COMSOL NEWS

A TECHNICAL COMPUTING MAGAZINE

Clearing the Air: Life Support for Space Exploration

MANUFACTURING:
MOLDING TECHNOLOGY
8

AUTOMOTIVE:
SENSOR DESIGN
30

COMSOL

COMSOL Multiphysics

Ten Years of Unlimited Simulation Capabilities!

In 1998 COMSOL Multiphysics® made its debut as the first commercial environment to enable scientists, engineers, and researchers to solve any system of coupled physics phenomena in the same simulation. Ever since, users have leveraged the insights of multiphysics modeling and simulation to work smarter.

In this issue of COMSOL News, you'll find 15 examples of how your colleagues use COMSOL to take on today's technological challenges. We have a report from a team at NASA Marshall Space Flight Center that's modeling next-generation life support systems for long-duration space habitation such as a lunar outpost and a roundtrip to Mars. Next, you can learn how multiphysics helps France's RocTool, which specializes in licensing its rapid molding technologies for the composites industry, customize molds for its clients' diverse needs. We also have two interesting examples of multiphysics in the consumer products industry: electric shavers from Philips and a full-color, photo-quality direct thermal printer from ZINK Imaging.

Odds are good that you will find many great examples of multiphysics modeling in this magazine, but it is just a sampling of the multiphysics universe. The Conference CD from last fall's worldwide user conferences has many more examples for you. In fact, the CD contains more than 250 technical papers, 190 user presentations, 40 downloadable models, and 90 video clips illustrating multiphysics modeling across all disciplines of science, industrial and space research, engineering, medical research, and education. Request your free-of-charge CD at **www.comsol.com**.

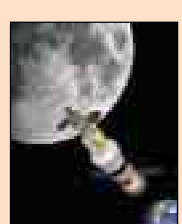
We're celebrating the 10th anniversary of COMSOL Multiphysics. And we have a busy year ahead with hands-on workshops around the world, the 2008 Conference featuring COMSOL 3.5, and much more. I hope to see you there!

Bernt Nilsson
Sr VP of Marketing
COMSOL, Inc.

CONTENTS // COMSOL NEWS 2008

FEATURES

DEPARTMENTS



On the Cover

This concept image depicts a lunar lander in transit from Earth to the Moon. COMSOL Multiphysics is part of the toolset used at NASA's Marshall Space Flight Center to develop robust life-support systems for future long-term space habitation. See page 4 for details.

Image courtesy of NASA Marshall Space Flight Center.

COMSOL NEWS

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

Clearing the Air:
Life Support for Space Exploration

Jim Knox and David Howard of the NASA Marshall Space Flight Center report on research into atmospheric revitalization systems for long-term space travel and the use of COMSOL Multiphysics to understand how thermal management and structured sorbents can improve the performance of adsorption processes.

An engineering requisite for all space travel is to minimize power, weight, and volume because all three translate to mass for any launch system. Compared to near-Earth missions such as the International Space Station, manned lunar outposts and long-duration space travel present additional constraints that stress system engineering. Chief among these constraints is that every system must be robust enough to operate for long periods of time without compromising crew safety, without resupply, and without launch-taxing extra mass such as spare parts or a glut of backup equipment. Life support systems are no exception.

At the Life Support Systems Development Team of NASA's Marshall Space Flight Center in Huntsville, Alabama, our task is to develop robust, yet mass-minimizing, life support systems for long-duration space travel, such as lunar exploration missions or a trip to Mars. Our extended team includes the adsorption experts at Vanderbilt University, led by M. Douglas LeVan, and at the University of South Carolina, led by James Ritter.

We are developing the next generation of atmosphere revitalization systems, which will reach for new levels of resource conservation via a high percentage of loop closure. For example, a high percentage of carbon dioxide (CO_2) exhaled by crewmembers can be converted by reaction into clean water, closing the loop from human metabolic waste to essential hydration and hygiene supplies. Adsorption processes play a lead role in these new closed loop systems. Engineered structured sorbent (ESS) technologies have attractive characteristics with the potential to reduce both complexity and overall resource needs.

One new ESS technology we are investigating involves coating thermally and electrically conductive (generally metallic) substrates with molecular sieve sorbents. Use of a metallic substrate allows for direct and efficient sorbent heating as well as the capability to reduce the negative impacts of the heat of adsorption on process efficiency.

But sorbent-coated metal technologies present a number of tradeoffs in terms of working capacity, mass, and volume. Thus, the question becomes, are they worth the effort? COMSOL Multiphysics simulation plays a key role in our design and analysis process as we investigate that question.

Conflicts with Heating and Cooling

That sorbent-coated metal ESS technologies may offer the reduced resource requirements needed for a long-term life support system becomes apparent in view of the physics underlying adsorption and desorption processes. Heat is produced during adsorption, yet the resulting higher temperatures reduce sorbent capacity and, therefore, inhibit adsorption. Yet, during desorption heat is lost and temperatures drop. While cooling increases sorbent capacity, it impedes desorption. The net effect of this heating and cooling byproduct of the adsorption process is a reduction in the working capacity of a regenerative revitalization system.

One potential solution lies in transferring the heat between adjacent adsorption and desorption beds to approach an isothermal process. This, along with the capability for direct resistive heating, led us to explore how Microlith substrates from Precision Combustion Inc. and Electron Beam Melting (EBM) manufactured substrates from Arcam behave when coated with zeolites.

Microlith is an expanded metal screen coated in a sorbent material (Figure 1). When electrically heated, the intimate contact of Microlith metal and sorbent

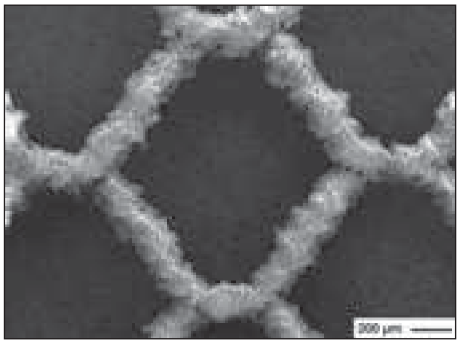


Figure 1: Micrograph of sorbent-coated Microlith.

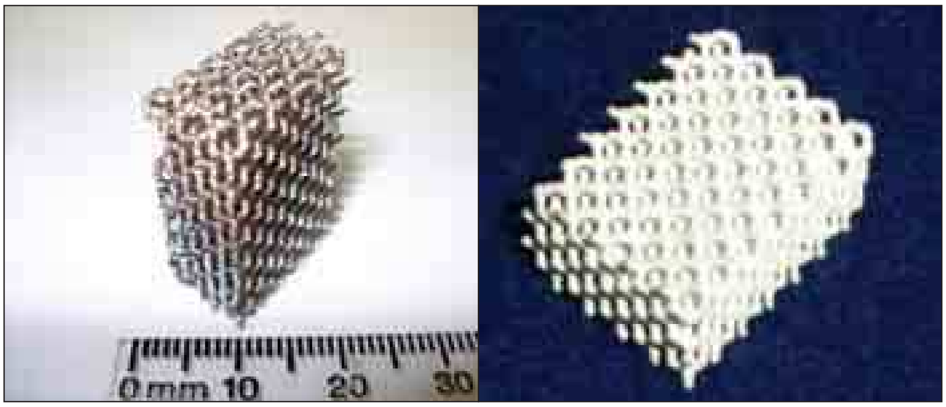


Figure 2: The interior lattice work (left) of the part built with an Arcam rapid manufacturing system at NASA Marshall Space Flight Center and coated with zeolite (right).

Intro Cov ToC

make for an efficient heat transport to the sorbent. Arcam's EBM rapid manufacturing process uses an electron beam to melt metal powder that then fuses, layer by layer, into a part that might otherwise be impossible to machine. Figure 2 shows a lattice produced by this process at the NASA Marshall Space Flight Center.

With these technologies appearing hopeful, the next challenge facing us is how to optimize the removal efficiency of a coated metal sorbent module, and thus reduce overall system volume. A second, related question is what sort of performance gains (and system size reductions) can be realized by removing the heat of adsorption during the CO_2 and humidity removal process? We address the second question first.

Hot Beds of Sorbent

We built models of sorbent beds using COMSOL Multiphysics to learn more about the thermal characteristics of various sorbents undergoing different adsorption processes. To derive the linear driver force (LDF) coefficient, which characterizes the rate of mass transfer from sorbent to gas and must be determined empirically for each sorbent-gas pair, we modeled isothermal adsorption testing conducted with a custom-built plate-finned heat exchanger packed with sorbent[1]. Due to the relatively constant temperature within the canister, the heat of adsorption could be neglected, allowing the mass transfer to be studied in isolation.

Testing began with a completely clean sorbent bed and the introduction of CO_2-laden nitrogen. Initially, no CO_2 exits the bed, but then the CO_2 outlet history emerges in the classic S-curve shape of a breakthrough curve. By adjusting the LDF coefficient, we obtained a match between the actual test data and the simulation data.

Since these simulations indicated our adsorption model was on the right path, our next step was to characterize the thermal characteristics of a sorbent canister and to determine the heat transfer coefficient between the fluid and the sorbent and the fluid and the wall.

Here, we were looking at the heat balance for the gas phase. This testing started with a clean bed of sorbent material and introduced 450 kelvin nitrogen, resulting in the large temperature swing shown in Figure 3. Modeling results following adjustment of the heat-transfer coefficients (also shown in Figure 3) provided a good match between the test results and the simulation. This gave us a usable characterization of the system.

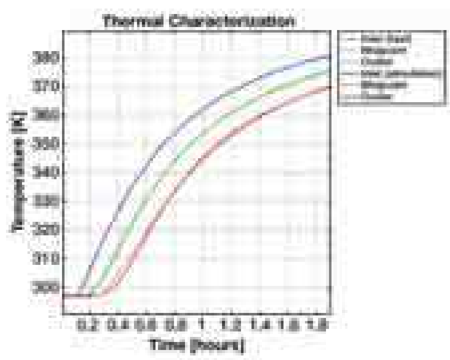


Figure 3: A comparison of test results and the COMSOL Multiphysics simulation characterized the heat transfer.

After some additional testing and simulations, we were able to determine that eliminating the heat of adsorption would delay the initial breakthrough by about an hour, not an insignificant amount of time. If we could adjust the actual adsorption cycle to take advantage of this delay, we could increase the adsorption performance and, hence, the working capacity.

In a subscale test rig (Figure 4), we proved that by recuperating the heat of adsorption with an adjacent, thermally linked desorbing bed during a vacuum swing sorption cycle, we could nearly eliminate the temperature swings of up to 26° Fahrenheit observed in thermally isolated beds. Thermally linking adjacent beds was achieved by packing granular silica gel in metallic foam filled beds. This approach allowed us to increase the adsorption period from 15 minutes to 60 minutes while maintaining a removal efficiency greater than 90% — a four-fold improvement in water adsorption.

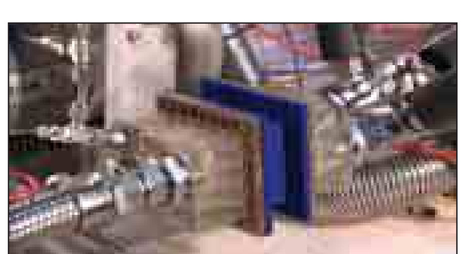


Figure 4: Subscale VSA test apparatus; results with a thermally linked bed showed a four-fold capacity improvement over thermally isolated sorbents beds.

Thus we confirmed that, for a process that approaches an isothermal vacuum swing process, significant performance benefits are realized during both adsorption and desorption. This is accomplished by inhibiting the temperature swings that result from the exothermic and endothermic nature of a cyclic sorption process.

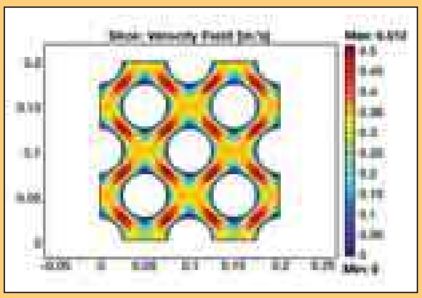
Modeling the EBM Component

These results encouraged us to optimize the removal efficiency of the coated metal sorbent and thus reduce overall system volume. Hardware and adsorption process optimization requires understanding the effect of varying substrate geometry (metal strand size and spacing), process (flow, desorption method, and cycle time), and canister design (sorbent types and quantities). Multiphysics simulation was clearly required here to capture the effects of changing these parameters on the fluid dynamics, transient mass transfer, and transient heat transfer during the adsorption process.

The top left image in Figure 5 shows a simplified geometry of the interior lattice of the EBM part to simulate alternative interior design featuring metal rods with a sorbent coating, with the rods connected thermally by a wall.

We then looked at a subset of this geometry (bottom left image Figure 5). The bottom left image in Figure 5 is a 2D simulation of a Navier-Stokes incompressible steady-state analysis of the flow field around the rods. The results obtained from COMSOL showed that, although the flow around the rods enters our adsorption chamber uniformly at y = 0, it quickly forms an established, repeatable flow field.

With this data, we could simplify our model and still obtain a reasonable answer. Next, we examined the boundary layer effects on the flow near the wall. The top right image in Figure 5 shows the 3D simulation of flow through a bed of the structured sorbent lattice. The similarity of the flow pattern at varying distances from the wall at the bottom indicates that



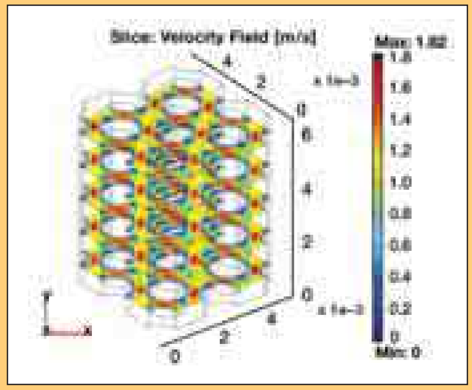


Figure 5: The wall in the middle connects a lattice of sorbent-coated metal rods (top left) thermally. The image on the bottom left shows a uniformity of fluid flow through a 2D structured sorbent lattice in the Y direction, while a 3D slice plot (top right) shows a uniformity of fluid flow through a structured sorbent lattice.

the wall effect diminishes quickly away from the wall.

Figure 6 shows the flow field in the two exit planes along with the streamlines. Again, simulation shows that the flow field becomes very consistent a short distance away from the wall. This means that we can use a small portion of the full lattice to study the effects of changing rod size, spacing, and geometry on the fluid flow. The ultimate goal is to maximize the mass transfer from the fluid to the sorbent while minimizing the pressure difference through the bed.

Where We Go From Here

So what does this all mean? It means we have much more work to do. For example, we plan to develop COMSOL Multiphysics simulations of existing subscale test articles, including EBM, Microlith, and other ESS configurations. The process parameters (cycle time, flow rate, etc.) as well as the design and structure of the coated metal latticework will require more optimization through simulation. Then we have to build and test designs based on our simulations, and compare ESS approaches against packed bed sorbents, the present standard in the industry.

In short, we have years of research prior to designing the atmospheric revitalization system for lunar outposts and the first human roundtrip to Mars. COMSOL Multiphysics has played a key role in our design and analysis process thus far, and our hope is to continue to use it extensively in the future. ■

Download the Presentation Slides at:

www.comsol.com/industry/papers/2451/

References

[1] NASA-CR-2277, "Development of Design Information for Molecular-Sieve Type Regenerative CO2 Removal Systems," R.M.Wright et. al., Los Angeles, 1973

[2] Mohamadinejad, H., Knox, J.C., and Smith, J. E. "Experimental and Numerical Investigation of Adsorption/Desorption in Packed Sorption Beds under Ideal and Nonideal Flows." Separation Science and Technology, 2000, 35(1), 1-22

Contacts

Arcam AB
www.arcam.com

Precision Combustion, Inc.
www.precision-combustion.com

Acknowledgments

Any opinions, findings, and conclusions expressed in this article are those of the author and do not necessarily reflect the views of NASA. Mention of any products or companies in this article should not be construed as an endorsement by NASA.

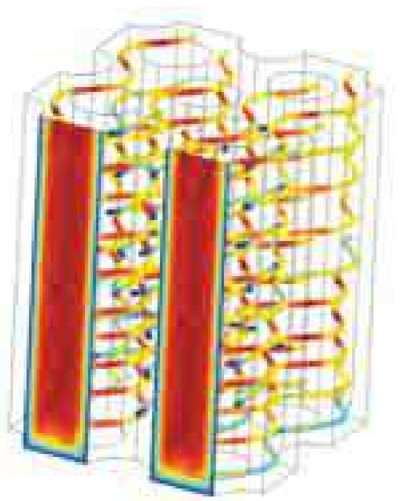


Figure 6: A simulation of the 3D fluid flow in COMSOL Multiphysics. The boundary layers at the separating wall are evident in the bottom of the exit planes. Streamlines show highest velocity in constricted areas.

About the Authors

Jim Knox (right) and David Howard at the Marshall Space Flight Center Environmental Control and Life Support test facility.

Jim Knox is NASA's technical manager of the Sorbent-Based Atmosphere Revitalization project, developing CO_2 and H_2O removal systems for the manned missions outlined in the U.S. Space Exploration Policy. Mr. Knox has over 20 years experience in flight system hardware development and R&D within the aerospace industry. David Howard is the Principle Investigator for testing and process development of Engineered Structured Sorbents. Mr. Howard has over 10 years experience in test, design, and analysis in the aerospace industry. The authors' present focus is evaluating and maturing emerging adsorption technologies for use in future manned habitat Atmosphere Revitalization systems.

Instrumentation Modeling for NASA's Next Mars Rover Mission

BY CATHLEEN LAMBERTSON

Scheduled to launch in the fall of 2009 with the goal of reaching Mars in October 2010, NASA's Mars Science Laboratory (MSL) is a robotic rover that will look for signs of habitable environments on the Red Planet. One of the instruments selected to fly aboard the MSL is the Chemistry and Mineralogy (CheMin) instrument. Capable of performing both x-ray diffraction and x-ray fluorescence analyses of powdered rock samples, CheMin will catalog the chemical and mineral composition of rocks it examines.

Concept illustration of NASA's Mars Science Laboratory (MSL).

To test the viability of CheMin, Dr. Talso Chui — a principal scientist in the Applied Low Temperature Physics Group at NASA's Jet Propulsion Laboratory (JPL) in Pasadena, CA — and his team used COMSOL Multiphysics to perform thermal modeling of the instrument. There were two important questions the group wanted answered: Do the electronic components overheat, and is the pressure too high after turning the x-ray source on? "We are interested in whether certain components are too hot," explained Dr. Chui. "The junction temperature should be kept below 120°C."

For the simulation, the model was structured into four components — one for each circuit board and one for the high voltage power supply (HVPS) can and mechanical structures. Using the command "File>Merge Component," all of the objects in a component were combined into a single composite object. The model featured 898,969 mesh elements, 282 domains, and 2,680 boundaries. The run time for the simulation was approximately 45 minutes.

"The COMSOL package took care of all of the different types of physics involved [in performing the simulation]," said Dr. Chui. "The software was very helpful because it can solve very complicated geometry." He found that using COMSOL Multiphysics was an economic way to explore various design options, since the simulation uncovered multiple problems. For example, the transformer potting material turned out to be above 80°C, which may cause hardening over time; the pressure was close to 100 psia, which is too high; and the pressure gauge was too hot at 120°C.

