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COMSOL NEWS

THE MULTIPHYSICS SIMULATION MAGAZINE

Commercializing Fusion Power

General Fusion reaches project milestone with multiphysics simulation

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COMSOL

Pharmaceutical and lab equipment supplier reduces prototyping with simulation-driven R&D

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Developing Cutting-Edge Technology for the Evolving World

As the world evolves, the products, tools, and workflows that shape the society we live in need to keep pace. Technological advancements that once seemed distant are now commonplace, such as listening to music on a speaker that also serves as a personal assistant or driving a car with autonomous capabilities. To stay ahead of the ever-changing landscape of technology and competitive markets, organizations globally continue to find ways to innovate faster, smarter, and at a lower cost.

We see nine great examples of such innovation in this year's edition of *COMSOL News*. On page 16, there is a story of how IAV developed a novel twin-battery design concept that opens up new possibilities for car manufacturers and battery designers. Another story focuses on how NASA used thermal modeling and experimental testing to develop next-generation carbon dioxide removal technology for astronauts living and working on the International Space Station. In the feature article, we cover General Fusion's use of simulation to design a large-scale fusion demonstration machine, which achieved first plasma in February 2025 and is now forming plasmas regularly.

Companies are serious about integrating simulation software into their core R&D process. For example, Sartorius, a life sciences company featured on page 13, built a brand new department dedicated to CAE. Staying ahead of ever-evolving technological demands calls for big ideas, ingenuity, and a willingness to push the limits. Modeling and simulation makes it easier to go from concept to reality.

Rachel Keatley
COMSOL, Inc.

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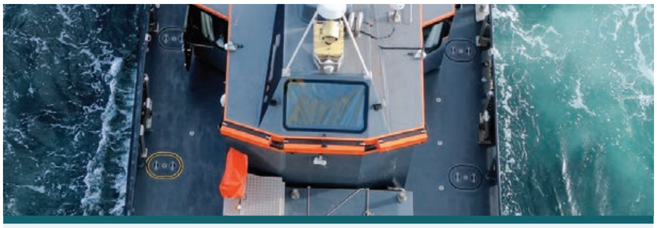

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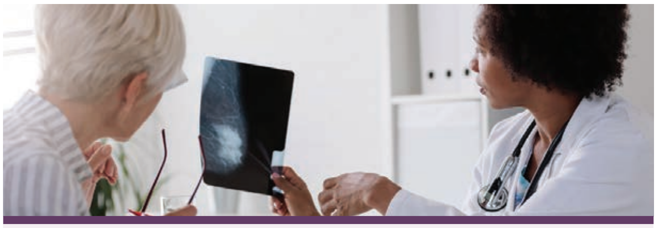


RESEARCH SPOTLIGHT

COMSOL, Massachusetts, USA

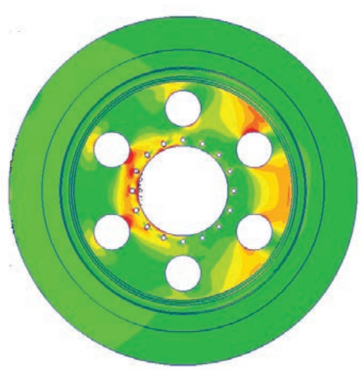
9 USES OF Modeling and Simulation Across Industries

by MACKENZIE MCCARTY

There are countless examples out there of organizations using multiphysics modeling and simulation apps to bring new innovations to life and optimize existing designs to make them more sustainable, cost effective, or simply better in some way. Read on to see nine industry examples that were presented at the COMSOL Conference.

Mine Hoists

The drum hoisting systems that ABB provides to mining companies around the world are composed of many parts, including a motor, control system, and drum system. Each one must meet efficiency, safety, and reliability requirements. To deliver on their promise, ABB engineers built a mechanical digital twin of its hoist systems to simulate stress distribution so they can identify potential areas of concern and optimize designs to avoid rope failure.



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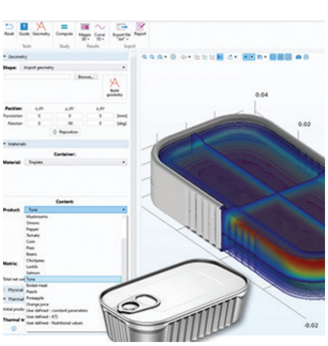

Food Safety

BE CAE & Test built a standalone simulation app for food engineers sterilizing canned food to predict bacteria reduction following a heat treatment, the efficiency of the process, and the heat distribution inside the can during the sterilization cycle. The app makes it easy for anyone to select the can shape, type of food product, and thermal treatment and visualize the results.

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Power Electronics Test Devices

In power electronics, components such as microelectronic chips are subjected to extreme temperature changes, which can cause degradation over time. KAI built a simulation app that can be used to upload the layout of a test device and quickly perform thermal simulations in the moment without direct assistance from the simulation specialist.

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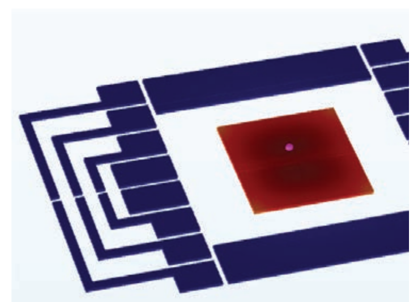

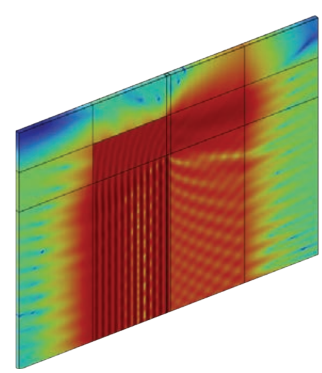

Traffic Noise Barrier

Phononic Vibes SRL and the University of Coimbra used numerical modeling to study the performance of ventilated acoustic noise barriers with the goal of mitigating traffic noise pollution. The teams modeled a unit cell design to compute sound transmission loss and analyze acoustic band-gap frequencies. This helped them design a barrier with effective sound reduction without compromising ventilation.

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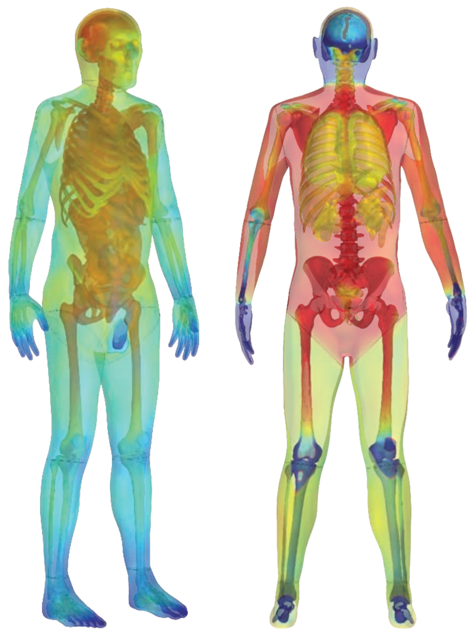

Frostbite Predictions

Existing guidelines for frostbite predictions were found to be overly simplistic. For more complete analyses of human thermoregulation, the United States Army Research Institute of Environmental Medicine used anatomically correct geometric representations that included layers of skin, fat, muscle, bones, and organs. The team was then able to more accurately predict frostbite onset based on skin site, protective clothing, sex, and exercise.

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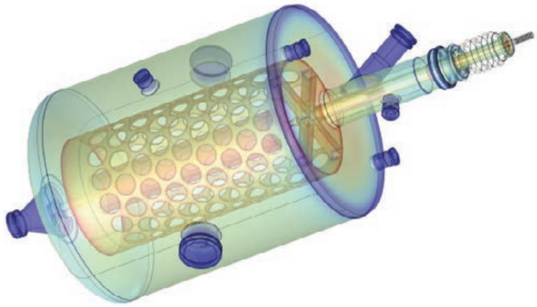

Energy Storage

The EU Horizon project HYSTORE is developing four different thermal energy storage system solutions. For this project, Inova Lab developed an innovative heating methodology that uses RF heating for thermochemical materials instead of the conventional microwave heating. The team used simulation to understand the system's power density distribution in order to optimize the performance of the electrodes.

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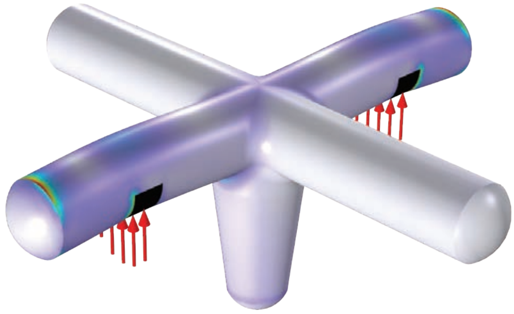

Cold Spray Additive Manufacturing

The cold spray process deposits multimaterial metal powder at high velocities, which enhances the fatigue performance of stainless steels. Triton Systems used modeling to predict the fatigue life of certain stainless steels with and without the multimaterial cold spray coating, significantly saving time and money compared to physical testing.

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Lightweight Flight Recorder

Serma Ingénierie developed a lightweight flight recorder that is compatible with light helicopters and complies with shock, crush, and fire standards. To ensure their design would pass the fire test, the team combined heat transfer modeling with experimental testing. Simulating flame exposure helped them find the optimal ratio for the internal material dimensions and efficiently test the system's ability to withstand fire. After that, the team used shape optimization to design a compact housing for the equipment.

