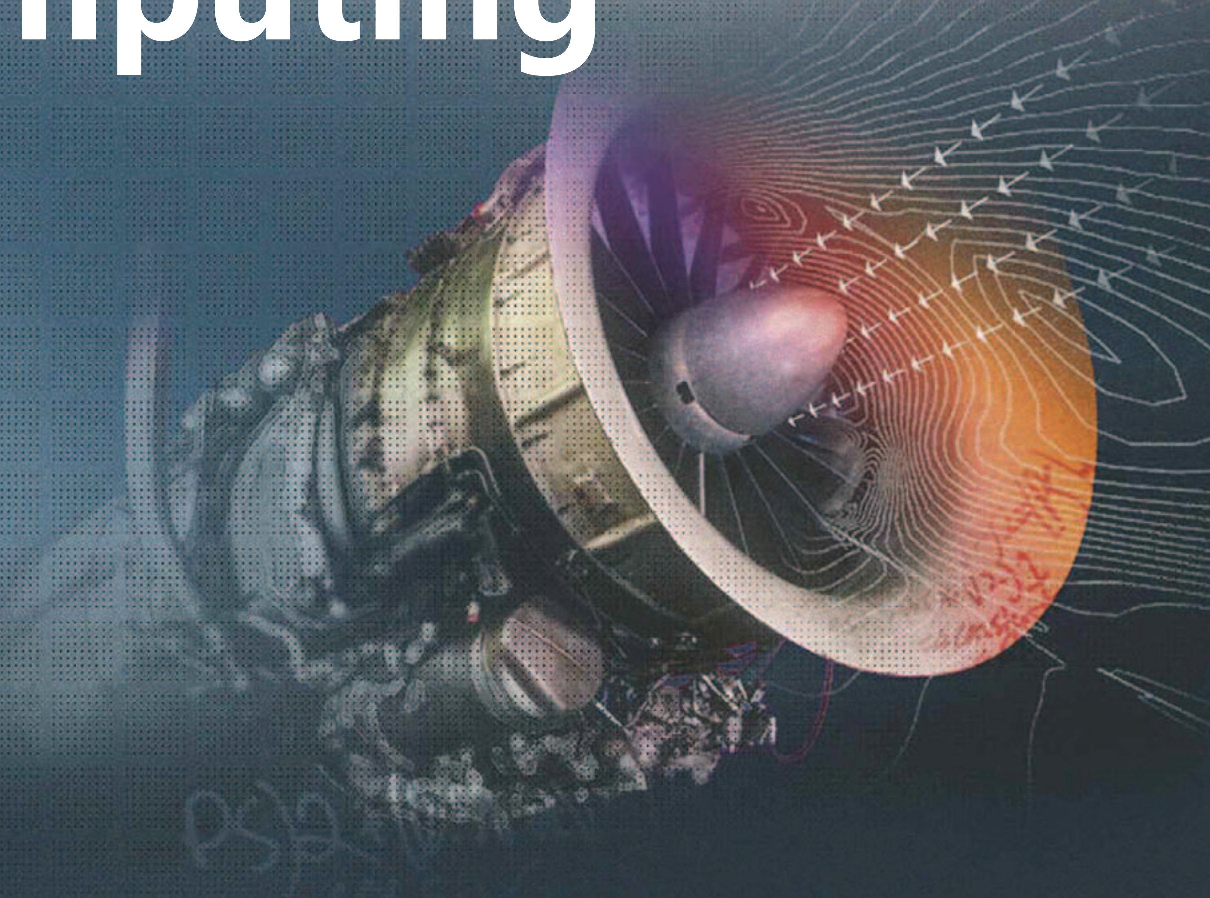
For the simulation, Dr. Ethridge used the RF Module to model the microwave power penetration and attenuation into the soil (Figure 3). When the model was running without error, the physics of heating and heat flow were added. A transient analysis was used to determine heating as a function of time. An AVI movie is available that shows lines of constant temperature as the heating progresses. "Development of an early experiment payload for a lunar lander mission requires the specification of the microwave frequency, power, and method of delivery of power. Developing experiments with several different microwave frequencies would require a significant investment of resources, manpower, and time to perform experiments," stated Dr. Ethridge. "COMSOL permits the calculation of microwave penetration and heating that could be expected with different experiment scenarios. This can reduce the time, labor, and cost to narrow the hardware requirements for the experiment."

The next step for Dr. Ethridge is to develop a model of the percolation of water vapor from the soil. Currently, Southern Research Institute (Birmingham, AL) is measuring the Darcy constant (describing the flow of a fluid through a porous medium) for lunar soil simulant. Once the data is generated, a model of the water vapor transport from the simulant will be developed.

AVI movie (3D animation showing how a 1KW microwave source entering from the top produces heating in a cubic meter simulated lunar soil.) **http://science.nasa.gov/science-news/science-at-nasa/2009/07oct_microwave/** ■

Dr. Edwin Ethridge showcasing the water extraction process.

High Productivity Computing



- Enhanced Productivity
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Baker Hughes engineers lower the AutoTrak™ LWD tool, fitted with an AziTrak™ module, into a well.

Modeling Tools for Formation Evaluation and Reservoir Navigation

Baker Hughes scientists turn to COMSOL Multiphysics to develop a reservoir navigation service more efficient and precise than ever before, saving customers millions of dollars.

DR. SUSHANT DUTTA AND DR. FEI LE, BAKER HUGHES

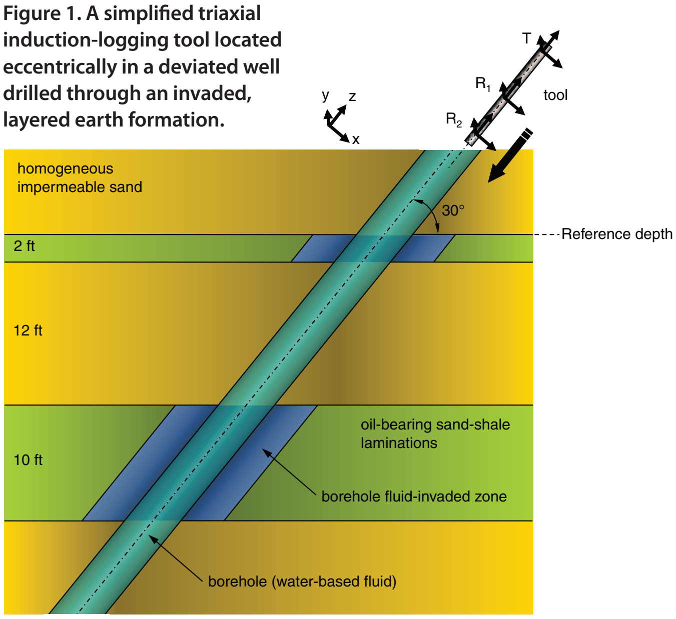
Headquartered in Houston, Texas, with operations in more than 90 countries, Baker Hughes is known around the world as a leading provider of products, services, and solutions for the petroleum and continuous-process industries. Formed in 1987 by the merging of Baker International Corp. (originally Baker Oil Tools, founded in 1907) and Hughes Tool Co. (founded in 1909), the company designs high-performance technologies aimed at creating value from oil and gas reservoirs for customers such as Shell, Exxon Mobil, Chevron, Marathon, Texaco, and Conoco.

Baker Hughes' global operations are backed by three product-line groups, which develop, manufacture, and support their advanced technologies. One of the groups — Drilling and Evaluation — offers real-time reservoir navigation and formation evaluation services during drilling in the form of logging-while-drilling (LWD) tools, and a complete range of wireline logging tools for detailed post-drilling formation evaluation in every environment. These services are designed to help customers drill more efficiently, evaluate geologic formations, place wells in productive zones within the reservoir, and perform petrophysical and geophysical data acquisition.

The Importance of "Sight"

Reservoir navigation and formation evaluation are important for the simple reason that drill operators need to "see" exactly where to place the well. While reservoir navigation is the matching of geological and resistivity models to drill along and through bed boundaries to precisely place wells, formation evaluation is the process of interpreting a combination of measurements taken inside a wellbore to detect and quantify oil and gas reserves

Figure 1. A simplified triaxial induction-logging tool located eccentrically in a deviated well drilled through an invaded, layered earth formation.



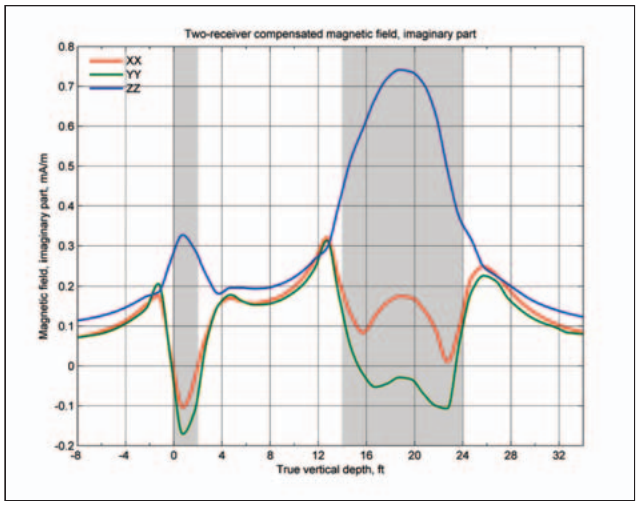


Figure 2. Imaginary magnetic fields, all three direct components, for frequency 20 kHz and when the tool is centered in the borehole. The lower frequency corresponds to a larger region of investigation. The gray shaded regions indicate the oil-bearing layers.

"Resistivity logging is the oldest systematic technique for formation evaluation, and is still the foremost technique in formation evaluation used for reservoir navigation."

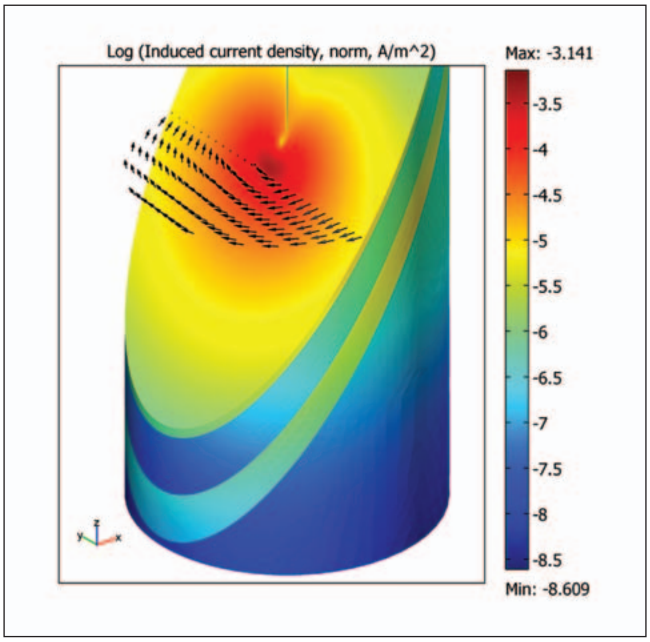


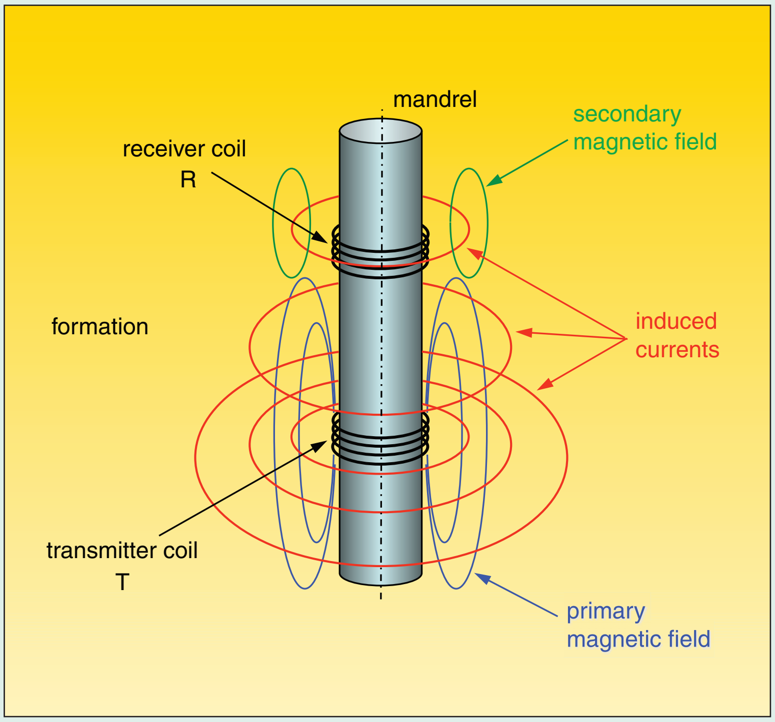
Figure 3. This image created with COMSOL Multiphysics shows a simulation result snapshot when the inductive logging tool's Z-transmitter is active at a depth of 8 feet. The subdomain colormap shows the magnitude of induced current density in the formation, while the arrows show the direction of flow of the induced currents. The colormap is log10 scaled for clarity.

in the rock adjacent to the well. The data from the evaluation is organized and interpreted by depth and represented on a graph called a log. "Baker Hughes' reservoir navigation tools routinely enable wells to be placed accurately by measuring and visualizing bed boundaries and oil-water contact zones and providing accurate geosteering information," said Sushant M. Dutta, Ph.D., a scientist in the Strategic Technology and Advanced Research group for the Drilling and Evaluation product line at Baker Hughes.

One such tool is Baker Hughes' AziTrak™ Deep Azimuthal Resistivity induction-logging tool. Resistivity logging is a method of well logging that works by characterizing the rock or sediment near a borehole by measuring its electrical resistivity. "Resistivity logging is the oldest systematic technique for formation evaluation, and is still the foremost technique in formation evaluation used for reservoir navigation. It is based on the

Induction Logging Explained

Consider a pipe mandrel with two multi-turn coils wound over it, surrounded by an earth formation. The transmitter coil T is fed an alternating current with a suitable frequency. The voltage (both amplitude and phase) across the receiver coil R is measured. This is a simple representation of an induction logging tool with coaxial transmitter/receiver. The current through the transmitter coil T generates an axial primary magnetic field (shown in blue). The alternating primary magnetic field induces electric current loops (shown in red) in the formation. These induced currents generate a secondary magnetic field (shown in green), which also crosses the receiver coil R in addition to the primary magnetic field. Thus, the signal generated in the receiver is in response to both the primary and secondary magnetic fields. The currents induced in the formation are a function of formation resistivity. Thus the receiver signal is an indicator of formation resistivity. Of course, the primary magnetic field is several orders of magnitude stronger than the secondary magnetic field. Hence, practical induction logging tools use multiple coil systems with hardware/software schemes to cancel the signal due to the primary magnetic field.



"COMSOL simulations for sensor design reduce prototyping costs. Solving forward problems helps us characterize new tools and build confidence in fast forward models for inversion."

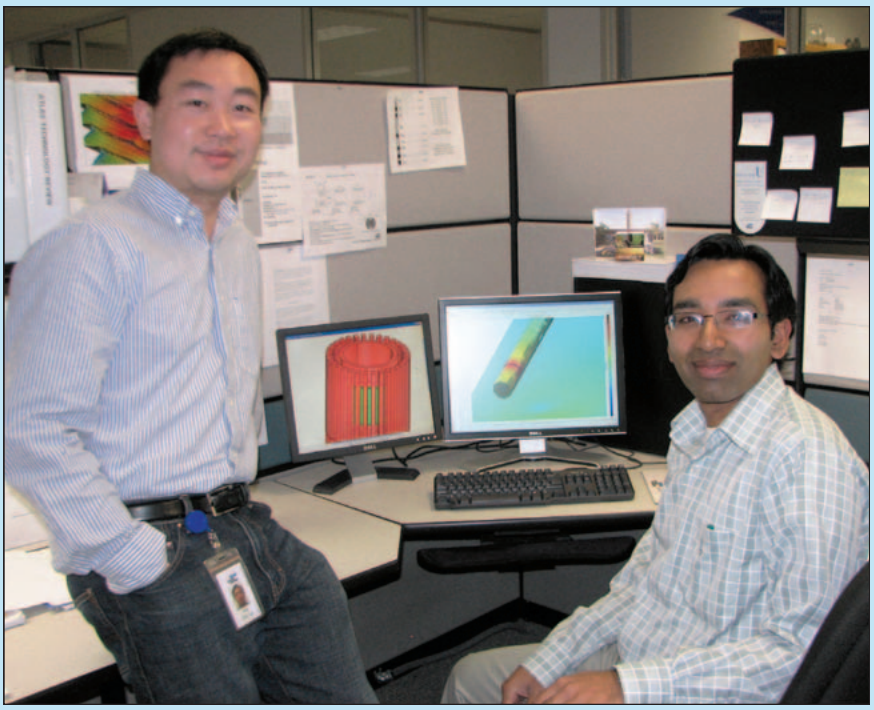
fact that oil and gas have a substantially higher electrical resistivity compared to (salt) water. Underground formations usually contain salt water in their pores. Hence, the bulk formation resistivity is higher if the pores contain oil or gas in addition to salt water," said Dr. Dutta.

Until recently, oil and gas operators had been limited in the types of real-time resistivity logging measurements they could use for reservoir navigation. Although deep-reading measurements provide information about approaching boundaries and fluid contacts, the azimuth of these boundaries and contacts is unknown. The AziTrak solves these issues by providing a 360° view of the downhole environment. It is capable of detecting, measuring, and visualizing bed boundaries and oil/water contact zones hours before they can be "seen" with conventional sensors.

Simulating the Tools

Dr. Dutta and his colleague, Dr. Fei Le, are using COMSOL Multiphysics to model induction logging tools, like the AziTrak, in a variety of situations. "Over the course of their continuous development, induction-logging tools have become increasingly difficult to characterize by the use of simple models. Similarly, with the advent of directional drilling, it has become imperative to model fully 3D formations," stated Dr. Dutta. And although Baker Hughes does possess in-house codes for true 3D models, there are limitations. "The lack of user interface and visualization capabilities motivated us to go for commercial packages. COMSOL Multiphysics is one of a suite of commercial FEM-based packages that we have been using for some time now."

To illustrate his use of COMSOL, Dr. Dutta described a simulation for a full 3D formation model with a simplified induction tool in a borehole: The formation (Figure 1) consists of five horizontal layers, with anisotropic oil-bearing layers invaded by the borehole fluid. The borehole makes a high angle with the vertical, which represents a realistic directional drilling scenario. The induction tool may or may not be centered inside the borehole. Furthermore, the induction tool transmitters and receivers are triaxial, which makes them capable of transmitting and measuring magnetic fields in each of three orthogonal directions, although they are modeled as simple wire loops. The induction tool operates at multiple frequencies. The results show (Figure 2) the direct magnetic fields in all three directions (imaginary parts) logged by the tool as a function of true vertical depth. The imaginary magnetic fields represent the voltage signals generated in the receivers that are in-phase with the transmitter currents. A 3D simulation (Figure 3) shows the induced currents in the formation when the Z-transmitter is active.


Fei Le (left) and Sushant Dutta studying their simulation results.

Looking Forward

Dr. Dutta continues to use COMSOL for sensor design, solving forward problems, validating experiments, and testing new design ideas. "COMSOL simulations for sensor design reduce prototyping costs. Solving forward problems helps us characterize new tools and build confidence in fast forward models for inversion," he said. And since directional drilling, reservoir navigation, and formation evaluation are areas of the oil and gas industry that use some of the most advanced technology in the world, "Baker Hughes' expertise in these areas often saves customers millions of dollars in improved productivity and time saved. The ability to accurately characterize induction-logging scenarios and to evaluate ideas for new and improved induction logging tools helps us keep that edge." ■

Covidien's ForceTriad™ energy platform and a few of the associated electrosurgical devices that use it as an energy source.

Simulating Energy-Tissue Interactions for Improved Patient Outcomes

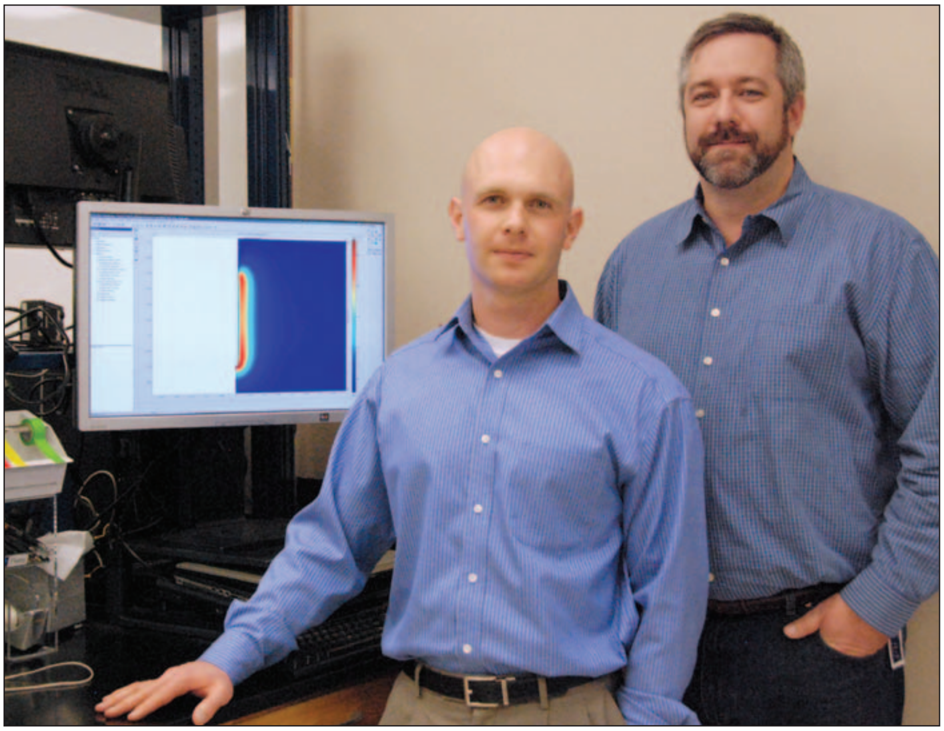
The first commercial electrosurgical generator is credited to Dr. William T. Bovie, who developed the instrument in 1920. Eventually, with advances in technology, solid-state generators replaced the original spark gap and vacuum tube models. In the early 1970s two companies, Valleylab and Electro Medical Systems (EMS), introduced the first solid-state electrosurgical generators, thereby establishing the modern era of isolated outputs, complex waveforms, increased safety, and more. Currently, electrosurgery is used in more than 90% of all surgeries performed in the United States.

CASEY LADTKOW AND ARLEN WARD, PE, COVIDIEN EBD

Electrosurgery is the application of high-frequency electric current to biological tissue as a means to cut through the tissue (vaporize) and/or stop bleeding (coagulate). These types of surgeries are performed using an electrosurgical generator and a hand piece that includes one or several electrodes. During electrosurgery procedures, current that passes though the tissue is converted to heat. The amount of heat generated determines if the tissue is vaporized or if coagulation occurs. This degree of control during surgery, as well as electrosurgery's precise cuts with limited blood loss, makes electrosurgical devices preferred over many alternative methods.

A leader in the energy-based medical treatment systems industry is Covidien Energy-based Devices (EbD, formerly Valleylab). Their systems include electrosurgical generators, accessories, argon enhanced electrosurgery systems, patient return electrodes, electrosurgical generators, and laparoscopic instruments.

With a goal toward advancing research and technology development for electrosurgery, vessel sealing, and tumor ablation, engineers at Covidien EbD employ computer simulations to describe the interaction between highly coupled physical effects where the application of energy changes tissue properties. According to Arlen Ward, a senior R&D Engineer at Covidien EbD, the simulations are used for understanding these complex interactions, demonstrating these effects to others both inside and outside the company, reducing prototyping costs, and investigating tighter energy control and subtle tissue effects. To this end, he and his colleagues have been using COMSOL Multiphysics.



Casey Ladtkow (left) and Arlen Ward demonstrate an electrosurgery simulation.

Optimizing the Energy Source

Mr. Ward explained how the simulation of energy-tissue interactions is a key part of the research performed at Covidien EbD to aid product development. “COMSOL has been applied to specific problems as a flexible tool by individuals within various research and development projects. As the benefits of using multiphysics simulations have become apparent, other groups have expressed a desire to incorporate simulation in their projects.” For example, Mr. Ward and his colleague at Covidien EbD, Senior R&D Engineer Casey Ladtkow, have been using COMSOL for about four years. While their projects are vastly different, they come together to share solutions to issues they have with the model itself.

> “COMSOL has been applied to specific problems as a flexible tool by individuals within various research and development projects. As the benefits of using multiphysics simulations have become apparent, other groups have expressed a desire to incorporate simulation in their projects.”

Electrosurgical generators produce a variety of electrical waveforms. As waveforms change, so do the corresponding tissue effects. Tissue heating rates determine whether one waveform cuts tissue and another stops bleeding. These are the two primary surgical effects that Mr. Ward is interested in — the ability to cut through tissue and the ability to control bleeding. “Knowing how much energy is used to vaporize the tissue (providing the cutting effect) and how much energy remains to provide hemostaisis (bleeding control) is key. You need to have a threshold amount of thermal margin to create the homeostasis, but you don’t want an excess of heating because you don’t want to damage the tissue unnecessarily.”

As the manufacturer of the energy source used in electrosurgery, Covidien EbD provides a platform that accepts a range of specialty surgery instruments, including those made by other manufacturers, and it is important that they understand the interactions of all types of devices to make sure the energy is applied in an appropriate way. Recently, Mr. Ward has been using COMSOL to investigate how energy delivered from one of Covidien’s products, the ForceTriad™ energy platform, works with other loop-shaped electrode devices used for removing prostate tissue during a surgical procedure called TURP (transurethral resection of the prostate). There are many small capillaries in the prostate and Mr. Ward uses COMSOL to model how much energy is required to cut through the prostate while providing enough extra energy to stop the bleeding (Figure 1). “We enter the prostate tissue properties, the geometries of the electrodes, and look at the way that we are applying energy in terms of electrical voltages or currents, and make sure we are putting in enough energy to vaporize the cut at that speed and that we are getting enough thermal margin to provide homeostasis, but also optimizing it to the correct amount,” he said. “The useful part is to be able to start with simple models — like coupling the electrical and thermal properties — and then once you’re satisfied that those are working together well, being able to add complexity to those models."

According to Mr. Ward, his primary challenge in modeling is the amount of available information. "As soon as we have to start defining the work in terms of differential equations and defining the interactions within simulations, it becomes apparent that we often need more information — whether it's tissue properties or perhaps discovering the physical mechanism that is driving the tissue effect. These are questions that have to be answered before you have a realistic model. We have had to iterate through that a number of times, but every time we do we gain more understanding and therefore make the next time we apply the model much easier."