Dr. Chui has used COMSOL software for a variety of other projects. He worked on the "world's most accurate clock," which uses a mercury ion lamp in its design. He chose COMSOL to simulate how hot the lamp can become. He also has used COMSOL for many different magnetic-shield modeling applications. "One thing I find particularly attractive with this package is that you learn the basics and then can apply it to different physics like magnetic modeling, superconducting shielding, and so on," he said. "These are totally different from thermal analysis, but once you learn the basic package, there is very little you need to learn in order to apply it to other areas." ■

COLLABORATION

TransTech Systems becomes COMSOL Certified Consultant

TransTech Systems will help you realize an idea and bring it to fruition. With world class service and a proven track record of turning ideas into products, TransTech can be an invaluable development resource to quickly analyze your concept, develop a prototype, enhance it through simulation and make it viable.

COMSOL certified consultant

A recent keynote speaker at the 2007 conference in Boston and a well respected person within the industry, Ronald Gamache is the leader of the COMSOL Certified Consultants group. Mr. Gamache has over thirty-five years experience in advanced sensing, measurement and control technologies. At TransTech, he is responsible for the development of electro-magnetic sensing solutions to material characterization problems.

Among many other applications, TransTech R&D includes specialists in:

- NDE Sensor Development
- Electrical Impedance Spectroscopy (EIS) and Tomography (EIT)
- Analog and Digital Electronics
- Electromagnetic Sensor Design
- Signal Processing
- Artificial Neural Networks
- Biomedical Engineering

For more information visit **www.transtech-RD.com** or email comsol@transtechsys.com.

Innovative Molding Technology

JOSÉ FEIGENBLUM, ROCTOOL, LE BOURGET DU LAC, FRANCE

Mathematical modeling is going far beyond the R&D lab and is starting to make a real difference in manufacturing processes. For instance, it's hard to imagine that RocTool's primary process, our rapid composite molding technology, would be here today without COMSOL Multiphysics. In fact, the success story of our company is linked closely to the capabilities of that software.

The process that makes up virtually all of our business today did not exist just five years ago. And it was only with the help of COMSOL that we were able to discover, understand and commercialize our Cage System technology. Today it would be virtually impossible to adapt our process to each client's requirements without the software.

RocTool is an innovative company that specializes in licensing its rapid molding technologies for the composites industry. Its customers include major automobile manufacturers plus their Tier 1 suppliers, the aircraft industry, as well as sports and leisure companies — all where lightweight yet strong composite materials are key components (Figure 1). The company does no manufacturing; rather, it helps clients set up production lines that integrate the Cage System inductive-heating method. With 15 employees and growing, RocTool last year had sales near 1.5 million euros, all from the licensing of its patents and in consulting.

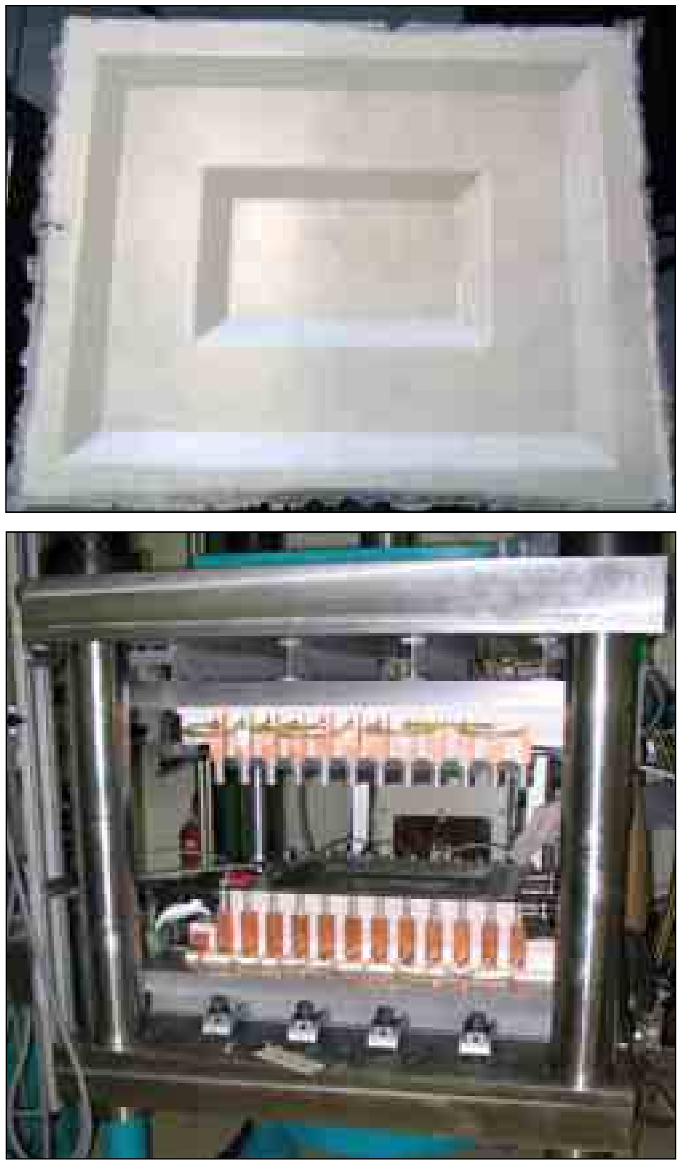


Figure 1: Example of a molded part and the molding apparatus used to create it. RocTool licenses its technology, which is used for many different types of molding. The materials, shapes and applications all differ greatly.

Better control of tooling-surface heat

When making composite parts in Resin Transfer Molding (RTM), a mold must be hot enough to cure the material, but not too hot during the injection phase. The mold generally consists of top and bottom surfaces separated by a few millimeters. Traditionally, molding sections are made of solid metal; these are heated by sending hot oil or water through small shafts bored through the mold, or by sitting the mold on a heating plate. This means that large volumes of metal are being continuously heated and, depending on the application and mold, the process can require 20 to 50 kW or more of power for 24 hours a day, 7 days a week. A complete injection/curing cycle varies with the requirements of the material being formed; for instance, with a thermoset such as an epoxy resin it can take 15 to 20 minutes at a constant temperature of 90°C.

We at RocTool knew there must be a better, faster way. I learned about COMSOL Multiphysics' capabilities during my PhD work and, when I joined RocTool five years ago, one of the first things I did was to tell engineering management that we had to have it. This turned out to be an excellent decision.

With COMSOL, we developed the Cage System, which we subsequently patented in 2004. This method involves surrounding both parts of the metal mold with an induction coil that is driven by a high-frequency signal of between 15 and 100 kHz. Because of skin effects, induced current stays within the outer 0.1 or 0.2 mm of the mold sections. The mold has a high magnetic permeability which induces strong eddy currents, and the material's high resistance results in locally heating the tooling surface in desired places. The other conductive surfaces on the exterior of the mold are made of nonmagnetic materials and do not contribute noticeably to the heating. Heating of the tooling surface starts immediately when the coil is activated, and requires 200 kW or more of power to quickly get from 40°C to 140°C. As a consequence the heating/cooling cycle drops to between 2 and 5 minutes (Figure 2).

The Cage System also gives process engineers much better control of the temperature cycle. For instance, the classical method to mold material such as resin epoxies uses a lower constant mold temperature during both injection and cur-

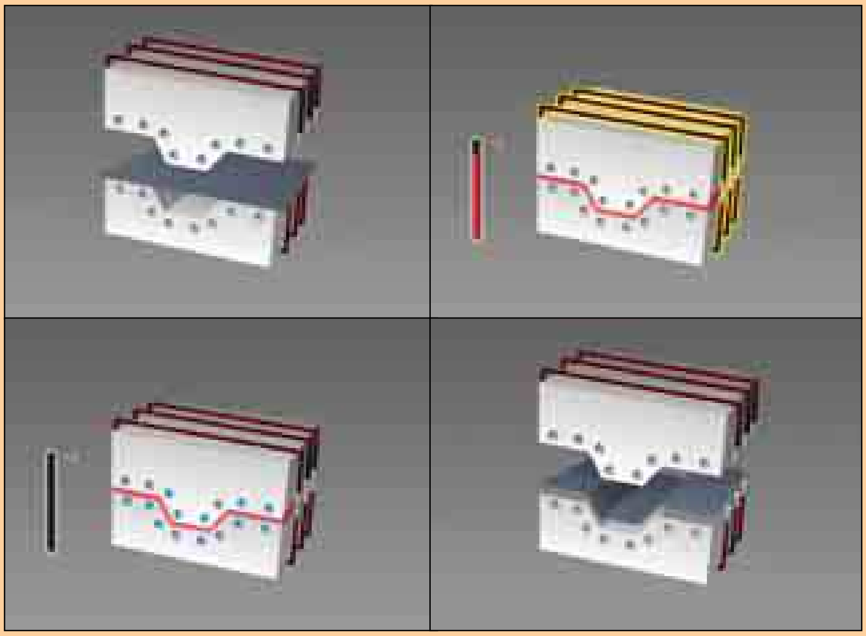


Figure 2: The molding process. The composite material is placed within the mold that then presses down on the material while induction currents heat the two surfaces of the mold. When the final shape has been taken, water flows through pipes to cool down the material. The final shape can then be removed.

ing. This lower mold temperature avoids cross-linking during injection, but the curing cycle takes a long time. The Cage System, on the other hand, preheats the mold to 40°C so that the epoxy resin has good viscosity for being injected, and the temperature can be quickly increased for the curing stage. In this way, it is possible to cut cycle times by a factor of two or three for many processes. Further, the Cage System is applicable to many molding processes that require fast heating and cooling, and it can be used in virtually all types of molding, such as blow, extrusion, injection, or compression molding.

A problem with using induction currents to heat the mold surfaces is the possibility of hot spots. The mold surface's shape can influence the magnetic field and thus the induced current, and for many shapes it is possible to see considerable temperature differences across the tooling surface. The material being transformed is therefore not heated homogeneously and a sharp curve can cause overheating where it is convex and underheating where it is concave. This is due both to higher current density on the convex radius and the fact that heat is concentrated in the area near the radius. However, with the Cage System, engineers can place surface inserts with lower magnetic properties in certain areas to closely regulate the heat distribution and to eliminate hot spots. Modeling is an integral part of determining the placement of these inserts.

Users indicate that while a molding machine using this process might cost 15 to 20% more than one using classical methods, manufacturing efficiencies then lower the cost of the final by 15 to 20%. For instance, the production of 20,000 automotive roofs using classical methods requires 2 production units and leads to a cost of 90 euro/ piece, which decreases to 45 euro/piece using the Cage System production unit. This is mostly due to a drastic reduction in the time cycle — by a factor 5 in this case (4 min as opposed to 20 min).

A model for every client

In the composite-molding business there is no such thing as a standard product; each mold must be designed individually based on the customer's material and product specifications. This is where COMSOL Multiphysics plays a crucial role. After reviewing the application with a client, RocTool creates a model that simulates the magnetic fields, eddy currents and Joule heating on the molding surface. The aim of the 3D model is to define the optimal inductor configuration and surface layer that creates efficient and homogeneous heating. We pay close attention to the selection of materials and the mold geometry, which we can determine effectively only through simulation. We use the AC/DC Module to first compute a quasi-static magnetic solution for the field due to the coil, and then use those results to find the heat distribution on the tooling surfaces (Figure 3).

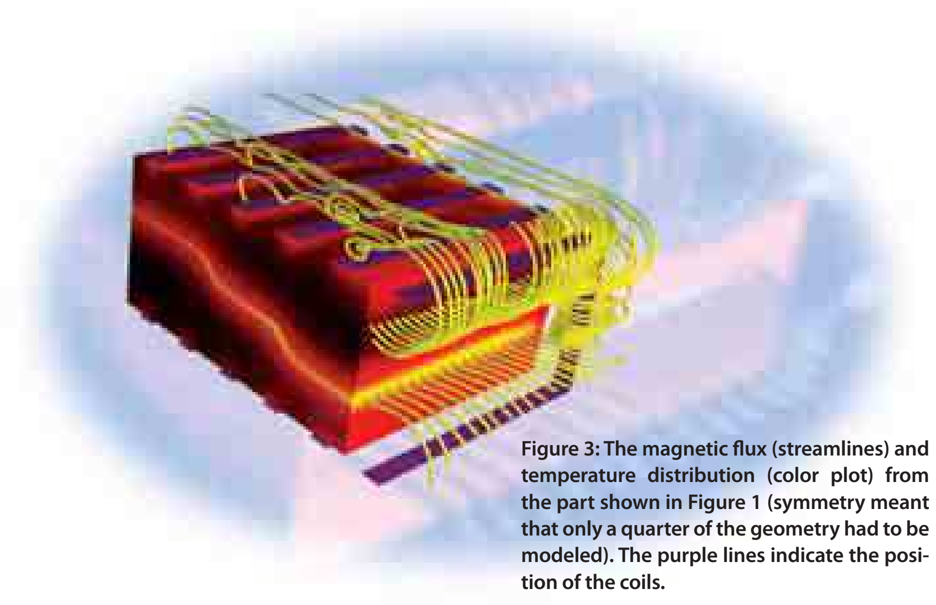


Figure 3: The magnetic flux (streamlines) and temperature distribution (color plot) from the part shown in Figure 1 (symmetry meant that only a quarter of the geometry had to be modeled). The purple lines indicate the position of the coils.

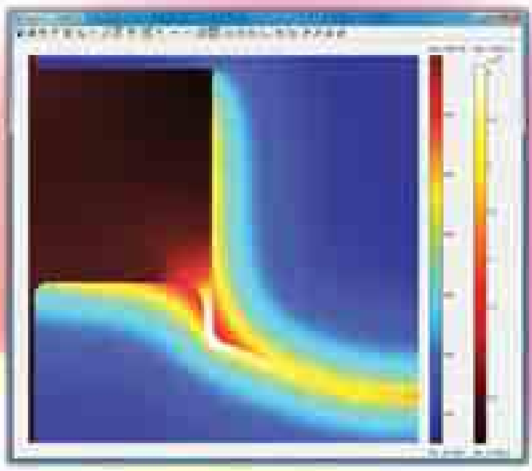


Figure 4: Close-up of a cross-section of the model of a mold. The 'hot' color scale shows the amount of current density inducing heat (A/m²), while the 'jet' color scale shows the localized temperature in the mold (K).

With this model, engineers can determine the optimal size of the coil, its placement, heating material properties and the optimized cycle time. We quickly learn how the number and placement of the turns in the inductor coil is crucial for homogeneous heating. Further, if the inductor is not long enough compared to the mold, cold areas can arise on the mold extremities where the magnetic field density is lower. After modeling, RocTool engineers can tell the client that the process will result in a given temperature cycle, that molding will take a given amount of time, and they can also give a reasonable estimate of what the parts will cost to manufacture.

Our latest research effort, which we are still in the process of commercializing, concentrates on determining how to best work with self thermally regulating materials (STRMs) to control hot spots. These materials are useful because when they reach their Curie temperature they become nonmagnetic and thus are no longer subject to inductive heating. Depending on the amount and placement of these materials, we can gain even better control of the temperature profile over the tooling surfaces. To model these materials in COMSOL, we create a 3D geometry and first solve for the magnetic field, then determine the materials' temperature. When these materials reach the Curie point, we re-run the magnetic field calculations and find the new temperatures.

CAD Import for a variety of clients

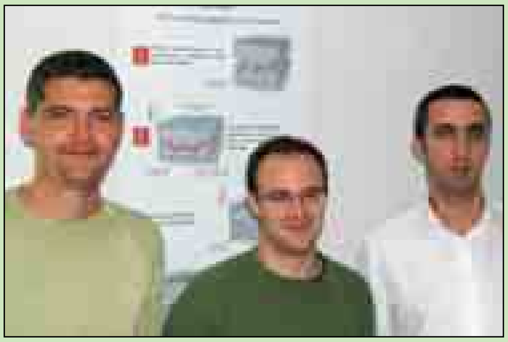
Another important aspect of the software is the CAD Import Module, as the tool designers must work with CAD data supplied by our clients. A large number of them, especially those in the automotive industry, work with the CATIA® CAD system and provide geometry data in either the IGES or STEP formats. Work with these imported geometries, from which the tooling engineers create the heating surfaces for the mold, is supported through the CAD Import Module. Part geometries can sometimes be quite complex, and the modelers use defeaturing tools to simplify the geometry to make the modeling more practical. They must strike a balance between model solution times and the detail of the results.

RocTool engineers are also very impressed with COMSOL's graphics capabilities, which make it easy to show results (Figure 4). For instance, a client once visited us and had some questions about how to improve his existing process. Within an hour, an engineer was able to create and solve a model and graphically show the improvements in the heating process — and before the customer left, he had made a commitment to order the next process improvement.

In general, though, the most attractive aspect of COMSOL Multiphysics is that it sets no limits on our R&D. It lets us see new approaches and opportunities, such as when we used it to develop the technology upon which RocTool's success depends. We can get by with far fewer prototypes because the models allow us to understand all the 3D phenomena going on inside this sophisticated process. Besides, running these COMSOL models is actually a lot of fun, especially when we can impress our clients as much as we do. ■

Author Biography:

Dr José Feigenblum has been the Research and Development Manager of RocTool in Le Bourget du Lac Cedex, France since 2004, after having acquired a Ph.D. in inductive processes. He is in charge of all technical developments at the company in areas such as induction, thermal, mechanical and mainly processes for plastic transformation.



The modeling group at RocTool: from left, Damien Perrier, Rémi Hemous and José Feigenblum

READ THE RESEARCH PAPER AT:
www.comsol.com/industry/papers/2577/

Fluid-Structure-Acoustic Interactions

BY DR. S.P. YUSHANOV, DR. J.S. CROMPTON, AND DR. K.C. KOPPENHOEFER, ACES OF COLUMBUS, LLC

Computational analysis of fluid-structure interactions (FSI) represents a considerable challenge for most computational analysis codes. Simple one-way coupled problems, in which the fluid pressure deforms a structure but does not substantially affect the fluid flow characteristics, can be solved by a variety of techniques. Solutions to the more complex two-way coupled fluid-structure interactions are more elusive. These occur when pressure of the flow of fluid deforms a structure in such a way that the resulting deformation alters the flow of fluid. The two-way coupled approach solves this problem and produces accurate, time dependent results.

Through the use of COMSOL Multiphysics, ACES of Columbus, LLC has developed practical solutions to realistic FSI problems across a wide range of applications in the biomedical, automotive and petrochemical industries. Examples of FSI problems in these industries include: blood flow through flexible systems, characteristic acoustic signatures of valve components, structural vibration due to intermittent transient flow through compressors and control of fluid cavitation around a vibrating structure.

COMSOL Multiphysics has been used to develop a specialized multiphysics model describing the response of a vibrating needle in a liquid. The vibration of the needle generates a pressure wave and causes bending of the flexible needle.

The FSI solution couples the continuum equations of solid mechanics with the Navier-Stokes equations of fluid mechanics. COMSOL Multiphysics solves these equations simultaneously over the same computational domain using an Arbitrary Lagrangian-Eulerian formulation (ALE). The moving mesh capabilities in the ALE formulation of COMSOL allow a stable solution while increasing the amounts of needle movement and deformation.