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Electric Vehicle Batteries

Veryst Engineering used multiphysics simulation to overcome the design challenges that are common in EV battery development as well as to gain insight into battery life. The team used simulation to test conditions for the lifetime performance, thermal management, and structural durability of a lithium-ion prismatic battery pack. This process cut down on testing time and helped the team determine an optimal thermal management strategy.

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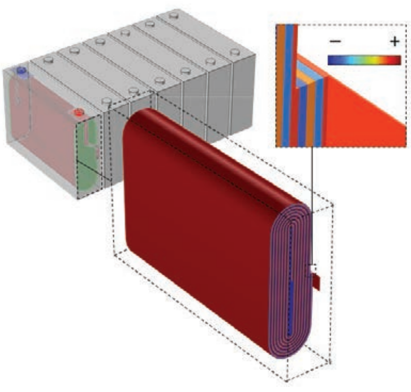

General Fusion, British Columbia, Canada

COMPRESSING THE TIMELINE TO A FUSION FUTURE

General Fusion worked with Veryst Engineering to simulate and better understand the Magnetized Target Fusion that occurs in a proof-of-concept fusion machine.

by **JOSEPH CAREW**

Magnetized Target Fusion (MTF) power plants have the potential to produce significant amounts of energy with comparatively inexpensive technology and without releasing carbon emissions. In a General Fusion MTF machine, hydrogen plasma (such as deuterium–tritium, or D-T) is injected into a liquid metal vessel formed inside the fusion machine. From there, an array of pistons compress and reshape the liquid metal vessel around the plasma, increasing the density and temperature of the plasma to fusion conditions — making fusion happen! It is a pulsed approach that repeats once per second in a commercial plant. The liquid metal wall of the vessel captures the energy of the neutrons, converts it to heat, and then carries it to a heat exchanger to create steam and ultimately produce electricity.

The engineers at General Fusion are using MTF to bring fusion power to the commercial power grid. This journey has reached a major milestone with the construction of Lawson Machine 26 (LM26), General Fusion's large-scale fusion demonstration machine. Through the use of multiphysics simulation, General Fusion has successfully designed and optimized LM26 and made a major step toward the team's fusion-powered vision for the future.

FIGURE 1 The team at General Fusion assembling LM26.

» LM26 RELIES ON ELECTROMAGNETIC COMPRESSION OF A LITHIUM LINER TO REACH FUSION CONDITIONS

In late 2024, LM26 (Figure 1) was built to derisk General Fusion's eventual large-scale

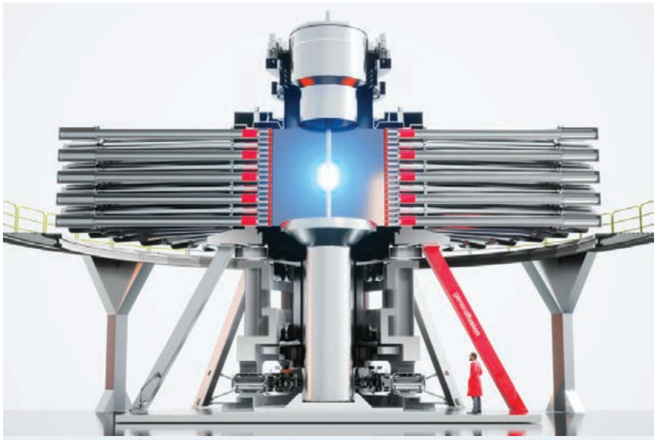

FIGURE 2 A rendering of General Fusion's commercial MTF machine design.

commercial MTF machine. The team's project goals for LM26 are to achieve 1 keV, then 10 keV, and finally, to achieve scientific breakeven equivalent.

LM26 is designed to inject a spherical tokamak plasma into the chamber and compress it using a solid lithium liner to reach fusion-relevant plasma temperatures. During the compression, a toroidal magnetic field is generated by an axial current flowing in the hourglass structure that keeps the plasma confined and stable. This process creates the plasma temperatures and densities that lead to the fusion of plasma ions and the release of energy in the form of neutrons.

In General Fusion's MTF power plant concept (Figure 2), pistons trigger the compression process instead of magnetic coils like in LM26. Pistons are unique to General Fusion's approach, as other fusion methods rely on superconducting coils, lasers, or other expensive equipment.

"For MTF, the larger the initial plasma volume, the more time it can stay hot, which gives us more time to compress the plasma to fusion conditions," said Jean-Sebastien Dick, an engineering analysis manager at General Fusion. "At General Fusion, we have been iterating on the process and developing a power plant operating point that is not only commercially viable but also very competitive against the other type of energies on the market."

» MODELING MAGNETOMECHANICAL COMPRESSION OF A SOLID LITHIUM LINER

LM26 is targeting the key temperature thresholds of 1 keV, 10 keV, and scientific breakeven equivalent by compression of a solid lithium liner. With the COMSOL Multiphysics® software, the team was able to model and measure the internal effects to predict the performance of the LM26 design (Figure 3).

"When I joined General Fusion, looking at the type of challenges we were facing, I thought that COMSOL Multiphysics would be a great tool to add to our list of software," Dick said. "This is what got us to interact with Veryst Engineering, who are well-known experts in the field of multiphysics. They know COMSOL very well."

Calibrating a Lithium Material Model with Help From Veryst Engineering

General Fusion's partnership with Veryst Engineering, a COMSOL Certified Consultant and engineering consulting company that specializes in highly nonlinear simulation and material modeling, was essential in the development of LM26. Sean Teller, a principal engineer at Veryst, worked alongside Dick to develop material models that enabled the team to accurately simulate the response of the lithium liner. This information was critical for accurate, predictive modeling of the LM26 liner trajectories, which enabled General Fusion to create and assemble LM26.

As Teller explained, "We used COMSOL Multiphysics simulation with integrated experimental plans and validation to enable the team at General Fusion to quickly iterate on designs of LM26. The predictive models are critical for

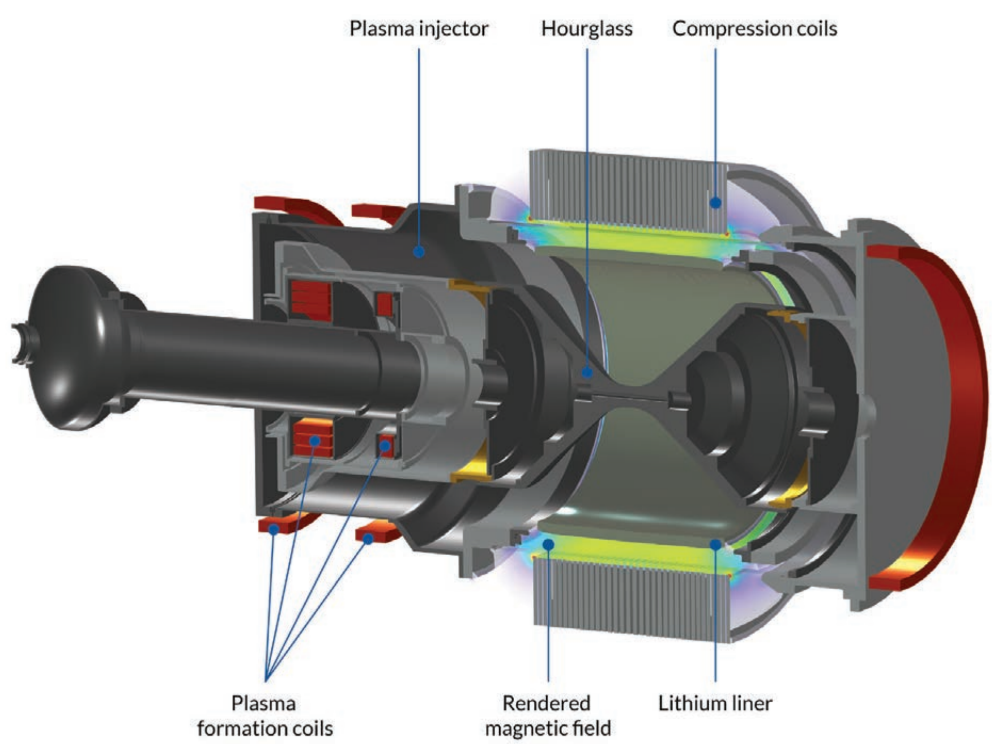

FIGURE 3 The LM26 geometry.

FIGURE 4 This experimental setup features a tensile test of the lithium (center, black with silver dots) between two black ceramic heaters.

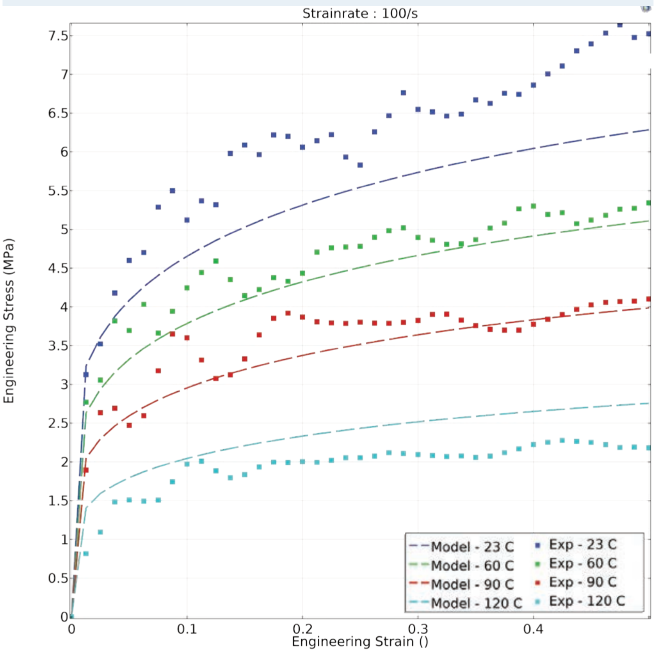

FIGURE 5 The plot shows the experimental data (square data points) as compared to the material model prediction (dashes).

achieving fusion conditions on the road to that viable and abundant clean fusion power."