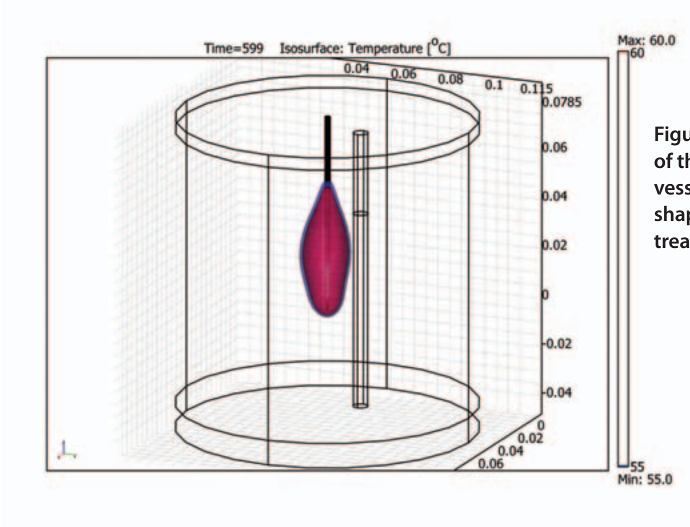


Figure 2. 3D COMSOL model of the impact of a large blood vessel on the ablation size and shape for a microwave tumor treatment.

Modeling Tumor Ablation

Mr. Ladtkow is heading another project employing COMSOL. He is examining Covidien EbD's tumor ablation line to review the differences between radio frequency (RF) and microwave (MW) instruments close to blood vessels.

Called the vessel effect model (Figure 2), Mr. Ladtkow uses three different tools to evaluate the issue: bench modeling with static tissue, preclinical testing with *in vivo* tissue, and modeling. These three tools are used to support each other in order to verify the findings. "The thing about the bench model and the *in vivo* model is that it's really time consuming, you don't get a lot of repeatability, and you don't get a lot of control over tissue properties. What the modeling brings is a measure of repeatability where you can test a wide variety of variables and scenarios quickly," he said.

The main challenge in designing RF and MW ablation products is tuning the energy delivery algorithm to a wide range of tissue conditions, explained Mr. Ladtkow. "Tissue is just so variable and it's so inhomogeneous, so you get results from tests where you can't really interpret what's going on because of the noise. I really think the opportunity for COMSOL is to overcome the noise you get from doing those experiments. I think it's larger than what you would find in other industries."

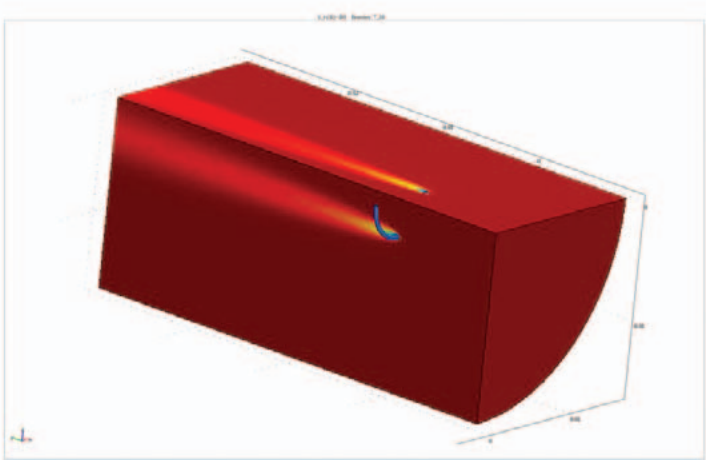
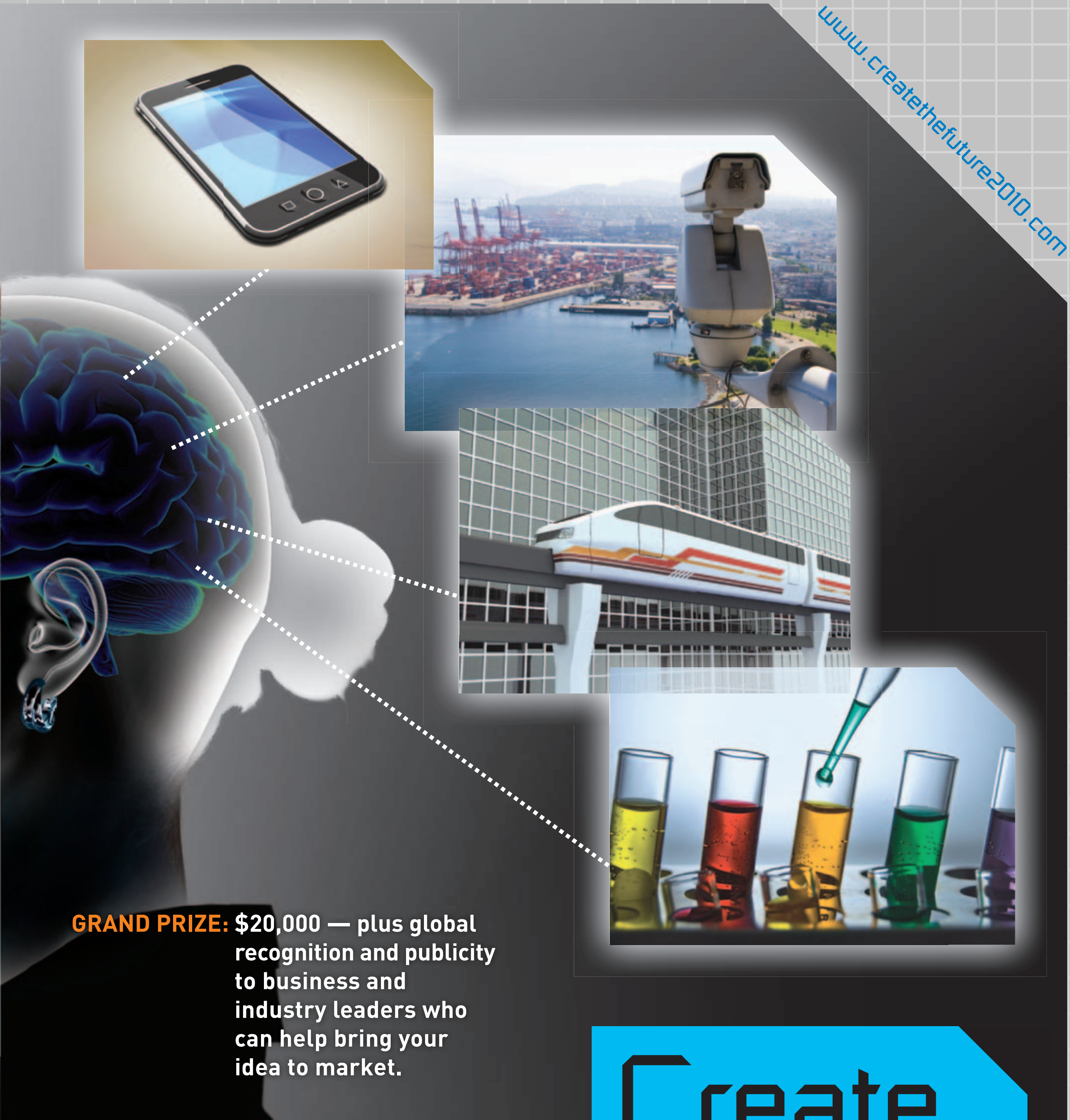


Figure 1. 2D axisymmetric COMSOL model of the cutting rate and thermal effects of a TURP loop electrode.

The Practical Advantages

While Mr. Ward and Mr. Ladtkow utilization of COMSOL varies greatly, they both agree that it offers exceptional compatibility with other software programs. For example, they both use COMSOL in conjunction with MATLAB®. Mr. Ladtkow mentioned how COMSOL has allowed for the simulation of a wide range of tissue conditions. "I think there is a lot of power to be able to use some of the toolboxes that come with MATLAB, like the genetic algorithms and additional search and optimization algorithms where you can couple it with COMSOL and you can optimize parameters in your model using some pretty sophisticated optimization algorithms. I think that is a really powerful thing to be able to do," he said.

While the primary output of the work done in COMSOL has been educational, key customer concerns have been addressed, thereby allowing Covidien EbD's devices to be used with more confidence and improved patient outcomes. "The end result of a better understanding of the relationship between the application of energy and the desired surgical effect and the ability to clearly demonstrate that relationship through images and animations increases everyone's understanding and comfort with new technologies and how they are best used in a surgical environment," asserted Mr. Ward. ■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Mixed Polymers Form Unique One-Piece Medical Implant

Mixing polymers for a medical implant while injecting them into a mold involves setting a wide range of parameters. When they ran into manufacturing problems, engineers developed a COMSOL Multiphysics model that uncovered the cause and have helped bring a similar novel polymeric implant based on this process to clinical trials.

BY DR. MARK YEOMAN, R&D DIRECTOR, CONTINUUM BLUE LTD.

Many soft tissue medical implants are only required for a number of months or years before the body's own tissue regenerates and heals. At this point it is sometimes desirable to remove them; however, this is not always possible. Such soft tissue medical implants have traditionally been made of fabrics or biotextiles, but with the advancement of specialized polymers there is a huge interest toward the use of hyper-elastic polymeric materials to produce implants that duplicate or augment the natural response of body tissues. Engineers at Continuum Blue Ltd. (UK) are taking that process a big step forward with the development of soft tissue implants made of biodegradable hyper-elastic elastomers that, when they have served their purpose, dissolve naturally within the body to eliminate the need for revision surgery to remove them.

Founded in 2004, Continuum Blue specializes in the research, development and analysis of medical devices and implants. It has worked with a number of international companies including Medtronic, Abbott Spine (now Zimmer), Synthes, NuVasive, Scient'X, British Technology Group, Ranier Technology, Aesculap and Blackstone Medical to name a few. The company focuses primarily on the orthopaedic and cardiovascular markets.

Novel new ligament implants act as would a rubber band to hold together and support bones while providing flexibility. However, they require anisotropic material properties to address various requirements. For instance, in a rotator cuff LARS (Ligament Replacement and Augmentation System, Figure 1), the implant must be flexible enough to give the patient ease of arm movement without restriction, and at the same time providing sufficient stability for functional use of the arm and shoulder region such as

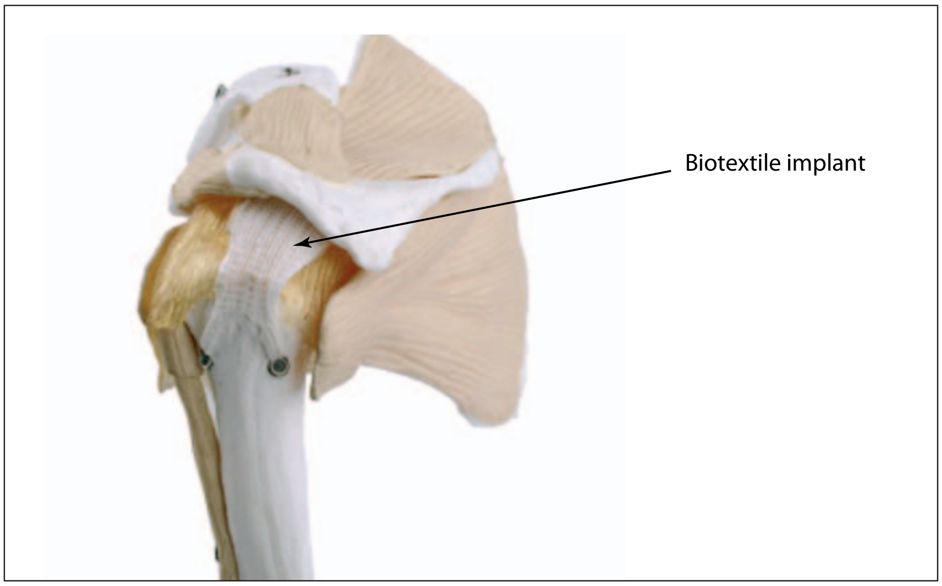


Figure 1. A fabric-based LARS implant shown in a shoulder joint. Note the two screws in the bone that anchor the fixation holes at one end of the implant. Continuum Blue is now working on a multi-elastomeric version of this implant that will biodegrade once the joint has been healed.

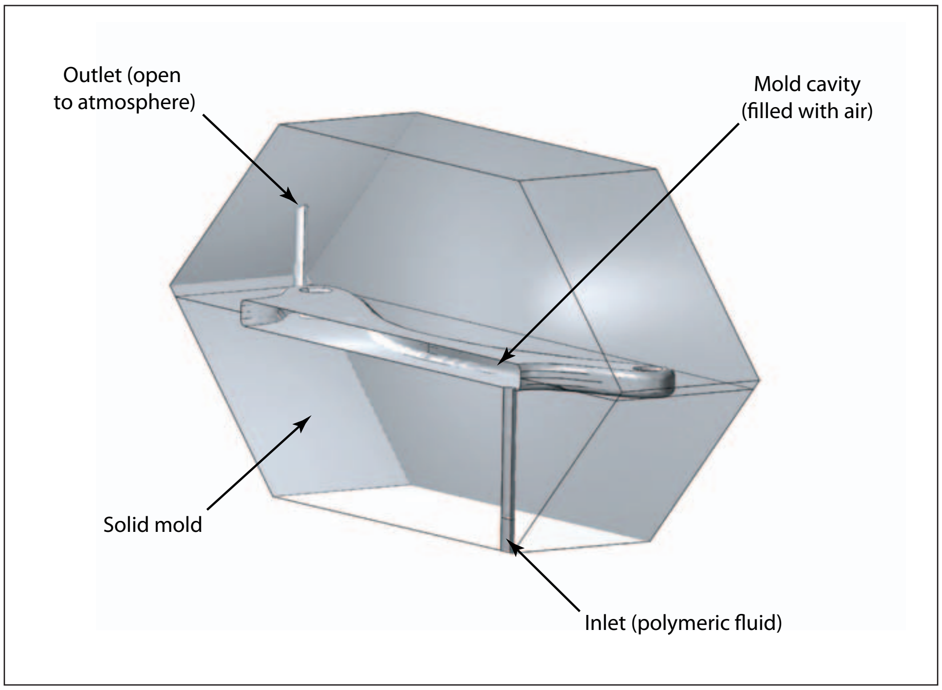


Figure 2. Modeling domain showing half the geometry for molding a dual-elastomer LARS. The polymer solution enters at the bottom and pushes air out through the top opening.

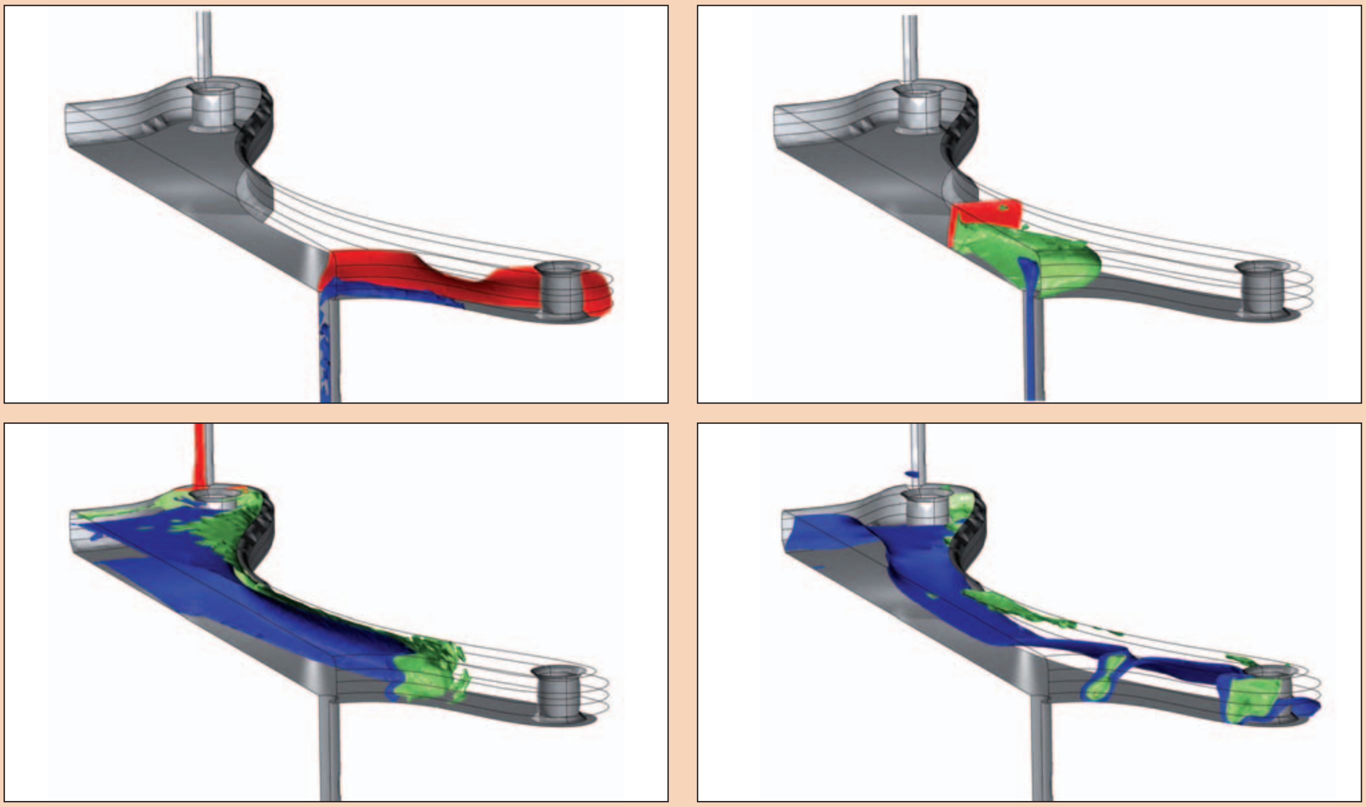


Figure 3. Simulation of the polymer as it fills the mold cavity after 20s, 40s, 100s and 3000s. The red isosurface indicates where the boundary between the polymer mixture and air occurs, the green isosurface indicates where the volume fraction between the two polymers is at 50%, while the blue isosurface is where the second polymer has a volume fraction of 100%. Note that some of the mold cavity walls have been removed for illustrative purposes.

where the patient wants to support or hold an object steady.

Mixing Polymers

A single elastomeric material cannot meet the desirable requirements of such a LARS. Our client developed a novel method of injecting two slow-curing polymers into a mold to create a one-piece implant with the desired anisotropic hyper-elastic properties. With a model, we were able to determine how to best manufacture the 3D implantable device in a single production process. This we have successfully done, and a product based on this process is now undergoing clinical trials. The next step is to add a third polymer that will add the desired biodegradable properties and contribute further to additional anisotropic hyper-elastic material properties.

Such polymer-based LARSs have many benefits. They're relatively inexpensive and quicker to produce than textile-based LARSs, which require multiple manufacturing steps. As there is human intervention in each of these manufacturing steps, each also requires extensive quality assurance (QA). In contrast, the polymeric implant requires just two steps: the molding and then the cleaning of the final product, thereby slashing manufacturing and QA costs.

Our first prototypes involved two elastomers that flow into the mold in the right concentration, at the right sequence, at the right speed, and under the right conditions. Each end of the molded product consists of 100% of one of the elastomers, and the regions in between have a continuous mix of the two. Our engineers must control the point of injection as well as the temperatures of the injected polymers, the overall mold, and the faces of the mold. Other aspects that must be controlled are when the polymer enters the mold and their combined volumes.

Determining the proper parameters for all of these variables is no easy task. In fact, when developing the first implant of this type, we encountered a manufacturing problem but could not identify the cause in the molding process. We then turned to simulation software to give us more insight into the process, and in the end it was only COMSOL Multiphysics that was up to the task. In particular, its capabilities to handle full 3D dual-polymer injection and control of the injection profile were not available in any of the

"We then turned to simulation software to give us more insight into the process, and in the end it was only COMSOL Multiphysics that was up to the task."

"COMSOL Multiphysics has been very valuable to finding a solution to this project, and its capabilities will certainly be beneficial and a key component to our future."

specialized injection-molding software alternatives we evaluated.

As for the model itself, it consists of three domains: a solid region for the mold cavity walls; a liquid region for the injected polymers; and a gas region for the air in the cavity. The co-injected polymers are mixed prior to entering the mold, which was simulated by including a boundary condition that describes the volume fractions of the two polymer solutions as a function of the injection rate. This description was very easy to define in COMSOL Multiphysics but almost impossible in other software.

To handle the complex interactions of the polymers with each other and the surrounding environment, we coupled three transient physics interfaces to each other. First, a two-phase flow phase field interface simulates the liquid flow front as it evacuates the air from the mold cavity. Second, a phase-field flow interface simulates the two dual injected polymer solutions in the liquid phase of the two-phase flow and their interactions with each other. Third, the convection and conduction application mode models the thermal changes. When the injection process comes to a stop, the filled cavity cools down. During that process, the two polymers' densities and viscosities change, and continued fluid-fluid interaction motion occurs until high viscosities are reached and all flow stops (Figure 3).

This model itself consists of roughly 50,000 elements and almost 300,000 degrees of freedom. It solves in 18 hours on a 2.8-GHz Intel Core 2 quad processor with 8 GB of memory running on Windows Vista.

Temperatures and Flows Correspond Nicely

The validation of the model was performed on a different complex three-dimensional body and cavity that cannot be fully disclosed in this article. However, we validated our model in three ways. First was a qualitative evaluation where we compared a video of the liquid-air flow front during the filling process with an animated visualization of the same process in COMSOL. We found that the model is very good at showing the fluid-air interface and the observed flow around various 3D features (such as walls and curved surfaces, including flow baffles) in the mold cavity at different injection rates.

Next, we placed three thermocouples inside the model at three locations to measure the temperature of the polymers as they flowed into the cavity and cooled. The thermocouples were located at the top, bottom and side of the mold cavity. The readings from these thermocouples were compared with the simulation. Figure 4 shows that there is a very good fit to the physical data. Concerning the discontinuities in the physical injection profile, they are due to the switching of the solenoids that control the polymer flow into the mold. In contrast, the model uses an ideal smooth flow function. For our purposes, these curves show excellent results from the model.

Third, once the mold had cooled and the polymer cured, sectional cuts were made in the device to look specifically

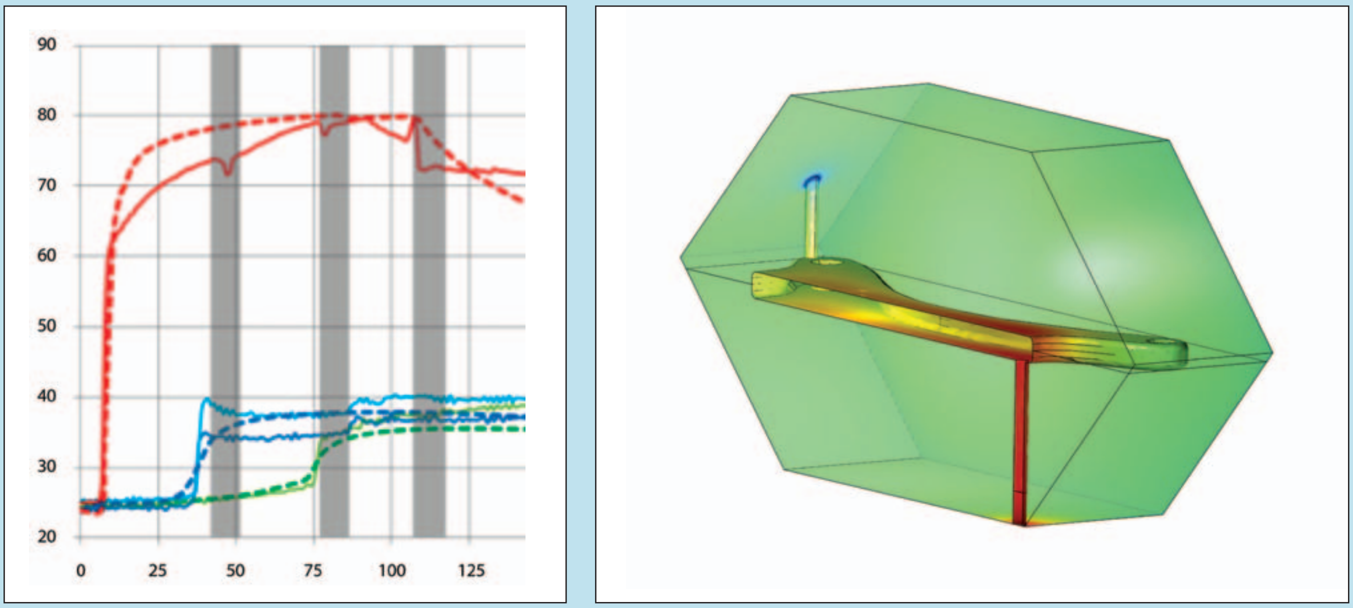


Figure 4. (left) Comparison of temperature readings inside the mold cavity during the filling process compared with model results. The solid lines represent measured data, and the dashed lines indicate the model data. The erratic sections in the measured data (represented by the grey regions in graph) are due to opening and closing solenoids to control the flow of the injected polymers. (right) Thermal plot of the mold cavity during filling.

at the boundary between the two polymer regions and compare them with the model. Once again, the model solution gives a very good estimation of the actual makeup of the implant (Figure 5, and note that this model shows a partial view of a 3D device different from the actual rotator cuff LARS).

With the model, it's now possible for us to investigate many mold variations in a reasonable time and cost. It is estimated that a single mold redesign and trial run with the model takes roughly 1.5 days and costs approximately GBP 850. In contrast, to do a physical sample run, where a specialized silicone mold costs approximately GBP 3000, the estimated total costs are almost GBP 9000, and the time to get the redesigned silicone mold is between 3 to 4 weeks.

Without COMSOL, finding the critical parameters that control polymer location would have taken much longer and would have cost in the order of 20 times more to do so. In addition to cost, due to the opaque nature of the molded implant samples, it is very difficult to easily define the polymer boundaries and graduated regions of the physical samples (as seen in Figure 5). In order to do so, microbubbles or dyes had to be added to the polymer solutions, changing the polymers' flow characteristics. Another more expensive option was to use mechanical-indent analysis to map physical material differences at points throughout the mold. In contrast the model gives far better insight into what is happening during the mold filling process, where the client can easily visualize the end product and the mixed regions between the two polymers. Having the COMSOL model and the resulting visualizations provide clear cost- and time-efficient benefits when convincing customers of the best mold process to provide a viable polymeric LARS solution.