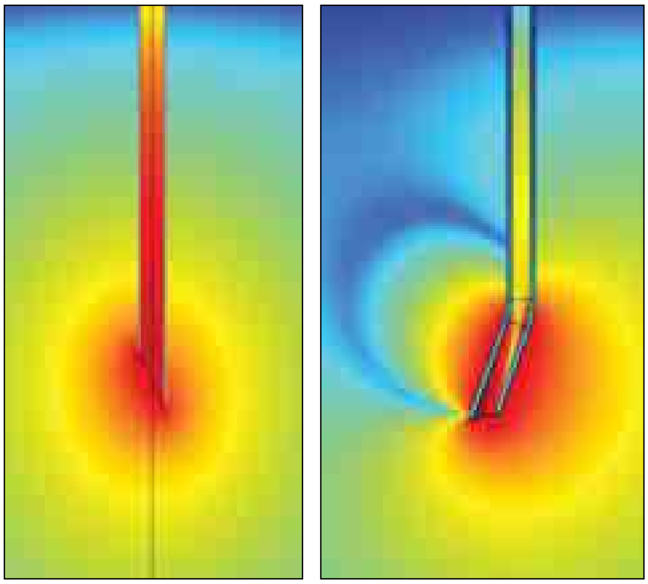


Figure 1. Sound pressure levels developed from two needle designs. These designs seek to maximize local pressure levels and minimize pressure at a specified distance.

Solutions of this type can quantify the influence of key design variables of the system. For example, the operating stress experienced by the needle, stream lines of the fluid flow, and the acoustic sound pressure levels developed (see Figure 1).

The results of fully coupled FSI analyses have allowed ACES to resolve performance issues with new products prior to mass production, significantly reducing the time and cost of new product development and manufacture.

This work was performed by Dr. S.P. Yushanov, Dr. J.S. Crompton, and Dr. K.C. Koppenhoefer using COMSOL Multiphysics. For more information please contact: K. Koppenhoefer, ACES of Columbus, 750E Cross Pointe Rd, Columbus, OH 43230, or visit ***www.acescolumbus.com****.* ■

Best Paper and Best Poster Awards — COMSOL Conference Boston and Grenoble 2007

Boston Best Paper Awards

- Acoustic Transparency of Non-homogeneous Plates (with repeating inclusions) using Periodic Structures Methodology, *Anthony Kalinowski, Naval Undersea Warfare Center, Newport, RI*
- Geometrical Optimization of Pyrophosphate Concentration in Thermosequencing Platform for DNA Sequencing, *Hessaam Esfandyarpour, Stanford University, Palo Alto, CA*
- A Model of Direct Thermal Printing, *W. T. Vetterling, ZINK Imaging, Inc., Waltham, MA*

Boston Popular Choice Best Poster Award

- Magnetic Particle Motion in a Gradient Field, *Usha K Veeramachaneni, West Virginia University, Morgantown, WV*
- Voltammetric Performance of Nanometer Interdigitated Electrodes, *Guigen Zhang, The University of Georgia, Athens, GA*

Grenoble Winners

- Catalyst Degradation in PEM Fuel Cells — Modeling Aspects, *Vaivars Guntars University of the Western Cape — South African Institute of Advanced Material Chemistry, South Africa*
- Coupled Electro Thermal and Fluid Dynamical Simulation of Axial Flux Permanent Magnet, Synchronous Machines, *Marignetti Fabrizio, Universitá degli Studi di Cassino, Italy*
- 3D Semiconductor detectors for medical imaging, *Ruat Marie, CEA Grenoble, France*
- Structural Shape Optimization Using Moving Mesh Method, *Liu Zhenyu, Universität Freiburg, Germany*

Electrochemical Machining in Appliance Manufacturing

To find the most efficient way to manufacture the caps for electric shavers, engineers at Philips use multiphysics modeling to study the best balance of process parameters.

DR. IR. REDMER VAN TIJUM, ROYAL PHILIPS ELECTRONICS NV, DRACHTEN, THE NETHERLANDS

Behind your clean, close shave there is an enormous amount of high technology, even in electric shavers that have been around for decades. Philips DAP is working with new materials for, among other components, the shaving cap that acts as a shell around the rotating cutter. On its next-generation shavers expected to reach the market in a couple of years, Philips is starting to use multiphysics modeling to optimize the process used to manufacture these caps.

In the manufacturing process, Philips first forms raw caps from transformation-induced plasticity (TRIP) steel. Because these are too thick and do not have the required precision shape, further manufacturing is required. For the low-end shaver range, Philips used electrical discharge machining (EDM) to finish the low-end shaver caps, but it required costly and regular replacement of the component electrodes and is therefore not applicable for complex shapes. High-end shavers also work with three cutters instead of one, so the cap has a much more sophisticated shape that requires a more complex manufacturing process (Figure 1). Philips turned towards electrochemical machining (ECM) to enable more complex shapes. Nowadays, the demand of more closeness requires improved process understanding. Computational simulations, rather than running costly experiments throughout the entire evaluation and optimization process can provide this vital information.

ECM consists of the managed electrochemical dissolution of an anode (the cap) by passing current between it and a pre-shaped cathode (the tool). At the cap surface, metal is dissolved into metallic ions by an electrochemical reaction. Placing the tool — whose shape is not altered by the reaction — and setting the applied voltage results in a cap with the desired accurate shape.

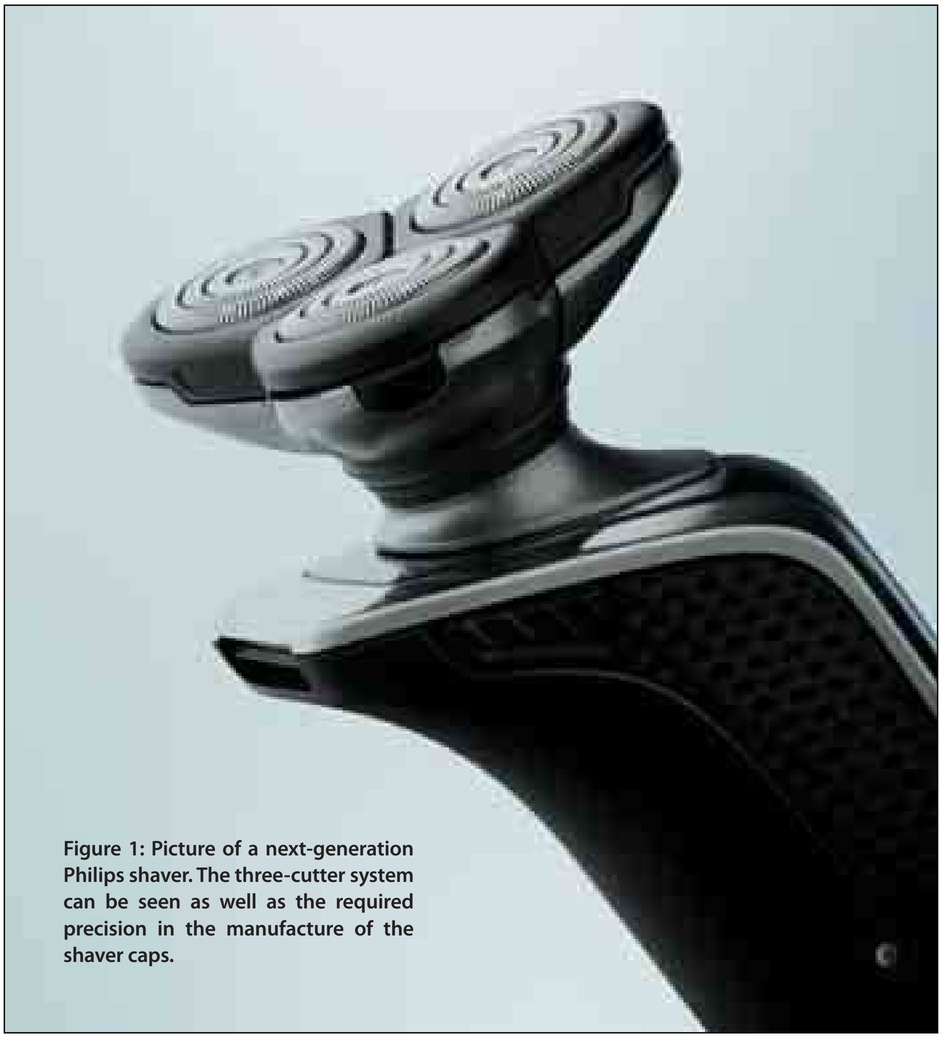


Figure 1: Picture of a next-generation Philips shaver. The three-cutter system can be seen as well as the required precision in the manufacture of the shaver caps.

Electrolyte flows between the cap and tool to remove metallic ions as well as a gas that evolves on the cap through a side reaction. The presence of this gas also contributes to the electrolyte's electrical resistance, and, along with the cap's changing surface area, the varying resistance must be compensated for by adjusting the system's voltage. A mass balance must also be considered to describe the electrochemical kinetics at the electrodes as well as adjust for material-based properties such as density in the fluid flow.

Here ECM works with high currents in thin materials and small electrolyte channels, which leads to high temperatures and even boiling if electrolyte flow is not adequate. This, along with the fact that the cap's structure also changes over time and is influenced by the high-pressure electrolyte flow, results in significant changes in the cap's structural integrity, where phenomena such as spring-back can occur. High temperatures also affect density in the fluid flow. In all, Philips has a complex multiphysics problem to investigate (Figure 2).

These highly interrelated effects make it virtually impossible to optimize the process through experimentation alone.

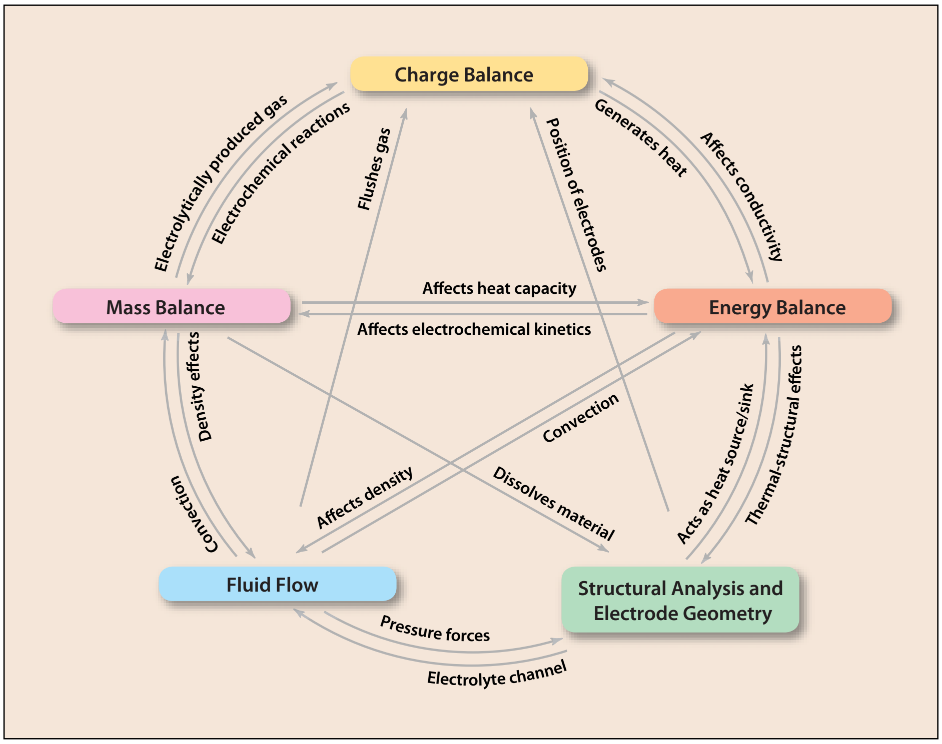


Figure 2: The various physics couplings in the multiphysics process that Philips must consider when modeling electrochemical machining (ECM).

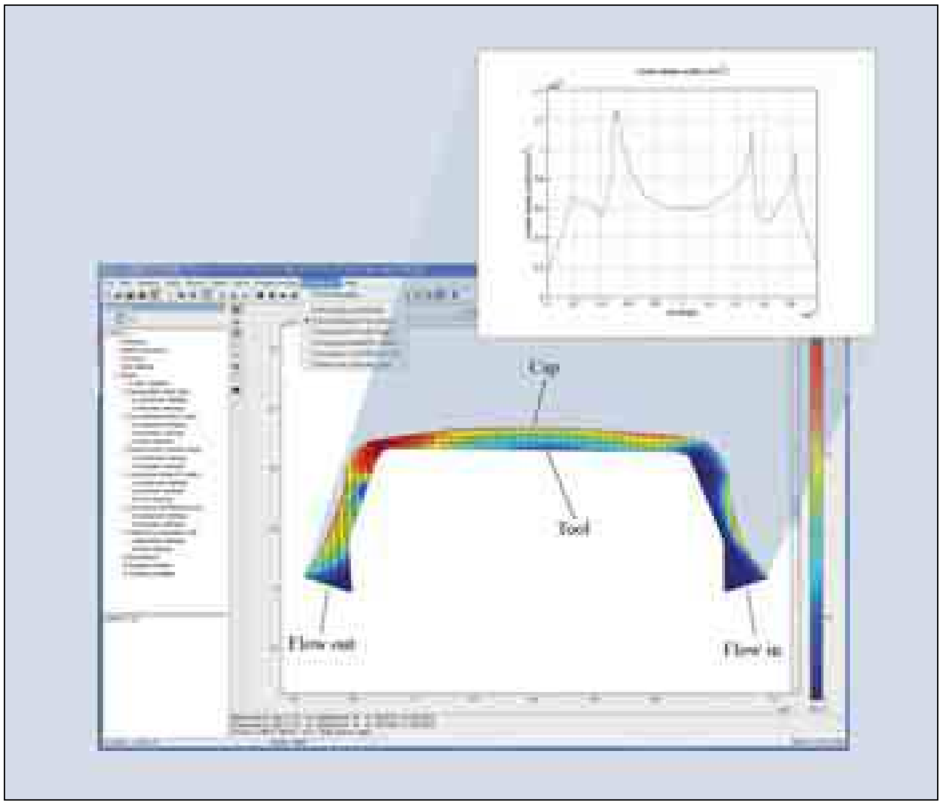


Figure 3: Results from a 2D model of a cut through the electrolyte channel between a shaver cap (top) and the tool (bottom). Electrolyte flows from right to left. Shown is the gas concentration (color plot) and velocity field (arrow plot). Noticeable is the effect that flow has on gas distribution as well as the accelerating effect that the gas impinges on the flow. Shown in the above plot is the distribution of current density along the cap's entire surface where peaks correlate to bends in the geometry and areas of greater dissolution.

Computational simulations were required, and Philips employed COMSOL Multiphysics. This package could handle all the interrelated physics while providing the ability to couple these physics. It also allowed models that would be easily understood by all people in the modeling and manufacturing processes.

To model this process, Philips needed to consider the physics of the electrical current. COMSOL Multiphysics contains a modeling interface for this, where electrochemical kinetics can be freely entered directly to simulate the reactions at the cap-electrolyte interface. Furthermore, COMSOL's interface also provides high flexibility whereby users can describe the conductivity that varies due to the presence of gas bubbles and heat. This was all then coupled directly to other modeling interfaces that describe the fluid flow (non-isothermal flow) and heat transfer (convection and conduction), where a source term in the heat transfer equations depends directly on the electrical current. An equation was also entered in the density term of the fluid-flow modeling interface to represent the effects of temperature and gas-mixture makeup. To save computational memory, heat flux was represented at the tool and cap interfaces with the electrolyte in order to simulate their energy storage capabilities.

The cap's structural geometry was also considered with respect to its effect on the other physics. The shape of the pre-formed cap was imported and could easily be updated during the modeling process based on intermediate model results. Furthermore, a special 'moving mesh' modeling interface was utilized for simulating the changing shape of the cap when it was coupled to the electrochemical reactions that simulated the dissolving TRIP steel. This resulted in an adequate description of the electrolyte channel and fluid flow.

With this model (Figure 3), Philips is well on the way to generating a manufacturing process for these new caps, to improve closeness. Validation studies are in progress, and then these models will become the driving force for improving the manufacturing process and the production lines. ■

Reduced Metal Consumption in Electroplating Saves Big Money

BY PHILIPPE GENDRE, PEM, SIAUGUES, FRANCE

Given the scarcity and price developments of today's metals, virtually all of them can be counted as being 'precious'. As a result, electroplating firms such as PEM always look for ways to reduce the amount of metals that are consumed as part of a process. Thanks to studies conducted using COMSOL Multiphysics, we have made significant advances, often including savings between 10% and 30% of the metal we deposit during electrolysis.

Components on reels

With sales of roughly 20 million euros in 2007, PEM is heavily involved in treating and finishing surfaces, and our specialty is reel-to-reel electroplating. The customer supplies a reel, which can be from several hundred to several thousand meters, and whose tape holds a continuous series of metal parts such as connectors for electronics systems. At our facilities, we unwind the tape or carrier strip from these reels, and send it through a sophisticated process consisting of cleaning, plating and rinsing stages. This happens at speeds from 1 to 20 m/min (Figure 1).

During the metal-plating stage, the tape passes through a reacting cell that is continuously replenished with electrolyte. The tape is made cathodic through contact to a voltage source, and the electrolyte completes the electrical circuit to anodes in the plating cell.

Getting a uniform plating layer is not simple. Consider that more metal tends to migrate towards the edges because if the tape (the cathode) is standing on end and the anodes are to its sides, the shape of the electric potential field follows the tape — up one side, around the top, and down the other side. Spikes in the current-density distribution occur where the tangential gradients for potential contribute, along with the normal gradients, to the overall ionic transport of species to and from the electrode surface (see blue trace in Figure 2). These are more commonly known as edge effects.

PEM's answer is to design a shield, a type of insulating screen or tray through which the tape travels as it passes through the plating reactor. Made with insulating materials that are chemically compatible with the bath, the shield is shaped so the lines of electric potential essentially run parallel along the entire width of the tape, and the gradient to the tape surface is even. The red trace in Figure 2 shows the benefits of adding such a shield.

Figure 1: Factory floor with a series of reel-to-reel electroplating units. Reels of solid or stamped metal plates are passed through the electroplating units, and metal is deposited over the whole or sections of the tape according to the application of electric current and the placement of shields.

Shield design without prototypes

The shield's shape varies with the components on the reel, the plating material and its thickness, electrolyte concentration, and tape traveling speed. Developing shields experimentally can require multiple time-consuming prototypes, so PEM started to use COMSOL Multiphysics to help us better understand the underlying phenomena and thereby come up with an appropriate shield for each process. These days, we are generally successful on the first try.

The multiphysics model accounts for several effects: conductive media for the electrical current, Navier-Stokes for the electrolyte flow, and electrokinetic flow to simulate the transport of species. For this, we use the Chemical Engineering Module along with the COMSOL Multiphysics modeling environment.

Author Biography:

Philippe Gendre is Head of R&D at PEM in Siaugues, France. He earned his Ph.D. in material chemistry from Pierre et Marie Curie (Paris VI) University. He has been working at PEM since 1997 on R&D topics related to developing new processes and materials for electrolysis.

Save even more material

We have successfully designed shields that handle most of the types of products we run through our process. Our next goal with COMSOL is to examine the effects of limiting currents so as to design our reactor cell with high fluid velocities near the cathode surface and thus increase process throughput. If you can replenish the metal ions better, you can raise the current density and thus production (Figure 3).