"One of these experimental tensile tests included measuring the material response of solid lithium. Using a high-speed camera and impact load cells, Veryst and General Fusion heated the lithium with a pair of ceramic heaters and pulled the sample to failure in order to measure the stress versus strain response (Figure 4). The results of these experiments were then used to calibrate a Johnson–Cook model (Figure 5).

"The full model is quite complex," Teller said. "It utilizes a moving mesh for the lithium and the compressed plasma, nonlinear solid mechanics and the Johnson–Cook material model, and EM forces from modeled circuits drive the compression of the lithium. The lithium liner impacts the hourglass device, so capturing the nonlinear contact is crucial to perform accurate predictions." To add to the complexity, heat transfer occurs between all of these model components.

Different LM26 designs were able to be weighed simultaneously and in the same space in the COMSOL® software. Veryst and General Fusion used a time-dependent, fully coupled solver and automatic remeshing to capture the large deformation and pressures inside LM26.

"All of this required tight integration between the physical tests and the finite element models to gain fundamental insights into this compressor design," Teller said.

During the validation campaign of the models, which led to the development of LM26, General Fusion compressed 40 lithium liners using electromagnetic compression to validate the COMSOL model. The team conducted physical experiments using a small-scale prototype of the compression system (Figure 6).

To measure the deformation of the liners, General Fusion developed a structured light reconstruction (SLR) technique. This involved the use of sheets of laser light to extract the velocity at multiple points in the liner. General Fusion also used photon Doppler velocimetry to measure the velocity of the center point of the lithium liner. This combination enabled General Fusion to recreate the deformation observed in the physical experiments and compare that to the simulation results for validation. They then used that rate- and temperature-dependent material model (Figure 5) in subsequent simulations of the plasma compressor and found good agreement between the test data and the data acquired through previous tests.

"The performance of the compressor would not have been possible without the insights gained from the early simulations and the multiphysics model, in particular, that helped drive this design," Teller said. "These validations increase confidence in future modeling efforts to further drive the devices to achieve the Lawson criterion and clean power."

Working with Compressor Impedance

One of the key components of LM26 is its electromagnetic compressor. This portion of the machine is responsible for the rapid compression of the magnetized plasma. A successful electromagnetic compressor design must be able to match its impedance with the compression time of the machine. When the impedance and compression follow the same time scale, that enables an "efficient compression", which is when the electrical energy is converted into kinetic energy. An "efficient compression" converts a significant fraction of the initial stored electrical energy into kinetic energy.

Modeling and simulation enabled General Fusion to adjust the impedance of the power supply, see how design alterations would impact the performance, and maximize the compression efficiency.

In order to tune the impedance, Dick used the software to make adjustments to the number of turns in the compressor's coils, altered the initial distance between the liner and the coils (known as the "air gap"), and altered how the liner was compressed over its trajectory. Additionally, the liner shape along the compression needs

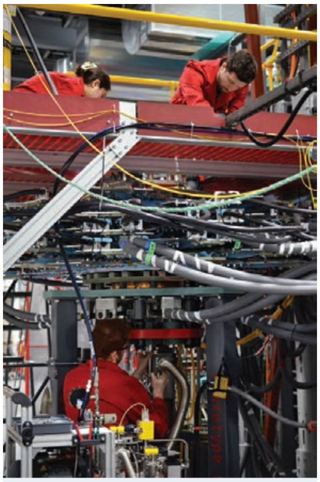

FIGURE 6 Prototype 0, the small-scale version of LM26's compression system.

to be controlled in order to ensure that the plasma stays stable, requiring iteration to the liner thickness and the axial spacing between the coils. Dick solved the model after making different design adjustments and compared the results to see if the machine could achieve a stable plasma compression.

"We have done multiple material characterization campaigns to make sure that this liner behaves as expected under the high strain rates and the high plastic strains we are experiencing in these compressors," Dick said.

Validating the Models

As with the experimental setups for the validation of the material characteristics, General Fusion performed internal validations to ensure that the advection of the magnetic field by the liner correctly matched the analytical predictions.

"We have done a separate test with each of these coils to tune their resistance and inductance in their circuits and make sure that they match as close as possible with what we measured with flux loops in our experiments," Dick said.

Dick relied on a 2D axisymmetric simulation (Figure 7) of the machine's operation in order to decrease the solving time.

» GAINING DATA POINTS WITH SIMULATION

"The framework of COMSOL has allowed us to incrementally build in complexity and build confidence in our design intentions and avoid having to reiterate the design phases," Dick said. "We have not had to change any major parts of these experiments. They were always behaving as intended."

The team at General Fusion is also able to run its simulations in a much shorter time frame. This is thanks to the team's use of the *Cluster Sweep* node in COMSOL Multiphysics, which makes it possible to create one large cluster job that spans a number of nodes. The more nodes that have been added directly relates to the amount of parameter values that are computed in parallel. General Fusion used this to tackle multiple parameters in a quicker fashion.

"In the past, running these simulations would have taken multiple weeks or even months, but now we are doing this in less than 24 hours," Dick said. "We are able to get hundreds of simulations done in that time span on our cluster."

The team was able to use the data from the simulation to develop a safe operating space for the machines with confidence.

» THE FUTURE OF SIMULATION AND FUSION POWER

Simulation enabled the General Fusion team to incrementally add in complexity as they developed their LM26 design, and combining real-life experimentation with multiphysics simulation was critical in the development of the proof-of-concept model. Multiphysics simulation and fusion research will continue to be inextricably linked as the team pushes fusion power to new heights.

LM26 achieved first plasma in February 2025 and is now forming plasmas regularly as General Fusion's team optimizes performance in preparation for its next step — compressing plasmas to create fusion and heating from compression.

"We are no longer just looking at aerodynamics or fluid dynamics or structural dynamics one sector at a time; we are putting everything together," Dick said. "I really like the way COMSOL is approaching the world of simulation. I like the canonical, incremental approach where you can build in complexity by assembling the physics like pieces of a puzzle. I believe that this is the way the future will go for simulation, because new innovations are very complex and require a lot of different physics to be involved together." ◎

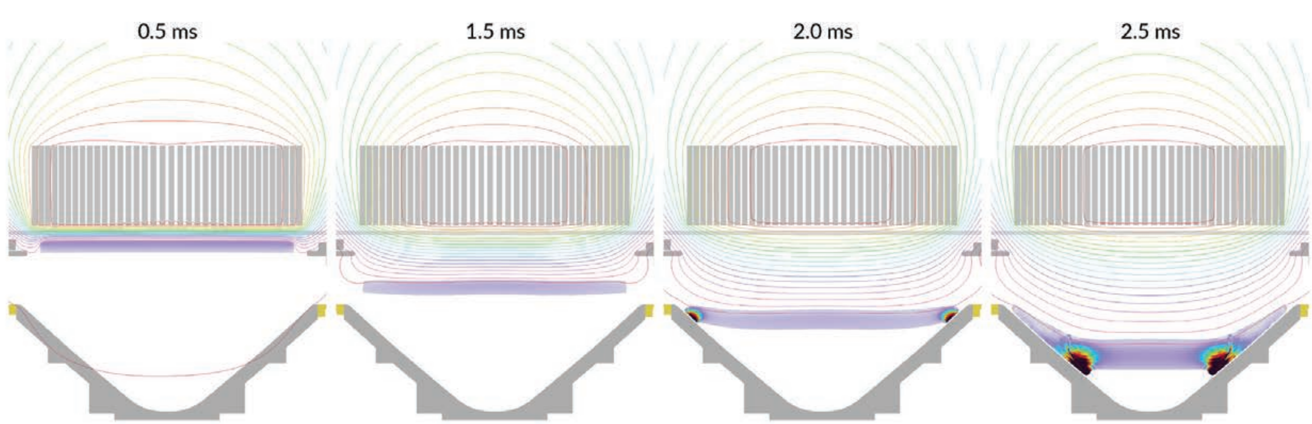

FIGURE 7 A 2D axisymmetric model of the machine, showing the hydrostatic pressure contours in the lithium and poloidal magnetic flux contours in all bodies. The central conducting cones are seen on the bottom, and the coils connected to the power supply are the gray bodies on top.

Baker Hughes, Texas, USA

MEETING QUALITY STANDARDS IN OIL AND GAS EXTRACTION WITH ULTRASONIC TRANSDUCERS

Baker Hughes saves 30% on prototyping costs by using 3D ultrasonic simulations to study acoustic wave propagation, capture experimental responses, and optimize their transducers used for testing extracted oil and gas.

by **MACKENZIE MCCARTY**

Before oil and gas can be used for heating homes, fueling cars, and generating electricity, they go through extensive refining, transporting, extracting, and testing processes. Baker Hughes focuses on the first step, also known as the upstream step, of this process, specifically using cement bond logging technology to assess gas quality. The company uses multiphysics simulation software to design and improve their ultrasonic transducers used during pulse-echo and pitch-catch testing, two commonly used methods for testing extracted oil and gas.