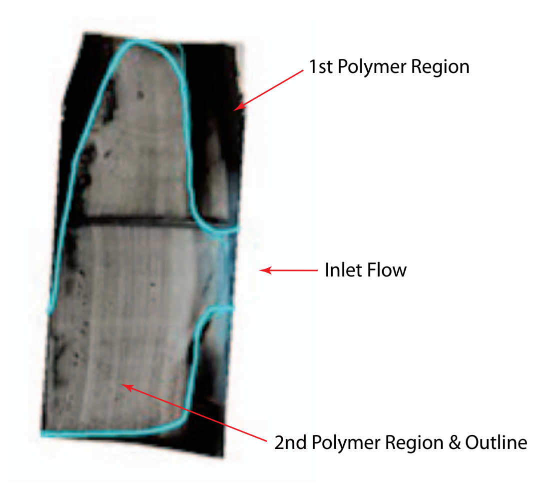


Figure 5. A cross-section from a validation sample compared to COMSOL results (blue line) shows that the outline of the second polymer matches very closely.

Adding Biodegradability

With the validated model in hand, our group has many projects in mind. First, we want to increase the number of injected polymers to allow for a biodegradable product. We also want to allow for multiple injection points.

Most ambitious of all is to add parameterization to the model so that the software can help us quickly find the process parameters for new products. It will be necessary to change the size and shape of a LARS implant to account for different anatomy, joint complications and disease. We thus hope to create an optimized model whereby we need only describe the end product's geometry, and the software will suggest the best mold design along with the process parameters that will result in the desired physical properties. The model will hopefully cater to any mold and material design change we might encounter.

In summary, COMSOL Multiphysics has been very valuable to finding a solution to this project, and its capabilities will certainly be beneficial and a key component to our future. ■

Acknowledgements

The author would like to thank Robert Snell at Ranier Technology for his assistance and help with this work.

The author, Mark Yeoman (right), receives an award from Svante Littmarck, President & CEO of COMSOL, Inc., during the Milan COMSOL Conference 2009.

About the Author

Dr. Mark Yeoman, R&D Director at Continuum Blue, is a medical-device development specialist with over 12 years of experience and expertise in this area. He has a PhD in computational modeling and applied mathematics, where his postgraduate studies focused on the design and optimization of cardiovascular implants using computational techniques and genetic algorithms for Medtronic. Dr. Yeoman has also worked for Disa Vascular, which specializes in stents. He also lectured at the graduate and undergraduate levels for a number of years on Dynamics and Computational Methods & Techniques.

Designing New Magnet Technology — A Multiphysics Challenge

Since 1995, Advanced Magnet Lab (AML) has provided revolutionary technology for the design and manufacture of advanced coils, magnets, and magnet systems for the energy, medical, defense, and research industries. The company's 3D coil-design software and automated construction processes enable rapid deployment of complex state-of-the-art magnets.

BY CATHLEEN LAMBERTSON

Recently, AML developed a new magnet topology — Direct Double-Helix™ (DDH) magnets — that allow for a significant increase in power density, performance in field generation, and field quality. The unique characteristics of the DDH magnets, part of the Double-Helix™ (DH) magnet family invented by AML's founder, Dr. Rainer Meinke, could lead to more affordable systems and potentially portable devices. The magnets have a large number of applications including high-speed generators and charged particle beam optics. AML's customers include the Department of Energy, NASA, the European Organization for Nuclear Research (CERN), Center for Advanced Power Systems (CAPS), National High Magnetic Field Laboratory (NHMFL) and GE Medical Systems.

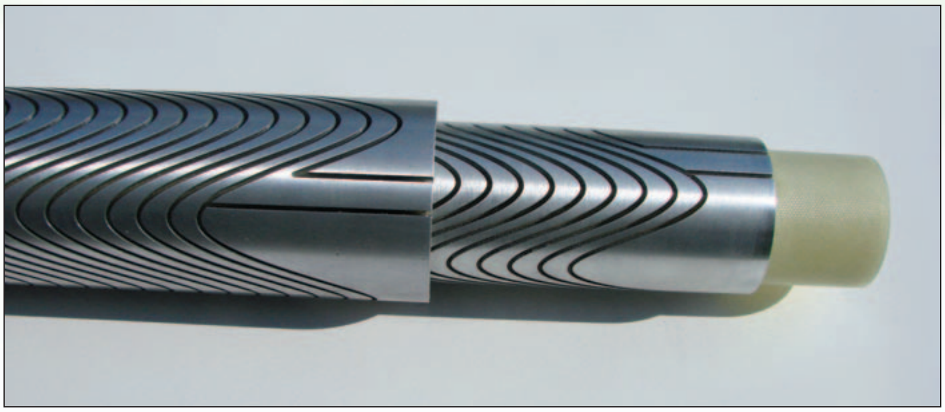


Figure 1. 2-layer multipole DDH magnet.

The Technology

Unlike conventional magnets based on saddle or racetrack coil configurations, AML's processes and designs enable magnets of any multipole fields with unmatched field homogeneity. Specifically, the DH and DDH magnets are composed of modulated tilted helices (Figure 1) that produce magnetic fields with very pure multipole content. However, while DH magnets are based on very accurate positioning of wire in machined grooves, DDH technology enables the design and manufacturing of magnet coils in one step without conventional conductor and winding processes.

"DDH magnets are created *in-situ* and conducting paths are machined directly out of a resistive object such as a conductive cylinder. The machined grooves serve as electrical insulation and follow a mathematical equation leading to non-uniform cross-section of the conductive paths," stated Dr. Philippe Masson, a Senior Research Scientist at AML. This results in a reduction of the total electrical resistance of a DDH magnet meaning more current can be flown into the conductor; hence, smaller magnets are produced. "Another great benefit is that each layer of a DDH magnet presents a large surface allowing for improved cooling. With a simple water-cooling system, small DDH coils can carry an excess of 200 A/mm^2 of peak current density in steady state."

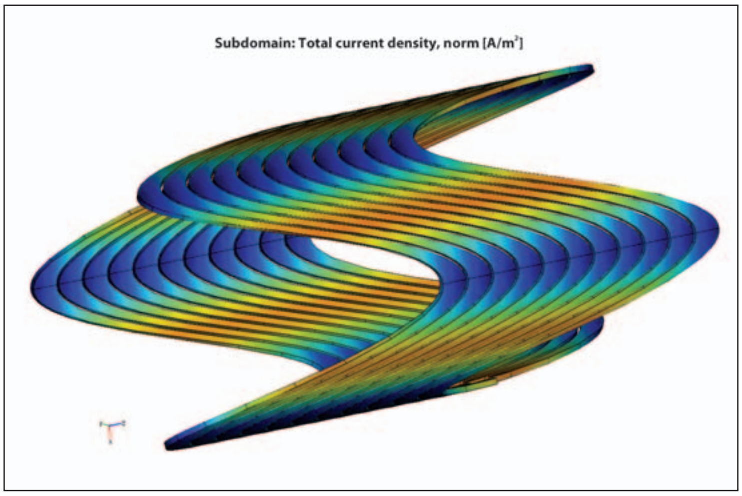


Figure 2. Current density distribution in a few turns of a 4-pole DDH magnet.

Optimized Magnet Design

According to Dr. Masson, when DDH was invented, the advantages were clear in concept — outstanding performances were obtained experimentally and applied

"With a simple water-cooling system, small DDH coils can carry an excess of 200 A/mm^2 of peak current density in steady state."

Senior Research Scientist Dr. Philippe J. Masson (left) and the creator of the Direct Double Helix magnet configuration, Chief Scientist Dr. Rainer Meinke, showcasing their breakthrough magnets.

"Using COMSOL Multiphysics allows for the design to be optimized numerically before anything is actually fabricated. All the trial and error can be performed through simulation, thus saving time and money."

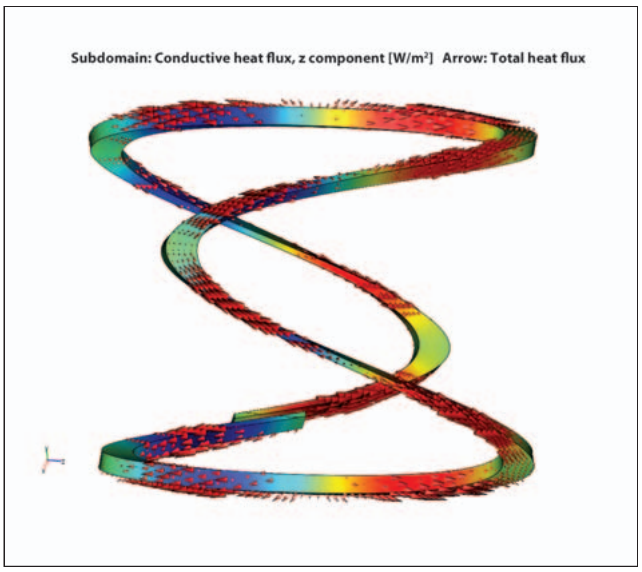


Figure 3. Heat flux distribution in one turn of a 4-pole DDH magnet.

to commercial products. "However, in order to really understand the physics behind the measurements, a detailed numerical analysis was required."

COMSOL Multiphysics was used to visualize the current distribution in the magnet (Figure 2) and to simulate the heat transfer in steady state operation through the coupling of the Conductive Media DC and General Heat Transfer physics interfaces. "The main question is, 'what is the limit of the technology?' Magnet design is a multiphysics process dealing with electromagnetism, thermal analysis, structural analysis, and fluid dynamics. The software allowed for all those aspects of the design to be simulated and moreover to be coupled together, making it the ideal tool for a magnet company," said Dr. Masson.

Since the resistance of the DDH coils strongly depends on the current density distribution, the first question Dr. Masson and his team needed to answer was how the current actually distributed in the conductor and how to accurately predict the resistance. Secondly, the team needed to figure out how the non-uniform distribution of current density in the conductor affected the field homogeneity. Finally, they worked on how the heat propagates in the coil and to the coolant. "All these questions were answered and the results are used to help push the limits of the technology and improve the coil design," stated Dr. Masson. "Using COMSOL Multiphysics allows for the design to be optimized numerically before anything is actually fabricated. All the trial and error can be performed through simulation, thus saving time and money." ■

Figure 1. The Compact Muon Solenoid (CMS) experiment at CERN.

Photo courtesy of CERN, photographer: Maximilien Brice

Cooling of the Largest Magnet in the World at CERN

Modeling has proved invaluable in understanding and optimizing the processes cooling the superconducting magnets needed in the world's most advanced particle accelerators, and COMSOL proves very attractive to researchers focused on the physics.

BY DR. BERTRAND BAUDOUY, CEA (FRENCH ATOMIC ENERGY COMMISSION)

In high-energy physics it's necessary to accelerate particles to incredible speeds while controlling their paths with extreme accuracy, and this is done with superconducting magnets. Their design is very complex, but various options can be examined and refined much more quickly with simulation software. Scientists at the French Atomic Energy Commission (CEA) have also discovered that COMSOL Multiphysics provides a good complement to in-house codes.

Largest Superconducting Magnets in the World

One quite famous example comes from the Large Hadron Collider at CERN (The European Organization for Nuclear Research), which is the world's largest scientific experiment. Located 100 meters underground in parts of both Switzerland and France, this collider has a circumference of 27 km. To accelerate its subatomic particles to 99.99% of the speed of light, the LHC uses more than 8000 superconducting magnets cooled with liquid helium. The cryogenic distribution system that circulates superfluid helium around the accelerator ring keeps the LHC at -271.3 °C (1.9 K), colder even than outer space. The Accelerator, Cryogeny and Magnetism Division of CEA located in Saclay, France — which includes roughly 120 employees, 30 of whom are active with simulation — have made frequent use of simulation software in their development of magnets and the processes for cooling them.

In particular, the Compact Muon Solenoid (CMS) particle detector in the LHC includes the largest superconducting magnets in the world, externally cooled with coils that carry two-phase helium operating at 4.2 K. They use natural convection to eliminate a pressurization system and the associated pumps with their costly maintenance and operation at low temperatures. This magnet, 7 meters in diameter and 12.5 meters long, consists of five independent modules, each cooled indirectly through a network of parallel tubes soldered onto the magnet casing. The modules are supplied with liquid helium through downward tubes from a reservoir that also serves as a phase separator.

The high current density of superconducting magnets makes it feasible to build them with the necessary magnetic field strength in a reasonable amount of space and with moderate energy consumption. Running the LHC requires 50 MW, half of this alone for the cryogenics system, and obtaining the precise cooling required is no easy task. Engineers must come up with designs that minimize the use of liquid helium, where the total helium inventory for the LHC is 700,000 liters, which equates to 2.6 million euros.

> "I can now design the cooling tubes for a superconducting magnet in a week or so, work that previously took two to three months."

For large detector magnets like those used in the CMS, the internal cooling

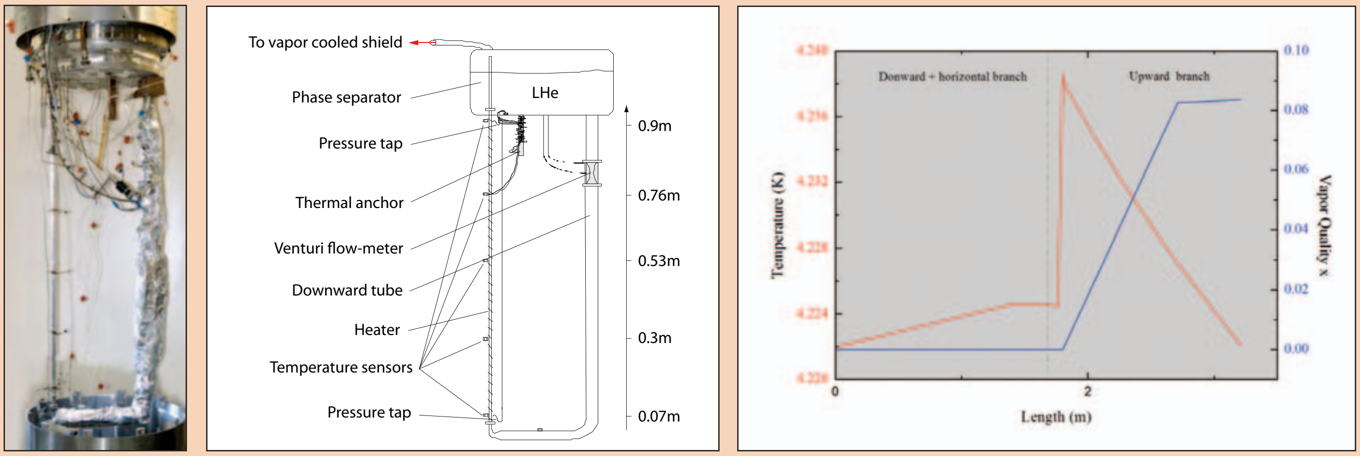


Figure 2. A photo of the small scale cooling loop (left) and a diagram illustrating its components (center). On the right are results from the 1D model show the temperature and vapour quality throughout the loop: 1- liquid helium tank; 2-downward and bottom pipe; 3-upward pipe.

has to be designed very carefully to ensure a proper cooling during normal operation as well as for scenarios such as quenching the magnet. Many variables come into play: the sizing and placement of the cooling tubes as well as the mass flow and pressure of the helium in the loops.

I wanted to investigate the cooling cycle with software that I could easily understand and experiment with as a complement to our highly specialized in-house code. I was delighted when I discovered COMSOL because with it I can see the physics rather than hundreds of lines of C or FORTRAN code. It is very easy to use and shows the physics immediately. You can use and modify the equations in the various modules or, as I did, enter your own equations. Meanwhile, I have become a true convert to COMSOL and people in my institute are calling me from other labs to ask about my experiences and how they might put it to use in their applications.

Design Improvements to Come

To get a deeper understanding of the helium two-phase thermosiphon open loop so as to optimize it for future projects, our group built a scale model where the test loop is 2 meters instead of 6 meters (Figure 2). To validate the concept we then simulated its operation with COMSOL Multiphysics and our results agreed very closely with the experiment. Now I have a tool that allows me to modify this loop for many other applications such as enlarging the loop or changing the geometry as well as modifying the effects of friction. Even better, I can now design the cooling tubes for a superconducting magnet in a week or so, work that previously took two to three months. My next step is to further expand the model to simulate a closed-loop cryocooler where the vapor is recondensed, which will allow the loops to be much smaller.

The work done in COMSOL Multiphysics will be extremely valuable in our current projects, just one being the development of the R3B superconducting magnet at the Facility for Antiproton and Ion Research (FAIR), Darmstadt, Germany. At its heart is a superconducting synchrotron double-ring facility with a circumference of about 1100 m, and it is planned for completion in 2011. Its cryogenics system is likewise based on the thermosiphon loop concept used in the CMS magnet but with horizontal cooling tubes. ■

About the Author

Dr. Bertrand Baudouy is a research scientist at the Accelerator, Cryogenics and Magnetism Division of CEA (the French Atomic Energy Commission), and he is currently leading the R&D activities in the Cryogenics Laboratory.

Intro Cov ToC

Simulation

Capture the Concept

COMSOL Multiphysics version 4.0 brings an unprecedented level of clarity to your simulation work by giving you both an organized model overview and a streamlined model-building process. The COMSOL user interface reduces clutter and redundant tasks, so your attention can be focused on the substance of your design studies resulting in increased productivity. Naturally COMSOL continues in its tradition of powerful solvers and flexibility in physics, but it is the new user interface that stands out the most.

New Products

The LiveLink suite is just the first in a series of products designed to help you get the most out of COMSOL. Version 4.0a, available this June, includes three new modules: CFD, Plasma, and Batteries & Fuel Cells. With this release we also consolidate the Chemical Engineering and the Reaction Engineering Modules to the Chemical Reaction Engineering Module.

Application Programming Interface

Version 4.1 will be unveiled at the users' conference this fall. This release will mark the first in an initiative to open up the COMSOL environment for building your own physics interfaces for others to use. At the conference, you will see a preview of what the API (Application Programming Interface) will look like.

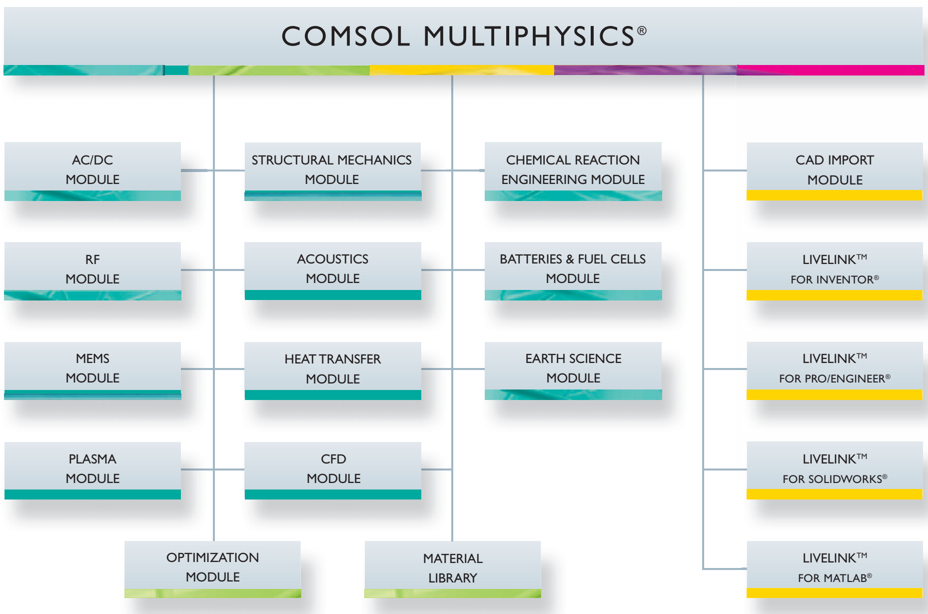
Hands-On Workshops and Training

To get a quick start using COMSOL and running your first simulation, attend a workshop. A one-day class is available for getting up to speed rapidly with version 4.0.

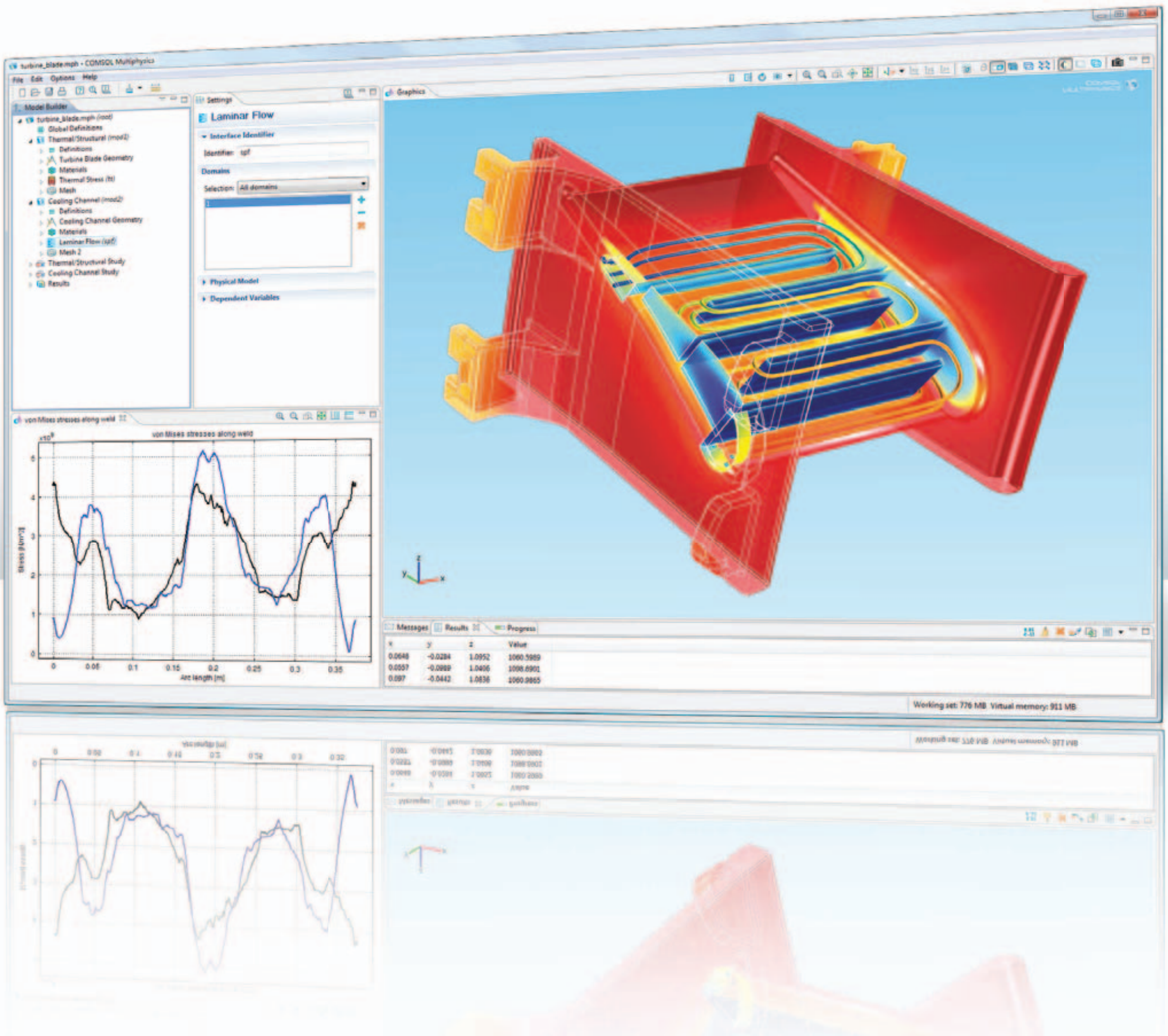
For worldwide dates and locations visit www.comsol.com/events.

COMSOL PRODUCT SUITE
The LiveLink suite opens a new dimension in your simulations by integrating your models with external CAD packages and MATLAB®.

We are also proud to introduce three application specific modules: CFD, Plasma and Batteries & Fuel Cells.



Highlights 2010



A stator blade in the turbine stage of a jet engine is heated by the combustion gases. To prevent the stator from melting, air is passed through a cooling duct in the blade. The resulting temperature gradients introduce significant stresses. Shown is the temperature distribution throughout the blade, as well as the von Mises stresses in both welds.

COMSOL

Modeling Continually Improves Advanced Materials for Automobiles

BHASKAR PATHAM, PH. D., KIRAN B. DESHPANDE, PH. D., AND SAMPATH K. VANIMISETTI
GENERAL MOTORS GLOBAL RESEARCH AND DEVELOPMENT, INDIA SCIENCE LAB, BANGALORE

Automakers such as General Motors are playing a key role in creating the science and technology that will help shape the global future in terms of personal transport. As GM focuses on developing automotive solutions that are sustainable in terms of energy and environment, reducing weight of the vehicle and electrification of the propulsion system have emerged as key priorities [1]. These solutions are driven by continual exploration of new materials and manufacturing processes — for example, multi-material solutions and composites for lightweighting and robust battery materials for electrification. Developing a fundamental understanding of these new material systems and the associated manufacturing processes therefore becomes very important and forms a key effort at the GM Global R&D. At the Material Characterization and Modeling Group, which is a part of the India Science Lab of the GM Global R&D, we are integral to this effort, with the mission to develop validated computational models applied to various products and sub-systems performance and the associated manufacturing processes. In this article, using three simple examples, we illustrate how computational tools help us in developing a fundamental understanding of materials and their processing, and in improving material and process performance.

Process-Property Interrelationships in Thermosets and Thermoset-Matrix Composites

Thermoset-matrix composites hold great potential as automotive materials because of their lower density (compared to metallic alloys such as steel), high specific strength, and good energy dissipation characteristics. With the right combination of suitable fibrous reinforcement and processing, thermoset-matrix composites have the potential for replacing ferrous materials in structural applications, thereby contributing to automotive lightweighting. In addition, thermoset resins, both unreinforced as well as reinforced, find wide applications in automotive component joining as adhesives.

Processing of thermoset resins and thermoset-matrix composites involves "cure," which converts them from their initial viscous fluid (or soft solid) state, through progressive crosslinking, into a stiffer solid. The curing process also typically involves application of heat, pressure (from a mold or in an autoclave), and constraints (globally, from a mold, or the components of a joining assembly, and at the local scales, from the reinforcing fibers). The versatility of thermoset chemistries allows the achievement, upon complete cure, of properties for the base resin that can range from rubbery to high stiffness for semi-structural applications (equivalent to engineering thermoplastics).

Processing of thermoset-composite parts and assembly with thermoset adhesives come with their own set of challenges. For example, while steels behave quite well during forming operations and show excellent retention of shape after being removed from a mold or press, this isn't easily achieved in the case of thermoset composites. This is because cure-induced residual stresses can result in springback of thermoset components after they are released from the mold or in shape-distortion effects in assemblies. Cure-induced residual stresses are driven by the evolution of the modulus of the crosslinking resin, combined with constraints that arise from the relative mismatch between the thermally or chemical-shrinkage induced deformations between the thermoset resin and the mold/components of the joining assembly/reinforcing fibers.