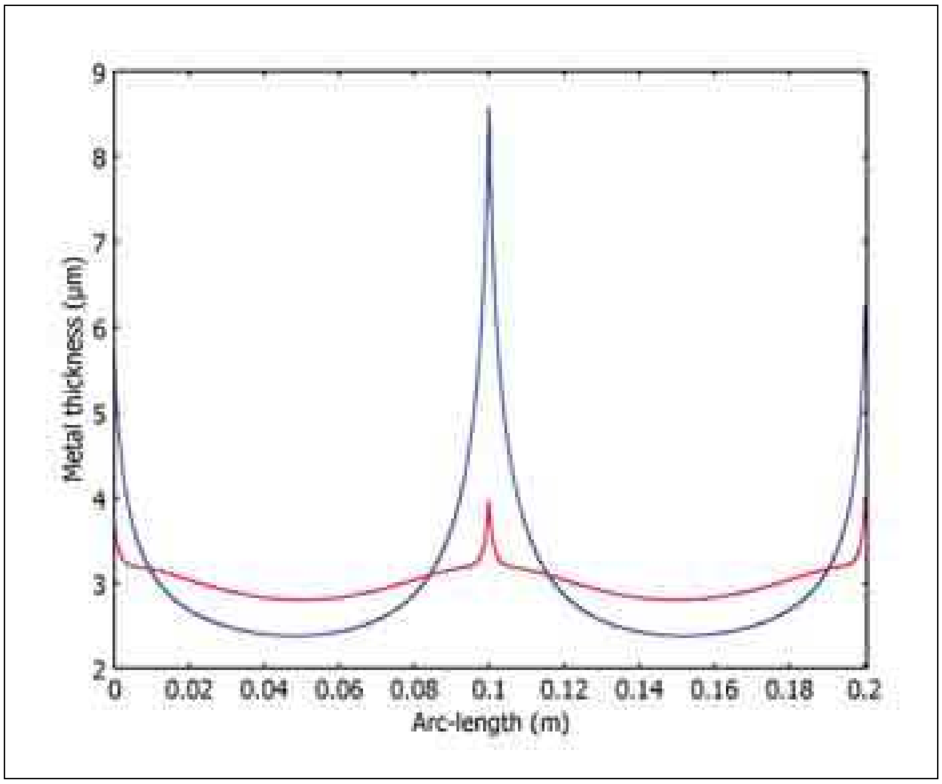


Figure 2: Comparison of plating thickness across both sides of the tape. The blue trace corresponds to metal thickness at the surface of the tape when the process does not use shields or screens. On the other hand, if edge effects are removed through the use of shields, then a far more even metal thickness distribution is achieved, as shown by the red trace.

Furthermore, the potential must be uniform throughout, so that there are no local secondary reactions such as the electrolyte electrolyzing to create hydrogen gas, leading to depleted areas of metal deposition or "tape burns." Thus, the tradeoff is to run the process as quickly as possible but where the entire surface is just below the current-limiting density. This type of modeling is particularly challenging because of the reactor size, as well as lateral and vertical oscillations due to tape movement with respect to the electrolyte injection holes. Yet, accurate predictions will have a major influence on future reactor designs.

One final aspect is that modeling is only a part of my job. Previously I had no real modeling experience, and my initial problems were not in learning COMSOL, as the software is very well designed and support is quite efficient, but rather mastering the underlying physics. Yet COMSOL allowed me to understand the physics quickly and I came to appreciate that you don't have to be a modeling expert to make good use of it. Anyone who is sufficiently curious and motivated can have great success. ■

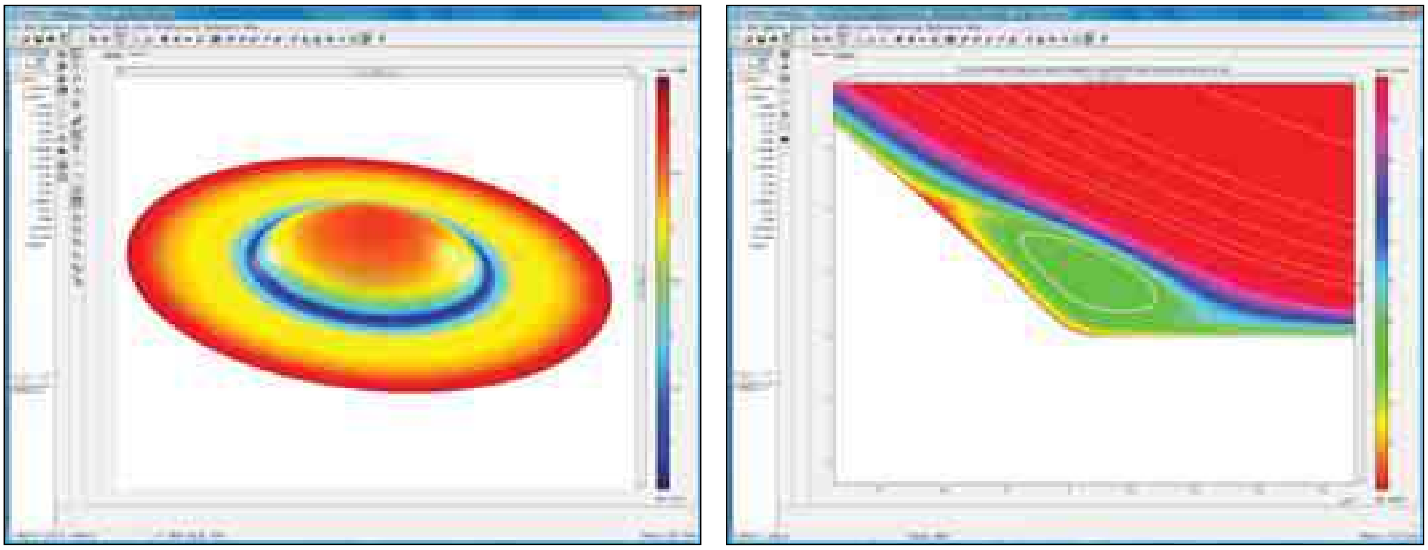


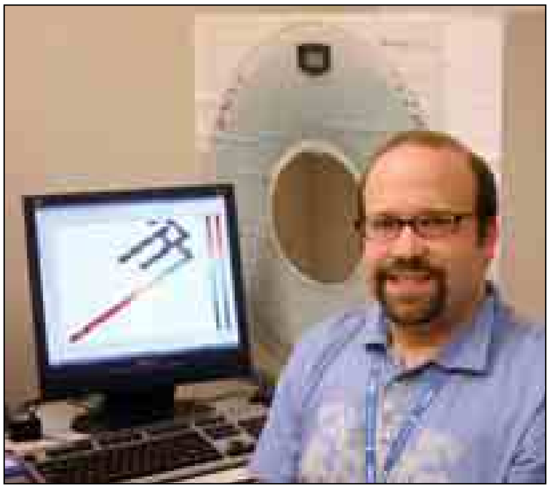
Figure 3: In order to understand the effect of geometry, fluid flow, and shield placement, a model such as this one is produced by PEM. The geometry is of a gold-plated contact for the automotive industry, which would sit on the tape moving through the electroplating unit. The first figure shows the extent of gold deposition on the contact, which is a maximum at the top of the contact, and a minimum where the contact is bent due to its rounded shape. Zooming in on the region of the bend, a 2D image indicates flow recirculation where the deposition is least, and therefore the concentration of gold ions is depleted. This is an area where secondary reactions can take place.

Faster, Safer Delivery of Therapeutic Substances

BY PAUL G. SCHREIER

Computer modeling has proven its value throughout the design, development, and deployment of new products. Such is the experience of John Kalafut, a principal research scientist in MEDRAD's Innovations Group (Indianola, Pennsylvania) who comments, "COMSOL Multiphysics has accompanied me throughout my career at MEDRAD, starting with systems engineering and today in R&D, even for products that won't be available for many years." Kalafut's experiences as a medical engineer show how multiphysics modeling is useful for solving an exceptionally wide range of problem.

MEDRAD, with sales of roughly $500 million, manufactures, sells, and services medical devices for diagnostic imaging and therapy in three main areas: cardiovascular diagnosis, magnetic resonance imaging (MRI), and computed tomography (CT). The company has 1700 employees worldwide, and physicians around the world use the company's products for more than 20 million medical procedures each year. One of the company's core competencies is intravascular fluid delivery such as supplying exact doses of medicine or contrast agents. The Innovations Group investigates novel technologies, business opportunities, and clinical applications to continue the company's >15% growth rate.



Dr John Kalafut MEDRAD's Innovations Group

Figure 1: A simplified model of the circulatory system from the point of entry for the contrast material leading to the heart. With this exploratory model, the engineers can determine which conditions give the optimal distribution.

Five engineers in the company use COMSOL software for a variety of tasks. Comments Kalafut, "COMSOL Multiphysics is a natural choice to support us during the investigation of concept feasibility, IP due diligence, and in research. This is a very powerful tool for the corporate biomedical engineer in research and development. Its true multiphysics capabilities mean that 'the sky's the limit' in terms of what we can tackle. COMSOL Multiphysics allows for the quick investigation of complex interactions — and a very affordable price."

From a modeling perspective, much of the firm's research deals with the most efficient yet safest way to deliver diagnostic fluids into a patient's body. And while fluid dynamics plays a crucial role in such studies, these models sometimes also involve heat transfer, electrostatics, chemical engineering, electromagnetics, and other physics.

Finding the best peak-enhancement curve

Speed of delivery plays an increasingly important role in improved CT scanners that allow for the acquisition of volumetric scans of the entire body in just seconds. To achieve the superb diagnostic images possible with modern CT scanners, the injection and delivery of the contrast material must be synchronized with the imaging procedure. One benefit of new CT scanners is that because the imaging takes a shorter amount of time, the total dose of contrast material can be reduced. The timing window is short, but in that time doctors want to make certain they have good insight into how the material travels throughout the body.

Fast injections alter the enhancement profile and, because the flow is transiting so quickly through the vasculature, the delivery peak is sometimes not well synchronized and the patient must be re-injected and scanned again. In addition, each patient presents a different flow profile (time-density curves), which complicates rational material-delivery schemes. The key question becomes how much contrast material must you inject to get good images of the blood vessels and the heart? At what rate? How long should the injection last?

As is the case with many systems developed at MEDRAD, here a major goal is to get the maximum amount of contrast material into the bloodstream and heart as quickly as possible. Researchers want to study the dynamic forces that arise from the insertion of a viscous fluid through a tube at rates from 0 to 6 or 7 ml/sec.

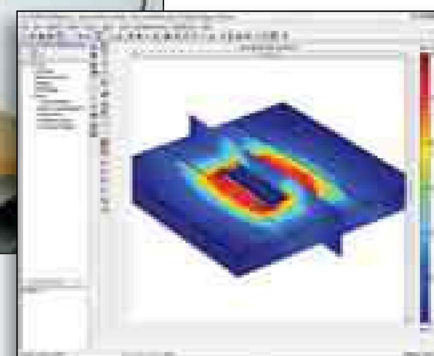
To address these questions, the company is developing smart injection systems where a doctor first performs an identification injection, and the system then determines the proper amount of contrast material. In the research and feasibility phase of this technology, a model of the human body would be preferable to benchtop in-vitro investigation or animal models. However, it would be impractical to do a full finite-element model of the entire body, so Kalafut and his team concentrated on the vessels going from the point of injection to the heart, so as to determine what happens to the drug on its way there (Figure 1).

They used COMSOL Multiphysics and the Chemical Engineering Module to better understand the early-time dynamics of the injection event. They coupled the Navier-Stokes application mode with the Convection & Diffusion application mode to gain insight into the distribution of the contrast agent through the peripheral vasculature into the heart. The early phase of the contrast's distribution in-vivo is difficult to determine non-invasively and is crucial for understanding the dynamics of contrast injection and propagation.

Knowledge gained by numerical modeling and simulation lends credence to assumptions made in global, compartmental models of the contrast material distribution after injection. One example of this model's application is in understanding the transit time from the injection site, typically a large bore angiocath needle inserted into an arm vein, to the heart. In some patients, due to possibly diseased venous systems, blocked veins, or even the position of the arm during injection, not all of the injected contrast material arrives as a well-defined bolus. Rather, the contrast material can become dispersed and arrive over a period of different times. Such a situation makes predictive control and contrast material delivery difficult, if not impossible to conduct.

The COMSOL models are playing a role in discovering which factors influence the dynamics of the contrast material. Because it is injected at rates much higher than typically encountered in healthcare (2-8 ml/s), an understanding of the processes at the injection site is also an area ripe for investigation with COMSOL Multiphysics. Figure 2 displays a 2D simulation depicting the injection of highly viscous fluid into a large bore "blood vessel." The results from this simulation are coupled with a material and physical model to better understand the relationship between injection rate and the dynamics at the needle-puncture site. This knowledge could ultimately aid clinicians when assessing the likelihood of an injection site failing (an uncommon but aggravating situation) during the administration of contrast material. This model leads to better use of the material, better scans, and better diagnosis.

(Above) Figure 3a: An MRI contrast-injection system consisting of a remote control panel that interfaces to the injection head located in the treatment room through a wireless link. A new phototransducer experienced electromagnetic interference and required shielding that was optimized using COMSOL Multiphysics.



(Below) Figure 3b: The COMSOL Multiphysics model of a phototransducer along with its shielding. The results show the E field around the final geometry. The goal was to shield the openings from an external E field greater than 20 V/m.

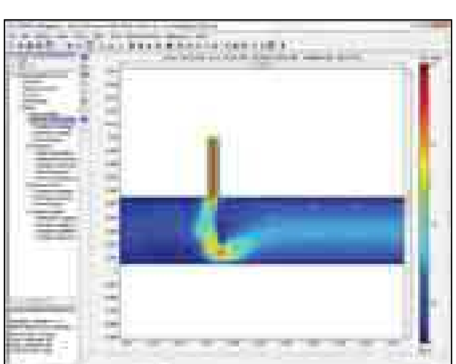


Figure 2: 2D model of a contrast material mixing with blood that allows for investigations of the dispersion of the material.

Shielding a communications link

One of the company's first serious experiences with finite-element modeling — and where they found that COMSOL Multiphysics makes modeling easy — came when fixing a problem that arose in an upgraded MRI contrast-injection system. That system uses an infrared link to communicate between the injection stand in the treatment room and the operator panel in a glassed-in control room (Figure 3a). Component obsolescence — an integrated circuit phototransducer taken out of production — required redesign of the communications link. The replacement part, however, brought with it some new problems; it was failing because it was more susceptible to electromagnetic interference from the MRI scanner and voltages inherent in the system.

The task then became one of determining how to reduce the effects of the electromagnetic fields on the phototransducer. Using COMSOL Multiphysics, Kalafut quickly replicated the problems that service engineers saw and concluded that a shielding structure around the transceiver structure would be a quick, cheap solution (Figure 3b). He explains, "we had to determine how thick the shielding should be and what shape it should have to do an adequate job, but also be as small as possible and fit in the existing equipment." Using COMSOL Multiphysics he set up a parametric solver to examine various geometries. "This approach saved us weeks of benchtop testing and technician time in building prototypes. In addition, the 3D plots we generated were quite useful in communicating the value of modeling with other engineers and with our management, who thereby first came to appreciate the value of virtual prototyping." ■

READ THE FULL ARTICLE AT:
www.comsol.com/stories

A Model of Direct Thermal Printing

Multiphysics helps researchers make full-color direct thermal printing a reality.

BY WILLIAM T. VETTERLING, ALEXEI AZAROV, BRIAN BUSCH, AND CHIEN LIU, ZINK IMAGING , MASSACHUSETTS, USA

ZINK — Zero Ink — technology prints full-color digital images without cartridges or ribbons. ZINK renders images using a single thermal print head that passes over a coated medium infused with layers of dye crystals. Using timed heat pulses and temperatures, ZINK melts these crystals to release colors that then combine to produce photographic-quality images.

The ZINK system consists of a thermal print head, the medium moving beneath the print head, and a rotating platen. The interplay between the mechanics, the thermal effects, and the chemical layers of the media structure is inherently a multiphysics problem. We used COMSOL Multiphysics to develop a model framework for direct thermal printing and applied the model to the ZINK media, demonstrating its ability to produce full-color photographic-quality images in a direct thermal printing process.

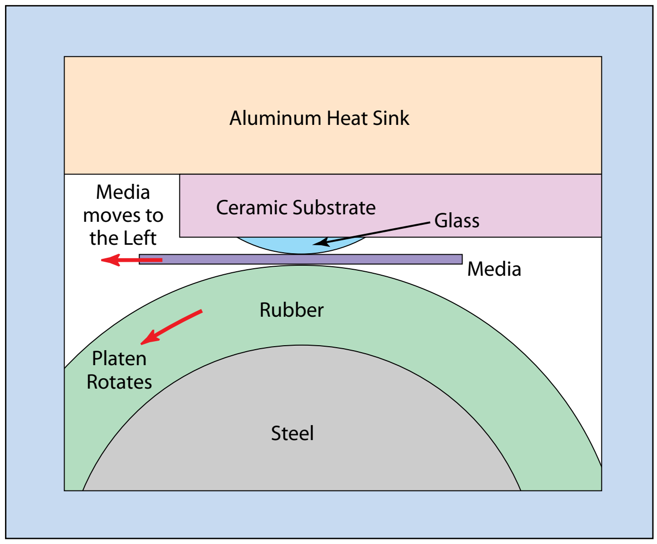


Figure 1: Model geometry showing the features of the ZINK print head.

Author Biography:

William T. Vetterling is a Research Fellow and Director of the Image Science Laboratory for ZINK Imaging, Inc., Alexei Azarov is Senior Scientist and Brian Busch and Chien Liu are Distinguished Scientists. To see a brief movie showing the COMSOL simulation of the time development of heat flows, go to: www.comsol.com/comsolnews/movie.

ZINK System Components

The ZINK print head is a linear array of heating elements, usually 300-600 per inch, sitting on an insulating glass bump that rides on a ceramic substrate attached to an aluminum heatsink (see Figure 1). The print medium is a layered structure made of three dye layers, two dye-separating layers, and a number of protective layers.

In our simulation, the medium was a single, uniform sheet with mechanical and thermal properties characteristic of the plastics used. We drew common material properties from the COMSOL Material Library and the rest from manufacturers, in-house measurements, or resources like MatWeb.

The platen is a rubber-coated roller that presses the print medium against the heating elements. Since the heaters are on a curved glass surface and the medium is flat, it is a function of the rubber to promote "wrapping" of the medium around the heaters, thus ensuring good thermal contact. The moving medium and platen carry heat away from the printing region, providing some additional cooling to the print head.

Models to Dye For

We used multiphysics modeling to model the mechanical and thermal behavior of our direct thermal printing process and to postprocess the data. The mechanical simulation investigated the compressive contact between the platen and the print medium as well as between the medium and print head. To avoid interpenetration of these components, we used the "contact pairs" feature of the Structural Mechanics Module.

Since we simulated a single heater of the print head, the mechanical constraint at the sides would be zero displacement normal to the boundaries. COMSOL enabled us to conserve memory by setting the material properties to be orthotropic with a Poisson ratio of zero in the normal direction, which had the effect of maintaining fixed walls.

Our thermal simulation subjected the structure to periodic thermal pulsing of the heater elements. One problem was the thin layer of air in the vicinity of the contact between the heating element and the medium, which can develop poor mesh quality under compression. Model set-up tools let us omit this air layer and use extrusion coupling to communicate the surrounding material surface temperatures and positions across the gap. This allowed independent evaluation of heat flow through the layer.