» EXPLORING OIL AND GAS EXTRACTION

When a hole is drilled into a well to extract gas in the upstream process, the well must be reinforced to control the flow of fluid within it. Cement bonding evaluation is an important procedure in this process. After drilling a borehole, cement is injected between the casing and the formation to prevent fluid communication between producing zones in the borehole. As Haiqi Wen, a lead scientist at Baker Hughes, explained, the cement sheath creates a hydraulic seal that prevents fluid communication and blocks the escape of fluid to the surface.

The two often used ultrasonic tools that are run on wireline into the well to gather accurate estimates of well integrity and fluid zone isolation are called cement-bonding logs (CBL) and variable-density logs (VDL). The results of the CBL are in the form of one waveform that can be used to determine the bonding quality between the casing and the cement based on the waveform's amplitude and decay coefficient. The VDL is "more like a visual representation of all the waveforms, and you can have more information for the bonding quality between the formation and the cement," said Wen.

Testing oil and gas at the point of extraction ensures that the product meets quality standards before continuing through the rest of the process. It identifies impurities that could affect the value or usability, and helps optimize production by analyzing composition and production rates, Wen explained. The testing also gathers data that allows operators to understand reservoir conditions, identify any safety concerns, and guide future improvements.

Piezoelectric transducers are used in the upstream, or testing, part of the process. Wen and his team used the COMSOL Multiphysics® software to model their piezoelectric transducers (Figure 1). Through the software's built-in multiphysics capabilities, they coupled fluid to the piezoelectric transducers, elastic waves to pressure acoustics, and an external electrical circuit to the terminal of the piezoelectric element. This allowed them to accurately examine how multiple physics interact and model the transformation of voltage signals to elastic waves, as well as fluid–structure interaction at the transducer's boundary with customized circuit parameters.

"I put absorbing layers at the boundary to absorb incoming waves," said Wen, before adding that "the boundary also performs frequency filtering and scanning functions. Only one eighth of the model is simulated to save time and energy, but by applying

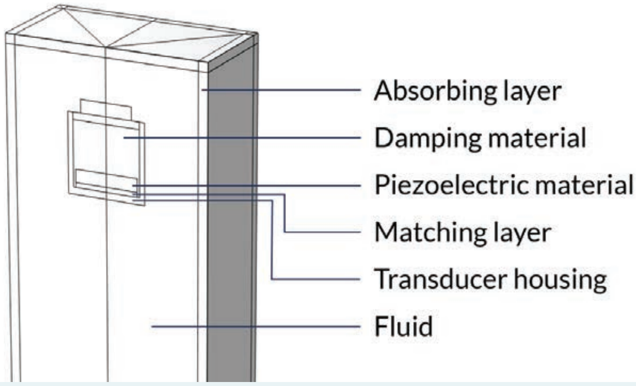

FIGURE 1 The piezoelectric transducer model geometry.

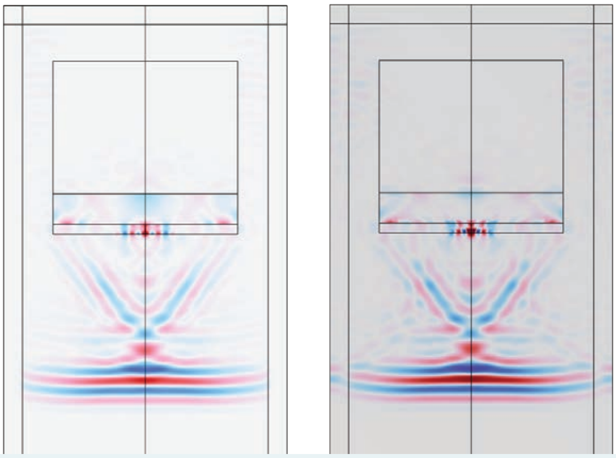

FIGURE 2 A short pulse signal is sent through the simple 2D axisymmetric model (left) and the 3D model (right), indicating that the wave propagation is nearly identical in the two models.

mirrored datasets, we can obtain the full model response and data."

A key component of transducer design is the thickness of the piezoelectric transducer compared to the wavelength and matching layer. In this design, the transducer thickness is set as half of the wavelength, while the matching layer thickness is set as one quarter of the wavelength.

Wen explored two different methods, form assembly versus form union, while building the transducer dimensions and mesh settings. Form assembly creates a discontinuous mesh at the interface, while form union creates a continuous mesh. "I think form union is usually a little bit more robust, but then you dump much finer elements at the interface so that might make your simulation just slightly slower in some cases," said Wen.

» REDUCING PROTOTYPING COSTS WITH SIMULATION

Wen built a simplified, axisymmetric 2D transducer model as well as a full 3D model (Figure 2) and validated both models against experimental testing. The simulation sends out a brief pulse signal that strikes the cement surface of the well. When the bonding

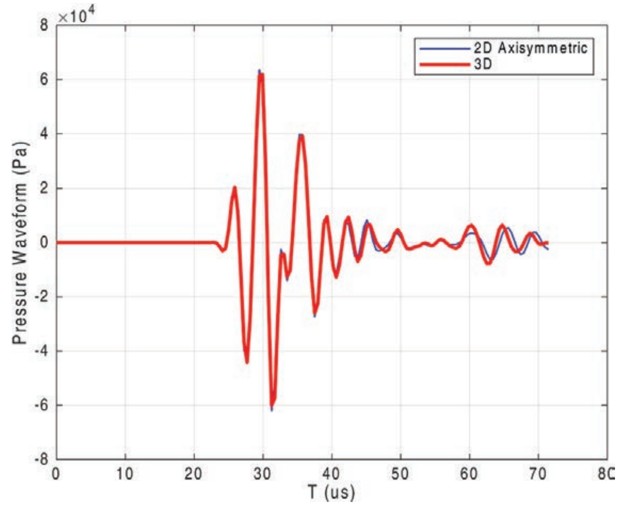

FIGURE 3 There is good agreement between the pressure probe responses of the 2D and 3D models.

quality is good, the receiver will not show many strong signals because the materials are all securely bonded without any voids or cracks between them. In this scenario, the signal passes through the surface. Conversely, if the bonding quality is poor, the receiver shows a reflected signal due to the signal hitting cracks or voids.

"In this work, I compared the wave propagation and the pressure response. As you can see, the wave propagation looks almost identical," said Wen. He went on to share that if the model is axisymmetric, they can use the 2D model for faster simulation results, otherwise they have to use the 3D model.

The 3D model results are obtained by evaluating the pressure response at the yz-cut plane, where x = 0 (shown at right in Figure 2). "For this pressure probe response, the 2D model is almost overlapping with the 3D model," said Wen. He compared the results using LiveLink™ *for* MATLAB®, an interfacing product that connects the COMSOL Multiphysics software with the MATLAB® software (Figure 3).

The COMSOL simulation results and measurement data align well at the near field, as shown in via LiveLink™ *for* MATLAB® (Figure 4). The results indicate that the maximum pressure is located on the axis, with the transducer's center frequency in this data being 280 kHz amplitude. However, as Wen pointed out, "there are some discrepancies we are trying to resolve." One example of this is the presence of side lobes in the measurement data, which were not present in the simulation results. Another inconsistency is the local cancellations observed in the simulation results, whereas the measurement data shows a continuous decay.

"I think the issue may be related to the modeling of the piezoelectric material because in the real application it is actually a composite material. However, in our current study, we are treating it as a homogeneous material," Wen said. "We are still trying to improve this."

"Overall, simulations have been saving us about 30% on prototyping costs," said Wen. "In the past, when we needed to order new transducers, we would usually order a batch of

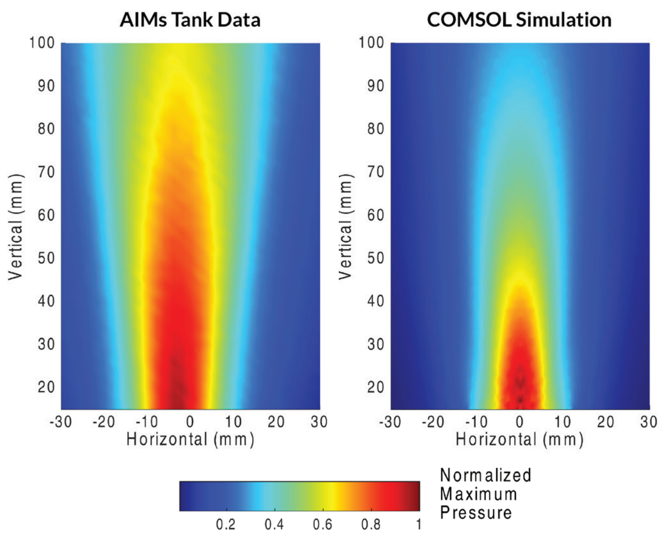

FIGURE 4 The peak pressure in the measurement data (left) and COMSOL simulation results (right) show good agreement at the near field.

different transducers with different specs. But now that we have been using simulation software like COMSOL®, we just need to verify that there are a few good designs in the batch. Then, we just need to order those designs instead of ordering all of the new transducer designs and testing which one performs the best," said Wen.