Process engineers may resort to a variety of strategies to minimize shape-distortion effects in thermoset systems: they can redesign the mold, modify the temperature-ramp during the cure-cycle, or modify the fibers and resins that make up the composite. Of course,

"COMSOL allows manipulation and redefinition of existing variables without resorting to complex user subroutines."

in the absence of a fundamental understanding of the various mechanisms that contribute to the development of residual stresses in a particular system, this would involve experimental trial and error, which would be a very expensive proposition. Simulations of residual-stress development in thermosets not only allow the systematic probing of various underlying mechanisms that may cause shape distortions, but also present an inexpensive alternative to experimental trial and error to arrive at optimal design and process modifications so as to mitigate the deleterious consequences of residual stresses.

In order to be able to use the estimates obtained from these simulations to formulate guidelines for process and design modifications, it is imperative to account for the cure-, temperature-, and time-dependence of the resin properties with utmost accuracy. As an example, the choice of material model — an elastic material model or a viscoelastic material model — can have significant impact on the predictions of residual stresses. Elastic models are simpler to set up, are computationally efficient, and give reasonable results in many scenarios. Viscoelastic models, on the other hand, capture the material properties much more faithfully and have higher accuracy, but they are not always easy to set up and are more expensive both in terms of computational memory and time requirements. Several prior studies have employed a viscoelastic model for thermosets, which has been implemented in user codes or as user subroutines in commercial FEM packages. While offering comprehensive models, these studies resorted to either elastic or viscoelastic models alone and did not make a quantitative comparison of the two approaches.

Our goal in this simple demonstration — involving the mold-constrained cure and subsequent springback behavior of a thick asymmetric 90°-elbow section of an unreinforced thermoset resin — was to develop equivalent elastic and viscoelastic models that can clearly pinpoint the differences between the two with regard to the time-, cure- and temperature-dependent evolution of stresses (For details, please see Ref [2]). It should be noted that cure of thick sections can result in significant exothermic heat release, resulting in large spatial gradients in temperature and degree of cure.

In Figure 1, the spatial distribution of stresses in the thick elbow section is shown at the end of the mold-constrained cure cycle, when the degree of cure and temperature are spatially uniform. It is clear from Figure 1 that the instantaneous stresses in a linear-elastic material are only governed by the instantaneous states of temperature and degree of cure, while the stresses in a viscoelastic material are strongly governed by the thermal history experienced by the resin. As seen in Figure 1, the spatial gradients in temperature and cure in thick sections (enhanced by the exothermic heat of reaction) can result in significant spatial variation of viscoelastic residual stresses even after equilibration of the temperature fields and achievement of uniform cure (as evident in a pronounced gradient in stresses along the diagonal of the elbow section).

These subtle details, captured by the viscoelastic model, also result in significantly different predictions of the springback behavior. As seen in Figure 2, the elastic material model does predict springback, but does not capture the shape-distortion details as clearly as the viscoelastic models. Thus, we conclude that the choice of the material model — elastic or viscoelastic — is equally, or more significant than the mold-part-interaction details in governing springback predictions.

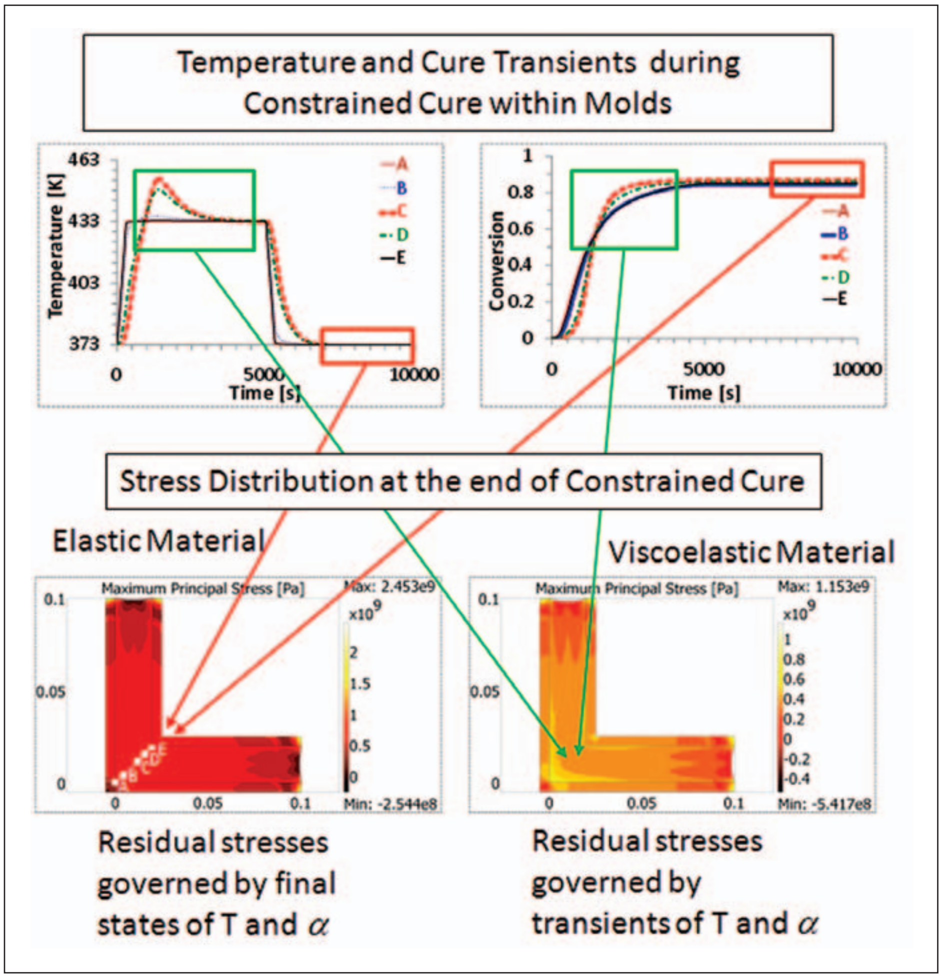


Figure 1. Residual stresses in an elastic material are only governed by the instantaneous states of temperature and degree of cure, while the stresses in a viscoelastic material are strongly governed by the thermal history experienced by the resin.

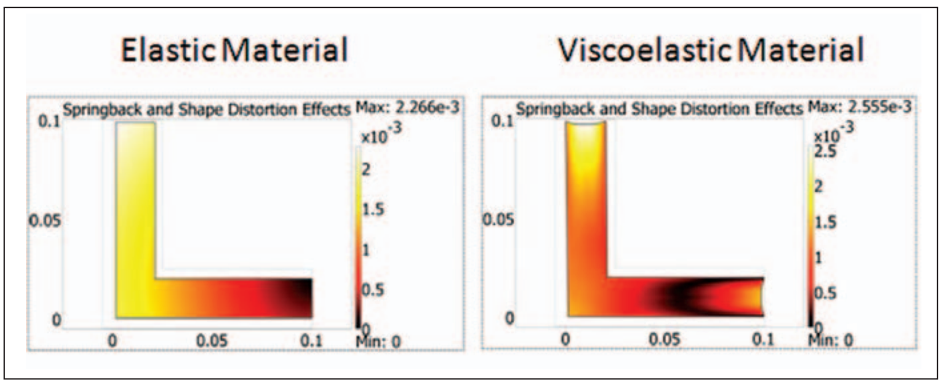


Figure 2. Viscoelastic model (right) captures the subtle influences of temperature and cure transients on the shape distortion effects.

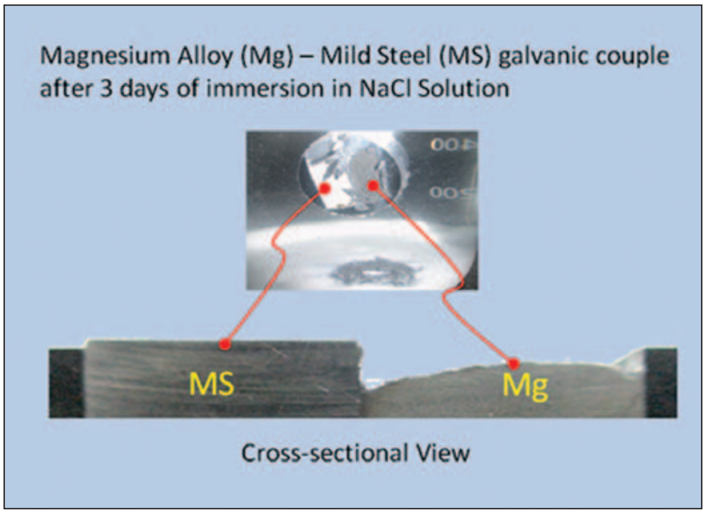


Figure 3. Corrosion of magnesium joined with steel when immersed in a salt solution.

We have thus been able to develop a model that accurately captures the evolution of residual stresses throughout the manufacturing process and determines their effect on the final shape of the composite part. For this application, COMSOL offers several advantages, as it allows manipulation and redefinition of existing variables without resorting to user subroutines and thus accommodates more complicated expressions for the evolution of the modulus apart from the basic viscoelastic model setup. The coupling between heat-transfer and diffusion analysis (to account for the exothermic heat of reaction) was readily available as a part of the standard variables offered in COMSOL. The coupling between diffusion and structural mechanics (to account for shrinkage strains), while not readily available as a part of standard variables, could be established in a systematic fashion without resorting to a complex user-defined routine because all the variables employed for the analysis are transparent to the user for easy modification.

Galvanic Corrosion in Multi-Material Assemblies

As noted earlier, a key thrust in the automotive industry is reducing vehicle mass. This has led to the exploration of multi-material solutions in the automotive structure, body, as well as powertrain. Magnesium is the lightest structural material, being 4 times lighter than steel and 1.5 times lighter than aluminum. However, the use of magnesium is quite limited today primarily due to its poor corrosion resistance. The corrosion behavior of magnesium, joined with steel and immersed in an electrolyte solution, is shown in Figure 3, in which it is possible to see that a considerable amount of material has been dissolved in the electrolyte from the magnesium's surface.

In order to quantify the dissolution rate (corrosion rate) of magnesium joined with steel, we developed a model using COMSOL Multiphysics. The polarization behavior of magnesium and steel, obtained individually from lab-scale polarization experiments, was used for the boundary conditions. Because the magnesium surface is continuously dissolving in the electrolyte, the galvanic corrosion becomes a moving boundary problem and was implemented using the Moving Mesh application mode. This numerical approach helps in the understanding of the corrosion mechanism, in the selection of materials based on galvanic-corrosion severity, and also in

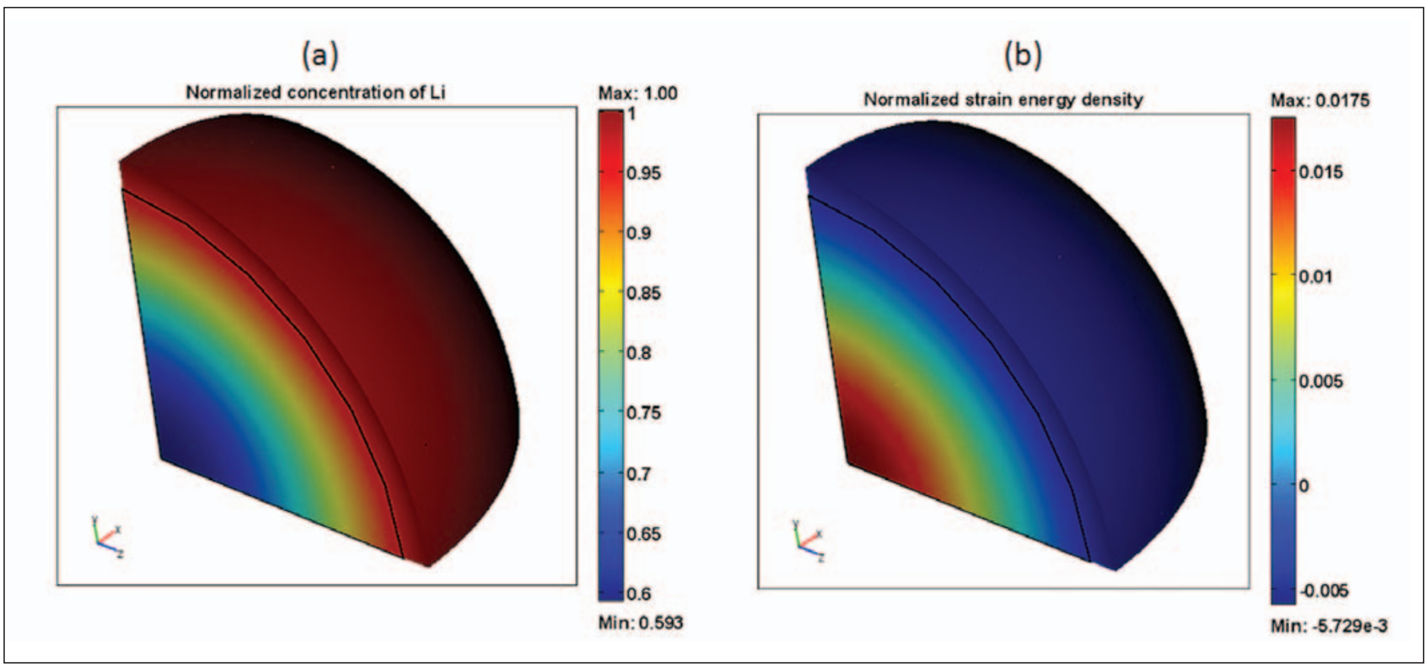


Figure 4. Typical 3D results from COMSOL Multiphysics simulations of a nodular battery electrode particle, idealized as a sphere. It shows the subdomain contours of (a) the normalized lithium concentration and (b) normalized strain energy density during intercalation of lithium into the host material while the battery is being charged or discharged. The black outline is indicative of the initial shape and size of the particle. Deformation is scaled for clarity.

providing design guidelines accounting for cathode-to-anode area ratio.

Mechanics of Advanced Battery Materials

In recent years, the electrification of vehicles has become an important strategic initiative. R&D activity in advanced electrochemical storage devices aims to offer a potentially robust and clean alternative to fossil fuels. Lithium-ion battery chemistry is the obvious choice for automotive energy storage due to its high gravimetric energy capacity and ability to deliver the power density necessary for driving the vehicular powertrain.

Lithium-ion batteries consist of two electrodes into which the lithium intercalates along with an electrolyte in which the lithium ion associates with the anions. Depending on whether the battery is charging or discharging, the lithium intercalates into or de-intercalates from either the positive or the negative electrode. Most electrode materials suffer from volume expansion due to lithium intercalation, which can be as high as 300% for some candidate materials. In addition, phase transformation in the lithiated compounds leads to formation of incoherent phases in the electrode particle that not only lead to misfit strains but also affect further lithiation. The transient in lithium diffusion, along with above aspects, leads to development of large mechanical stresses in the electrode particles. Cyclic intercalation and de-intercalation may cause cracking or accumulation of damage over time in the electrode particle.

It is widely reported that this mechanical degradation of the battery electrode material is associated with capacity fading due to loss of active lithium in the formation of SEI (Solid Electrolyte Interphase) on the damaged surface or electronic isolation. The study of diffusion-induced stresses in electrode particles due to lithium intercalation forms a part of our group's fundamental investigation to understand the impact of electrode design parameters on the performance of the battery.

To this end, we created a 3D model in COMSOL by taking advantage of its multiphysics and customization capabilities. The aspects related to diffusion from the Chemical Engineering Module were combined with 3D stress analysis from the Structural Mechanics Module. We developed a special solution scheme to couple the lithium concentration with mechanical strain and subsequently used that to estimate quasi-static equilibrium stresses in the particle. We then used results from the 3D finite element simulations (Figure 4) to understand the effect of microstructural aspects on the possibility of mechanical degradation of the battery materials.

Future improvements to the model aim to incorporate a more realistic description of the host material by addressing phase transformation due to lithium intercalation, anisotropy and polycrystallinity. Eventually, the study aims to offer clues to mitigate detrimental stresses and improve battery durability. ■

About the Authors

Bhaskar Patham is a researcher at the General Motors R&D, India Science Lab, Bangalore. His research interests are in the areas of experimental and analytical rheology, complex fluids, polymer and composites processing, and processing-structure-property interrelationships in multi-phase polymeric systems and polymeric matrix composites. He holds a Ph.D. in Chemical Engineering and Materials Science from Michigan State University. Prior to joining GM R&D, he was a research engineer with the General Electric Global Research Center at Bangalore.

Kiran B. Deshpande is a researcher at the General Motors R&D, India Science Lab, Bangalore, where he is involved in modeling of galvanic corrosion and its mitigation strategies. He holds a Ph.D. in Chemical Engineering from University of Sheffield. Prior to joining GM R&D, he was a Knowledge Transfer Program associate with University of Sheffield and MHT Technology Ltd., UK. He has contributed a chapter in the book titled *Multiphysics Modeling with Finite Element Methods* by Prof. WBJ Zimmerman.

(From left to right) Bhaskar Patham, Kiran B. Deshpande, and Sampath K. Vanimisetti.

Sampath K. Vanimisetti is a researcher at the General Motors R&D, India Science Lab, Bangalore. His field of expertise is in the area of computational mechanics of materials with specific emphasis on damage and fatigue. At GM R&D he is employing modeling techniques in COMSOL to understand diffusion-induced stresses responsible for fragmentation in battery electrode materials. Proir to GM R&D, Sampath was a research engineer at GE Global Research Center. He holds a M.Sc.(Engg.) degree in Mechanical Engineering from the Indian Institute of Science, Bengaluru (India).

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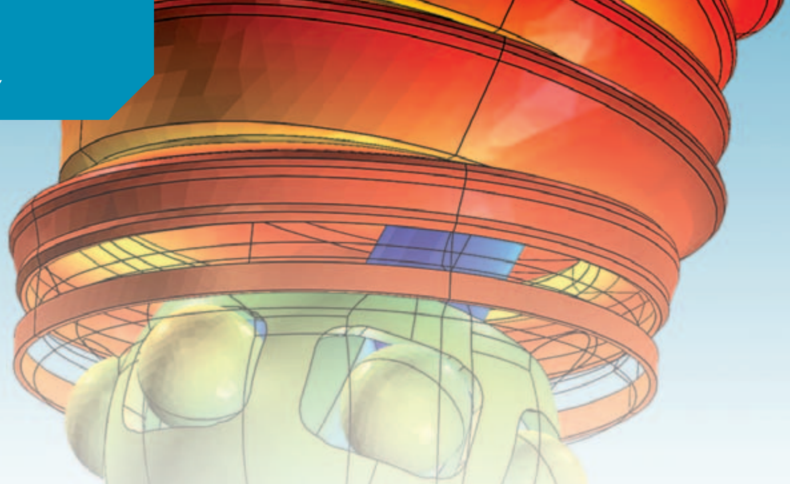
Intro Cov ToC



Simulation Software Makes Major Contributions to Multiple Aspects of Auto-Part Design and Manufacturing

BY FABIO GATELLI AND LUCA ARMELLIN, METELLI S.P.A.

As a major supplier of automobile components, Metelli S.p.A. (Cologne, Italy) designs and manufactures brake parts, engine parts, transmission components and water pumps for OEMs as well as for the aftermarket. Our R&D team has been using modeling software for a decade, but a few years ago we ran into a situation where the software we had been using was inadequate. We then found that COMSOL Multiphysics could handle the job — and in the meantime, we have successfully used COMSOL in an increasing number of projects.

Upgrading From a 2D FEM Tool

We first turned to COMSOL to study the magnetic field in an inverse electromagnetic clutch, which works with a floating disk that is attracted by a magnetic field generated by a permanent magnet; the mechanism is then disengaged through a coil. This project had produced some prototypes designed using a 2D FEM tool. However, we felt the need for a 3D FEM tool both to check the correctness of the simplifications introduced in the 2D model and to be able to manage complex 3D geometries. We chose COMSOL with the AC/DC Module due to good agreement between the model and experiment, which meant that no changes were required to start manufacture of the clutch pre-production samples. We subsequently used COMSOL to examine how the magnetic field flux flows through the steel parts because if this is insufficient, there is no separation between the parts, and the clutch won't work.

Figure 1 shows the norm of the magnetic flux density where the maximum value is approximately 2.64 Tesla. We also compared this value with the clutch magnetic flux saturation limit because a greater value would mean that we would have to redesign the component geometry. In this case, though, 2.64 Tesla was an acceptable value, and so we knew the geometry would function as desired.

With that experience under our belt, we started looking at fluid flow in a vacuum-actuated water pump, specifically to check the maximum actuation time. Of course, we wanted to design a unit that met specifications while building the minimum number of prototypes, each of which can cost 10,000 euros each and take 2 to 3 months to make. In contrast, model simulations could give us answers to our design questions in just a week or two. We turned to COMSOL because we needed reliable results from a model before we started building prototypes.

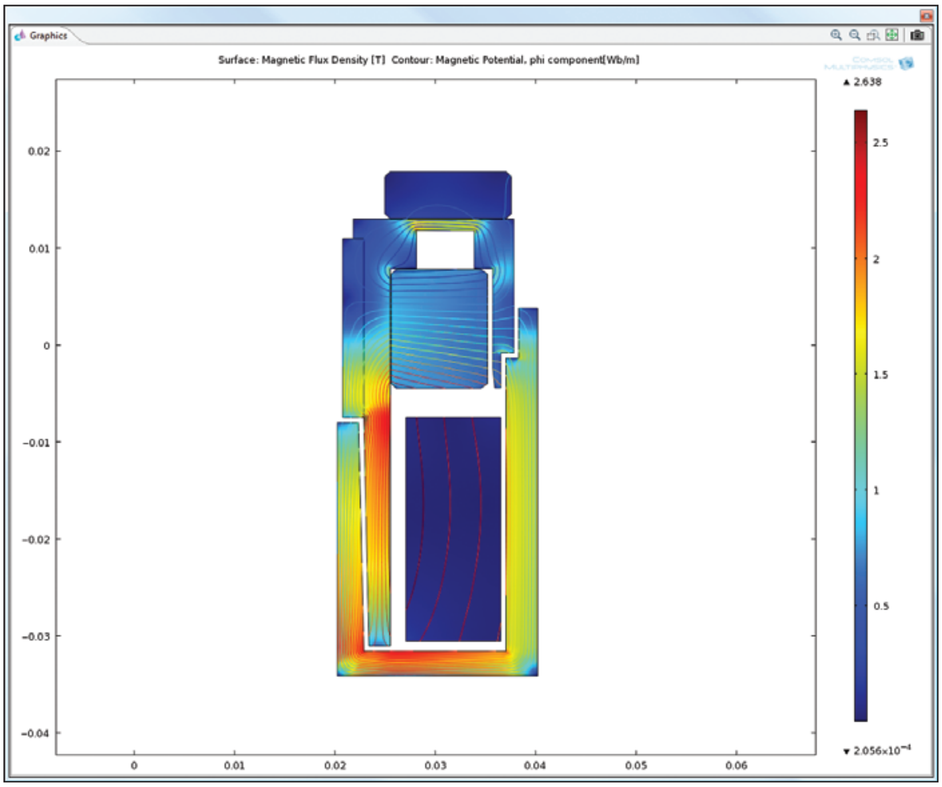


Figure 1. Surface plot of the norm of the magnetic flux density and contour plot of the magnetic potential in a clutch.

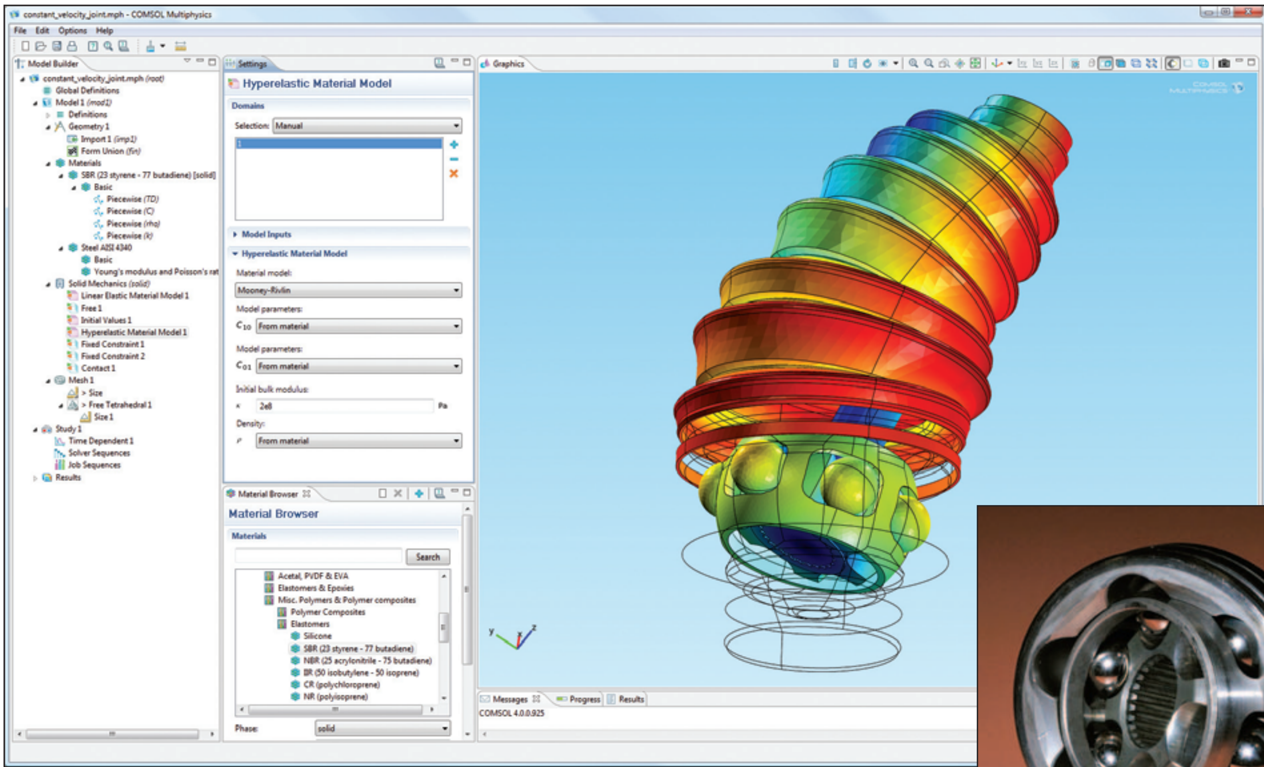


Figure 2. A Rzeppa CV joint (right) and the simulation (above) showing the final configuration and the absolute displacements of the joint when the shaft reaches the maximum angle with respect to the original configuration.