Another concern was that both the media and platen move and transport heat. COMSOL helped us with this by letting us apply a linear convective term with the velocity of the medium and a cylindrical convective term with the velocity of the platen. To represent the medium entering the printer at ambient temperature and leaving warmer, we set a fixed-temperature boundary condition at the entrance and a convective boundary condition at exit.

With these features in place, we ran a time-dependent thermal simulation with a pulsing heat source on the compressed geometry.

Colorful Postprocessing

Our main interest was the temperatures in a crystal dye layer a fixed distance below the heated medium's surface, so we traced a time history of the temperature at points in the layer fixed to the medium. Since we used a convective term to simulate the media motion, our results referenced points fixed in the global coordinates.

Armed with the temperature and time history of every point in the layer, we used a "media model" to determine the opacity of the dye at each point in the medium. Here, we considered a so-called "amorphochromic" dye developed for ZINK that consists of colorless crystals that become colored upon melting. Since a point in the medium heated above a crystal's melting point gets colored, applying the media model meant comparing the temperature history of each point to a threshold melting temperature.

The surface plot in Figure 2 shows the temperatures in the components following a thermal pulse and as the system cools to the heat-sink temperature as the heated media exits the printing region. It's apparent that the print medium carries away heat, cooling the center of the heater, and that the platen also carries away heat.

Post-processed data shows the maximum temperatures reached by points in a plane below the medium's heated surface (see Figure 3). If you place a layer of dye crystals at these points and heat it, you get a regular array of colored dots. If you apply pulses of higher energy, temperature peaks rise and exceed threshold temperatures over a wide area, producing larger dots, increased color density, and even a layer of solid color.

Our simulations showed us how the temperature peaks diffuse away from the heat source. A comparison of the peak temperatures at various planes of the media indicated that we could produce bichrome images by intermixing short, high-power pulses and long, low-power pulses to melt crystals at different layers and with dissimilar melting points. With this knowledge, we knew we could position three dye layers to make a full-color medium and obtain photographic-quality images with one pass of the medium under the thermal print head.

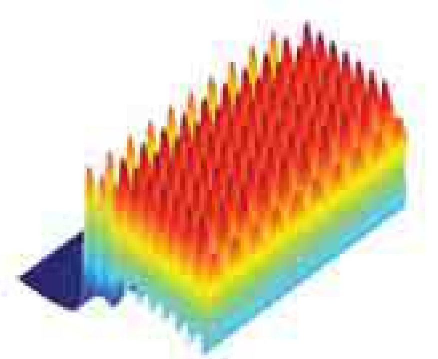


Figure 3: A surface plot showing the maximum temperatures reached at points in a 2D plane lying 3 microns below the heated surface medium after the medium was heated with 3 ms pulses, spaced by 33 ms. The temperature at the peaks is 436 K (163° C).

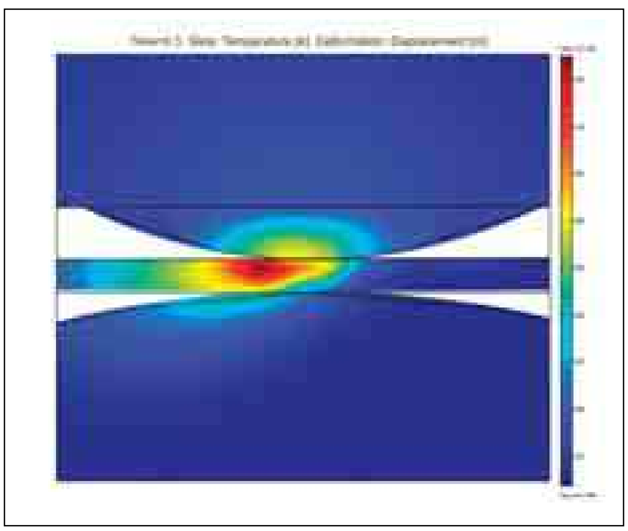


Figure 2: Temperature profile following a heat pulse. The color indicates temperature, with a scale going from 273 K to 315 K.

William Vetterling (second from right) Research Fellow and Director of the Image Science Lab at ZINK Imaging with, from left to right team members Alexei Azarov, Chien Liu, and Brian Busch. Vetterling, Busch, and Liu are among the co-inventors of the ZINK technology.

Future Considerations

As a component of our ZINK thermal printing development, we make frequent use of COMSOL Multiphysics tools. Moving from product invention to product development, and then to manufacturing, we have touched on many engineering fields — mechanical, thermal, chemical, and fluid dynamics. The combination of all these fields in a single approachable tool with a single user interface has significantly lowered the barriers to the use of modeling as a daily tool rather than a special enterprise.

In the future, we will, of course, refine our models and use optimization to find the most favorable material properties for extending our color palette. As we enter the manufacturing phase of our project, in which we work with high-speed commercial coaters and driers, the additional capabilities of the Chemical Engineering Module in fluid dynamics and process design become very attractive as possible additions to our toolset. Beyond that, our modeling will be guided by the imagination of our customers! ■

Contact Information

ZINK Imaging
www.zink.com

MatWeb
www.matweb.com

Application Brief:

Temperature Dependent Material Properties

BY JOHN SELVERIAN, JAHM SOFTWARE, INC. , MASSACHUSETTS, USA

While setting up the governing equations, geometry, and mesh consumes the most simulation time, usually little time or effort is devoted to obtaining accurate material properties. Frequently, scientists and engineers obtain material data from a handbook or web site, which often provide limited data. For example, these resources typically do not specify the test and material conditions, and a reference to the original data source is not provided. It is common to use data at room temperature in a simulation because elevated temperature data could not be found. However, the effects of temperature on a given material property can be quite large and ignoring the temperature effects can lead to erroneous and misleading simulation results.

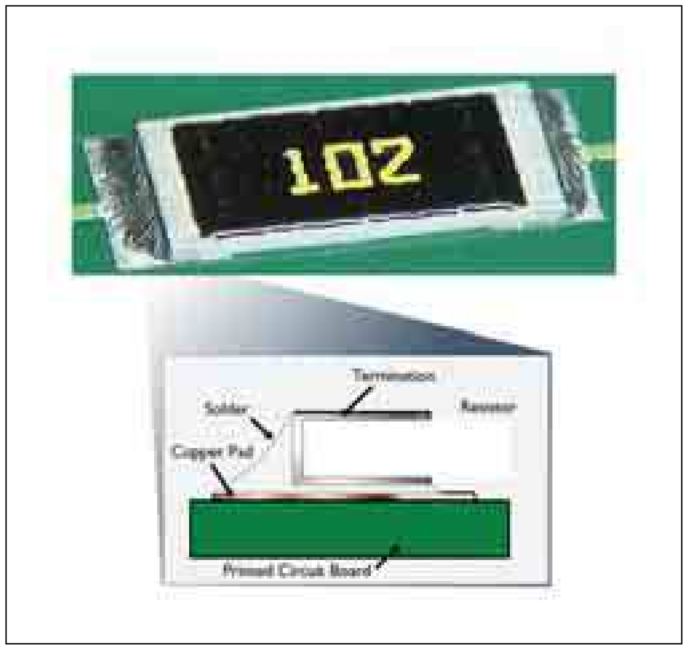


Figure 1. Depiction of the surface resistor problem. The resistor is made from aluminum oxide (Al_2O_3).

Faster model set-up using the Material Library

Finding the right material properties to use in simulations can be time-consuming and expensive. The best method is to measure the properties you need on an actual sample of the material. Often, however, this is not possible, as material tests can cost tens of thousands of dollars and take several weeks if not longer to complete.

In light of these practical limitations, users of COMSOL can now turn to the Material Library for access to 2,500 materials, all of which fully integrate into the COMSOL Multiphysics modeling and simulation environment. This new product provides a database of temperature-dependent material properties that can be added to your models at the click of a button. Even if the material is not available at the exact conditions you are using it, physical properties can be estimated from similar materials. For example, if your copper alloy does not match a material in the database exactly, you can select one that is as close as possible in composition, its heat treatment, or some other relevant aspect.

A thermal stress study

An example of a surface mounted resistor* (Figure 1) demonstrates the importance of temperature dependence and material plasticity on analysis results. Electrical current flowing through the resistor leads to energy dissipation which results in an increase in temperature. Electrical and therefore thermal cycling can lead to cracks propagating through the solder joints, resulting in premature failure. The failure is caused by the difference in thermal expansion coefficient between neighboring materials. A multiphysics simulation would consider heat transport, along with structural stresses and deforma-

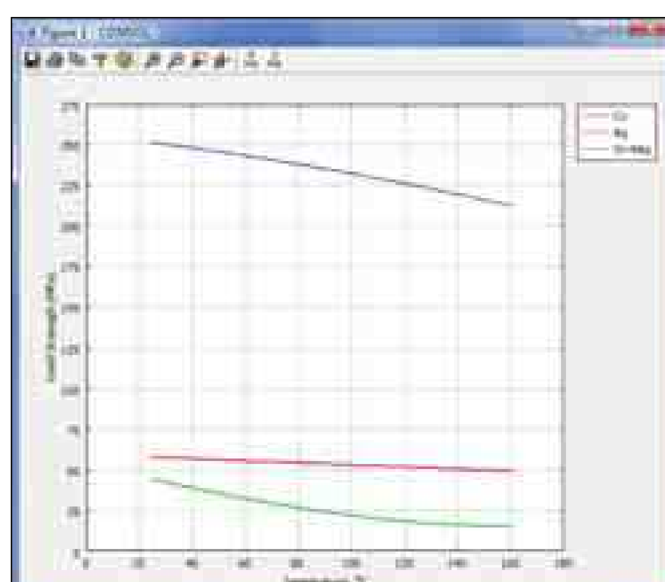


Figure 2. Temperature dependence of the yield strength of the materials.

Author Information:

John Selverian, JAHM Software, Inc., has been involved in materials science for almost thirty years. He received his B.Sc. in Metallurgy in 1983, and then his M.Sc. (1985) and Ph.D (1988) in Materials Science and Engineering from Lehigh University in Bethlehem, PA. Dr Selverian started building his Material Properties Databases (MPDB) in 1998 when he was involved in high-temperature materials research. During the subsequent years, he has produced more than 20 papers and other publications, two US patents and one European patent.

tions. In this case, the resistor body is modeled using aluminum oxide (Al_2O_3) as the material, while the termination is made from silver, the solder from the Sn-4Ag alloy, and the circuit board from FR-4. Four different simulations are performed using combinations of room temperature versus temperature-dependent material data with elastic versus elastic-plastic deformation.

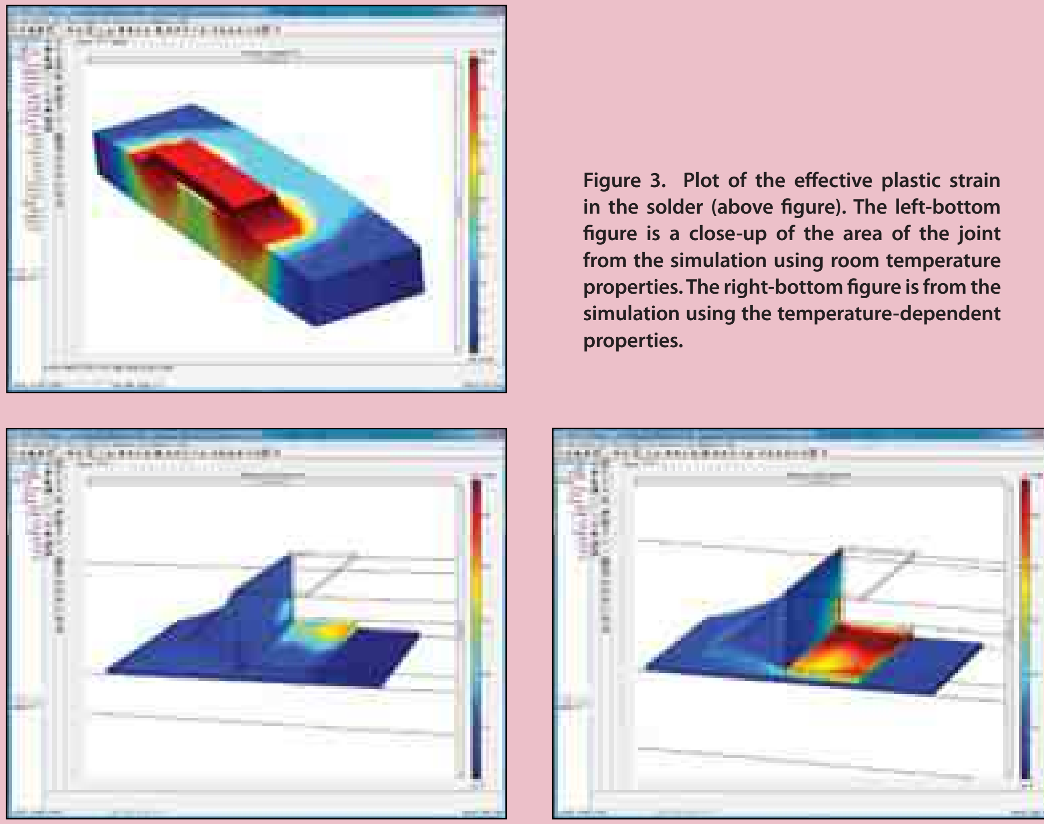


Figure 3. Plot of the effective plastic strain in the solder (above figure). The left-bottom figure is a close-up of the area of the joint from the simulation using room temperature properties. The right-bottom figure is from the simulation using the temperature-dependent properties.

The model consists of 78,000 degrees of freedom and 3,732 elements. The same mesh and boundary conditions were used for all four analyses, where only the material properties and the plasticity model were changed: plastic deformation was defined to be perfectly-plastic. Figure 2 shows the temperature dependence of the yield strength from 20°C to 160°C. The yield strength of Sn-4Ag is a factor of 2 lower at 160°C than at 20°C. This effect must be accounted for in any realistic simulation.

Three main conclusions can be drawn. First, plasticity must be included in the material model for realistic results. Second, over the temperature range of this problem, the temperature dependence of the thermal properties is not significant. The only material with substantial dependency on the thermal conductivity is Al_2O_3. However, this simulation applies a volumetric thermal load so that the thermal conductivity of Al_2O_3 does not influence the results. Third, the temperature dependence of the yield strength of the Sn-4Ag solder is very significant.

Results from the simulation show the maximum effective plastic strain in the solder increasing from 0.0194 to 0.0563, and the maximum tensile stress in the resistor decreasing from 341 MPa to 221 MPa, when the temperature dependency of the yield strength is taken into account (Table 1). Since many of the solder-reliability predictive equations use the plastic strain as a critical parameter, including temperature effects is very important when developing predictive correlations. Basing a design decision on the model performed using the room temperature data would result in a non-conservative design; i.e., the actual part would perform worse than the simulation predicts. Whenever possible, any uncertainty should lead to overdesign of the component, not underdesign.

The new Material Library database is designed to give more accurate simulation results from which better design decisions can be made. The ease at which the data can be imported into COMSOL makes the database an important tool for improved simulations with faster turnaround time. ■

Table I. Summary of the results.

SIMULATION TYPE	MAXIMUM TEMPERATURE (°C)	MAXIMUM PRINCIPAL STRESS IN RESISTOR (MPa)	MAXIMUM EFFECTIVE PLASTIC STRAIN IN SOLDER
Room temperature material data and elastic deformation	160	749	—
Room temperature material data and elastic-plastic deformation †	160	341	0.0194
Temperature dependent material data and elastic deformation	161	711	—
Temperature dependent material data and elastic-plastic deformation †	160	221	0.0563

† plastic deformation was defined to be perfectly plastic

*** THE MODEL CAN BE DOWNLOADED AT:**
www.comsol.com/industry/papers/3519/

©U.S. Air Force photo/Senior Airman James Croxon

Multiphysics Electrifies Modeling in Many Scales

The world's largest companies are typically involved in many areas of business, and their engineers find that multiphysics modeling can play an important role in many of them. These two examples from the Saab Group — one dealing with the heating of aircraft composite materials after a lightning strike, and the other addressing electromagnetic shielding around a power substation — show the wide variety of such applications and the growing importance of virtual prototyping and simulations to firms of all sizes.

BY GÖRAN ERIKSSON, THE SAAB GROUP, LINKÖPING, SWEDEN

With sales in 2007 of roughly 2.5 billion Euros, the Saab Group is a leader in many of the diverse areas it covers in its 17 business units, which are split into defense & security, systems & products, and aeronautics. Over the years, our company has taken advantage of the many paradigm shifts that have taken place in engineering analysis, one example being our ability to implement comprehensive engineering methodologies that combine traditional experiments and testing with newer tools such as computer modeling and simulation. In fact, back in the 80's, Saab became one of the pioneers in applying large-scale computer simulations, which we used early on to verify the lightning-protection components in the wings of the famous Gripen fighter aircraft.

Lightning heats aircraft composites

Several years ago, one of the Saab divisions was working with the Swedish Defense Material Administration, and engineers in that division asked my group to perform a conceptual study on what happens to airplane materials when struck by lightning. Because weight is a major consideration in aeronautic design, these wings are made of light-weight yet strong composite materials. These materials are made up of several layers of different composites, and in these layers the materials often have a different orientation to increase strength. But, because these modern composites exhibit strongly anisotropic electrical and thermal conductivities and because they have low conductivity compared to metals, when the high electric currents due to a lightning strike flow through them, they experience a high temperature rise and are vulnerable to heating damage. The heat flowing through the composite structure also has an effect on aircraft parts close to the location of the strike.

The anisotropic, layered nature of these composites demands a 3D analysis. In addition, the underlying physics are strongly coupled because the heating, and thus temperature, depends on the current distribution, which in turn is influenced by the fact that the composites' electrical conductivity is temperature dependent. Any attempt to analyze the temperature rise becomes a non-trivial multiphysics problem.

In our first attempts at modeling this effect, we tried manipulating our own in-house codes and commercial codes so they would include these multiphysics phenomena. However, this proved extremely difficult because none of the codes were built for simultaneously solving the electromagnetic and temperature fields together.

Then, in 2002, I heard about COMSOL Multiphysics and attended one of the company's seminars. Here I learned about a simulation tool whose fundamental structure was built around coupling physics and solving them together easily and intuitively. This was, at the time, almost unheard of in codes for electromagnetic simulations, which basically analyzed just the electromagnetic fields; if other physics were to be involved in the modeling application, we had to integrate their effect in an empirical or approximate fashion.

When we discovered COMSOL Multiphysics, it represented the latest paradigm shift in my field. We saw that this software was built around the physics-coupling approach, and it suddenly made the modeling of lightning strikes on an airplane very easy and affordable. In particular, modeling this effect with COM-

Author Biography:

Dr. Göran Eriksson completed his PhD at Uppsala University, Sweden, where his research concerned the study of fusion plasma physics. Eriksson continued as a researcher and senior lecturer in this field at Uppsala University until he moved to the Saab Group in Linköping, where he now specializes in simulating electromagnetic phenomena and applications.