» PULSE-ECHO AND PITCH-CATCH TESTING

Furthering their work, Wen and his team used COMSOL Multiphysics to simulate and optimize pulse-echo and pitch-catch testing. Their pulse-echo simulation highlights an ultrasonic nondestructive testing (NDT) technique that sends out ultrasonic pulse waves to identify defects in materials or analyze the reflective waveforms for information. Wen and his team sent out waves that were reflected by a metal casing, with the transducer acting as both a transmitter and receiver. The waveform data can be analyzed after being measured by a point probe.

Wen uses the Hilbert transform to extract the waveform envelope. Then, "you can take the FFT [fast Fourier transform] off of it to get one of the frequency peaks, and that peak is actually corresponding to the internal reflection within the casing. When you send the signal, there is the first reflection, but there is actually internal reflection," Wen explained. The casing measurements can then be calculated based on the frequency.

> "Overall, simulations have been saving us about 30% on prototyping costs."
>
> — HAIQI WEN, A LEAD SCIENTIST AT BAKER HUGHES

The Hilbert transform can also be used to extract the envelope of the wavelength in pitch-catch testing, which would allow you to track the amplitude of the peaks. The peaks in this study are represented by the blue and red dots at specific points in Figure 5. Wen plotted the wave amplitude as a function of the transducer spacing, which then allows the exponential curve to fit (note that this is not shown in Figure 5). He compared the different results between the free pipe water and foam cement to understand the material properties within the domain.

"The challenge is that you can see the peak of fairly low amplitude. In real applications, it is going to be very challenging because you will naturally suffer from poor signal-to-noise ratio, especially if you go to higher frequencies," said Wen. He explains that it will be harder to capture meaningful signals when the acoustic waves are being sent and received very quickly.

Simulating the two testing methods in COMSOL Multiphysics allows for increased efficiency in gathering data from the ultrasonic pulse waves, and modeling the transducer conserves resources while optimizing the design. Simulation helps Wen and his team explore how the wave propagates through different materials and determine what causes the final waveform to look the way it does. "That's really something that simulation can provide where we can't get information out of the test experiments," Wen explained. Ultimately, this helps Baker Hughes improve efficiency and accuracy in the upstream step of the oil and gas production process. ◎

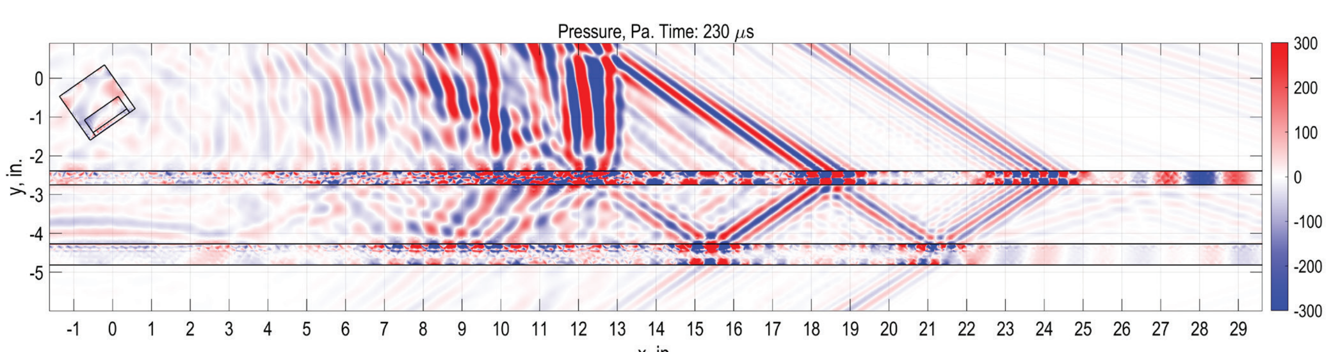

FIGURE 5 Pitch-catch simulation of pressure waves in free pipe water and foam cement, where the two horizontal bands represent casings. Note the peaks at (18.5, -2.5); (21, -4.5); (23.5, -2.5); and (28, -2.5).

Sartorius, Germany

LIFE SCIENCES COMPANY ACCELERATES BIOPHARMACEUTICAL R&D WITH A DEDICATED CAE DEPARTMENT

Sartorius leans on its Computer-Aided Engineering department to optimize devices that enable the creation of biopharmaceuticals.

by JOSEPH CAREW

Biopharmaceuticals can be effective treatments for illnesses such as cancer, multiple sclerosis, and rheumatism. These novel drug products are highly complex, and their production requires bioreactors, biotechnological processes, and a significant investment in time and resources. The Computer-Aided Engineering (CAE) department at Sartorius, an international pharmaceutical and laboratory equipment supplier, found that using the COMSOL Multiphysics® software helped them overcome common production challenges by speeding up development, reducing prototypes, supporting innovation, and optimizing testing.

» MAKING THE ONE IN TEN THOUSAND: MANUFACTURING A SUCCESSFUL BIOPHARMACEUTICAL

A biopharmaceutical is any pharmaceutical drug product that has been manufactured in, extracted from, or synthesized from biological sources. Unlike chemical-based drugs, biopharmaceuticals can be customized to target specific cells and include vaccines, somatic cells, tissues, and whole blood among other examples. A recent, notable biopharmaceutical success story is the COVID-19 vaccine. While biopharmaceuticals can boast strong capabilities, the development process is not without challenges.

"Only one of ten thousand new drug candidates reach the market," explained Dr. Friedrich Maier, a senior scientist of CAE simulation at Sartorius. "One drug is above a 2-billion-euro investment in development costs, not to mention the significant time investment as well." (Figure 1)

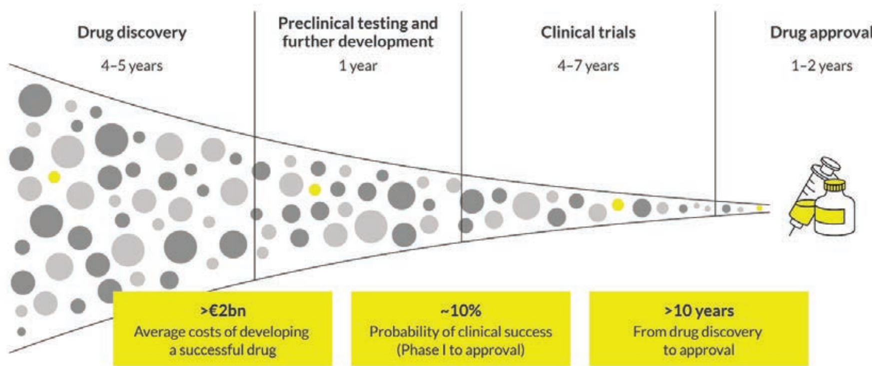

FIGURE 1 Out of all the drug candidates, only one in ten thousand make it to market after a long and costly development process.

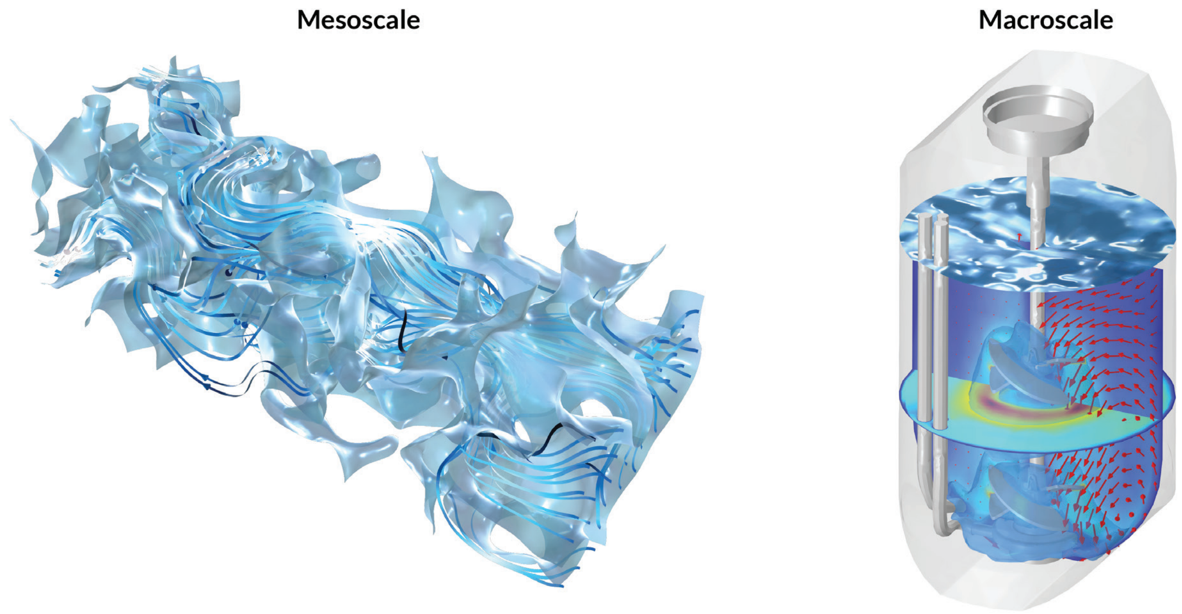

FIGURE 2 Models at the mesoscale visualize flow through smaller components (left), while macroscale models make it possible to assess device performance (right).