A key factor is that we have more than 600 types of water pumps. When designing a new one to a customer's requirements, we often want to use existing impellers. With our models, we can safely and quickly compare the performance of a new impeller versus an existing one. With COMSOL's abilities to model fluid-structure interaction, the next goal in these kinds of simulations will be to determine if the blade thickness is sufficient to achieve the desired hydraulic action and yet stand up to the stresses.

Moving to Multiphysics

Many of our new designs are multiphysics problems. In our inverse clutch, for instance, it's necessary to estimate the temperature of components surrounding the magnet because if the magnet gets too hot, it loses its magnetic properties and the clutch fails. So not only did we look at heat generation and transport through the various components, we also added fluid flow to determine the cooling effects as they moved at various rotational speeds.

In our latest project, we have started investigating the stresses in a Rzeppa Constant-Velocity (CV) joint, which uses steel spheres to transmit torque at variable shaft angles instead of gears with teeth. Although CV joints have been around for a long time, they are still very difficult to manufacture and simulate (due to multiple contacts among all components, highly stressed parts and heat-treated steel). In particular, the different components undergo varying levels of stress and require different materials. For instance, the inner race is heavily stressed and a high-performing, expensive alloyed steel is required; the outer race experiences slightly lower stress and it is possible to use a less expensive steel. With a model, we can check that the selected materials can withstand the stresses they experience and to estimate their capability to resist them at the maximum loads applicable with a minimum safety factor.

"A key factor is that we have more than 600 types of water pumps. When designing a new one to a customer's requirements, we often want to use existing impellers. With COMSOL, we can safely and quickly compare the performance of a new impeller versus an existing one."

The first step was to perform a kinematic study of the displacement between the inner and outer race. Figure 2 illustrates the total displacement at the final stage of the transient analysis in which the joint is first rotated with an initially increasing velocity that, after 0.05 seconds, is constantly maintained for 0.1 seconds while the internal shaft is rotated by 30 degrees. In this model we are also looking at the stress level in the spheres and other metal parts as well as the behavior of the boot against the angular displacement of the shaft.

Now that we have investigated mechanical contact with untreated "generic" steel's mechanical properties, our next goal is to include the effects of specific steels as well as performing fatigue analyses. Another investigation path will be the correct simulation of the lubricant among the components; in real joints, lubrication is crucial and most times it is the key factor that makes the difference between a working application and an early failure. These steps are particularly important because while the inner race and balls are made of case-hardened steel, the outer race is made of induction-hardened steel.

"We are constantly using COMSOL, and it's safe to say that we are saving thousands of euros per year in engineering and development costs because of it."

In this process, which uses electromagnetic induction and resistive losses to harden only certain locations on a part, the results depend a great deal on the frequency of the alternating magnetic field and the resulting currents. Add to this the fact that it is extremely difficult to examine the residual stresses on a part treated in this way, and simulations become vital. So our goal is to create one multiphysics model that will allow us to examine all the effects — kinematics, stresses, lubrication and the effects of different material properties with their specific heat treatment.

An Expanding Universe of Applications

What these examples show is that following our first experiences of studying electromagnetic effects with COMSOL, we discovered the software's considerable flexibility and how open it is to use. We soon started using it to examine fluid flow, fluid-structure interaction and, lately, structural mechanics. Now we can examine many different aspects of the one product without the need to change to a different software environment. We can also investigate interactions between the physics. Further, we like the fact that it is so customizable. It is a great plus for us being able to enter our own equations in contrast to other closed packages where you cannot modify the physics.

We use COMSOL for both new parts and aftermarket parts. In the design of new parts, we want to make sure that our designs will meet or exceed customer's requirements. When designing aftermarket parts, we often want to re-engineer an existing product to meet specific specifications while keeping costs down. In both cases, we rely heavily on simulations to come up with designs that meet requirements before creating the first prototype, thus saving money.

We are constantly using COMSOL, and it's safe to say that we are saving thousands of euros per year in engineering and development costs because of it. Additionally, it allows us to respond to customer questions more quickly and get products to market faster while completely adhering to specifications. ■

About the Authors

Luca Armellin (left) joined Metelli S.p.A. in 2001, from 2004 being the Technical Manager and from mid-2009, full-time in the R&D department. Prior to this, he received his degree in mechanical engineering from the Università degli Studi di Brescia, worked as a 3D CAD consultant at OCS Technology Srl, and then joined the auto water pump manufacturer, GRAF SpA, as a Chief Designer.

Fabio Gatelli has been in the R&D department at Metelli S.p.A. since 2006. He earned a degree in electronic engineering at the Politecnico di Milano, after which he joined the European Space Research Agency. He moved on to ABB to work on switchgear protection and control, and then headed up electronic design at Brandt Italia, a manufacturer of household appliances.

Simulation Helps Develop Better Household Products

Modeling saves time and money manufacturing and shipping household products.

BY VINCENZO GUIDA, PROCTER & GAMBLE, POMEZIA, ITALY

My role as an R&D process design engineer in Procter & Gamble, Fabric and Home Care Division, is to design reliable and cost-effective manufacturing processes for large volumes of detergents and laundry additive products. Complex multi-component mixtures with chemical and physical properties requiring detailed processes to manufacture properly, the household products have complicated and anomalous behaviors that pose many challenging engineering problems.

Modeling tools that are easy to use and provide accurate results quickly are essential to the effective and rapid development of new products. Because detergents are complex, I need to be able to develop customized models that couple multiple physics and use unconventional constitutive relations, not generally found in off-the-shelf modeling software, to close mass, energy, and momentum balances. COMSOL provides me with the ability to develop my models quickly, experiment with constitutive equations, compare models with experimental results, and spend my time making the physics right, rather than writing code and identifying algorithms for fast convergence.

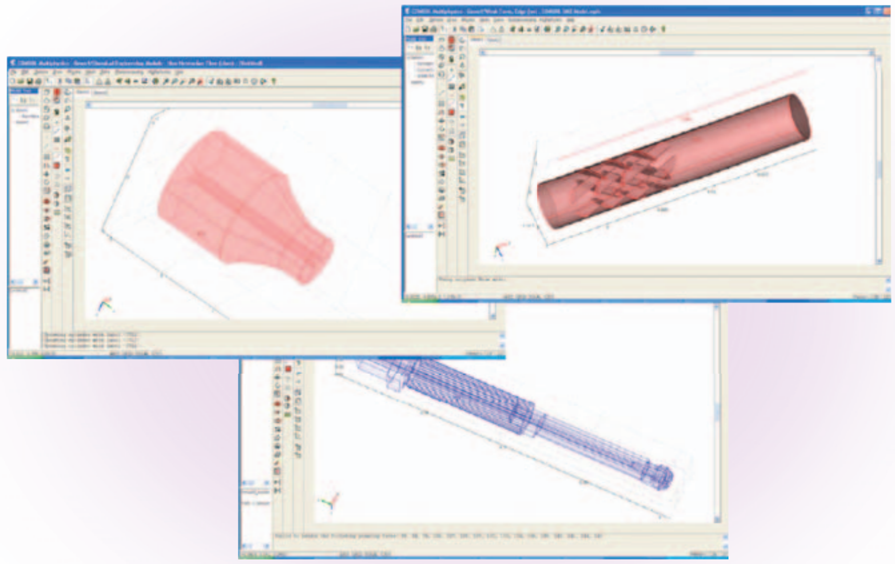


Figure 1. Geometry of some components in the liquid detergent manufacturing process.

"COMSOL provides me with the ability to develop my models quickly, experiment with constitutive equations, compare models with experimental results, and spend my time making the physics right, rather than writing code and identifying algorithms for fast convergence."

Don't Stress the Product

In my first study, I examined the stress history on structured liquid detergents. Some liquid detergents are structured fluids that owe their rheological and physical properties to the presence of tiny rod-like crystalline particles that in modeling result in high aspect ratios. To make liquid detergents properly, it is essential not only to control their chemical composition but also their microstructure so that the crystals are dispersed in the matrix homogeneously and, if required, oriented correctly. These crystals provide a gel structure to the product, which produces the desired rheological properties and preserves product integrity over aging.

Microstructures can be controlled via shear history during the manufacturing process. Shear forces are applied through static or dynamic mixers, pumps, nozzles, or pipes. All of these processes break up and recombine the flow in different streams as ingredients are added and mixed. Shear forces are essential to incorporating ingredients into the finished product that is put into a bottle, but too much stress is detrimental to product microstructure. Overshearing will destroy the gel structure, leading to the product physically separating over its shelf life and to undesirably low product thickness. Consumers find an over-sheared product difficult to use and often dislike its appearance.

To avoid placing so much strain on the product, the amount of stress during the manufacturing process must be quantified so that you can predict its effect on microstructural breakdown. This

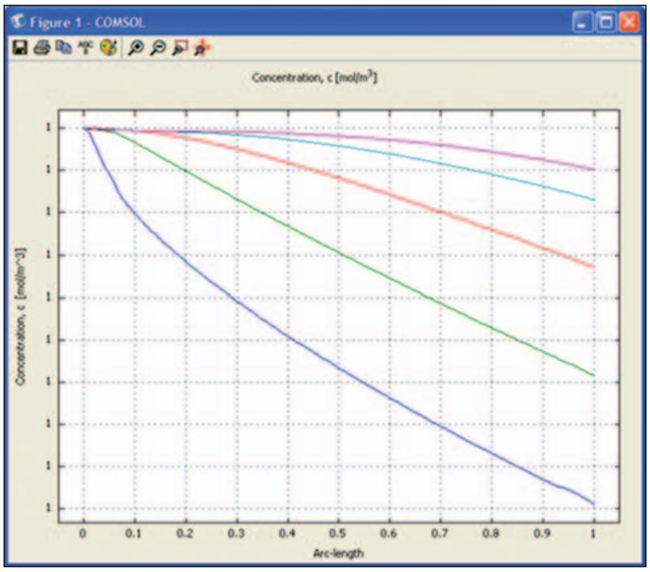


Figure 2. Plot of the structure factor through a pipe for various flow rates.

"COMSOL provides me, as a non-modeling expert, the capability to work with unusual combinations of physics on my own, relatively quickly."

information helps Procter & Gamble size mixers, pumps, and pipelines as well as being used to calculate the pressure drop in mixing devices, packing, nozzles, manifolds, and other elements.

To obtain this information, we created a hybrid model that required defining a pseudo structure factor, which describes its breakdown kinetics as a function of shear intensity.

Figure 1 shows the geometry of some of the types of devices modeled. Figure 2 is a plot of the structure factor along the arc length of a piece of piping at various flowrates. It shows that as the product flows through the pipe the factor decreases indicating microstructural breakdown. This enables engineers to modify design factors while answering questions such as "how long can the pipe be without destroying more than 10% of the structure?"

Because a product's structure changes over time, engineers cannot work with standard fluid-flow equations such as Navier-Stokes. Before we implemented COMSOL, our engineers mostly used physical experiments and empirical results. Sometimes they turned to finite-element software to model fluid dynamics and the shear stresses, while not being able to couple these properties to the structural breakdown. COMSOL provides me, as a non-modeling expert, the capability to work with unusual combinations of physics on my own, relatively quickly.

The benefits have been significant. For example, to set up a pilot plant to test a possible process and its operating parameters usually takes at least a week and costs several thousand euros. However, with COMSOL models, I can examine a process design within an hour — an effective acceleration of my learning phase. I have also found that the models are quite effective in convincing skeptical people as to the benefits of certain proposed processes. I can run repeated experiments and show them the results. Once I demonstrate that the modeling results closely correspond to reality, they take our results much more seriously.

Avoiding Heat Buildup

A second example of our use of COMSOL looks at preventing thermal runaway decomposition of dry laundry additives. This can occur during storage and shipping following manufacturing but prior to being put on store shelves. If a product undergoes thermal runaway, it loses its effectiveness and can no longer be sold, resulting in potentially millions of euros in wasted goods.

Consider the case of the laundry additive Ariel Stain Remover (in the US sold under the Tide brand). This laundry additive contains a bleaching ingredient, known as sodium percarbonate, that naturally decomposes exothermically over time. If this product is stored in large quantities, at too high of a temperature, its decomposition heat results in a temperature increase and an exponential increase of its decomposition rate. This is known as thermal runaway.

The problem in a nutshell: The heat generated is proportional to the volume, and the heat dissipated is proportional to the surface area. When the material is in storage, the best-case scenario is for it to reach thermal equilibrium. But as the volume of stored material goes up — whether in one large container or many small containers placed together — the surface/volume ratio goes down, potentially leading to thermal runaway. In a manufacturing environment this can lead to dangerous situations where inadequate ventilation could result in a fire. Fire does not occur

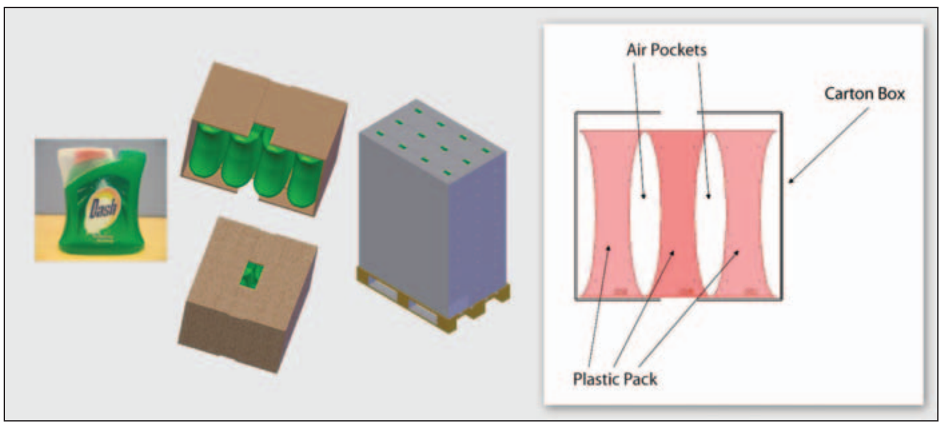


Figure 3. When consumer packages of a laundry additive are put into cartons and then packaged and placed on pallets (left), air pockets form that can potentially lead to thermal runaway.

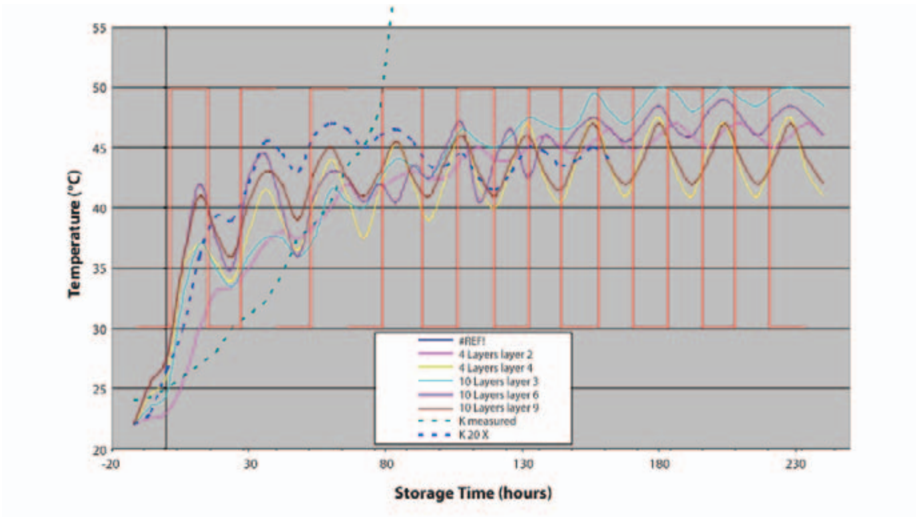


Figure 5. Comparison of actual temperature (solid lines) with model results (blue dotted line); the red pulse shows the cycling of the oven temperature.

in consumer packages, but the problem is still that product loses its activity and becomes ineffective.

Because of possible thermal runaway, the maximum amount of product that can be put on a pallet is limited, especially if the product is stored in an unventilated warehouse or when transferred in regions with very hot climates. With such a range of storage scenarios, it's not feasible to conduct physical testing for each possible problem.

To analyze thermal runaway risks for all possible scenarios, a COMSOL model was created, which, in addition to the heat build-up, studied the fluid dynamics of natural convection in air pockets around the packages (Figure 3).

Together with the University of Naples, a thermal runaway model to predict the risk of thermal runaway was developed. This model describes the energy balance for the pallet, including natural convection in air pockets. The model couples non-isothermal fluid dynamics and heat transfer physics over a complex 3D geometry.

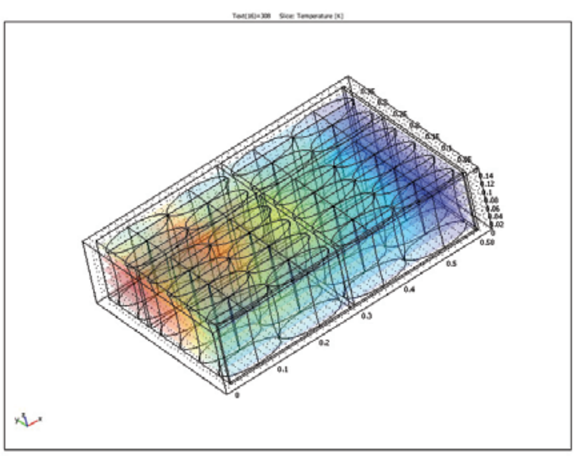


Figure 4. Temperature profile of palletized products.

For model validation, physical tests with pallets of various configurations using products with different thermal activities and other physical properties were conducted. The pallet was subjected to 13 days of heat cycling in an oven, alternating between 30 and 50 °C.

Once the model was validated we were able to establish a maximum safe storage temperature, the induction time for runaway as a function of pallet configuration and total load, and product thermal activity.

Once we validated the thermal-stability model and refined it, recommendations on the number of layers of pallets that can be stacked could be made. The optimized pallet configuration produced a multi-million euros logistic cost saving and helped reduce the environmental impact of logistic chain. Additionally, the results of this study enabled us to make better decisions as to temperatures that must be maintained in the supply chain, and helped Procter & Gamble preserve product quality and effectiveness for consumers.

COMSOL proved to be the perfect tool to do this work. The COMSOL model is robust enough to handle many different simulation conditions (transient, steady state, highly nonlinear constitutive equations for heat flow, high temperature gradients, etc.), yet can be run on a standard four-processor workstation with 8 GB of memory. Additionally, the model can provide real-time results in less than an hour, and the user-friendly COMSOL interface has also been used to design a tool for plant safety managers, enabling them to independently run simulations to assess thermal runaway risks in their own plants. ■

About the Author

Vincenzo Guida is a chemical engineer in the Fabric Care Division at Procter & Gamble, Pomezia, Italy. He holds a masters degree from the University of Naples. His research interests include the rheology of structured fluids, chemistry of bleaching systems, and stability (chemical, physical) modeling. Guida is responsible for designing and scaling up liquid detergents and laundry additives products.

Excellent Sound to Every Seat in the House

Arrays of speakers for public venues must have wavefronts that combine to work as if they were a single speaker. Modeling helps in the design of an acoustic lens and dramatically shortens the time needed to find the best design.

BY MATTIA COBIANCHI AND ROBERTO MAGALOTTI, B&C SPEAKERS S.P.A.

Projecting high-quality sound to large audiences often involves a linear array of speakers. However, to make sure that every audience member hears every word clearly and every sound with full fidelity, the wavefronts from the individual speakers inside the array must be in phase with each other, and the frequency response must be as smooth as possible — ideally flat. The traditional method has been to combine megaphone-variant horns in a coherent array, but even the best such horns produce unintended side effects such as diffraction, reflection and distortion. These waveguides leave considerable room for improvement when trying to combine multiple loudspeaker enclosures in arrays without destroying the coherency of the wavefront.

In an ideal waveguide, the signal throughout the driver outlet arrives in phase. Over the years, speaker manufacturers have employed a variety of techniques to achieve that effect such as by shaping the waveguides a certain way or by using variable-density foam. With the help of COMSOL Multiphysics and the Acoustics Module, our research team at B&C Speakers S.p.A. has taken a new approach by designing an acoustic lens in a waveguide (Figure 1, left) that achieves the required phase coherence in the output sound field. This allows a line array of individual speakers (Figure 1, right) to work together as an extended sound source, which is particularly important for the high frequencies from roughly 1 to 20 kHz. The final design of our waveguide is now patented in Europe and patent pending in China.

Getting Line Arrays to Function as One

In a line array, a series of speaker modules are stacked on top of each other, and the slot in the center projects the higher frequencies. This high-frequency source is nearly as tall as the entire module so that stacked modules in essence form an uninterrupted line from top to bottom and function as a single source. They must have phase coherence so that the sound field outside the waveguide outlet is isophasic (that is, the sound at all frequencies presents a flat waveform upon exiting the horn).

One issue is that our compression drivers consist of a membrane with a plug-like transformer, and the exit at the end of the

Figure 1. A B&C waveguide undergoing acoustic testing (left). A line array using this type of waveguide (right) consists of several speakers each with one or more compression drivers stacked so the thin rectangular exit at the center of each is aligned to form an extended sound source going from top to bottom. Photo courtesy of LSS Advanced Speaker Systems — Italy. Employing 90 people, B&C Speakers is one of largest and most prestigious manufacturers of professional loudspeaker transducers in the world, and our core business is in professional audio for large systems intended for nightclubs, concert halls and stadiums. Besides designing and distributing components under our own brand name, we also supply OEM components to most of the top professional audio brands in the market today.

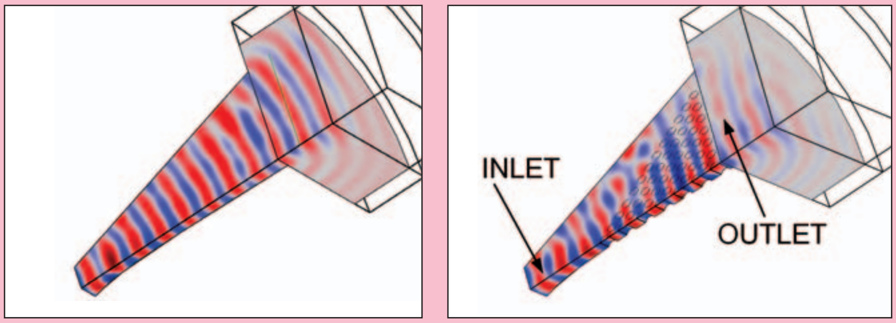


Figure 2. These images, created with the Acoustics Module for COMSOL, show the sound pressure level at 16 kHz through the waveguide. Here the two cases solved for are: no acoustic lens embedded (left), and the final prototype with the lens showing how the wavefront is almost perfectly planar at the waveguide outlet.

> "I was also particularly impressed with COMSOL's support to help us get the most out of the software. We were able to get significant results in our first month, and it's just been better ever since."

plug is circular. However, the sound energy must be transformed so that it exits out of the rectangular slit. Our waveguide is thus made of two elements. First is a waveguide shell whose cross section changes smoothly from a circle with a diameter of 36 mm to a rectangle measuring 153 x 25 mm; second, that shell is filled with almond-shaped pegs forming an acoustic lens that delays the central part of the wavefront so sound from the upper and lower parts of the transducer can catch up and achieve the required phase coherence. With our model, we can easily study the waveguide's geometry and optimize the number and distribution of the pegs.

We first simulated the empty waveguide to estimate the amount of phase correction needed. The left image in Figure 2 shows that considerable work was needed, and we determined that the most troublesome frequencies were the highest ones. We compared our model to experimental results and found that a good fit was achieved.

Figure 2 shows the sound pressure through the waveguide at 16 kHz in an empty waveguide (left) and in the final prototype (right). Note in the final prototype how the wavefront is almost perfectly planar at the rectangular waveguide's outlet. In these first investigations we learned a great deal about what is happening inside the waveguide as opposed to simply placing objects in an anechoic chamber.

The power of the model lies not just in reduced design time but in the information we have been able to gather about future designs. Beyond that, this finite element analysis allows us to evaluate some quantities in certain parts of a system that we cannot reasonably access with instruments or by taking physical measurements. It allows us to learn so much about the behavior of a device that this invaluable wisdom can then be employed in the development of similar products and devices with deeper knowledge and awareness.

These days we seldom need more than one prototype. We save two months of engineering time that would have been involved in creating CAD models and trial-and-error design refinements, and we ultimately get to market that much more quickly. As we push forward the complexity of the models in the next few months, we'll likely be able to save even more time and costs.

We chose COMSOL Multiphysics because it is very user-friendly, provides for multiphysics couplings and is affordable — competitive software can cost five times as much for more limited application potential. I was also particularly impressed with COMSOL's support to help us get the most out of the software. We were able to get significant results in our first month, and it's just been better ever since. We have meanwhile studied magnetic effects in speakers, motors and some mechanical simulation for the moving parts and suspension within drivers as well as acoustic-structural interactions to predict the sound pressure level and frequency response of our compression drivers. ■

About the Authors

For the past year, Mattia Cobianchi (left) has been a research engineer at B&C Speakers, Bagno a Ripoli, Italy, where he is responsible for activities including FEA modeling and new measurement techniques.

Roberto Magalotti (right) joined the Research & Development Lab of B&C Speakers in 2001 and is currently in charge of research activities within the lab.

COMSOL Acoustics Module Finite Element Modeling for Infrasound Propagation

Remote monitoring of a suite of sources, both man-made and naturally occurring, are of interest to military and other government agencies. One such monitoring technology uses infrasound, or sub-audible acoustics, which can propagate tens to thousands of kilometers depending on source strength without losing signal character. The following discussion highlights the feasibility of methods for the modeling of infrasound propagation.

BY DR. MIHAN H. MCKENNA, U.S. ARMY ENGINEER RESEARCH & DEVELOPMENT CENTER

Generally classified as sound between 0.05 and 20 Hz, infrasound cannot be heard by human beings, but can be detected on specialized sub-audible microphones, which operate on the principle of a vibrating pressure field generating recordable electronic impulses. Classical infrasound monitoring focuses on source-to-receiver distances greater than 250 km, where more recent infrasound monitoring research has focused on distances closer than 150 km, bridging the distance between long-range acoustics and true infrasound monitoring.

Historically, parabolic equation (PE) methods have been developed for the numerical solution of long-range (> 500 km) infrasound propagation in a layered atmosphere. This technique can be powerful for long-range propagation due to its simple numerical implementation and limited use of computational resources. PE techniques are analogous to frequency-wavenumber investigations in observed data, predicting how trapped energy and spherical wave front phenomena interact not only in arrival times but also in the attenuation of the observed amplitude. The PE method approximates the wave equation by modeling energy propagation along a cone oriented in a preferred direction. This approximation provides reasonable accuracy over long propagation distances. However, for short-range propagation (< 50 km), the mathematical formulations used in the PE method break down and do not provide sufficient accuracy needed for precise measurements and predictions.