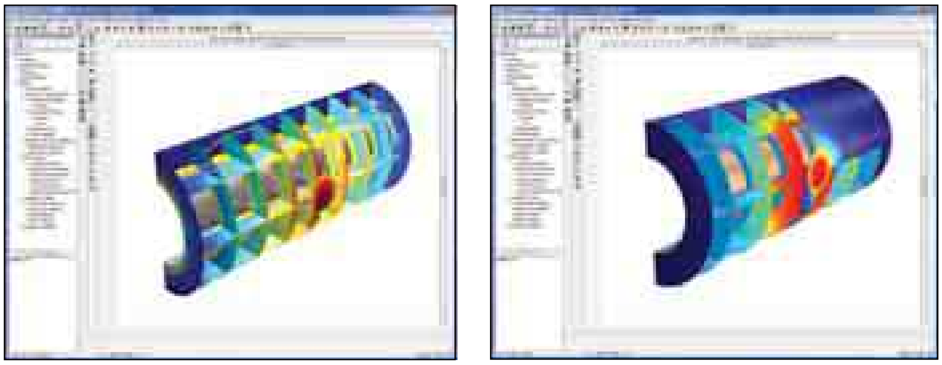


Figure 1: Model of lightning striking an airplane wing. On the left: the slice plot shows current density and the streamlines show current path. On the right: the slice plot shows the temperature, and the boundary plot shows the electric potential from the lightning strike.

SOL Multiphysics is possible thanks to the software's ability to solve virtually any set of coupled differential equations. In addition, we can easily add other physical effects such as wind cooling and black-body radiation heating that arises from the hot lightning channel, which is the 1-cm thick channel of ionized hot air (10,000-20,000°C) where the lightning discharge flows onto an airplane wing.

Figure 1 shows the results of one such simulation of the heating caused by a current pulse from lightning injected into the leading edge of a wing that consists of two layers of different anisotropic and homogeneous composite materials[1]. The current is injected across a small circular area in the front.

The figure shows the distribution of current density on a number of vertical and horizontal slices through the structure at an instant in time just after the lightning has struck. In the left image, the slice plot shows current density while streamlines indicate the current's path. In the figure on the right, the slice plot describes the temperature, and the boundary plot in the middle of the geometry shows the electric potential.

The figure on the right shows where the temperature distribution reaches the material's melting temperature, 300°C. It is evident that the outer material layer, which has the lowest electrical conductivity, is severely damaged by the temperature rise while the inner layer is not. Furthermore, it is easy to study how the extent of the damage is influenced by the degree of material anisotropies.

We validated this methodology for simulating lightning strikes against actual test results and found excellent agreement. We also learned that radiative heating from the lightning channel also plays an important role. The findings from these simulations had a major impact on construction techniques and provided useful design rules for the next generation of advanced materials for aircraft structures.

Meanwhile, we have used electromagnetic simulations to analyze a variety of other aircraft-related applications such as antenna diagrams, antenna-to-antenna couplings, radar cross-sections, interference propagation, printed circuit board designs, and test setup optimization.

As I started learning the other advantages of COMSOL Multiphysics, I began using it more and more in other simulation projects. I have found it very easy to use with a short learning curve. Any user can get right into the details of modeling immediately, particularly with the help of its Model Libraries. I also found the company's support team to be the best I have ever come across.

Tricks for handling conductive layers

Another project where COMSOL Multiphysics played a key role concerned one of our external customers, ABB. In this case we were modeling the electromagnetic effects on the casing (the electromagnetic shielding) surrounding a voltage substation. These electricity-distribution systems are used to transform voltages between different forms and levels and thus provide the link between high-voltage transmission lines and the domestic electricity supply. Substations contain many components such as switches, transformers, and reactor coils that generate electromagnetic fields. The strong fields emanating from the transformers must frequently be shielded so as to protect other equip-

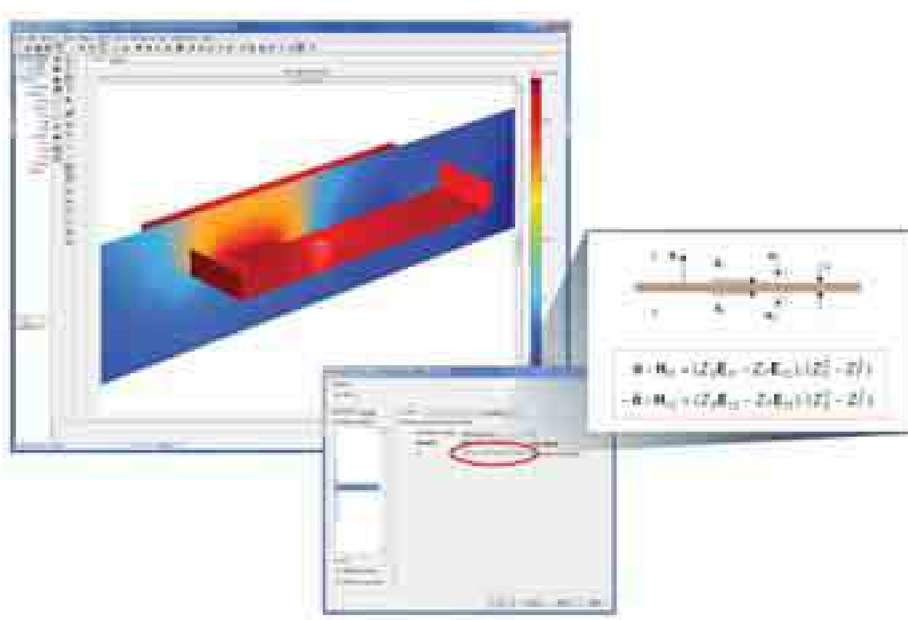


Figure 2: COMSOL Multiphysics allows users to implement an expression for a conducting layer so the software treats a 3D structure as a 2D surface but nonetheless simulates the 3D behavior. Such can be useful for simulating thin internal borders, such as possible shielding layers modifying the near-field from a cellular phone.

ment and systems in and around the substation. In this process, however, the enclosure or shield walls are subject to eddy currents, which can heat the wall material enough to lead to melting.

In this application we easily modeled the multiphysics coupling between heat and electromagnetics with COMSOL, but in this model a different problem arose. An important parameter in electromagnetic shielding is the ratio of the layer thickness, d, to the penetration (skin) depth, δ. In many situations $d \geq \delta$, particularly at higher frequencies or for very thick layers.

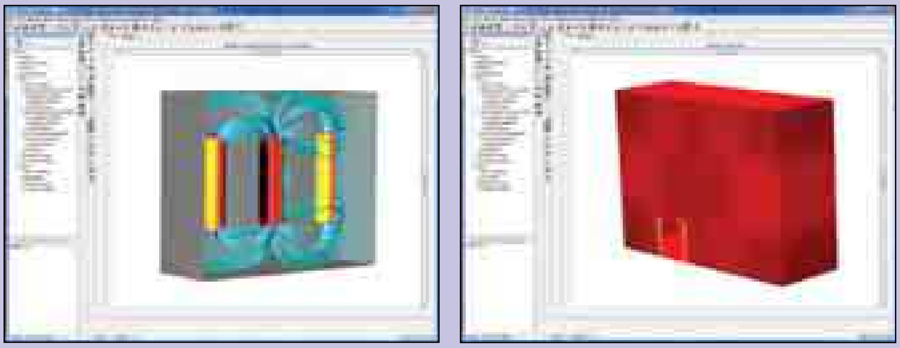


Figure 3: Model of three current-carrying coils of different phase (left) and the inductive heating in the electromagnetic shield (right).

The finite element method (FEM) is very well suited for modeling arbitrary shapes and coupled phenomena, but it often requires a very fine mesh if it is to resolve the interior of very thin structures such as a metal wall as in the case of these shields. With standard grid shapes, modeling such walls and other, thin conducting layers in three dimensions often leads to an excessive number of mesh elements. One approach to reduce the number of elements is to work with scaled or elongated objects, but in many cases this still leads to a number of elements that is difficult or slow to handle.

With the tools in COMSOL Multiphysics I found a far better solution. The software lets me implement an expression for the conducting layer, and while it treats the 3D structure as a 2D surface, it nonetheless simulates the layer's 3D behavior[2,3]. To include the influence of the layer on the electromagnetic fields in the surrounding 3D domain, I applied appropriate boundary conditions across the surface (Figure 2). Thus, while I was able to significantly reduce the amount of memory needed and the solution time by treating the wall layer as a 2D boundary, I could still simulate the substation enclosure's inductive wall heating and the shielding efficiency. These methods have been applied to simulate such cases within microwave phenomena[2] and electromagnetic compatibility[3], where an equation at the boundary replaces the need to model the thin domain. An added advantage is that this system of equations can also simulate internal borders such as shielding layers modifying the near-field in a cellular phone such as between the antenna and other components (Figure 2).

Including these equations in the description of the 2D layer or boundary condition was very intuitive; I simply typed them directly into the graphical user interface. This unique feature of the software eliminates the need for time-consuming low level code programming. The implementation and validation of this boundary-condition formulation for thin conducting layers is reported in Ref. 4.

In our specific application, we developed a model of an enclosed substation with three current-carrying coils designed to reduce reactive power, that is, to minimize the phase shift between current and voltage. In this situation, the currents induced in the wall are very strong, leading to high temperatures. In particular, current density in the regions near openings and slits can become so high that the temperature reaches the metal's melting point. The model results indeed show that the heating is greatest around the porthole at the front of the electromagnetic shield. Figure 3 (left) shows simulation results for three current-carrying coils of different phases and reveals the size and direction of the magnetic flux. The figure on the right illustrates inductive heating in the electromagnetic shield. The model uses aluminum as the shielding material, and the results confirm that heating is greatest around the porthole at the front of the electromagnetic shield. Adjustments in the design are likely necessary in order to reduce the maximum temperature.

State-of-the-future technologies

For more than four decades, Saab has provided qualified, cutting-edge expertise aimed at creating solutions for the future. Modeling has been an integral part of achieving this and has ensured that we can offer our customers solutions utilizing state-of-the-art, or even state-of-the-future, technologies at minimal risk. Finding and then mastering COMSOL Multiphysics has helped me greatly in my work for modeling the future. ■

About the Saab Group

The Saab Group provides the global market with world-leading products, services and solutions ranging from aviation aircraft and military defense to civil security and communications. With over 13,600 employees throughout the world and annual sales of EUR 2.5 billion ($US 3.7 billion), research and development corresponds to about 20% of Saab's annual sales. **www.saabgroup.se**

References

[1] Eriksson G., Proc. Intl. Conf. on Lightning and Static Electricity (ICOLSE 2005), Seattle, 2005.
[2] Horton R., et al., Electron. Lett., Vol. 7, no. 17, pp. 490-491, Aug. 1971.
[3] Sarto M.S., IEEE Trans. Electromagn. Compat., Vol. 41, no. 4, pp. 298-306, Nov. 1999.
[4] Eriksson G., Proc. 2007 IEEE Intl Symp. Electromagnetic Compatibility, Honolulu, 2007.

support@comsol.com

Linus Andersson, COMSOL Support

The Support Team is here to help you get the most out of your COMSOL products. We strive to provide speedy service, and we try to make it easy for you to find the information you need fast.

The Support Team also maintains a database of almost 1,000 demonstration models that can help you learn how to fully simulate your application. And, if your application is so unique that a ready model is not available, we can guide you through the model set up.

Speed Up Your Simulations with Parallel Processing

The more processors you use for computing, the quicker your simulations run. By allowing for multicore processing of your COMSOL Multiphysics models, you can achieve a significant speedup in 3D meshing, assembly, and solving. Here are some tips to help you better leverage your multicore platform for multiphysics modeling.

To run COMSOL Multiphysics with multicore processor support on Linux or Sun platforms, use the command:

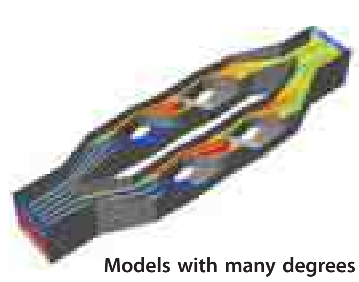
```
comsol -np n
```

where `n` is the number of processor cores you want to use.

In Windows, COMSOL Multiphysics will use all available cores by default. You can use the same command if you want to reserve some cores for a separate COMSOL session or for other tasks.

In a multicore environment, COMSOL distributes meshing between cores subdomain by subdomain. To maximize performance, use more subdomains than the physics of your model would otherwise dictate. Say, for instance, that you have a quad-core processor, and you would like to speed up the meshing process in a model with a complex geometry but nominally only one subdomain. Try splitting the geometry into four subdomains, each with similar size and complexity, and then do your meshing.

In the solution process, the degree of parallelization mostly depends on which solver you use. Generally, the solver that benefits most from multicore processing is the PARDISO direct solver. All iterative solvers and smoothers except Incomplete LU are also parallelized. ■



Models with many degrees of freedom, such as this static micromixer, benefit greatly from multicore parallel processing.

Q&A

Questions & Answers from the Support Desk

Here are a few snippets from entries in the COMSOL Knowledge Base. Visit **www.comsol.com/support/** for answers to your questions or contact the Support Desk at support@comsol.com.

Q1: I am modeling in the frequency domain. How can I define materials with losses?

A1: No matter what physics you are modeling, you can always represent losses as a complex material property with a *negative* imaginary part. For instance, in optics, setting the refractive index to `2.1-0.5*i` will give you a lossy material. Often, you will have other options as well, such as setting a flow resistivity in acoustics, a non-zero conductivity in electromagnetics, or a loss factor in structural mechanics. If, on the other hand, you want to model a material with gain, you can do that with a positive imaginary part. To learn more about how to do this, see Knowledge Base Solution 1009.

Q2: I'd like to track the interface between two immiscible fluids. I have heard of several techniques such as Volume of Fluids, Level Sets, and ALE. What is the difference between them and which one should I use?

A2: While the Volume of Fluid method uses a discrete function to trace the interface, the Level Set method represents the interface as the contour of a smooth function. Typically, the Level Set method gives the surface tension and position of the interface with far better accuracy, but it does *not* guarantee mass conservation. COMSOL Multiphysics, however, uses an enhanced version of the Level Set method that also adjusts your models to provide good mass conservation.

Model of droplet breakup created with the Level Set method.

The ALE method continuously deforms the computational mesh to adapt it to the current shape of each fluid domain. ALE can be advantageous in cases without topological changes, and it is also useful for fluid-structure interactions. See Knowledge Base Solution 1025 to read more about the differences between each of these methods.

Q3: When I increase the frequency in my induction heating model, the skin effect forces my currents toward the surface. I can't afford a mesh that is fine enough to resolve them.

A3: Use the impedance boundary condition. This means you exclude the interior of your metals from your model and treat all induced currents as surface currents. This is a good approximation whenever your metal domains are much thicker than the skin depth. Find out more in Knowledge Base Solution 1004, which provides a concise description of impedance boundary conditions.

Improving Prediction of Semiconductor Lifetimes

BY F. CACHO AND V. FIORI, STMICROELECTRONICS , CROLLES, FRANCE

We want our electronic gadgets to function properly for long periods of time, and service lifetimes are particularly critical where systems must work reliably far longer. It is thus important to know how long integrated circuits (ICs) will function properly. It's not practical to test ICs in the reality conditions and thus wait years to find out when failures start to occur naturally or through operation. Semiconductor engineers have consequently developed accelerated life-cycle tests, which place components under high current stress and temperature. This helps predict their useful lifetimes by extrapolation. Based on such experiments we have also started to develop models that predict semiconductor lifetimes.

These models don't predict when a specific device will fail, but can predict, with reasonable certainty, the rate of failure under specific conditions. And semiconductor companies are expending a great deal of effort to make these models as accurate as possible. In order to do so, process engineers need a better understanding of the underlying failure mechanisms. With the help of COMSOL Multiphysics, myself and others at the $10 billion company STMicroelectronics are studying the mechanisms that bring about one of the primary causes for IC failure, electromigration in interconnects.

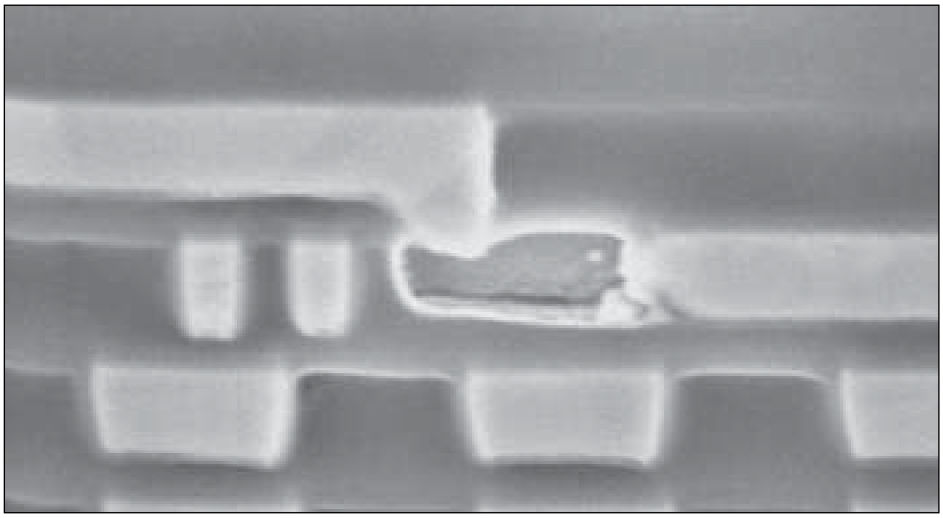


Figure 1: A scanning electron microscopy image of a copper line interconnect where a void has developed due to vacancy accumulation. This has led to a broken circuit.

A complex multiphysics problem

With the scaling down of semiconductor devices, current density in the metal interconnects joining individual transistors increases. Up to now, lifetime models have been based on empirical methods. Thus, an evaluation of potential failure modes is very important as STMicroelectronics brings new advanced CMOS technologies onto the market.

In devices fabricated with these process technologies, interconnect copper lines can be just 100nm thick and roughly the same height. The prevalent failure mode for interconnects is electromigration, which is the net transport of material caused by conducting electrons colliding with metal ions. Over time, a number of metal atoms are knocked from their original positions due to this phenomenon commonly known as an "electron wind." The subsequent vacancies or holes in the crystal structure are due to the migration of metal atoms, and over time, these can accumulate to form minute voids that lead to open circuits and device failure, see Figure 1. Vacancy flux depends on several driving forces including the gradients of the hydrostatic stress, temperature and electric potential.

Several characteristics of the metal interconnect have a strong influence on their lifespan. These include the conductor's dimensions, the material properties, the electrochemical deposition process, and the chemical mechanical planarization (CMP) process used to fabricate the interconnects.

When our reliability engineers perform accelerated life tests, they want to work with worst-case conditions. With the deeper understanding of electromigration we gain with our multiphysics model, we can be much more certain that we have actually stipulated the worst-case conditions.

Realistic simulation of the microstructure

We chose COMSOL Multiphysics because it was able to efficiently handle all

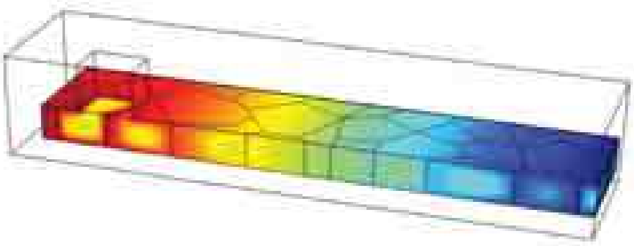


Figure 2: The extent of relative vacancy concentration through a copper interconnect line connected to the via and embedded in oxide. The higher relative vacancy occurs in the vicinity of the via, which is to be expected. Yet, areas of relative vacancy concentration are also prevalent at the boundaries between grains.