Biopharmaceuticals are expensive to develop largely because of their complex molecular structure, the specialized manufacturing processes they require, as well as the regulatory requirements on the industry. Physical experiments, in particular, are expensive investments. Modeling and simulation eases this burden and reduces the reliance on those experiments, but it can be a challenge to get the models right. That is because the biological processes that need to be replicated are complex, have high fluctuations, and are not easy to replicate. Sartorius supports their biopharma and life science customers by meticulously integrating the biological processes into their devices, aiming to minimize error propagation and maximize product yield.

» ONBOARDING A CAE DEPARTMENT AND OPTIMIZING COLLABORATION AND DEVELOPMENT

In 2019, Sartorius introduced an in-house CAE department to help resolve production challenges, and Maier knew exactly where to start: "Our first step was to define the tools we wanted to use," he shared.

Maier and his team were looking to improve the sharing of insights and results between the engineers developing the devices and the scientists looking at the process. The team decided to use the COMSOL Multiphysics software, which has since become an important tool in the CAE toolkit and a key ingredient for successful communication and problem solving.

The CAE department trained engineering colleagues on how to use simulation software to create an internal simulation community that can provide quality checks for the company's projects. "Our problems are defined by the physics, the process, the dimension in space and time, and by the materials or material interactions you need to consider in the modeling approaches," said Maier.

Now, years into the CAE department operating at Sartorius, the team has an established development process that combines a CAE and V-model development approach. "In the idea phase, we look at a cost level, and we break it down to the main item, and then, once we understand the processes inside, we build up to the system level again," said Maier. This approach extends across the whole production chain, including the mature stages when experts are brought in to optimize the design, share ideas on how to improve

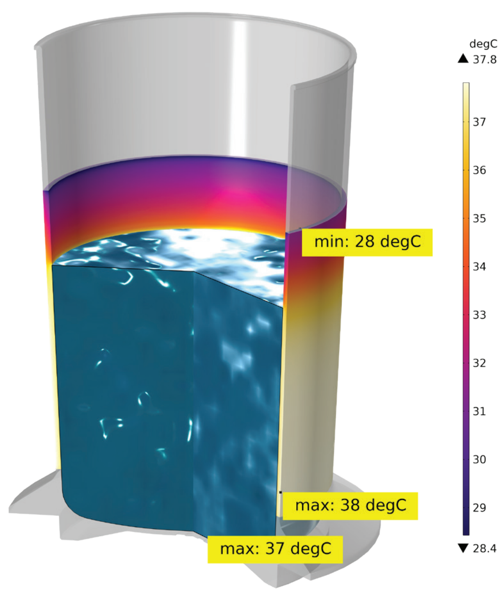

FIGURE 3 The model captures the transient behavior of the heat jacket, revealing temperature distribution, sensor and switch performance, heating efficiency, and identifying potential hot spots that could impact material integrity.

the products, and ultimately produce a digital prototype.

The CAE department at Sartorius is engaged in a diverse array of projects, spanning various scale levels and encompassing a wide range of biopharmaceutical devices. Each project operates independently, allowing for focused innovation. In one initiative, the team developed a bioreactor. Simultaneously, they pursued research on the 3D modeling of membrane structures at the mesoscale, which was a study undertaken independently of the bioreactor project. However, insights from this mesoscale model enhance the design of filters, which are integral components in bioreactor assemblies and other biopharmaceutical devices (Figure 2).

The majority of their simulations are in that macroscale, but Maier and the CAE team also explore system interactions. "Looking at the whole value chain from the raw material to the drug, there is a multitude of requests on our desks dealing from pipettes, over mixers, the downstream area, and then a lot of filtration chromatography steps, freezing and final filling until we reach the drug dose," Maier said. With such a wide swath of projects, the CAE team needs to be able to model multiple physics areas.

"Biopharma is multiphysical," Maier said. "For our products, we have to focus on structural mechanics that ensure the robustness, but we also have to look at the computational fluid dynamics, and we need to know the performance. It is liquid systems everywhere...and here COMSOL Multiphysics is definitely very helpful."

» MOVING FROM MODEL TO MANUFACTURED DEVICE

Sartorius' CAE department has often used COMSOL Multiphysics for specialized CFD applications such as mixers and porous media. Additionally, they have worked on projects that needed to account for freezing, welding, reactive transport, heat transfer processes, and fluid–structure interaction (FSI). Through the use of equation-based modeling, Maier has also incorporated controls and control processes to improve design performance, shorten development timelines, and reduce prototyping.

The CAE department's simulations have provided experts throughout the broader organization with detailed insight into diverse phenomena. When it comes to root cause analysis, the experts can strengthen their knowledge with insights not possible with physical testing, such as when it is impossible to look inside the device. Simulation also helps Sartorius' designers with their testing processes.

"We challenge the tests and the tests challenge us. So, it is a back and forth," Maier explained. The results can show uncertainties in the tests as well as in the simulations. From there, the team can extend the tests with additional simulations or metrics that are difficult to measure and optimize their testing efforts.

FIGURE 4 The Univessel® SU with the heat jacket seamlessly installed.

» DEVELOPING A BIOREACTOR ACCESSORY WITH A SINGLE PROTOTYPE

During the COVID-19 pandemic, the Univessel® SU bioreactor portfolio proved the need for high-quality products to manufacture biopharmaceuticals. The original Univessel® SU bioreactor was a key component in BioNTech's production of their first COVID-19 vaccine, and based on its success, Sartorius decided to update it by adding more functions and sizes to it. One of the functions is an important bioreactor accessory: a heat jacket. The heat jacket development represents the CAE department's typical approach. The team began their investigation with an off-the-shelf heat jacket they found on the market that lacked efficiency and decided to model the design to come up with a better one. Building the model representing the new heat jacket design (Figure 3) involved CFD, heat transfer, and equation-based modeling to account for the sensors, switches, and controllers. Maier said that the results provided the development team with clear recommendations, such as where to put switches and sensors and how to distribute the heating, which helps lead them to smart designs.

"We got a nice transient-controlled simulation out of it, and we were able to derive an optimized design," Maier said. The simulation and the real-life experiments saw temperatures meet in perfect agreement, and the team only needed to create one prototype of their design (Figure 4).

Thanks to the tools available to Sartorius' CAE team, the organization has established an efficient and high-performing department that is overcoming the challenges of biopharmaceutical production, with one goal in mind: "We want to empower scientists and engineers to simplify and accelerate progress in life science and bioprocessing and enable them to develop new, better, and more affordable medicines," explained Maier.

IAV, Germany

DRIVING EV DEVELOPMENT WITH A TWIN-BATTERY APPROACH

Considering energy efficiency, energy density, and environmental concerns, IAV combined complementary sodium-ion and solid-state lithium iron phosphate battery technologies in a twin-battery system optimized and validated with multiphysics simulation that opens up new possibilities for car manufacturers and battery designers.

by JOSEPH CAREW

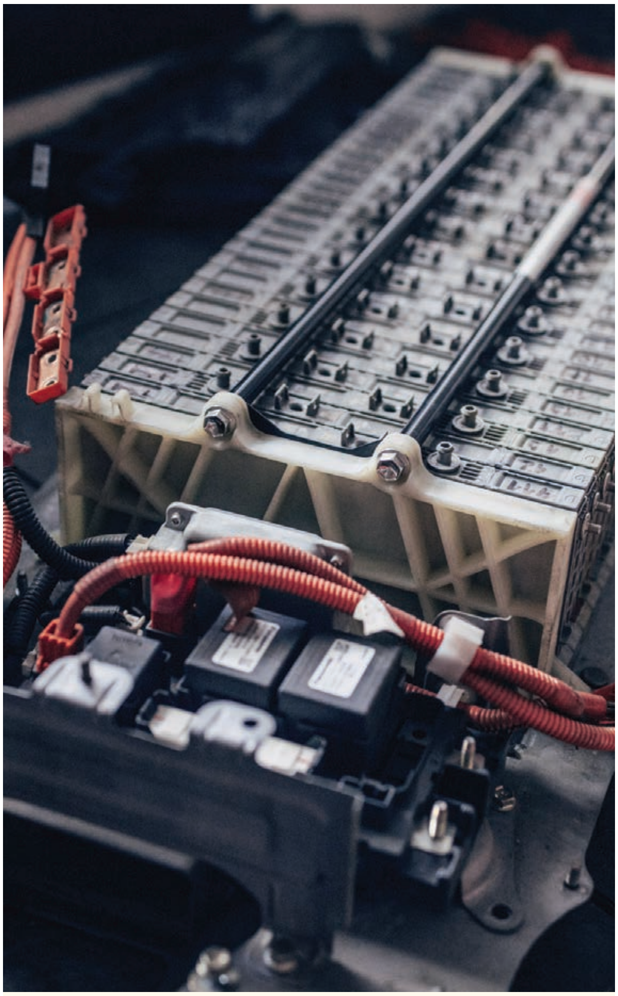

FIGURE 1 Lithium-ion batteries in a repair shop.

Avoiding the rare raw materials required for the production of traditional batteries without sacrificing energy density is a major goal for those looking to electrify the world. Lithium-ion batteries power most of today's electric vehicles (EVs) but are associated with high costs as well as sustainability and environmental concerns. Engineers and developers in the battery industry are investigating alternative chemistries and designs to find new approaches that address these concerns and reduce costs while fulfilling the demands of most lithium-ion applications.

IAV is one of the world's largest engineering companies. Within an extensive portfolio geared toward the future of mobility, battery development plays a critical role. A team of IAV engineers including Jakob Hilgert, a technical consultant at the company, felt that, with the right approach, IAV could achieve better battery designs. The team leaned on its understanding of what makes existing single-chemistry designs successful — as well as what holds each back — to develop a novel approach to solving battery energy density, sustainability, and thermal management issues: a twin-battery design.