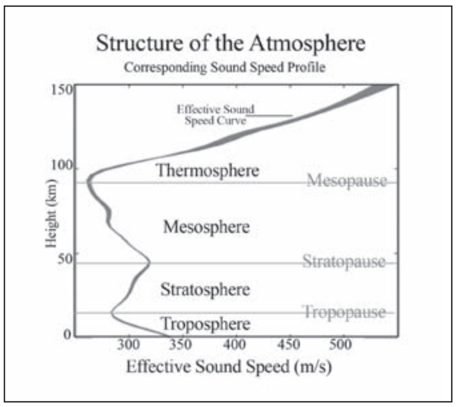


Figure 1. Idealized atmospheric structure with a linear trend in the troposphere.

Figure 2. Space Shuttle *Columbia* on takeoff. *Photo courtesy of NASA.*

To produce high-fidelity propagation modeling coupled to complex source functions, the author worked in conjunction with Dr. Kyle Koppenhoefer and Dr. Jeffrey Crompton of AltaSim Technologies to develop finite element method (FEM) based acoustic solutions, such as those implemented in COMSOL Multiphysics, to accurately represent the propagation of acoustic waves without the approximations in the PE method. These solutions can be used to provide accurate solutions for short-range propagation acoustic waves where the PE method is not well suited. However, FEM methods require large computational resources (i.e., memory and cpu time) to solve long-range propagation problems making accurate solutions difficult. Thus, FEM and PE methods complement each other for the solution of infrasound propagation in layered atmospheres; FEM-based solution providing accuracy in the short range and PE-based solutions accurately simulating behavior at large distances. To validate the use of COMSOL's FEM acoustics code, we present two cases where the PE and FEM methods are evaluated.

Infrasound Propagation

Infrasound propagation depends on the effective sound speed (C_{eff}) of the atmosphere through which it travels, so it is imperative to properly characterize the atmospheric conditions as close to the time and location of the propagation pathway as possible. The propagation pathways are governed by effective sound speed profiles, calculated by: $C_{eff} = C_t + n \cdot v$, where $C_t \sim 20.07(T)^{1/2}$, T is absolute temperature in Kelvin, and $n \cdot v$ is the component of wind speed in the propagation direction. Temperature is the dominant factor in calculating the effective sound speed; wind speed and direction are only secondary factors. In order for up-going infrasonic energy to be observed at Earth's surface, it must reach an area of higher sound velocity than at the point of origin. If this occurs, the energy turns and then returns to the surface of the earth. Figure 1 shows the sample effective sound speed profile with the regions of the atmosphere labeled.

How the atmosphere is quantified for data analysis and modeling depends on the particular areas of the atmosphere through which the infrasound propagates. For source-to-receiver paths of less than 200 km, local meteorological information is imperative to accurately characterize the propagation medium. Surface measurements are inadequate to properly characterize the whole height of the atmospheric profile through which the infrasound propagates. It is necessary to use radiosonde, weather balloon or equivalent measurements for the temperature and wind profiles to create the C_{eff} used in modeling.

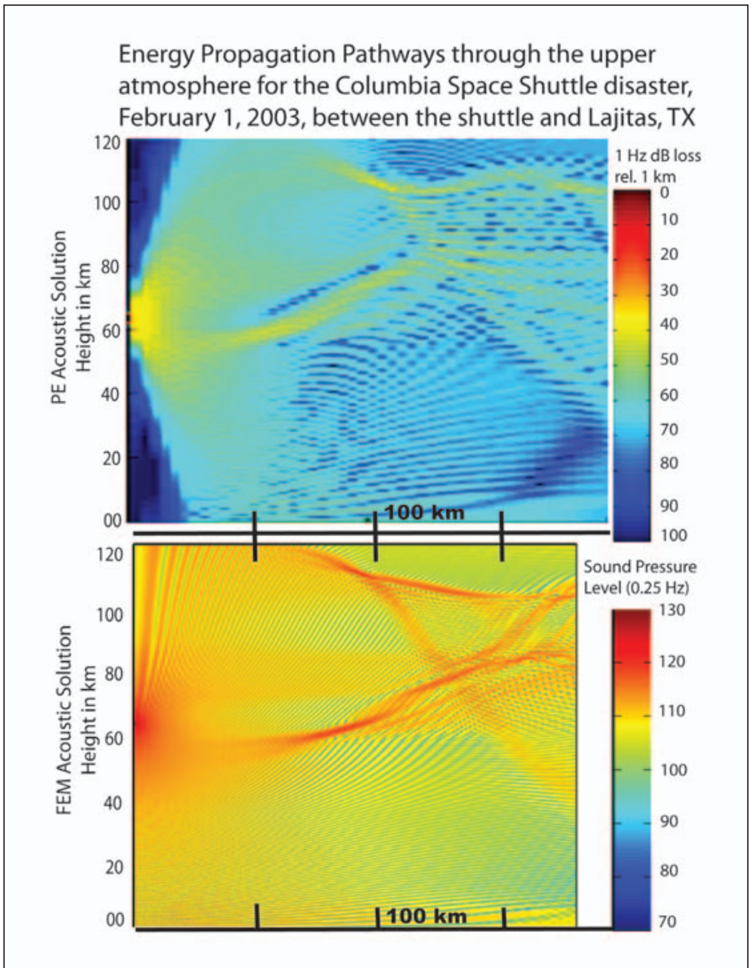


Figure 3. The PE solution for the Columbia, above. 1 Hz was taken to be the dominant frequency for modeling, determined from the observed data. COMSOL FEM Acoustics Module solution, below, for the effective sound speed profile seen in figure 2, 0.25 Hz dominant frequency.

For distances greater than 200 km from the source to the receiver, the signal may travel via highly variable energy pathways that travel primarily through the upper atmosphere, the thermosphere, and propagate vast distances though a medium that changes little over the time span of months. Most of these sources are either large (such as energy from the Krakatoa volcano eruption in 1883, which reverberated around the world eight times before dying out), from substantial vertical seismic displacements from earthquakes, or occur in the upper atmosphere, such as meteorites.

Despite the linear depiction of the tropospheric effective sound speed profile from Figure 1, the tropospheric structure is sometimes governed by fast moving weather systems and is considerably more variable than the atmosphere above the tropopause. Short-lived temperature inversions can create ephemeral ducts with higher sound speed velocities than are found at the ground. Being able to accurately quantify these ducts in time and space is imperative for remote monitoring using infrasound by developing computational methods to effectively manage discontinuities and rapid changes in temperature and wind with altitude.

Long-Range Infrasound Propagation

Worldwide infrasound arrays observe a variety of sources at variable distances. Earthquakes, volcanoes, mining explosions, and man-made atmospheric explosions are some of the most common signals observed on infrasound arrays, but bolides (meteors) and shuttle reentries are also recorded at very long propagation distances, hundreds to thousands of kilometers.

Observations from supersonic atmospheric sources, such as space shuttle re-entries, have been recorded on the

"COMSOL provides highly accurate solutions by solving the partial differential equation for acoustic wave propagation without the approximations used in the PE method."

infrasound arrays from initial installation and have been subject to intense study over the years. As early as 1971, infrasound signals were observed from the Apollo spacecraft flights and recordings continue through today.

The events of the February 1, 2003 Columbia space shuttle re-entry failure provide the first case where an explosion at altitude has a known location in four-dimensional space and time, as well as a well-characterized atmospheric profile in addition to being recorded on an infrasound array approximately 600 km away in Lajitas, Texas. The three-dimensional shuttle path was recorded by NASA and the timing of the events that led to the disintegration was known; the trajectory and timing can then be combined with a well-characterized atmospheric profile to produce a graphical representation of the paths the acoustic energy takes through the atmosphere.

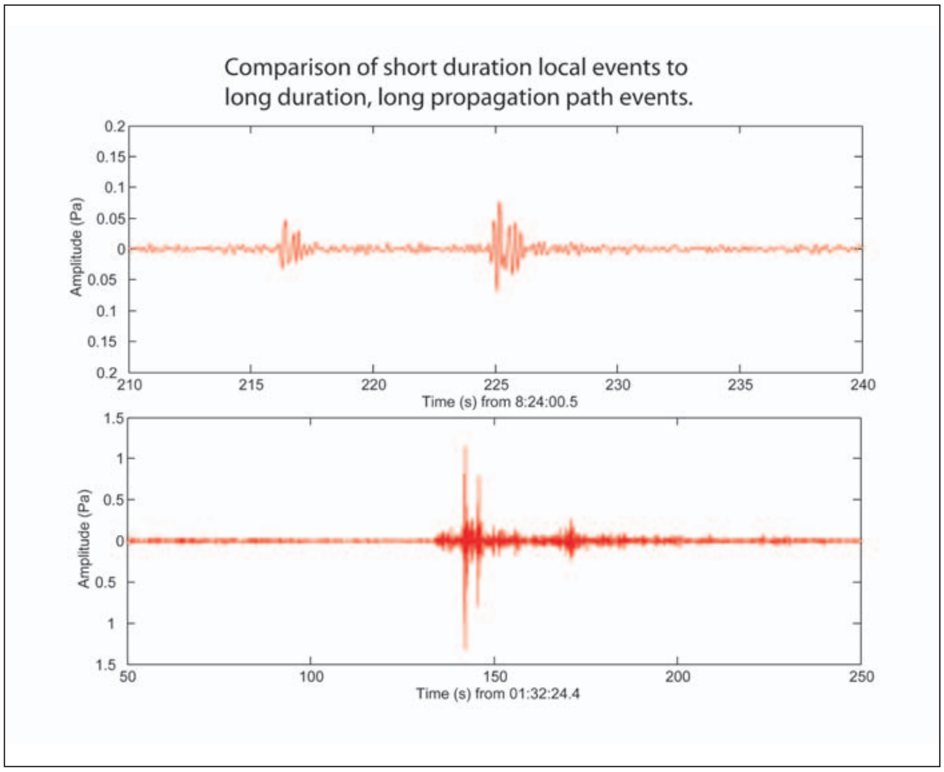


Figure 4. Variable signal character between near-regional and long-range (tele-infrasonic) propagation pathways.

Originally adapted from underwater acoustic studies, PE (Parabolic Equation) modeling provides a field solution for a complete vertical plane at one frequency. An infrasound monitoring community standard PE code was compared in this effort, and it steps forward from a source and calculates an attenuation field for predicting amplitudes along the vertical slice. In using the PE codes, it is imperative that the computational atmosphere be deep enough to include all viable energy pathways. This depth of field required for PE modeling is where the high-accuracy advantage of finite element modeling breaks down. The PE run in Figure 3 took minutes to execute on a laptop system and utilized the effective sound speed profile provided by the Naval Research Laboratory using data from the time of the Columbia disintegration from the NOAA Global Forecast System (GFS), NASA Goddard Space Flight Center (GFSC), and Goddard Earth Observing System (GEOS) system for the 0 to 55 km region, with the explosion located at 62.2 km elevation.

In contrast, the FEM solution seen in Figure 3 for the same atmospheric profile took five days to run on a 16 GB quadcore Mac Pro, for 0.25 Hz, and only propagated out to 200 km, rather than the full distance of 600 km (not pictured). The two results correlate well over the distances executed in the FEM model, bearing in mind the change in frequency content from 1 Hz to 0.25 Hz and associated change in wavelength. While accurate, the computational resources required to produce equivalent solutions to the PE codes at these distances indicate that the PE solutions would be more efficient.

Figure 5. Above ground detonation of 100 lbs of ANFO from calibration experimentation.

Short-Range Infrasound Propagation

At shorter ranges, the advantage of COMSOL's FE method is readily apparent. Recently, infrasound propagation over short range, less than 100 km, has become of greater interest. At long distances, such as the Columbia propagation pathways, the fine-scale source structure found in the propagating energy is smeared in the observed signal. At the shorter distances of 30-100 km presented below, retaining source character becomes more important, as there is less smearing in the observed signal. The difference in signal character from small, near-regional impulsive sources, and energy that has traveled much greater distances can be seen in Figure 4. Note the difference in time scale between the recordings, where the near-regional signals last on the order of a few seconds, and the diffuse tele-infrasonic recording lasts on the order of tens to hundreds of seconds.

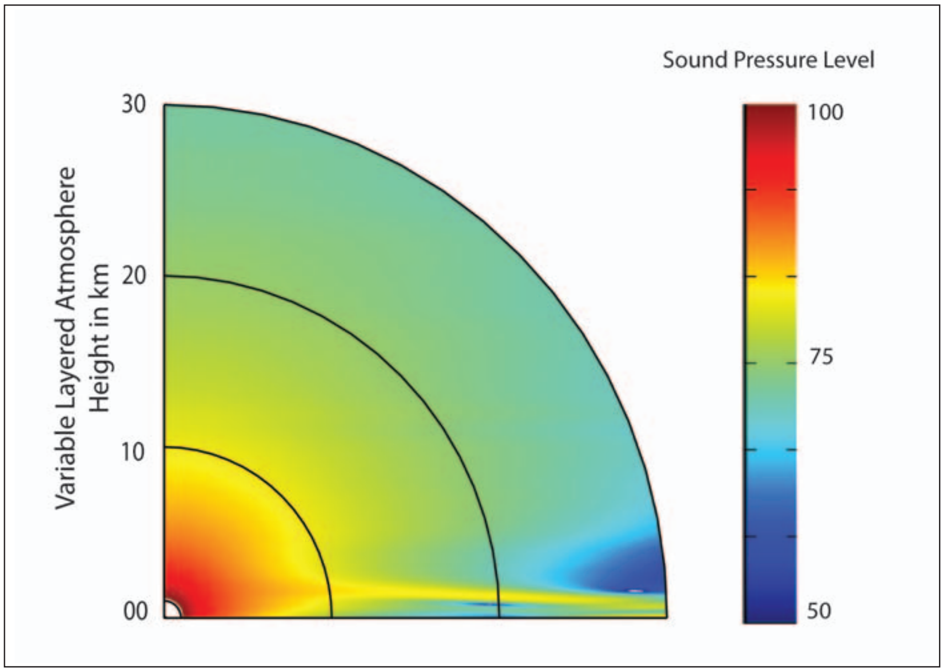


Figure 6. Energy propagation pathways through the lower atmosphere for regional propagation at 2 Hz.

COMSOL provides highly accurate solutions by solving the partial differential equation for acoustic wave propagation without the approximations used in the PE method. Thus, the full characteristics of the source will be included in the solution. Modeling sources as diverse as point explosions, as shown in Figure 4, or structural emanations, COMSOL supports integrating the source and propagation functions in the same model. This flexibility enables infrasound modeling of many conditions that were previously difficult to solve. Thus, COMSOL offers advantages beyond the additional accuracy found in the FEM solutions. It opens up the study of infrasound to a much broader range of sources while permitting the study of infrasound in the near field.

COMSOL also provides the capability to develop transient and time-harmonic solutions. The transient solution most accurately represents short duration sources, such as point source explosions shown in Figure 5.

Figure 6 shows the propagation of a 2 Hz signal over 30 km produced using COMSOL's Acoustics Module. The variation of sound speed through the layers of the atmosphere strongly influences the propagation of this signal. When the atmospheric conditions are favorable the acoustic energy refracts to the Earth's surface. The duct at approximately 2 km traps the acoustic energy necessary to produce favorable likelihood for observing infrasound energy from source to receiver.

While future research to optimize boundary conditions and mesh sizes to minimize run time and computational resources is ongoing, COMSOL's Acoustic Module offers the long-range acoustics and near-regional infrasound monitoring community a very effective tool to produce highly accurate, high-resolution propagation modeling for situations where integrating complex sources is important. ■

ACKNOWLEDGEMENTS

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Mihan H. McKenna, Ph.D.

About the Author

Since July of 2005, Dr. McKenna has been a Research Geophysicist in the Structural Engineering Branch of the Geotechnical and Structures Laboratory at the U.S. Army Engineer Research and Development Center (ERDC), a group of 7 R&D laboratories for the US Corps of Engineers (USACE) and the US Army.

Dr. McKenna's area of expertise is acquiring, interpreting, and numerically modeling seismic, acoustic, and infrasound source and propagation phenomenology to support tactical decision making for forward deployed expeditionary forces. She directs the Denied Area Monitoring and Exploitation Systems working group at ERDC, which has ongoing integrated high-performance computing modeling and experimental research with the Department of Defense, Department of Energy, Defense Intelligence Agency, Los Alamos National Laboratory and academic institutions. She supports several ongoing DARPA and DTRA programs concerned with hard target defeat and strategic imaging and monitoring of trans-national threats. In addition, Dr. McKenna is a federally certified bridge inspector and conducts structural monitoring of transportation infrastructure from remote stand-off.

Modeling Nuclear Fuel Behavior for Enhanced Reactor Performance and Safety

Nuclear energy offers a green solution for electric power generation. Researchers at Royal Military College in Canada show how to get the most out of nuclear fuel.

BRENT LEWIS, KHALED SHAHEEN, AND MICHAEL J. WELLAND

Nuclear energy is gaining attention across the globe as a practical alternative-energy solution. In comparison to thermal sources where fossil fuels are burned to create energy, nuclear power can be considered a clean form of energy because there is no combustion during the nuclear reaction. Hence, nuclear energy does not emit greenhouse gases, acidic gases, or particulates, all issues related to global warming and environmental damage. Additionally, the high-energy density of nuclear fission reduces the use of natural resources, not to mention the impact of extracting those resources. Finally, nuclear fuel can be reprocessed to extract even more of the unused energy from the fuel, making it recyclable. All reasons why research into how to efficiently and safely get the most out of nuclear fuel can be considered of great importance.

One country that has been utilizing nuclear power generation for some time is Canada, where nuclear energy generates 15% of Canada's electric power. To help further Canada's nuclear technology domestically and throughout the world, nuclear energy research is supported at the university level, including at the Royal Military College (RMC) of Canada in Ontario. According to Brent Lewis, Ph.D., Industrial Research Chair (IRC) in Nuclear Fuel at RMC, the university's work will help support the CANDU (CANada Deuterium Uranium) nuclear industry for improved reactor operational support, fuel performance prediction, and reactor safety code analysis. "This research is of particular importance in light of the need for increased capacity and the realization of next-generation reactors, which can offset the greenhouse gas footprint," said Dr. Lewis.

The Research Team

Since nuclear fuel is a key enabling technology for the enhancement of reactor safety, performance, and economics, Dr. Lewis and his team at RMC are conducting research on nuclear fuel behavior. Dr. Lewis explained how the main goals of the IRC in nuclear fuel are to better understand nuclear fuel performance during normal and reactor accident conditions, including the behavior of advanced and next-generation fuel designs.

Because of its multiphysics capabilities, Dr. Lewis chose COMSOL for his team to model the complexities of nuclear fuel behavior (Figure 2). "COMSOL allows us to quickly focus on the model development and given application with its multiphysics capa-

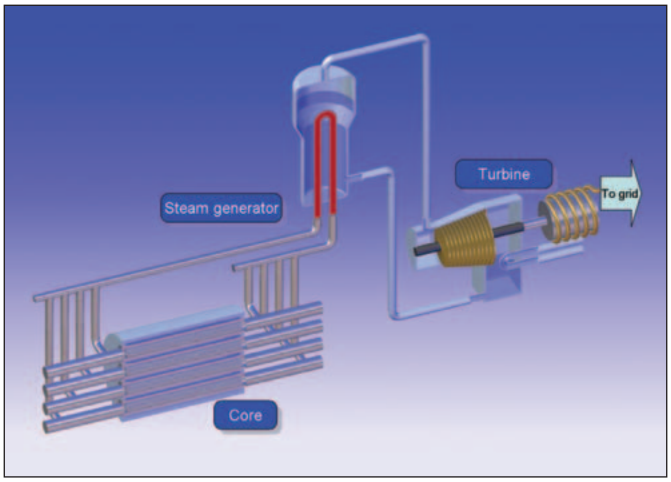


Figure 1. Schematic of a CANDU plant. *Used with permission from A. El-Jaby.*

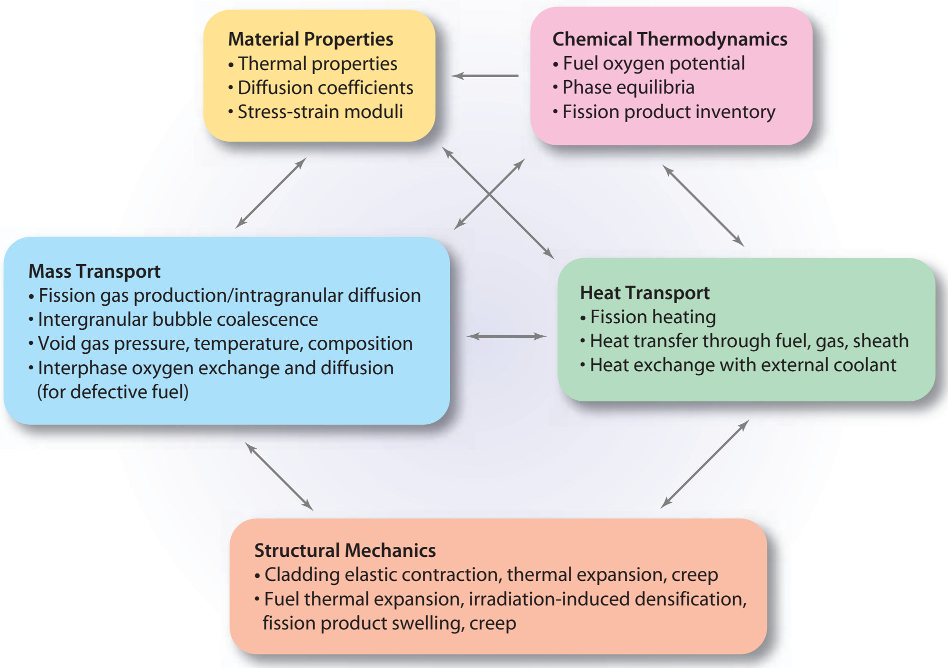


Figure 2. Summary of coupled phenomena and properties governing nuclear fuel performance.

bility and its ability for numerical solution of the governing (coupled) partial differential equations for heat and mass transport," said Dr. Lewis. "Since COMSOL is used and tested by many people in the world, we trust its solver and therefore can specifically focus on the model development."

Accurately Modeling the Fuel Element

One of Dr. Lewis's Ph.D. students, Khaled Shaheen, M.A.Sc., is currently modeling the behavior of a nuclear fuel element — intact or defective — during reactor operation. "There are many considerations that must be taken into account in order to simulate the reactor temperature under varying circumstances — material composition and properties that are changing over time, and a geometry that is evolving in response to the physics of the system," said Mr. Shaheen. For example, Dr. Lewis explained how, "The Structural Mechanics Module allows us to develop mechanistically-based models for describing the thermo-mechanical behavior of nuclear fuel. The multiphysics platform allows us to couple governing partial and ordinary differential equations." It is these sophisticated models that Mr. Shaheen relies on in order to accurately predict all of these coupled phenomena together.

One specific challenge Mr. Shaheen discussed about his work was how geometry and fission gas behavior affect the heat transport within the fuel rod. The heat transport simultaneously affects the physical deformation of the rod, and the production and release of fission gases, which makes modeling fuel performance a highly-coupled problem. "The multiphysics capability of COMSOL, and the ability to implement two-way coupling between the different physics interfaces and the moving mesh interface, are key to being able to solve this problem. Adding new effects to a model is straightforward, which means that we can always add new and more detailed physics to increase the accuracy, sophistication, and applicability of our code," said Mr. Shaheen. "Also significant is the ability to control meshing parameters. As we expand our models to multiple dimensions, the different scales make it very important to deal with aspect ratios, meaning that we need the flexibility in customizing meshes," he added.

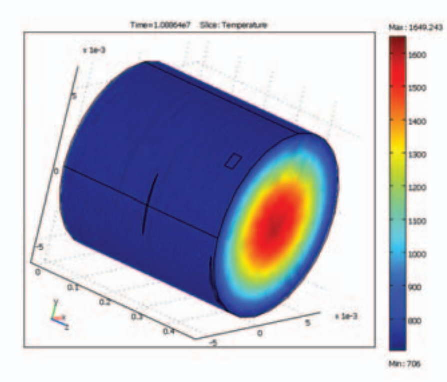


Figure 3. Temperature profile of oxidized defective fuel. Fuel element temperature slice plot in degrees Kelvin.

Combining Models

While Mr. Shaheen was working on nuclear fuel behavior during normal reactor conditions, his colleague Michael J. Welland, Ph.D. — currently a research fellow at the JRC- Institute for Transuranium Elements in Karlsruhe, Germany — was completing his Ph.D. thesis at RMC concentrating on fuel during reactor accident conditions, specifically fuel melting. "The fuel melting model work was conducted to improve the understanding of the melting process and what might be expected should it occur. As such, it contributes to the safe and efficient operation of the modern reactors and may help in the design of the next-generation reactors," stated Dr. Welland.

If a fuel rod becomes defective, the coolant could make contact with the fuel and oxidize it, explained Dr. Welland. Oxidized fuel has a reduced thermal conductivity and a lower initial melting temperature. This has the effect of increasing the temperature in the center of the fuel, and the potential for centerline melting under upset conditions (Figure 3). In reactor operation, the melting of the fuel is forbidden as it can challenge the structural integrity of the reactor core. A limit is therefore imposed on the power at which the reactor can be safely operated.

The team at RMC had a fuel oxidation model that was used to simulate ten cases of defective fuel oxidation that had occurred during real power reactor operation. "It was possible to take features from the model used to predict oxidation and integrate them, with some modification, into the fuel-melting model," said Mr. Shaheen.

Dr. Welland pointed out that while the initial model for fuel oxidation was developed for normal operating conditions and therefore required some modifying, this required little more than copying and pasting the appropriate expressions. "As both models were in COMSOL, we were able to truly combine them, rather than coupling them as one would have to do were they developed as separate modules or standalone codes. The result was that this could happen quickly and easily and that the resulting model is of good quality," he said.

Ongoing Efforts

The team at RMC is also modeling Zircaloy hydriding, iodine-induced stress corrosion cracking, and fission product transport in defective fuel and to plan and design an instrumented out-reactor fuel test to provide data for model validation. "The COMSOL numerical platform can be easily learned by students and the programs passed on to other students for ongoing and continued research development," said Dr. Lewis. " This software allows us to quickly develop and test models in a number of graduate theses within a reasonable timeframe. These models can then be used by the industry after they have been conceptually developed and tested at the university." ■

The modeling team (left to right) Brent Lewis, Khaled Shaheen, and Michael J. Welland.