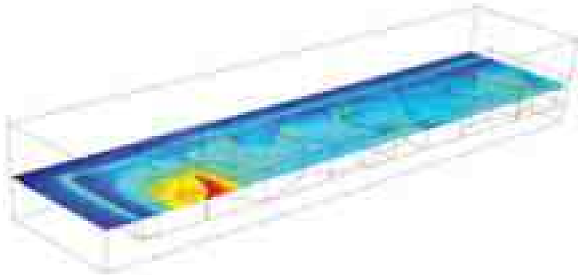


Figure 3: von Mises stresses in a slice through the copper interconnect line. Areas of greatest stress occur close to the via at the first grain boundary.

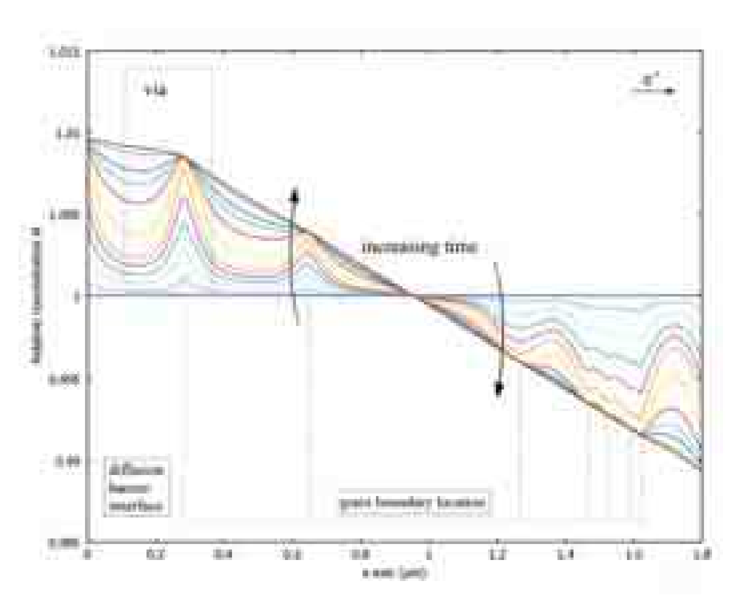


Figure 4: The evolution of relative vacancy concentration along a line through the center of the model. The peaks occur close to the via and in the vicinity of the grain boundaries.

the physical factors that influence electron migration in metallic interconnects. Our model couples the transport of vacancies with structural mechanics and thermal diffusion. We started with a 2D model that enabled us to benchmark the solution and gain confidence in the approach. However, realistic diffusion paths involve multiple metal/metal interfaces, which drove us to create a 3D model, where we studied the transient vacancy transport with realistic microstructure and kinetic paths, see Figure 2.

The model couples several physics: standard diffusion due to concentration gradients; the "electron wind" driven by a chemical potential difference; hydrostatic stress and heat-induced atomic diffusion. COMSOL Multiphysics provides a number of tools for modeling such phenomena: the ease of creating a geometry that accounts for crystal grains and interfaces between different components, such as interconnects and vias; the ease of modeling different coefficients (for both electromigration and structural mechanics); and the ease of modeling multiphysics phenomenon (coupling the diffusion equations from the DC current to the physics of structural mechanics and heat transfer), see Figure 3.

After studying the model results, we learned that, as a first approximation, the location of the void nucleation can be determined by the occurrence of a critical vacancy concentration. The model enables us to predict that maximum concentration as a function of applied current, initial stress, temperature and, above all, the line's geometry. As a result, we now have a preliminary predictive model for the lifetime of metal interconnects, see Figure 4.

These modeling results are important to our reliability teams because our accelerated tests must be very predictive and accurate. However, there are many physical effects engineers don't yet fully understand. We are currently using COMSOL Multiphysics to develop better predictive failure models so that we can save time in our qualification process and also be sure that we are indeed using worst-case scenarios. With the help of these models we also get insight into process design rules that define, for instance, the minimum size for interconnects.

The modeling team

Hired by STMicroelectronics specifically to do mechanical and thermal simulation, the two authors are part of the modeling team at the company's site in Crolles, France. They spend roughly 60% of their time simulating semiconductor aspects such as thermal effects and Joule heating, as well as nonlinear mechanical effects. ■

READ THE RESEARCH PAPER AT:
comsol.com/industry/papers/2892/

About the Authors

Florian Cacho received his Ph.D. in Material Science from l'Ecole des Mines de Paris. Since 2005, he has been a mechanical & thermal engineer in the Technology Modeling Department at STMicroelectronics in Crolles, France.

Vincent Fiori has a masters degree in Mechanical Engineering from the National Institute of Applied Science, Lyon. He joined STMicroelectronics in 2000 and currently leads projects on mechanical and thermal modeling activities. These are particularly focused on the front-end technology development of semiconductor production.

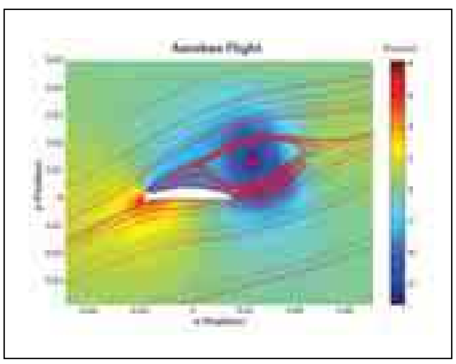
The modeling team at STMicroelectronics standing outside their facility in Crolles, France. From left: Sébastien Gallois, Romuald Roucou, Vincent Fiori and Florian Cacho.

In the Classroom:

Rensselaer Polytechnic Institute Puts COMSOL to the Test

BY CATHLEEN LAMBERTSON

As a professor in the Department of Chemical and Biological Engineering at Rensselaer Polytechnic Institute in Troy, NY, and author of the textbook, *Transport Phenomena Fundamentals*, Joel L. Plawsky has been using COMSOL Multiphysics for more than five years. "As a research tool, COMSOL has simplified our lives quite a bit. Instead



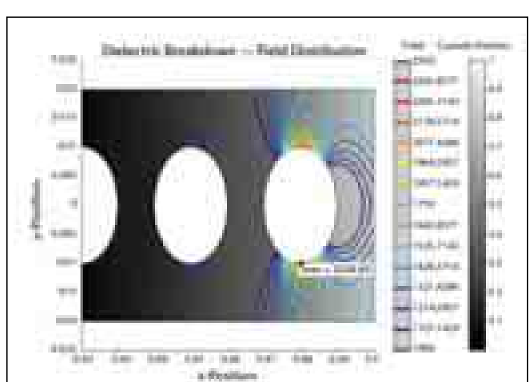
This figure shows the pressure distribution and flow streamlines about an aerobee flying ring at the point where the forward stagnation point is very near the lower tip of the aerobee. The tremendous lift generated contributes to the long distance flying ability of the ring.

of having to write code and laboriously work to visualize the solutions, we are now able to be much more efficient and productive. COMSOL enables us to spend less time solving the problem and more time understanding the underlying physical phenomena and analyzing the results," he said.

Professor Plawsky's research team recently has been investigating gate and interconnect dielectric reliability as a function of operating temperature and the electric field applied to the structure. They are interested in how metal ions injected into the dielectric affect the time required for the devices to fail. COMSOL was used to simulate a dielectric breakdown in a transistor that led his team to uncover some new physics about how that process works. Professor Plawsky added, "Using COMSOL, we've done things at Rensselaer such as simulating a whole piece of pilot scale equipment that we built to make coated aerogel superinsulation for NASA. We've also simulated temperature profiles in the active region of LEDs, the performance of wickless micro heat pipes, and the flow around an Aerobee flying ring."

According to Professor Plawsky, modeling and simulation software is an essential part of the modern-day engineer's toolkit, which is why integrating software into the curriculum at Rensselaer is a priority. He first began using COMSOL as a teaching tool for transport phenomena: "There are many finite element packages out there and many packages that do one or the other of the transport processes chemical engineers need; however, it turns out that for transport processes and especially for coupled transport processes, COMSOL is the best program available."

Currently, COMSOL is used in the undergraduate and graduate transport processes sequence as well as in the graduate math methods course at Rensselaer. "COMSOL is something that chemical engineers can jump right into and read-



This figure shows a contour plot of the electric field generated by copper ion diffusion in a porous low dielectric constant material. Failure occurs when the electric field crosses a threshold value shown by the maximum point on the figure. This point occurs very near the classical boundary separation point in flow over a cylinder.

Joel L. Plawsky is a professor in the Department of Chemical and Biological Engineering at Rensselaer Polytechnic Institute in Troy, NY, and author of the textbook, *Transport Phenomena Fundamentals*.

ily use. The equations and the jargon that the program uses are nearly identical to how we teach the discipline in our courses. So the software becomes a natural extension of what we do in the classroom and something students will want to use," said Plawsky.

As for the text used in the classroom, a second edition of Professor Plawsky's book (published by Taylor & Francis) is due out for the 2009/2010 academic year and will make extensive use of COMSOL as a teaching tool. "COMSOL gets integrated with the book from the very beginning as both examples and homework problems. Some of the introductory concepts in the book are some of the easiest things to simulate in COMSOL, so students who are unfamiliar with the program can start out working some modules early on," he said. "Using the textbook, students can get a feel for how the program works, and then as we build up in complexity in the textbook, we begin to build up in complexity with COMSOL by introducing new features and new phenomena." ■

DOWNLOAD MODELS FROM THE TEXTBOOK "TRANSPORT PHENOMENA FUNDAMENTALS" AT:

www.comsol.com/academic/resources/

Engineers Advance Skills

Associate Professor Ernesto Gutierrez-Miravete of the Department of Engineering Science at Rensselaer at Hartford explains why COMSOL is a natural fit in the continuing engineering education classroom.

Keeping your engineering skills up to date and career on track requires constant learning. When it comes to continuing education for professional engineers, perhaps no institution offers a greater degree of engineering expertise and flexibility than Rensselaer at Hartford, Connecticut, a branch campus of the technology-based education and academic research leader Rensselaer Polytechnic Institute.

Ernesto Gutierrez-Miravete (far right) finds that his many of continuing engineering education students at Rensselaer at Hartford use COMSOL Multiphysics to create models of real-world systems they work with daily. From left to right in the front row are Eric Rogers, Douglas Blake, and Gutierrez-Miravete.

Associate Professor Gutierrez-Miravete of the Department of Engineering Science uses COMSOL Multiphysics to help him teach multiphysics phenomena and the practical applications of partial differential equations (PDEs) to engineers from such high-tech heavyweights as Pratt & Whitney and United Technologies. We asked Professor Gutierrez-Miravete about the role COMSOL Multiphysics plays expanding the skills of practicing engineers.

COMSOL News: Professor Ernesto Gutierrez-Miravete, what courses do you teach?

Gutierrez-Miravete: I teach a broad variety of courses, including Advanced Engineering Mathematics, Mechanics of Solid Materials, Mathematical Modeling of Manufacturing Processes, and Stochastic Simulation.

COMSOL News: Tell us a little about your students.

Gutierrez-Miravete: Practically all our students are successful, practicing engineers. On average, they have 5-7 years of experience in the field, and many are in their late 20s or early 30s. Most are degree-seeking. In my department, most of the students are mechanical engineers, but we also get aero-astro, industrial and materials engineers, as well as some physicists. A significant number of older students also attend Rensselaer, most seeking a follow-up management degree but also some after a second engineering degree.

COMSOL News: How does COMSOL Multiphysics fit into your classroom?

Gutierrez-Miravete: COMSOL is a natural fit, as it constitutes an excellent teaching aid that uses the language analytical engineers are comfortable with. I very much appreciate the short learning curve and the ability to let students focus on the examination of results rather than on programming details.

COMSOL News: How does COMSOL Multiphysics help you teach about the relationship of multiple physics phenomena?

> "COMSOL constitutes an excellent teaching aid that uses the language analytical engineers are comfortable with."
>
> — Ernesto Gutierrez-Miravete, Rensselaer at Hartford

Gutierrez-Miravete: Many engineering problems are truly multiphysics. For instance, one examines flow in turbine airfoils, among other reasons, because of their effect on the temperature and stress in the foil; tool wear in titanium machining is due to cobalt diffusion which in turn depends on the temperature of the tool; a magnetic field produces forces in a liquid metal that drive fluid flow.

COMSOL News: How do your students react to COMSOL Multiphysics? Does it help them understand the practical application of PDEs to their work life?

Gutierrez-Miravete: Most students find COMSOL easy to learn; they also like to be able to formulate their models using the language of differential equations. Several of my students are now using COMSOL to create models of real-world systems they work with on a daily basis. ■

Rensselaer at Hartford

Rensselaer at Hartford offers an educational experience for students who need to balance their professional, academic, and personal lives. It offers graduate and specialized programs, several graduate certificates, professional development programs, and a variety of additional educational opportunities. For more information, visit Rensselaer at Hartford on the web at www.ewp.rpi.edu/hartford. Links to examples of his students' work **www.comsol.com/academic/resources/courses/**.

Rapid Developments of Sensors in Vehicle Design

BY MARTIN SÁS, CONTINENTAL CORPORATION (FORMERLY SIEMENS VDO), FRENSTAT, CZECH REPUBLIC

As a major worldwide supplier, Continental manufactures a wide range of products for all types of cars, trucks or motorcycles. At our factory, these products include sensors, switches, and printed-circuit assemblies for measuring temperatures, pressures, fluid levels and flows, and vehicle speeds, while also controlling many of the accessories in these vehicles. Our customers are in a continual, unrelenting process of upgrading their existing vehicle designs or introducing new models — and the requirements for components change just as frequently. It is only with the help of computer modeling and simulations that we can keep up with the demand for all these new designs on a timely basis.

Author Biography:

Martin Sás has been a modeling engineer at Continental (formerly Siemens VDO) since 2006. Prior to this he worked in quality, mechanical design and development in the automotive industry and was involved with high-precision testing and standards. Sás received his MSc. in Mechanical Engineering from the Slovak Technical University. Parallel to his work with Continental, he is completing his Ph.D in heat transfer and high-precision temperature measurement techniques.

Continental's factory in Frenstat, Czech Republic, has roughly 2,200 employees, with 60 working in the R&D department, of which three of us develop simulations. Before I joined the company, when it was known as Siemens VDO, the R&D department was just starting to use simulation software. Prior to that, the simulations for new products were provided by external consultants.

I came to Continental with a bit of experience from modeling and designing with finite-element analysis and CAD software. The company hired me with the charter of bringing full-scale modeling to the product-development process where we could analyze far more than just structural integrity. COMSOL Multiphysics had newly arrived at the department, and I started by applying it to model heat-transfer, structural applications and also fluid flow.

Learning more about a well-studied sensor

One of the first fluid-flow investigations I took on was the analysis of a mass airflow sensor, which is fitted to an air-intake system where air must pass through a filter and into the automobile engine. A typical sensor measures flows as high as 50 m/s. The engine computer uses data from this and other sensors to adjust the amount of fuel injected into the engine. In this case, I used COMSOL to evaluate the software's computational abilities by comparing results from the software (Figure 1) with previous experimental calculations from colleagues who develop such sensors. I was pleased to find close agreement between experimental data and simulation results, which gave me confidence in COMSOL Multiphysics.

In Figure 1, the inverted "U" tube incorporates a hot-film anemometer whose output is directly related to air flow. The model solves the turbulent flow using COMSOL Multiphysics' k-ε application mode and describes the flow that enters the chamber. The color plot indicates magnitude of the velocity while the streamlines show the velocity field.

The simulation of components such as this has become an integral part of our overall development cycle. We now use COMSOL to investigate existing designs in order to improve them, better utilize them or better implement them, and we then pass this advice on to our R&D Department. Those engineers, working in Pro/ENGINEER®, then come back to us with improved designs or sometimes even completely new designs based on our results and specifications from our customers. Sometimes they supply us with a variety of alternate designs for a given product that we then simulate,

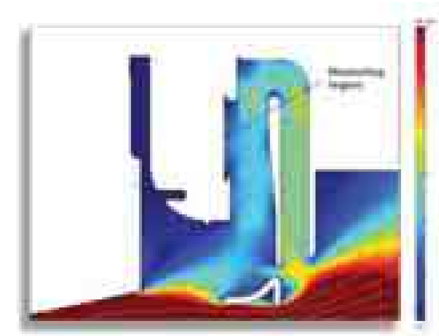


Figure 1: Model of a mass airflow sensor. The inverted "U" tube incorporates a hot-film anemometer whose output is directly related to air flow.

allowing them to select the most appropriate one for which to then build a prototype. Our Testing Department takes this prototype and evaluates the component's behavior in real-life conditions, taking measurements on a number of relevant parameters such as the mechanical and thermal loads applied in the vehicle.

This inter-team collaboration leads to better model parameters for more accurate simulations as well as better testing procedures. It is vital that we verify our models with their experimental results and that we calibrate our models with their data and procedures.

Shaving seconds from response time

Figure 2 illustrates a further example of how COMSOL has made a positive contribution to our joint efforts. It shows a 3D model of a sensor that measures the electrical resistance that changes with temperature. In order to give a fast temperature reading, though, the sensor must accurately account for the response time its transducer material needs to reach to the surrounding environment's temperature. Of course, the sensor must be accurate too.

The first step was to import the assembly geometry from Pro/ENGINEER using COMSOL's CAD Import Module. During that step, we removed some of the small geometry features that were unimportant for our analysis but that would have led to an unnecessarily large mesh. We next assigned material properties and boundary conditions to simulate the sensor's surrounding environment and operating conditions. By modeling the transient temperature distribution in this component, and especially the part that measures electrical resistance, we can then calculate the response time.

It was very simple to set up and solve this model, which revealed invaluable knowledge about the sensor's overall design and its operating parameters. Figure 2 shows a photograph and an X-ray image of the resistance-based temperature sensor. The model plot shows the temperature distribution in the sensor 70 s after the temperature has changed from 25 to 90°C.

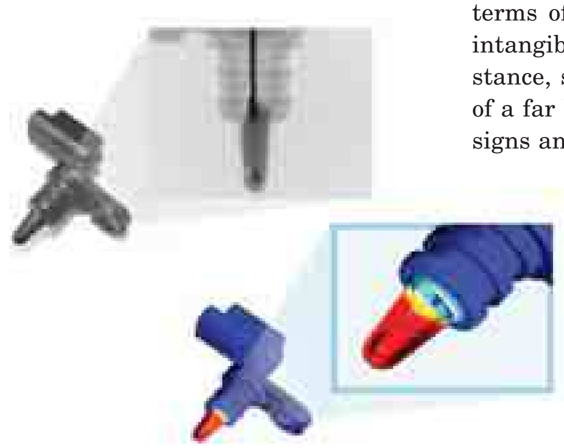


Figure 2: A photograph and X-ray picture of a temperature sensor and a model plot of temperature distribution over the whole of the sensor and on the sensing element inside the cap.

To gain confidence in our model, we ran experiments and compared the results, which were virtually the same for both experiments and the model. Figure 3 illustrates the response time for a step change in the temperature in the model (red line) and an experimental benchmarking test (blue line) based on the ISO 4113 standard.

Some benefits: priceless

As we learned through these and many other examples, the benefits of introducing COMSOL Multiphysics to the development cycle have been many and varied. While some can be quantified in terms of cost savings, others are more intangible but just as important. For instance, such "priceless" benefits consist of a far better understanding of our designs and materials along with how the operating parameters and surrounding environment affects them. Where we once received information only about components' structural properties, we now have information about feedback times, eigenfrequencies, temperature distributions, flow fields and the impact of different materials. Soon we will also investigate how cyclic thermal loads and aging degrade materials and sensor characteristics and will also research the multiphysics phenomenon of the transient interaction of temperature with flow.