Instead of turning solely to lithium-ion cells, IAV engineers thought a pair of alternative battery chemistries could be combined to form a less expensive and more ecofriendly system that could handle EV applications. With this approach in mind, IAV turned to multiphysics simulation to successfully design and validate its twin-battery solution.

» AVOIDING LITHIUM-ION BATTERY PAIN POINTS

While lithium-ion batteries (Figure 1) are often used for their high energy density, their creation can have environmental drawbacks. Open-pit mining for lithium removes vegetation, creates toxic soil, and releases dust that elevates the risk of illness in humans and animals. Producing these batteries is also an expensive prospect and reliant on a relatively rare material. IAV engineers looked to avoid these concerns when choosing the technologies to be included in their twin-battery approach.

"We need to be prepared for batteries that have a larger focus on recycling and resources," Hilgert said. "We cannot always take the highest-energy-density cell that is theoretically possible and use that as our solution."

Instead, the team at IAV chose to pair a sodium-ion battery (SIB) and a lithium iron phosphate (LFP) solid-state battery (SSB) for its design because of the chemistries' unique ability to complement one another. SIBs are typically cheaper, more sustainable to source, and easier to recycle than conventional lithium-ion batteries; however, they tend to have comparatively lower energy density and a shorter cycle life. Meanwhile, traditional LFPs are known for their stability and long cycle life but also lack in energy density when compared to conventional lithium-ion batteries. Finally, SSBs are known for having higher energy density than traditional lithium-ion battery chemistries. By combining an SIB with an LFP-SSB, the resulting design should theoretically have an improved environmental footprint (Figure 2), cost less money to create, and feature a relatively strong energy density for demanding applications such as powering EVs.

"The development of batteries for automotive use is progressing rapidly. It goes hand in hand with a rising demand for scarce raw materials," Hilgert said. "Diversification of cell chemistries is a promising approach to respond to market fluctuations and at the same time minimize system costs."

Creating Thermal Compatibility

IAV's twin-battery design was also developed, in part, to test the thermal compatibility between an SIB and LFP-SSB. The idea was that channeling the waste heat from the SIB into the LFP-SSB would rapidly activate the latter's solid-state cells and push them into the higher temperature ranges where they perform best — while simultaneously keeping the SIB from exceeding its maximum operating temperature and increasing the system's overall energy efficiency.

"If we have some cells that can operate at high temperatures and some cells that can operate at low temperatures, it is beneficial to take the exhaust heat of the higher-running cells

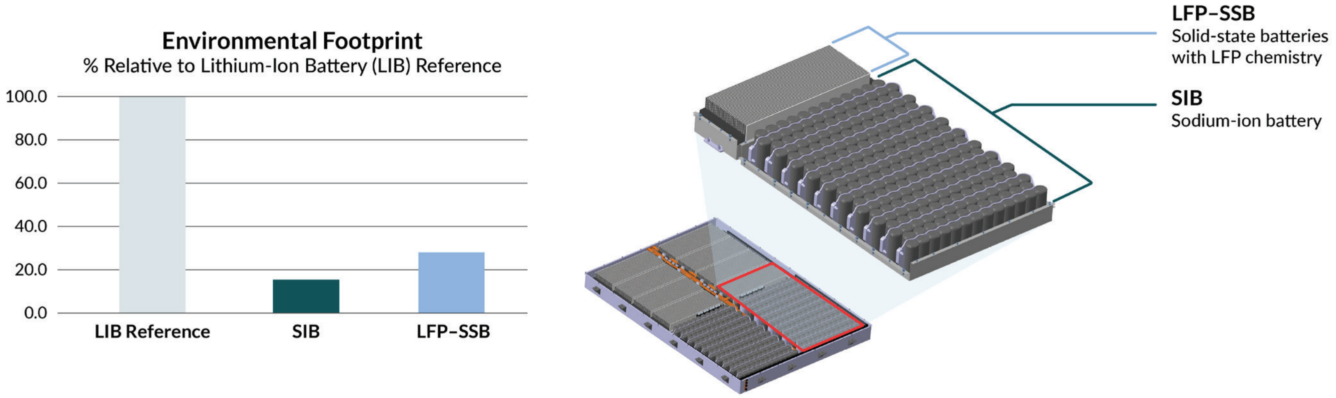

FIGURE 2 A comparison of the two battery technologies used in the twin-battery approach.

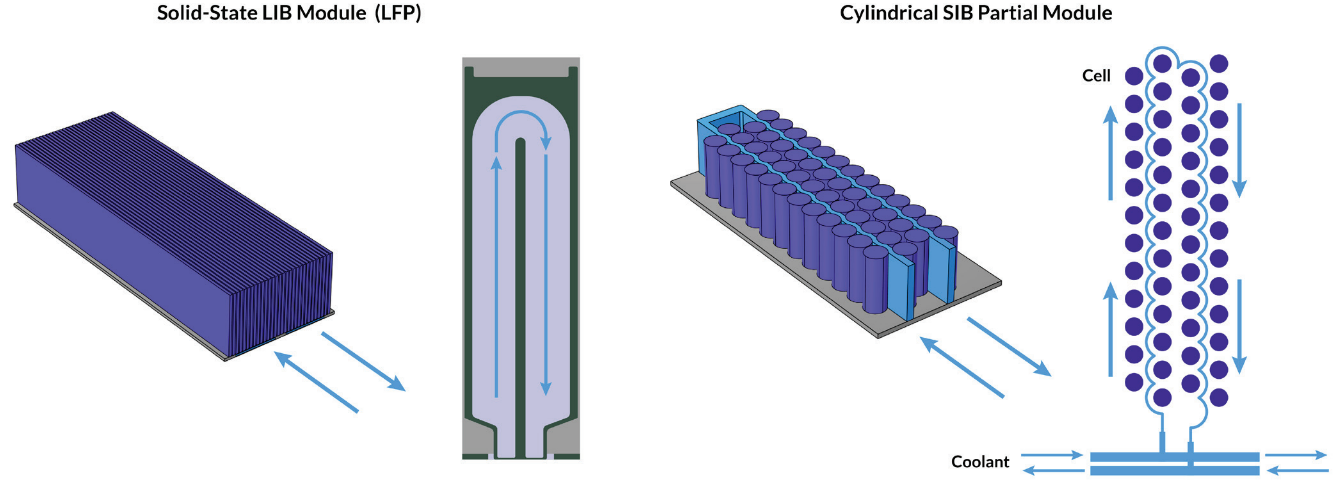

FIGURE 3 The two battery technologies as they appear in the COMSOL model.

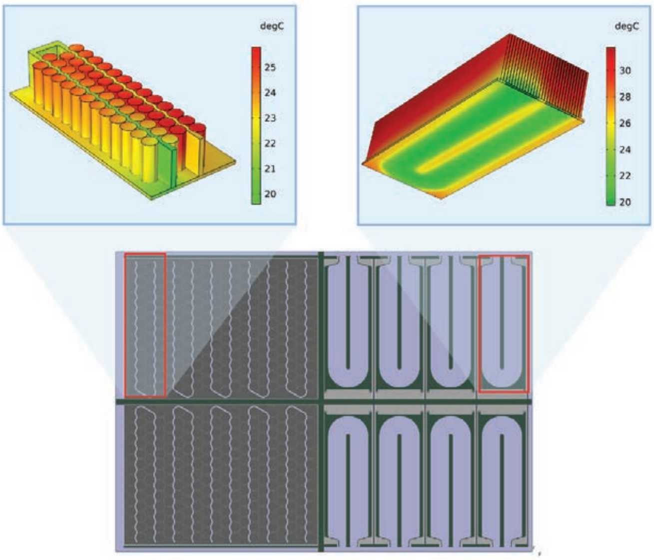

FIGURE 4 The two battery technologies working as one system.

to heat up the lower-running cells, and vice versa," Hilgert said. "That's why we came up with a cooling system that shifts the energy from cells that want to be in a cooler state to cells that want to be in a hotter state."

Cells with liquid electrolyte have limited thermal stability and require cooling (true for both sodium and lithium cells), and temperatures above ~60°C need to be avoided. Solid-state cells can operate at higher temperatures because of their solid electrolyte, and these need an elevated temperature to reach usable ion conductivity. Therefore, the SIB cells in this concept need cooling while the SSB cells need heating, and both cells benefit from the mutual heat exchange. IAV engineers knew that this interaction in particular would be a significant optimization challenge and felt that modeling and simulation would be essential to easing the complexity. For this, the team turned to the COMSOL Multiphysics® software.

» DESIGNING THE BATTERY SYSTEM

IAV first began using the COMSOL Multiphysics software more than a decade ago to improve its design workflow.

"We were using a large quantity of different specialized tools for different specialized topics," Hilgert said. "When we started working with batteries, it was time to say, 'We need one tool to deal with all of these topics.'"

The platform's comprehensive workspace gives IAV the opportunity to avoid building unnecessary prototypes for clients and easily optimize its designs. With the twin-battery model, IAV engineers can tweak different parameters (whether, for example, they impact the cooling of particular circuits or the maximum power that cells at a certain temperature produce) and alter the design to ensure that any real-world creation is as efficient as possible.