Nordic Researchers Model Deep Geologic Repository of Nuclear Waste

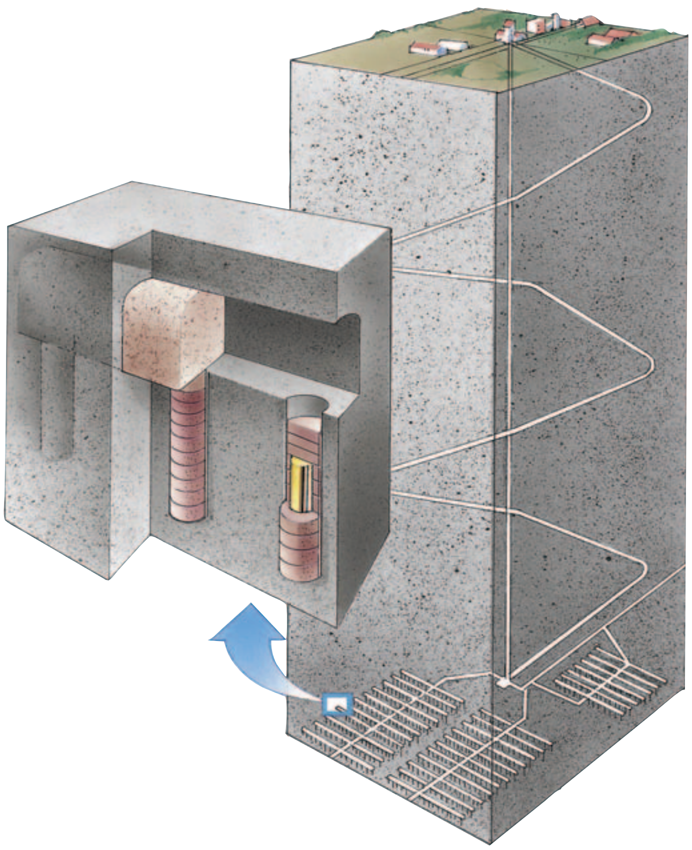
BY PHIL BYRNE, COMSOL

Nuclear energy has been touted as being one possible source of alternative clean energy to carbon-based energy, where the gains in the reduction of greenhouse gases from burning fossil fuel is evident. Yet, while producing this energy, the nuclear industry is also committed to safe waste management, and is now reaping the benefits from half a century of advanced research and billions of Euros in investment in robust geological repositories.

The scientific consensus is that the disposal of spent nuclear fuel rods in deep geological structures is an acceptable and safe method for long-term management of them. Many sites throughout the world, which have remained geologically stable for millions of years and are likely to do so in the future, are being considered as repositories.

Sweden and Finland are the two countries that have progressed furthest with respect to developing such repositories. And the work is indeed immense. Nuclear power companies in Sweden jointly established the Swedish Nuclear Fuel and Waste Management Company (SKB) in the 1970s and a fund to finance it in 1982. Companies that use radioactive fuel that will someday be placed in their repositories pay an annual fee to this fund, which, in 2008, was almost 3 billion Swedish kronor (300 MEUR). At the beginning of 2010,

Figure 1. Schematic illustration of a final repository. Spent nuclear fuel bundles are placed within a copper canister that can measure 8 meters in height. This is then surrounded by the bentonite buffer material, along with filler material and placed in the final repository, 500 meters under the Earth's surface. *Copyright© SKB. Illustrator: Jan M Rojmar — Grafiska Illustrationer.*



"As time goes on, more research groups and institutions will turn to modeling to adequately simulate the behaviour of their nuclear waste and repositories."

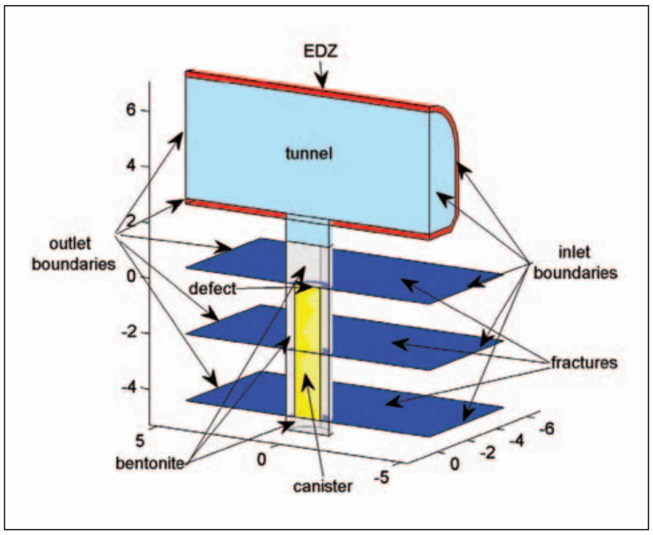


Figure 2. Modeling domains. Radionuclides seep from a defect in the canister and are transported by diffusion through the bentonite, rock fractures, the tunnel and the excavation damaged zone (EDZ).

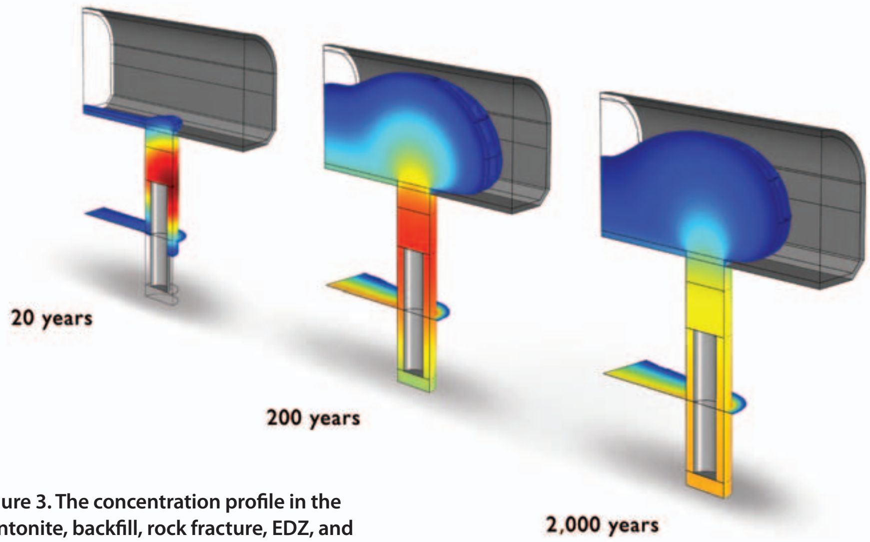


Figure 3. The concentration profile in the bentonite, backfill, rock fracture, EDZ, and tunnel after 20, 200 and 2,000 years.

the fund was worth approximately SEK 42 billion. Finland through her equivalent, Posiva Oy, assumes that the total cost of their repositories and maintenance will also be in the scale of billions of Euros.

The repositories consist of, among others, two important containment barriers, each contributing to the required long-term isolation of the nuclear waste from the biosphere (see Figure 1). One is the containers or canisters that protect the waste and prevent any water reaching it for hundreds of thousands of years. Made of copper and specially welded and treated, a lot of research has been made on the choice of material and design. Another is the bentonite buffer material that protects the canisters, preventing water from flowing through to them, as well as mitigating any deep-earth movement, and binding any radionuclides that eventually escape from the canisters.

Bentonite has long been used in the drilling and mining engineering industries due to its unique rheological properties. It is a naturally occurring type of clay that expands when coming into contact with water, but on the other hand, allows almost no water flow through it at all. Expanding bentonite fills the space surrounding the final disposal canisters; cracks that already exist and cracks that may open up in the future. It also behaves somewhat like modeling clay by buckling when necessary, and recovering its shape because of its elasticity. In the event of a possible canister leak, it also retards the radioactive substances from coming into contact with the rock through its sizable resistance to radionuclide diffusion.

$$2\mathrm{NaX} + \mathrm{Ca}^{2+} \leftrightarrow \mathrm{CaX}_2 + 2\mathrm{Na}^+ \quad \log K_{\mathrm{NaCa}} = -0.20$$

$$K_{\mathrm{NaCa}} = \frac{\beta_{\mathrm{Ca}}[\mathrm{Na}^+]^2}{\beta_{\mathrm{Na}}^2 \gamma_0^2 [\mathrm{Ca}^+]} = 0.62$$

$$\mathrm{NaCl}_{(aq)} \leftrightarrow \mathrm{Na}^+ + \mathrm{Cl}^- \quad \log K_{\mathrm{NaCl}} = 0.78$$

$$K_{\mathrm{NaCl}} = \frac{\gamma_0^2[\mathrm{Na}^+][\mathrm{Cl}^-]}{[\mathrm{NaCl}_{(aq)}]} = 6.0$$

$$\mathrm{CaCl}^+ \leftrightarrow \mathrm{Ca}^{2+} + \mathrm{Cl}^- \quad \log K_{\mathrm{CaCl}} = 0.79$$

$$K_{\mathrm{CaCl}} = \frac{\gamma_0^4[\mathrm{Ca}^{2+}][\mathrm{Cl}^-]}{[\mathrm{CaCl}^+]} = 5.0$$

$$c_{\mathrm{Na}} = [\mathrm{Na}^+] + [\mathrm{NaCl}_{(aq)}] + c_{\mathrm{NaX}}$$

$$c_{\mathrm{Ca}} = [\mathrm{Ca}^+] + [\mathrm{CaCl}^+] + c_{\mathrm{CaX}_2}$$

$$c_{\mathrm{Cl}} = [\mathrm{Cl}^-] + [\mathrm{NaCl}_{(aq)}] + [\mathrm{CaCl}^+]$$

$$[\mathrm{Na}^+] + 2[\mathrm{Ca}^{2+}] + [\mathrm{CaCl}^+] = [\mathrm{Cl}^-]$$

$$\log\gamma_0 = -0.51 \times \left(\frac{\sqrt{I}}{1+\sqrt{I}} - 0.3I\right)$$

$$I = ½([\mathrm{Na}^+] + 4[\mathrm{Ca}^{2+}] + [\mathrm{CaCl}^+] + [\mathrm{Cl}^-])$$

Figure 4. Chemical reactions and equations involved in describing the transfer of sodium and calcium ions between the bentonite and water.

A number of research groups throughout the world are studying the effectiveness of bentonite as a barrier of containment. These activities consist of work with mathematical models, since testing is extremely difficult due to the the time-scales involved. Both SKB and its Finnish equivalent, Posiva Oy, have collaborated with several research groups in Sweden and Finland to model and study the repositories. These include a group led by Docent Markus Olin at VTT Technical Research Centre of Finland (VTT), and a group led by Professor Ivars Neretnieks and Dr. Luis Moreno at the Division of Chemical Engineering at the Royal Institute of Technology, Sweden (KTH).

Markus Olin and his colleagues at VTT have a number of different phenomena that they are looking at. If we were to consider the application according to time-scales, three significant stages occur. They are investigating what happens during the excavation of the tunnels and placement of the canisters (days to months), the saturation of bentonite by water (months to hundreds of years), and the long-term safety where breaches can occur such that the surrounding system will have to retard radioactive material reaching the biosphere (many thousands of years). They are also considering a number of different but interacting physical phenomena that influence the repositories; hydrological, thermal, mechanical and chemical phenomena.

Veli-Matti Pulkkanen at VTT has produced 3D models over the whole bentonite and surrounding rock including fractures that cut through it where a hypothetical leak of radionuclides from a canister is simulated. When the tunnels and holes are excavated, a thin layer of bedrock surrounding them may be damaged (known as the excavation damaged zone — EDZ), and it is easier for water to flow through the small pores and fractures that have resulted from this excavation. It may be even easier for fluid to flow in the EDZ than through the original tunnel, which has been backfilled with bedrock (see Figure 2).

COMSOL Multiphysics is particularly useful in his modeling as he is able to define the source of radionuclide leaking from the canister using a simple 1D initial boundary-value problem, and couple this to the natural 3D geometry. The same technique is also used to define the flow physics in 2D for thin fractures and couple this to 3D flow. This ability to couple physics defined in different dimensions comes as an automatic interface in the software and requires nothing more than specifying the relevant material properties — the coupling between the different geometries is done automatically and the meshing is simple to manipulate. His results indicate that the bentonite layer is an important hindrance to the transport of leaking radionuclides (see Figure 3).

On another level, Markus Olin at VTT has simulated the chemical stability of bentonite using the Reaction Engineering Module. The susceptibility of bentonite to dissolve in relatively low-saline water, which could reach the repositories after postglacial periods, is far greater if its cation makeup is dominated by sodium ions as opposed to calcium ions. Even if the bentonite is in contact with saline water, the exchange of calcium ions with sodium ions can also occur.

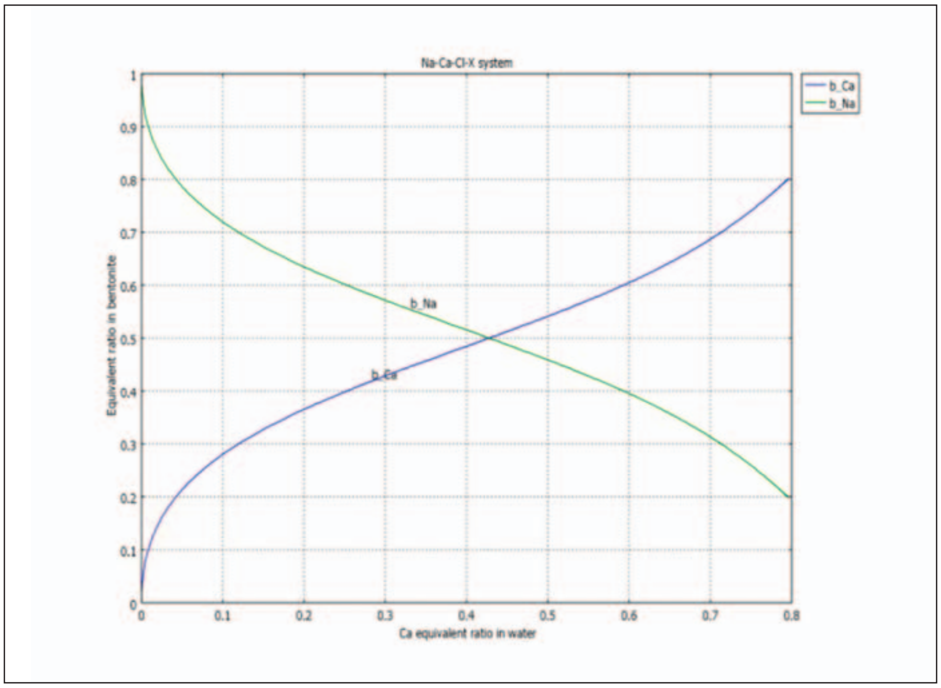


Figure 5. The equivalent ratio of sodium ions (green line) and calcium ions (blue line) in bentonite in relationship to the equivalent ratio of calcium ions in the external water. When the water is low in calcium ion concentation, then the amount of calcium in the bentonite is also low, leading to the increased risk of bentonite dissolution as colloids.

He was able to define and simultaneously solve three chemical equations and their corresponding non-linear mass-action laws, three mass balance equations, two charge balance equations and an activity coefficient model (see Figure 4). From this simplest possible chemical model of bentonite, he was able to determine the equivalents of the two ions in the bentonite as a function of the equivalent of calcium ions in water, and show that the relationship is nonlinear — a property that must be considered when considering transport models of the system (see Figure 5). Olin hopes to later incorporate his reaction model into a model of transport between a fracture and the bentonite by also the structural behaviour of saturated and swelling bentonite.

The research group at VTT consists of Anniina Seppälä, Veli-Matti Pulkkanen and Markus Olin.

The group led by Ivars Neretnieks is investigating how the structural properties of bentonite affect its dissolution. When bentonite in contact with a water stream dissolves in this stream, it reduces its material volume. Yet, because bentonite expands in the presence of water, it will also continue to replenish its volume, as other parts come in contact with the water. It therefore grows towards the region of dissolution and promotes its own dissolution. Being able to couple these mechanisms has required the flexibility of COMSOL Multiphysics.

As time goes on, more research groups and institutions will turn to modeling to adequately simulate the behaviour of their nuclear waste and repositories. The time-scales associated with the behaviour make experiments and testing rather limited, so that highly accurate estimations of the future consequences are required. The more physics you can incorporate into a model, the more accurate it will become. And by keeping the models equation-based, just as COMSOL Multiphysics does, and not hidden in the intricacies of code, then this will allow future generations to build on the simulations that are being conducted today. ■

Modeling Thermal Runaway for Safer Lithium Ion Batteries

Simulation reveals the heating conditions that can lead to thermal ignition.

TATSUYA YAMAUE, PHD, KOBELCO RESEARCH INSTITUTE, INC.

In the development of lithium ion batteries, safety design and evaluation play an important role in preventing problems such as ignition due to thermal runaway. We use simulation technologies such as COMSOL Multiphysics to understand the various phenomena that affect lithium ion batteries and to estimate battery safety. This paper describes a modeling methodology for testing the safety of chemical reaction heating in lithium ion batteries.

Our study focused on heating tests using thermal analysis to evaluate thermal runaway conditions. Three types of heating are considered:

- External heating using an oven or accelerating rate calorimeter (ARC),
- Internal heat generated by chemical reaction (thermo degradation reaction, combustion, etc.), and
- Heat release (heat transfer, radiation).

If the heat release is greater than the heat generated by external and internal heating, the battery will be thermally stable. If heat release is less, then temperatures rise steadily and lead to thermal runaway. In the heating test simulations, external heating is supplied using an oven.

If the heat release is greater than the heat generated by external and internal heating, the battery will be thermally stable. If heat release is less, then temperatures rise steadily and lead to thermal runaway.

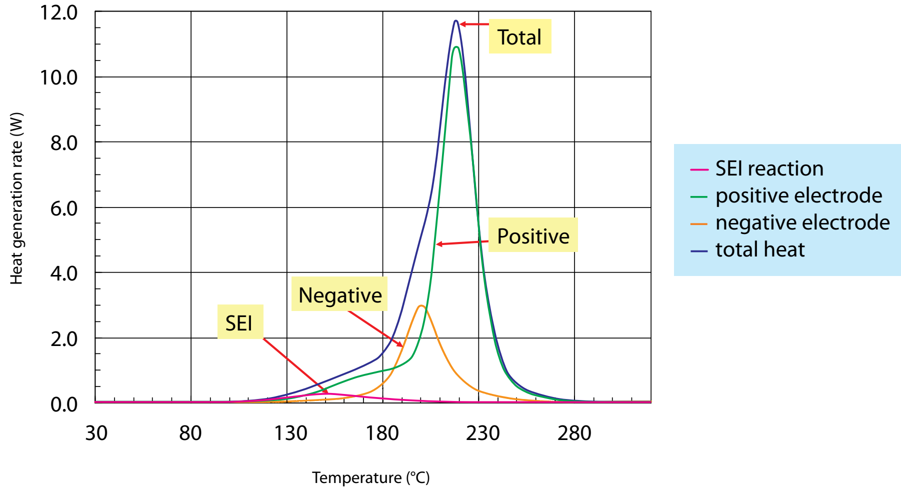


Figure 1. DSC measurements of heat reaction of active materials

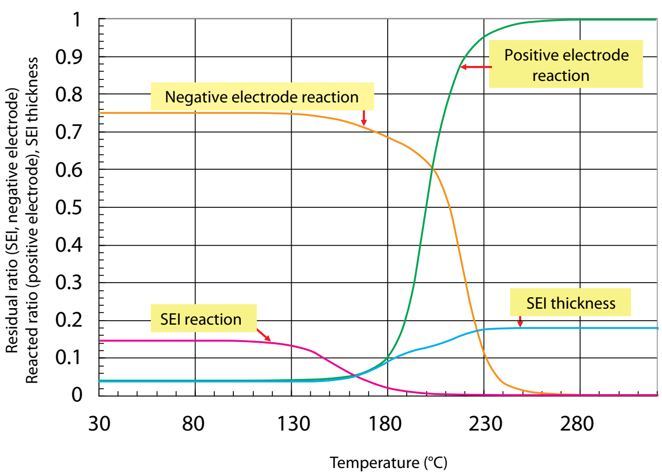


Figure 2. Analysis of reacted ratio under temperature elevation process (5°C/min) using reaction rate formula.

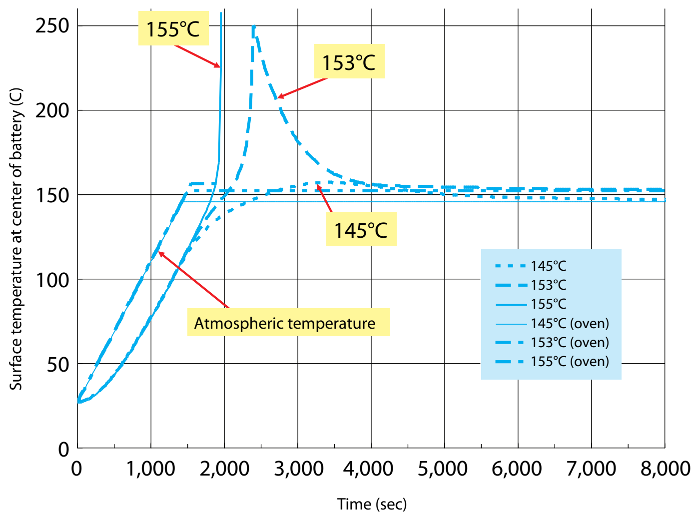


Figure 3. Change in battery surface temperature over time in heating test simulations at target temperatures: 145°C, 153°C, and 155°C.

Dimensions (18650 cylindrical battery)	Length 65 (mm), Radius 9 (mm)
Positive electrode active material mass	12 (g)
Negative electrode active material mass	6 (g)
Axial coefficient of thermal conductivity	14 (W/m K)
Radial coefficient of thermal conductivity	3.4 (W/m K)
Specific heat (battery average)	830 (J/kg K)
Density (battery average)	2580 (kg/m^3)
Heat transfer coefficient	Established by radiation test
Thermal emissivity	Established by radiation test

Table 1. Analysis conditions (18650 cylindrical battery).

A Reaction Heat Model

When modeling internal heating by chemical reactions, several physical phenomena must be accounted for. The first is thermal degradation of the separators and electrolyte, which affects conductivity. Second is the negative electrode-electrolyte reaction, which involves multiple reaction processes that cannot be described using a single reaction formula. Here, the reaction is divided into two parts: the solid-electrolyte interface (SEI) reaction and the negative electrode-electrolyte reaction through the SEI. Finally, the positive electrolyte reaction is included in the model.

To obtain the reaction heat model, we ran a series of Differential Scanning Calorimeter (DSC) measurements at a constant rate of temperature rise for each of the chemical reactions to obtain parameter fitting. Figure 1 shows an example of DSC measurements for a 1-hour temperature elevation process (5°C/min) where the positive electrode is $LiCoO_2$, the negative electrode is carbon, and the electrolyte is a mixture of EC (ethylene carbonate) and DEC (diethyl carbonate).

From the results of DSC measurements in Figure 1, the heat generation rate coefficient — i.e., the amount of heat generation per unit volume and unit time — and its dependence on temperature T were drawn.

Figure 2 shows the reacted ratio of each material under the temperature elevation process, analyzed using the reaction rate formula determined by peak fitting from the experiments. The first reaction to occur was in the SEI and the negative electrode, followed by the electrode-electrolyte reaction in the temperature range 100°C to 200°C. The thickness of the SEI suppresses the rate of the negative electrode reactions, but the rate still increases as the reaction progresses (150°C to 200°C), where the reaction then participates in a direct reaction with the electrolyte and is greatly increased (200°C – 250°C).

Safety Test Simulations

We conducted a suite of simulations using the obtained reaction rate formula. The battery analyzed was an 18650 cylindrical battery with a $LiCoO_2$ positive electrode, a carbon negative electrode, and a mixture of EC and DEC electrolyte.

For these simulations, the material property values for density, specific heat, heat transfer coefficient within the electrode surface, and other materials were the average of measured values for the positive electrode plate, negative electrode plate, and separators. For the area perpendicular to the electrode surface, we used the thermal diffusivity coefficient of the laminated film. We express heat release from the surface of the battery as the sum of heat transfer and thermal radiation. The heat transfer coefficient depends on atmospheric conditions, and thermal radiation depends on the material of the surface. We determined the coefficients of heat transfer and thermal radiation by fitting the change in surface temperature measured in oven tests. Table 1 lists the analysis conditions.

Figure 3 shows the results of the heating test simulations. The atmospheric temperature was raised to and maintained at various target temperatures. At a target temperature of 145°C, we observed some self-heating, but the temperature stabilized and did not produce a thermal runaway. At 155°C, however, thermal runaway occurred and the surface temperature increased sharply. At a target temperature of 153°C, the surface temperature increased but thereafter stabilized. Yet, as the chemical reaction progressed, surface temperature increased by more than 100°C, which we judged to effectively constitute thermal runaway.

Figure 4 shows the internal temperature distribution and negative electrode reacted ratio distribution at the time when thermal runaway commenced at the target temperature of 155°C. The central portion of the battery was the

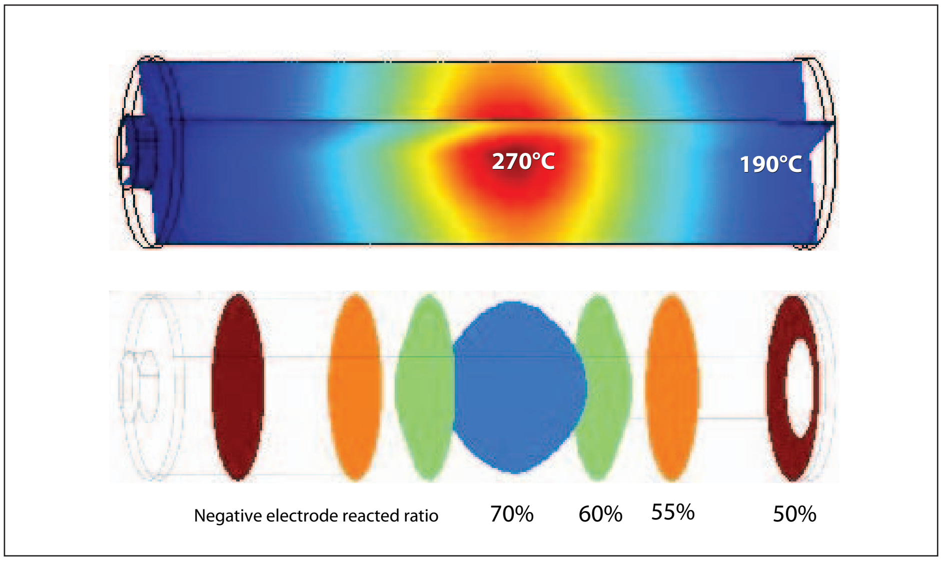


Figure 4. Internal temperature at start of thermal runaway for target temperature of 155°C (190–270°C) (above) and isosurface of negative electrode reacted ratio (below).

"COMSOL Multiphysics seems to be the ideal platform for battery analysis."

hottest, and the temperature difference between the ends and center of the battery reached 80°C.