The Development Department also uses our models to communicate with our customers and suppliers, leading to improvements in the specifications they provide us with. When our customers have a better understanding of the components and how each one reacts in its operating environment, then we receive even better specifications from them. Model result also increases their confidence in our products and capabilities.

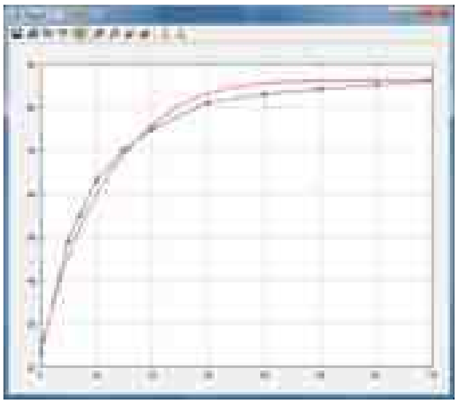


Figure 3: Comparison of modeled values (red line) and experimental values (blue line) for the response time of a temperature sensor.

Another benefit from simulating our product designs is a reduction in the number of physical prototypes. Instead of producing five to ten prototypes when testing a component, we now only produce two, and sometimes even a single prototype is sufficient. While an initial prototype made through stereolithography can cost as much as $140 for each component, the time spent testing it incurs costs far in excess of this.

The ease with which we can set up models using COMSOL Multiphysics, along with the fact that the software can simulate all the phenomena and physics we need, has opened up a whole new world of possibilities in improving our designs. Instead of modeling just one step in the development process, modeling has become an integral part in all of the steps of the development process. ■

READ THE RESEARCH PAPER AT:
www.comsol.com/industry/papers/2775/

About Continental Corporation

The Continental Corporation is one of the top five automotive suppliers worldwide, manufacturing gasoline and diesel systems, hybrid electric drives, breaking systems, power train control units, and a large variety of sensors and actuators. With its purchase of Siemens VDO in December 2007, Continental now realizes aggregate annual sales of roughly 25 billion euros with a worldwide workforce of close to 140,000.

Continental Team. From left David Kafka, Petr Beran, Martin Sás, Rostislav Slavik, and Jan Haag.

Environmentally Friendly Flameless Furnace

GIULIANO CAMMARATA AND GIUSEPPE PETRONE, UNIVERSITY OF CATANIA, ITALY

We naturally associate flames with fire, but every school child also learns about slowly occurring flameless oxidation such as when iron rusts or wood rots. Meanwhile researchers have learned that even continuous rapid oxidation need not have a visible flame, and a major benefit of furnaces based on flameless combustion is the extremely low amounts of environmentally damaging nitrogen oxides (NOx) they create. In such furnaces, incoming fuel and air must mix with exhaust gases throughout the chamber. Getting the exhaust gases to recirculate to achieve the proper mix is a key to successful operation, so researchers are using multiphysics simulations to help them design and optimize the furnace components responsible for gas recirculation.

NOx also means NOxious

The reduction of NOx has taken on great importance in an environmentally conscious world. NOx contributes to the formation of ozone, it can also cause cardiovascular and respiratory diseases and harm other parts of the body, and it contributes to global warming. Along with sulfur dioxide, it is a major cause of acid rain and can harm the soil.

NOx generation during combustion is typically due to hot spots with high temperature differentials. In a conventional furnace, combustion typically takes place in the range from 1200 to 2500 K, and the gradient between the flame nozzle and other parts of the chamber can reach 700 or 800 K. Yet, while a flameless furnace might have a temperature near 2000 K, the temperature is roughly equal throughout, so no hot spots arise and thus the production of NOx is negligible.

Although reduced NOx emissions are the primary motivation for applying flameless combustion, other benefits include a homogenous temperature distribution throughout the entire combustion chamber and thus less thermal stress on the system for higher reliability, greatly reduced noise (especially important in home furnaces), and fewer restrictions on the types of fuels, because no flame stability is required.

Operating principles

In flameless combustion, air and fuel entering the chamber are mixed with high-temperature recirculated exhaust gases that provide the activation energy needed to initiate and maintain the reaction throughout the chamber. The luminescence of a flame cannot be seen because the reaction does not take place in a specific region, although the primary region of mixing is subject to a higher rate of product formation.

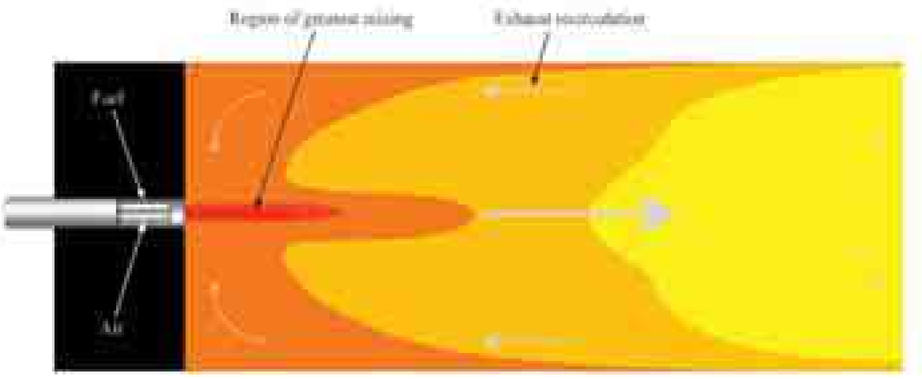


Figure 1: The operation of a flameless-combustion furnace. The recirculation of exhaust gases ensures a flameless combustion and reduces the levels of NOx.

It is important that the fuel and air are injected in such a way that they force recirculation evenly throughout the chamber. This is sometimes achieved with a swirl burner that consists of a series of guided vanes that generate a spiral motion (Figure 2). But with the gases swirling around inside the chamber, what brings them back towards the nozzle area so that they can mix properly with the incoming fuel and air? As the products pass through the swirler at high speeds, their resulting motion generates a low-pressure region inside a spiral field, here called the reverse flow zone (RFZ), that resembles the eye of a hurricane. This low-pressure zone attracts the recirculating gases towards the nozzle to aid in mixing.

Figure 2: Geometry of the axial swirler.

Simple geometry, complex aerodynamics

Even though a swirl burner might have a relatively simple geometry, the resulting aerodynamics are very complex due to the high level of turbulence. Also note that the spiraling behavior cannot be reproduced by a 2D simulation, so we created one based on fully developed 3D spiral motion.

The first step was to import the geometry of the axial swirler, which was created with SolidWorks® and saved as an IGES file; we brought this drawing into COMSOL Multiphysics with the CAD Import Module. We then divided the geometry

Author Biography:

Giuliano Cammarata is a professor of applied thermodynamics and heat transfer at the University of Catania (Italy). From 1994 to 2002 he was Director of the Institute of Technical Physics. He uses CFD tools extensively in his research fields, which include energy distributions in buildings, room acoustics, solar energy, combustion analysis and waste incineration.

Giuseppe Petrone is a researcher in the Department of Industrial and Mechanical Engineering at the University of Catania (Italy). He earned his BSc in Mechanical Engineering at that school and then his Ph.D. at the University of Marne-la-Vallee (France). His primary focus is the use of numerical methods and modeling in fluid dynamics, applied thermodynamics and heat transfer.

into two sections: one dealing with the inlet duct where the swirler is located, and the second representing the initial part of the circular combustion reactor. Then, when meshing the geometry, we used a non-structured mesh made of tetrahedral elements with finer elements close to the swirler zone so we could get more detailed results in that region.

The first step of setting up the model physics dealt with the fluid dynamics of the injection system. The aerodynamics of swirling turbulent jets combine the characteristics of rotating motion and the free turbulence phenomena encountered in jets and wake flows. For this, we used the k-ε turbulence model application mode.

Next, we implemented the oxidation reaction by defining several diffusion-transport equations where the source term drives the chemical kinetics. The maximum value of reaction rate is observed very close to the end of the inlet channels where the combustive material and fuel meet and where oxidation starts. However, the oxidizing agent is present with a high concentration along the entire volume of the cylindrical combustion chamber.

We then focused on the thermal analysis by using the general heat transfer application mode to relate a source term to the reaction enthalpy and product concentration. Because the gases are extremely hot, they become participating absorbers of radiation, an effect that COMSOL can handle through including expressions in the radiating term in the heat transfer application mode.

In order to estimate heat transfer in the participating media, we assumed that we had an optically thick medium (one through which a photon can travel only a short distance without being absorbed). With such a medium it is possible to express the radiating term as an equivalent diffusive term by introducing a value for global conductivity that takes into account both real conductive and equivalent radiating flux. For the system under study, the radiating properties of the medium satisfy the criterion of an optically thick medium very well, so we could adopt the diffusion approximation in solving the energy equation. The results showed a flat temperature field inside the cylindrical furnace, as expected.

Finally, we solved this nonlinear problem using the UMFPACK solver.

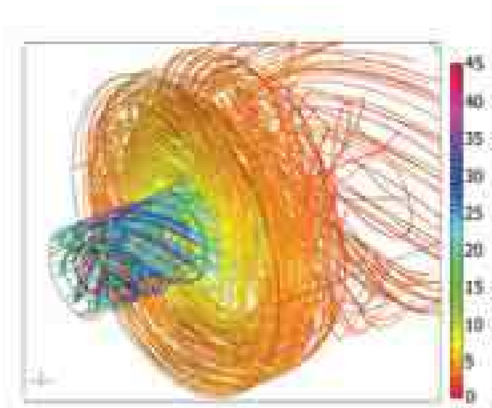


Figure 3: Spiral motion (m/s) imparted to the incoming fluid to spur recirculation.

Looking inside the furnace

With COMSOL's imaging capabilities, we were able to see how the fluid accelerates when it moves through the swirler. In addition, when the fluid enters the reactor, it expands. With velocity streamlines we observed the spiral motion imparted to the fluid by the swirler (Figure 3). As noted earlier, the pressure gradients in the spiral core region set up the reverse flow zone, which is clearly visible when you plot the axial velocity isosurfaces as in Figure 4. In that figure, note the bulb located in the central core. It corresponds to the negative values of axial velocity, which means the fluid is recirculated towards the burner outlet. The RFZ is highest close to the outlet and decreases as the fluid reaches the reactor's central zone.

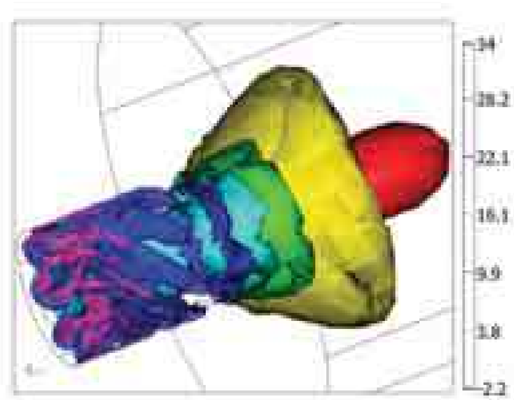


Figure 4: Plot of axial velocity. The bulb in the central core corresponds to the reverse flow zone (RFZ).

The swirler under examination here has proven sufficient for the development of the RFZ, and the recirculation effects reported by the COMSOL model reflect actual swirl-burner behavior. This thermal distribution is in good agreement with experimental data, thereby proving the reliability and effectiveness of the modeling approach. The model is also in good agreement with the literature in terms of both the fluid-dynamic and thermal results. Recall that the main mechanism responsible for the formation of NOx is related to a high temperature gradient during combustion. Because the model shows a temperature field inside the reactor as being almost isothermal, it is safe to assume that NOx formation is significantly hindered.

With this model verified, we can now expand our work to simulate other operating conditions. For example, we plan to perform virtual experiments with other fluids or other inlet velocities without having to conduct expensive experiments. We can also study how the combustion reaction can influence the velocity and pressure fields. ■

READ THE RESEARCH PAPER AT:
comsol.com/industry/papers/1168/

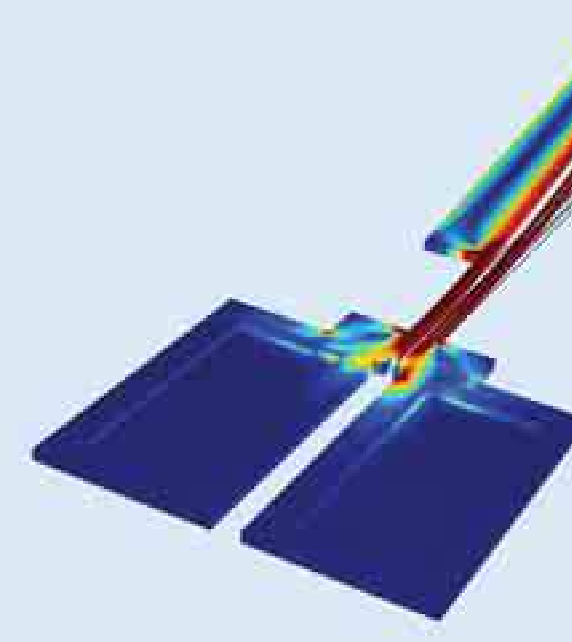
Benchmarking COMSOL Multiphysics

BY ED FONTES, COMSOL

COMSOL continues to push the curve in delivering the utmost performance and accuracy in solving multiphysics problems. The most recent release, version 3.4, brought support for multicore computers and introduced fast segregated solvers. Users praise the boost in simulation speed, and a new benchmark study by Dr. Darrell W. Pepper of the University of Nevada, Las Vegas, and Dr. Xiuling Wang of Purdue University-Calumet seems to indicate that users have good reasons for their praise.

The report, *Benchmarking COMSOL Multiphysics 3.4*, summarizes the results of Dr. Pepper and Dr. Wang's recently concluded benchmark project in which they compared COMSOL Multiphysics 3.4 to five leading, widely deployed physics applications. "The purpose of this benchmarking project," write Dr. Wang and Dr. Pepper, "was to solve four 3D standard benchmark problems using COMSOL Multiphysics 3.4 as well as other well-known commercial packages in the related areas and to compare performances in the CPU time and memory consumption required to reach a given accuracy in the modeling results."

Dr. Pepper and Dr. Wang determined the selection of the benchmark problems and conducted the benchmark tests at the Nevada Center for Advanced Computational Methods. The four benchmark tests simulated fluid-structure interaction (FSI), fully coupled electronic current conduction with thermal and structural analysis, electromagnetic wave propagation, and the magnetic fields around and inside a rotating electric generator.



A MEMS actuator is one out of four benchmark problems studied in the report Benchmarking COMSOL Multiphysics 3.4 by Dr. Wang and Dr. Pepper. Download the full report at **femcodes.nscee.edu.**

The 46-page *Benchmarking COMSOL Multiphysics 3.4* provides complete descriptions of all benchmark problem definitions as well as the testing criteria, environment, and individual test methodologies. Scientific literature and experimental data are well annotated and compared with simulation results whenever possible. Simulation results include extensive comparison tables as well as a rich complement of full-color charts and screens shots for each benchmark test.

To download a free copy of *Benchmarking COMSOL Multiphysics 3.4* by Dr. Darrell W. Pepper and Dr. Xiuling Wang, go to **femcodes.nscee.edu** ■

COLLABORATION

rbMIT ©MIT Software for COMSOL

The software rbMIT(*) is a package for rapid and reliable prediction of engineering outputs associated with parameterized partial differential equations. The software is particularly well suited to the many query and real-time contexts.

At present, the software treats parameterized (scalar and vector) elliptic and parabolic linear coercive partial differential equations in planar and axisymmetric two-dimensional geometries. Parameters can be introduced to describe the domain geometry, the coefficients of the PDE, the sources, the boundary conditions, and the initial conditions. Applications include steady and unsteady heat transfer and convection-diffusion, and linear elasticity for isotropic and orthotropic media.

COMSOL Multiphysics users can invoke the COMSOL platform — adaptive mesh generation, finite element discretization, and matrix assembly/solution capabilities — to generate the necessary rbMIT offline database. Once the offline database is created, the user can apply the rbMIT online codes: for any given parameter value, the online evaluator provides the desired output and rigorous output error bound (relative to the finite element model) very rapidly. Online visualization is also possible.

The rbMIT Software and associated documentation for elliptic and parabolic problems can be downloaded at **augustine.mit.edu**. A collection of model problems is also provided to illustrate various capabilities of the software and to allow "learning by example".

(*) ©Technology Licensing Office of M.I.T., Case 12600.

Dr. Kipp earned his Ph.D. in Inorganic Chemistry in 1988 at Northwestern University where he studied aluminum oxides. Since 1996, Dr. Kipp has been with MatWeb, where he is responsible for collecting, categorizing, and transferring engineering raw materials data.

GUEST EDITORIAL

Materials Selection in the Information Age

We are now in the so-called "Information Age" in which increased computing power, storage, and networking speed/availability have transformed the way industry operates. Changes in how scientists, engineers, and designers use the materials selection processes exemplify this transformation.

A short time ago, the material selection tool of choice was a dog-eared handbook, or sales literature, or simply human experience. Engineers desiring multiple criteria for searching, sorting, and comparing materials would have been fortunate if they had access to any digital database at all, even a costly one with a limited set of materials and clunky search algorithms.

> Improved IT has created benefits beyond the materials selection process through integration into the management and transfer of materials data.

Then, in the span of a few years, Internet access rose from negligible to nearly universal. Simultaneously, engineers, scientists, and designers gained online access to powerful and content-rich materials resources. Tech-savvy professionals then began demanding that the manufacturers and distributors they patronized provide real-time access to online tech data and robust selection tools. Manufacturers responded with web sites containing technical property databases as sales aides and tech support facilitators.

The technical community also demanded and received online reference sources unconnected to any specific raw material vendor. Today, these reference sources cover the informational spectrum from broad to narrow, deep to shallow, and free to subscription-based. Excellent free databases with impressive depth of information have been assembled by professional societies as well as by trade groups promoting their products, such as the Global Powder Metallurgy Database.

More useful for the selection of new materials during product design are comprehensive databases, such as MatWeb. MatWeb, which offers comprehensive information across all categories of structural materials and is free for most capabilities, disseminates some 40,000 data sheets daily to its 23,000 users. Fee-based data resources, such as Granta's library of reference data, are also available for those needing greater depth than they can get from the free resources.

Global design and manufacturing is another trend driving demand for tech data on specific material grades from a growing number of manufacturers. It is not unusual today for a part to be designed in the USA and manufactured in China using plastic from a German raw material producer. In such an international environment, it is vital that product data for the *exact* raw material be readily available through all phases of the production process because "generic" material information is insufficient. Fortunately, the companies maintaining material databases have kept up with the explosive growth of unique material grades manufactured and used worldwide.

Beyond Materials Selection

Improved IT has created benefits beyond the materials selection process through integration into the management and transfer of materials data. A prime example is the capability for users to transfer data seamlessly from MatWeb's 65,000 data sheets into their COMSOL Multiphysics simulation. This feature saves users time (therefore money) and eliminates errors introduced during transcription or unit conversion, while making the exact material grade available to the model. Through their web sites, proactive raw materials producers such as Quadrant EPP also make seamless data transfer into COMSOL Multiphysics possible.

OEMs collect vast amounts of raw materials data during the course of their manufacturing processes, much of which is proprietary information. Data derived from testing unique material grades, developmental materials, and specific lots is obviously not available from third-party data resources. Yet, the ability to dynamically aggregate, protect, search, and integrate real-time materials data is vital in the fast-paced manufacturing marketplace. ■