Results from the ARC tests with the same type of battery showed that self-heating was observed from 73°C onwards and thermal runaway began at 150°C. These results indicate that the temperature predictions for thermal runaway obtained in the simulation were valid.

Figure 5 shows an extended safety study where we simulated a calamity resulting from an internal short circuit. Shown over a period of time are the temperature distributions during thermal runaway and the isosurfaces of reacted ratio of the negative electrode at 20W and 100W heat sources, respectively, from the short circuit. For several tens of seconds, a wide reaction zone was observed to move from the vicinity of the nail towards the end of the battery.

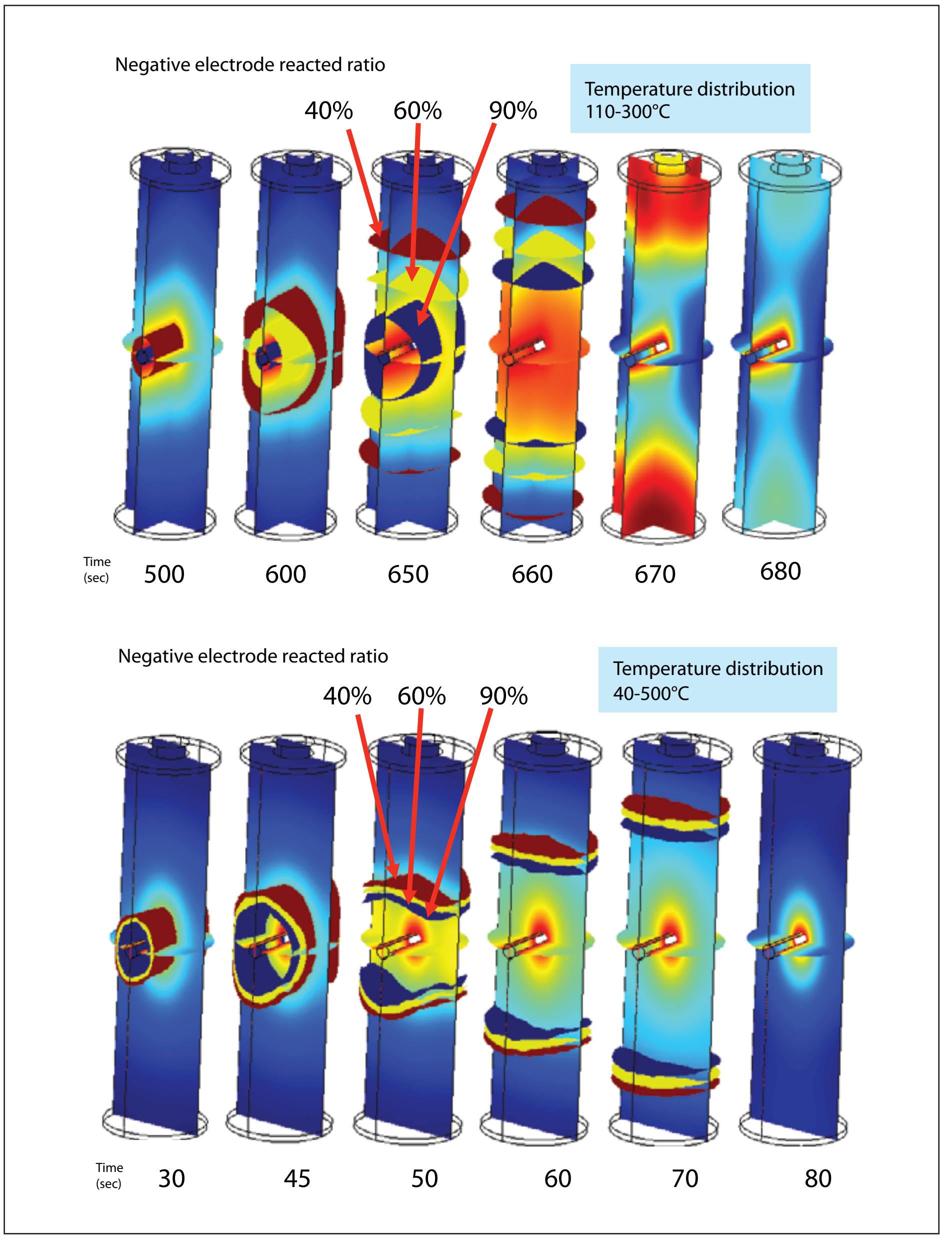


Figure 5. Change over time of temperature distribution (color contours) and isosurfaces of reacted ratio of the negative electrode during thermal runaway for an internal short circuit heat generation of 20W (upper row) and 100W (lower row).

Extended Battery Analysis

COMSOL Multiphysics seems to be the ideal platform for battery analysis, which requires the analysis of complex physical phenomena on different scales, such as the modification of chemical reaction model formulae, the application of integral boundary conditions for current distribution analysis, and the analysis of different physical phenomena for each domain. By being able to model all the phenomena related to heating and cooling a lithium ion battery properly, we are then able to extend our investigations to possible catastrophes.

Kobelco Research Institute, Inc. has devised not only the macro safety test simulations described in this paper but multilevel modeling and simulations, including charge and discharge cycle test, ionic transport within the electrodes, and nano-simulations of electrode surface reactions, using COMSOL Multiphysics and several other applications relating to molecular dynamics and ab-initio molecular dynamics. We use simulation technology with validation tests and measurements from material design and selection to battery design and evaluation. ■

About the Author

Tatsuya Yamaue, PhD, conducts his research at the Kobelco Research Institute, Inc.'s Engineering Mechanics Division, Technology Headquarters.

Modeling Finds the Minimum Energy for the Best Weld

BY DR. FRÉDÉRIC ROGER, ÉCOLE NATIONALE SUPÉRIEURE DE TECHNIQUES AVANCÉES PARISTECH

The next generation of nuclear power plants will likely have a design life of 60 years or more according to researchers at EPRI (Reference 1). Improved welding and fabrication practices will be essential in achieving this increased life expectancy and minimizing the potential for unexpected and costly repairs and maintenance. This report also indicates that most material failures in operating plants occur in or near welds, and evaluations showed that many of these failures resulted from less than optimum welding, fabrication, or surface-conditioning practices.

To improve welding and fabrication practices and thus ensure that new nuclear plants will operate reliably over their designed 60-year lifetimes, many companies are turning to simulation software. For instance, the École Nationale Supérieure de Techniques Avancées Paristech

> "Our COMSOL model takes into account all the factors that lead to fluid flow including gravity, electromagnetic forces, arc pressure and the Marangoni effect, which is the induced convection resulting from surface-tension gradients along the weld pool's surface."

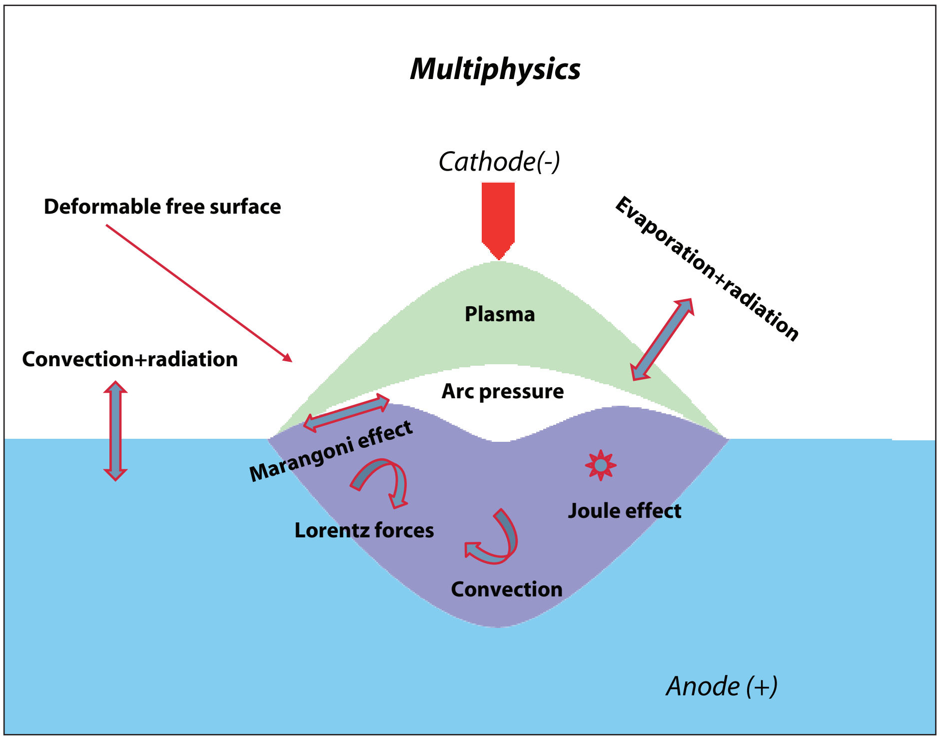


Figure 1. The primary physical phenomena in arc welding. Fluid flow in the pool is driven and influenced by a combination of buoyancy, electromagnetic forces, surface tension and arc pressure.

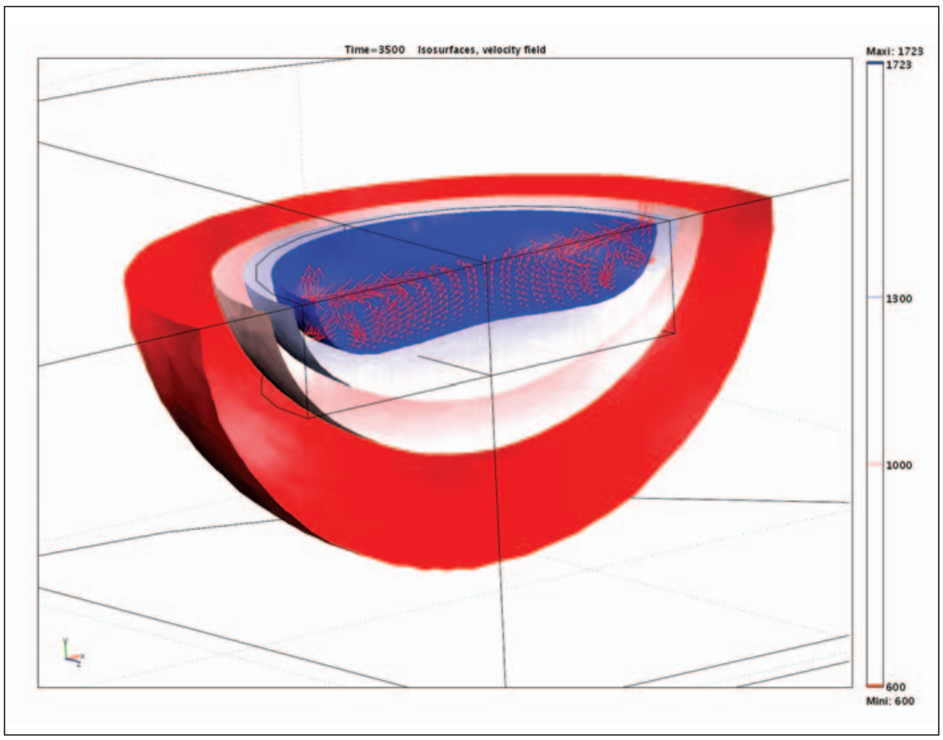


Figure 2. 3D representation of the weld pool at the end of the heating duration and some iso-thermal lines.

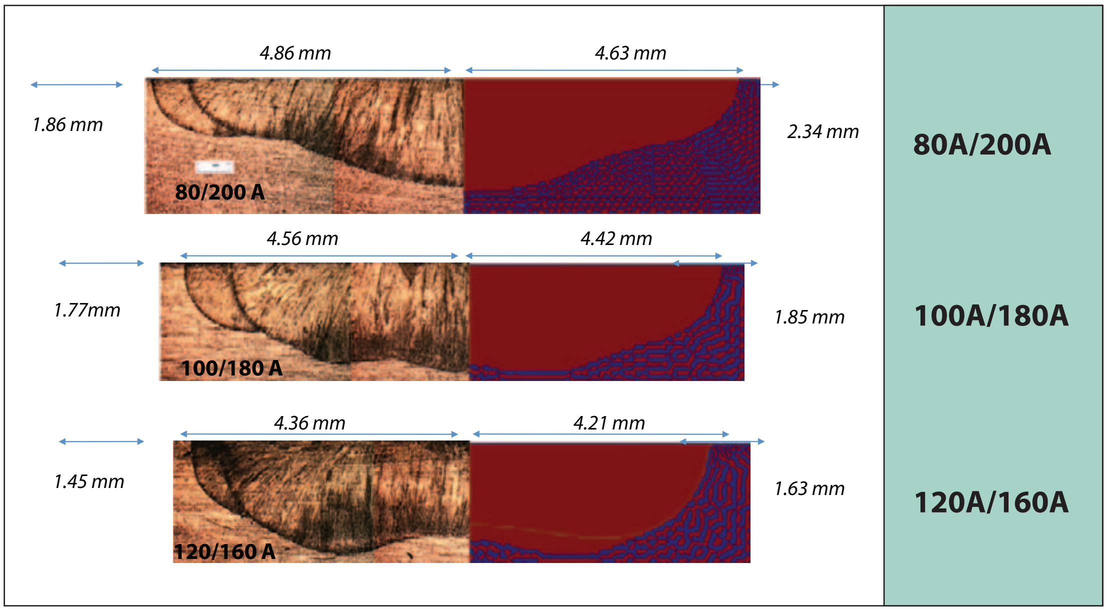


Figure 3. Comparison between the experimental macrographies of the three pulsed current cases (left) and the predicted weld pool shape after solidification (right), which shows very good agreement in both shape and dimensions.

(ENSTA Paristech) in Paris has set up a group in its Mechanical Engineering Unit to study welding. ENSTA is a public institution under the supervision of the French Department of Defense, and one of the welding group's major sponsors is AREVA NP, the world leader in the global nuclear power industry.

Effects of Phase Transformations

In the process of melting and reforming metal, welding generates heat gradients that are very localized and lead to the occurrence of residual stress and strain fields that play an important role in the prediction of fatigue life. Further, thermal cycles induced by welding or heat-treatment operations can generate solid phase transformations within the material.

Looking at the Weld Pool

In an initial study, we examined how to optimize operating parameters for the pulsed-current variation of GTA (gas tungsten arc) welding. This method allows for greater control of the weld pool, and operators can increase weld penetration, welding speed and quality. The process has been reported to have great advantages such as improving arc stability, avoiding weld cracks and reducing thermal distortions and residual stress due to the reduction of the total heat input. In fact, for a given shape of the weld pool, pulsed-current GTA welding can reduce the welding energy by 22% compared to constant-current GTA welding.

This is possible because the welding current rapidly alternates between two levels. During the period of peak current, the weld area is heated and fusion occurs; upon dropping to the background current, the weld area is allowed to cool and solidify.

The welder's goal is to choose the best parameters to maximize welding penetration and minimize thermal gradients to reduce residual distortion and stresses (Figure 2). However, these parameters — which include the values of the peak/background current as well as the pulse frequency — are more complex to define. Until now, their choice was based on empirical studies, but mathematical models can now help us understand the effect of various parameters on fluid flow in the weld pool, the final weld shape and thermal gradients.

Simulation of the Arc Welding Process

Our COMSOL model takes into account all the factors that lead to fluid flow including gravity, electromagnetic forces, arc pressure and the Marangoni effect, which is the induced convection resulting from surface-tension gradients along the weld pool's surface. Arc heating makes the temperature of the pool surface significantly higher at the center than at the edge. Surface tension decreases with increasing temperature, so the melt at the pool surface flows outward from the center to the edge.

The flow is positive until temperature reaches a critical value and then it becomes negative. Consider Figure 4, which shows the time evolution of the calculated weld pool at the end of each background time and each peak time (0.5 s each) for the total heating duration. It is important to note in each figure that two vortex fields are clearly visible; a clockwise vortex near the center of the weld pool resulting in an outward fluid flow at the surface; and a

About the Author

Since 2001, Dr. Frédéric Roger has been an Assistant Professor in the Mechanical Engineering Department at ENSTA (École Nationale Supérieure de Techniques Avancées) in Paris, he received his PhD at the Ecole Polytechnique in the Solid Mechanics Laboratory.

The pulsed GTAW simulations have been realized with Abderrazak Traidia, PhD Student at ENSTA, in collaboration with AREVA NP.

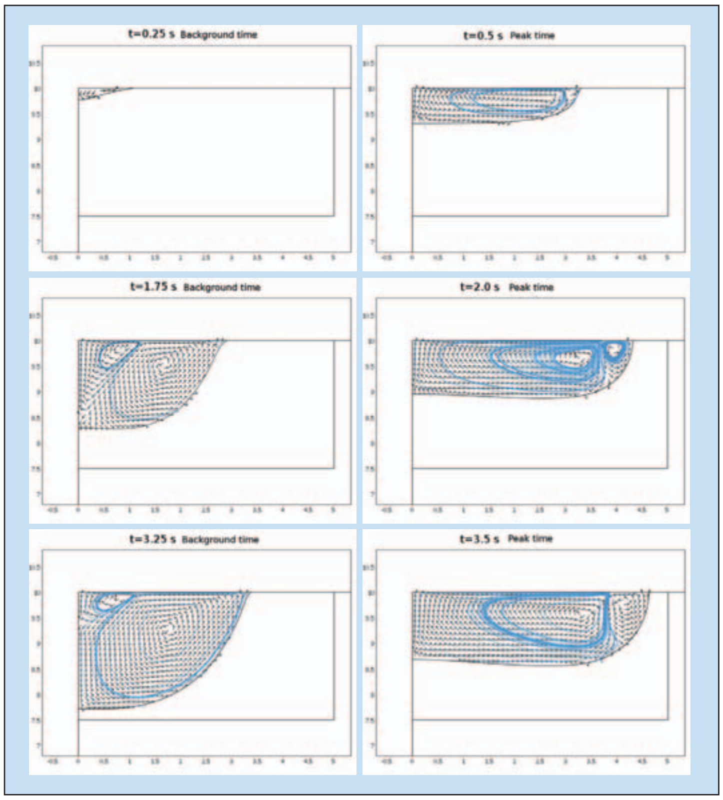


Figure 4. Time evolution of the calculated weld pool. The graph shows the case where the application of current occurs through pulses of 0.5 s each. The background currents occurs at 0.25 s, 0.75 s, etc.., while the peak current occurs at 0.5 s, 1.0 s, etc.…

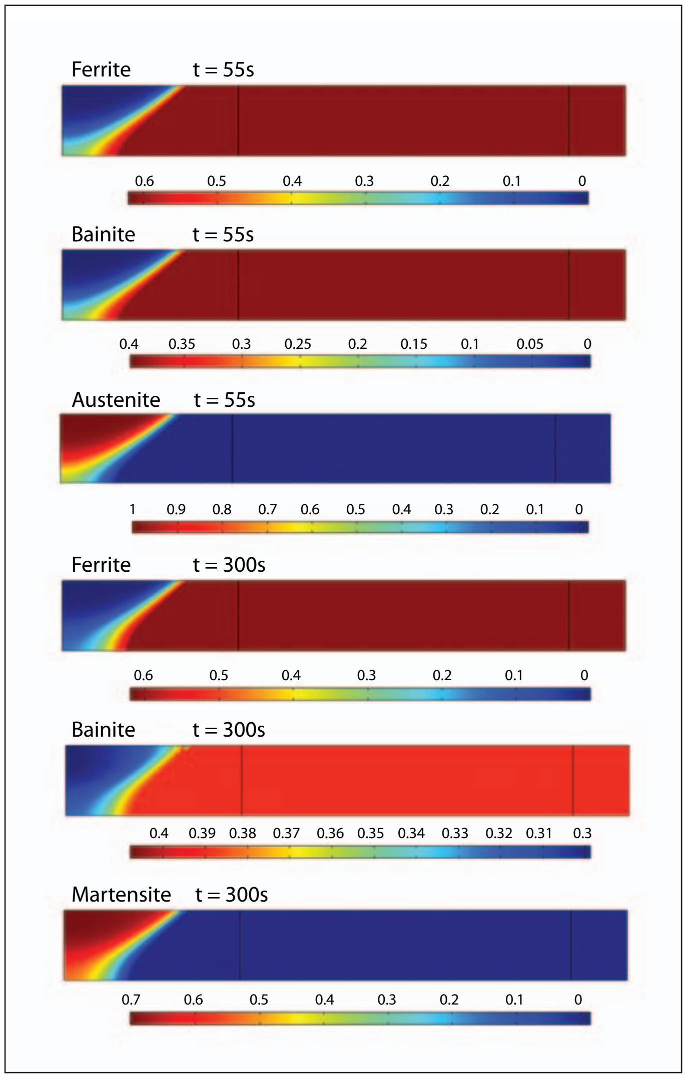


Figure 5. Phase fields in a steel disk at the end of heating (t = 55 s) and after cooling (t = 300 s). In the beginning, the ferritic part and bainitic part at the center were transformed directly into austenite, while after cooling a mixture of martensite and bainite is obtained.

counterclockwise vortex near the solidification point, resulting in an inward fluid flow at the surface of the weld pool. At each background time, the counterclockwise vortex is clearly dominant and goes towards creating a deeper weld pool. In converse, at each peak time, the clockwise vortex is dominant, which creates a wider, although shallower, weld pool.

Our first key result is that pulsed welding produces a deeper and wider weld pool than using a mean current. We also found that the pulsed cases induce a higher temperature at the center of the plate, leading to higher thermal gradients. Thus, an optimal choice must be made between the weld pool penetration and the induced thermal gradients.

We next studied the effect of the current's frequency on the shape of the weld pool using 2, 4 and 6 Hz. The 2-Hz case produced a wider and deeper weld pool than the other cases. Also, increasing the frequency brings the weld pool dimensions closer to those for a mean current, which means that pulsed welding can produce the same weld pool shape as continuous current with less welding energy. Furthermore, using pulsed current limits the heat transferred to the metal plate and thus reduces residual stress and distortions.

When the Weld has Solidified

After the weld has solidified, it is necessary to determine residual strains and stresses in the welded structure by modeling and investigating the thermal, metallurgical and mechanical phenomena as well as their interactions. To simulate a weld, we studied a metal disc heated with a laser both experimentally and in our models (Figure 5). Stresses occur between the different solid phases as they have different crystalline structures, where these residual stresses are more pronounced in areas of high thermal gradients.

The model was able to simulate the experimental results and we were then able to put it to use by studying the low-alloy ferritic steel welds used in the manufacture of pressurized-water nuclear reactor vessels. Depending on the cooling rate, several types of metallurgical structures can be obtained, each with different thermomechanical characteristics. ■

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High-Performance Computing for the Masses

Continued from back cover

a report. But in this respect, each operating system places fairly strict borders around its workflow. Clearly, this model for scaling up computing power is not sustainable in the long term.

Microsoft entered the HPC market more than 4 years ago with the goal of enabling Windows desktops to offload compute-intensive tasks onto a cluster of Windows servers. This would enable engineers to stay within their Windows desktop at all times, while compute-intensive tasks like COMSOL sent all their heavy computational jobs to the cluster. The cluster, managed by the same IT staff maintaining the rest of the Windows infrastructure, would use the same identity and access technology as the e-mail, file, and print servers. Microsoft's vision was for all Windows desktops to be empowered by a few scalable, central resources for heavy computations, similar in concept to centralized storage systems.

> "For scientific and engineering software companies like COMSOL, the Windows HPC server represents an out-of-the-box solution."

For scientific and engineering software companies like COMSOL, the Windows HPC server represents an out-of-the-box solution containing everything their users need for cluster computations, including a server operating system, a job scheduler, MPI library, and management tools. Previously, such a solution had to be built with products from a number of different vendors and even open source communities, which often left your total cluster solution without complete support.

The Windows HPC server is completely based on Windows Server and, like all Windows products, comes with a 10-year support commitment. Together with the rich support for parallel development in Visual Studio, this makes the Windows platform the most efficient and economical solution for developers of compute-intense scientific software by far. For the end-user, this translates into having many affordable HPC applications such as COMSOL available in a familiar Windows desktop environment, along with an almost unlimited ability to scale-out on the commodity hardware and server operating system. ■

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GUEST EDITORIAL

High-Performance Computing for the Masses

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Raw computing power is one of the most important assets for competitive organizations. If you can compute more efficiently than your competitors, you are likely to outcompete them by having faster access to more accurate information about the problem. In areas ranging from automotive aerodynamics to oil exploration reservoir simulation and stock portfolio management, we are witnessing a technological escalation where companies are buying more compute power to compete more effectively and efficiently — and this trend is spreading quickly across most industries. For example, I know a software company that had a turn-around time of 24 hours for its "daily" builds. By purchasing 100 compute servers, this company cut down its turnaround time to just 15 minutes — a dramatic shortening of its time-to-market.

The continual and exponential increase in CPU clock frequencies over the last 20 years has been a key contributor to the success of the IT industry because it enables software developers to leverage higher abstractions. But recently this performance increase has almost come to a stop due to limitations in physics, which is why we rarely see clock frequencies above 3 GHz. Today, the only way to increase compute power is to use parallel computing — distributing compute tasks over several CPUs, often spread over several physical computers — usually called High-Performance Computing (HPC).

The use of HPC in science and engineering is well established. Among the most widely deployed applications are simulations of different physical phenomena such as computational fluid dynamics, structural mechanics, and electromagnetics. A significant performance boost is achieved through parametric simulations, a form of simulation that allows for optimal scalability by solving the same problem in parallel for a wide range of parameter values. COMSOL Multiphysics version 4.0 supports all of these uses of HPC.

Microsoft entered the IT industry with the vision of one computer on every desk, a vision now more than fulfilled. In disciplines such as scientific computing or engineering, users are often double blessed by having two computers on their desk. The first computer is typically used for e-mail, reporting, and routine day-to-day work using Microsoft Office with Excel, Word, Outlook, and similar applications. The second computer is reserved for heavy computations, simulations, compilations, renderings, or similar time- and resource-intensive tasks.

There are many reasons for having two computers: You may need different operating systems for certain applications, and some applications require so many resources they cannot co-exist with other applications. Or maybe you simply want double the computing power. The key benefit of two computers is that it gives you the opportunity to work on parallel tasks, such as writing a report on your current experiment while simulating the next experiment.

From a productivity perspective however, there are no advantages to using several operating systems simultaneously — quite the opposite, in fact, because your workflow gets disturbed. While you may want to do things in parallel, you also need to be able to interact between tasks, say, cutting and pasting live data from a simulation into

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Henrik Steepler earned his PhD in Computer Science in 1999 at Chalmers University, Sweden. Since 2003, he has been working at Microsoft on emerging markets like Security, Virtualization, and since 2007 on their High Performance Computing (HPC) initiative. He is now managing the partner network for Microsoft in Europe, the Middle East, and Africa around HPC.

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