"If you have this knowledge and you do not have to guess at all of these parameters, then the technology readiness level of the prototype will be a lot higher," Hilgert said.

Because of the multiphysics nature of battery modeling, the COMSOL® software's capabilities were well-suited for the twin-battery system (Figure 3) development project: Designing operational batteries requires proper thermal management, an understanding of how the materials of different cells are going to perform within their modules, knowledge of the varying pressures within the internal processes in the battery, as well as an electrochemical understanding of the whole. There also needs to be an understanding of how swelling or contraction during charging and discharging can impact the mechanics of these systems.

"A highly integrated model-based development process can be used to investigate the potential of different cell chemistries, designs, and cooling concepts," Hilgert said. "It reduces the need for physical prototypes and allows for performance optimization toward typical requirements of automotive applications."

» HEATING, COOLING, AND DESIGN OPTIMIZATION

Engineers at IAV were able to verify the performance of its twin-battery concept using coupled multiscale and multidomain simulation (Figure 4). The team found that the design worked as desired during concept development, paving a path forward for better battery design. The model showed very fast on-demand activation of solid-state cells, with partial preconditioning done by the SIB's waste heat. The team has optimized the thermal management of the two cells and shortened the time and energy input needed for SSB activation in cold conditions.

"The simulations showed that it is actually possible to do what we had in mind," Hilgert said. "The waste heat actually can be transported by the cooling system, and the amount of heat is sufficient to heat up the other part of the battery."

IAV was able to run different scenarios, comparing various levels of sensitivity for different surrounding conditions or parameter selections with its model, which functions as a virtual prototype. The team successfully integrated 3D cell temperature distributions, pseudo-2D (P2D) electrochemical modeling, and 1D cooling circuit dynamics into a comprehensive electric powertrain model.

» DEMOCRATIZING THE TWIN-BATTERY MODEL WITH APPS

Once IAV's simulation specialists have developed a white-box model for a customer, they often use the Application Builder in COMSOL Multiphysics to additionally package its functionality into a simulation app, a custom-configured user interface with restricted inputs and outputs that the customer can distribute internally to colleagues in different domains who use it to run simulations and evaluate results in their respective contexts. App users do not need in-depth knowledge of the underlying complex model; instead, simulation apps are designed to be easy to use and hard to break, making them ideal for IAV's many customers who "want to distribute these simulation tasks to people that usually do not do modeling," as Hilgert put it.

"Having COMSOL Compiler as a distribution option is a great benefit for our work. We can use our own models for some simulation or profiling tests just by compiling some apps and then having other people do their jobs, without having to wait for the licenses."

— JAKOB HILGERT, IAV TECHNICAL CONSULTANT

"We can start with the basic functionality and hand it out to everybody, and nobody will have a problem using it. Later on, if things get more detailed, we can have the apps grow with the application and add more physics, more options, more buttons," shared Hilgert.

IAV engineers use COMSOL Compiler™ to turn their simulation apps into standalone executable files that they send to their customers alongside the white-box versions of the underlying models, who can then run them without a COMSOL license. This makes it easier to run simulations in distributed development environments. In the case of the twin-battery design, cooling system engineers can run parallel optimization calculations without COMSOL licenses. Streamlined access to simulation results leads to more efficient development processes and has greatly improved the acceptance of model-based development both internally and among IAV's customers.

"Having COMSOL Compiler as a distribution option is a great benefit for our work," Hilgert said. "We can use our own models for some simulation or profiling tests just by compiling some apps and then having other people do their jobs, without having to wait for the licenses."

Interfacing Java code is used to provide remote control of the apps that IAV builds thanks to the COMSOL software's API. This remote control allows users to automate repetitive modeling steps. The team also implements Functional Mock-up Unit (FMU) interfaces, which it couples to vehicle simulation environments in third-party software for cosimulation.

Users of the twin-battery app are given the voltage, state of charge (SOC), temperatures, and power dissipation as inputs to the battery management system and cooling system. Design engineers can view the internal cell states through these apps and make changes to the cooling system as they evaluate the varying battery performance.

Using Apps Internally

Apps that are used internally at IAV are often designed for cosimulation with COMSOL Multiphysics and external toolchains and are routed through IAV's virtual test bench interface. Figure 5 shows an example battery module app used for cosimulation, which provides basic user feedback about the internal states of the models like current, voltage, temperatures, etc. App results are provided as a real-time data stream to other programs in the cosimulation framework, where detailed evaluation of results is performed.

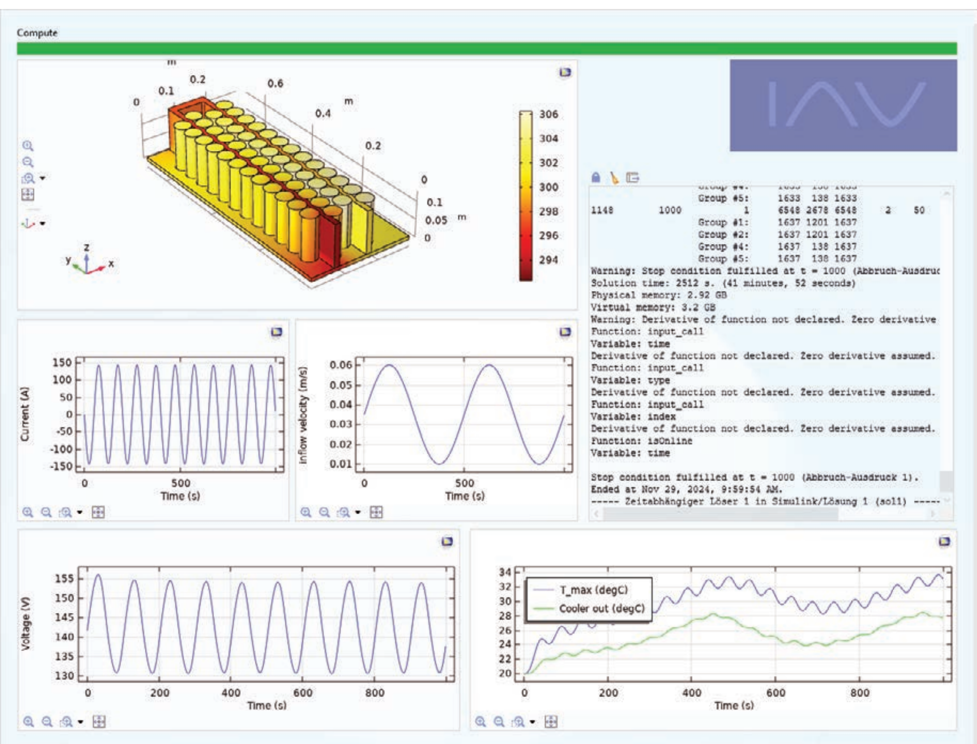

FIGURE 5 In IAV's battery module app, output graphs provide the user with convenient visual feedback on the state of the model during execution.

» (T)WINNING THE BATTLE FOR A BETTER BATTERY

IAV hopes that its twin-battery design concept will function as a showcase to others in the battery industry that, even if you have demands that are contradicting, there can still be a solution.

"The twin-battery approach gives the car manufacturer or the battery designer more options to solve their problems," Hilgert said. "It also shows that there is a way of integrating future technologies with very different principles into existing frameworks." ◎

COMSOL, Massachusetts, USA

ENHANCING GENERATIVE DESIGN WITH TOPOLOGY OPTIMIZATION

FIGURE 1 Top: The topology optimization functionality in COMSOL Multiphysics® with the add-on Optimization Module can be used to generate a drone model with good performance. Bottom: The model is shown with the displacement magnitude to help us visualize the optimization process.

Generative design and topology optimization automate the design process, making design iteration more efficient. There are benefits to both approaches, and by using the methods in combination, designers can create a product that balances the benefits of both.

by **BETH BEAUDRY**

Generative design facilitates more freedom in manufacturing by automating design processes. While topology optimization can be considered a form of generative design, its distinct nature makes it well suited for incorporating into a hybrid approach combining the two processes that can be used to improve products, particularly in terms of performance.

The main similarity between generative design and topology optimization is that they both involve using computational software to generate designs based on criteria defined by the designer, as opposed to the designer manually creating each design iteration. However, a generative design process differs from topology optimization in that it places more emphasis on the designer's requirements for the end product's presentation. For this reason, it is often called a rule-based process; the designer defines values for the design, and the software adheres to them. Topology optimization, on the other hand, is employed more often when the focus is on product performance rather than presentation. Furthermore, it is more physics-based than rule-based, meaning the optimization adheres to the physics of the problem rather than primarily following the rules set by the designer.

With one process prioritizing presentation and the other prioritizing performance, taking a hybrid approach that combines generative design and topology optimization allows for producing an end result with sufficient performance and optimal presentation. In addition, incorporating topology optimization rather than using a purely generative approach can result in an end product that is more sustainable, as designs created with topology optimization are based on objective criteria and thus tend to be timeless.

A hybrid approach could look like using generative design and topology optimization for different components of one larger product. Most commonly, a majority of the components would be produced traditionally, and then generative design and topology optimization would be added for only a few, specific components. It would fall to the designer to decide how to balance the needs of different components, such as determining which parts could sacrifice presentation for stronger performance, and vice versa.

» TAKING A CLOSER LOOK AT TOPOLOGY OPTIMIZATION

When using topology optimization, designers create a geometric virtual space (often a box-like frame) for their design and input some required parameters into the software. The software then fills out the design by iteratively removing and adding material, producing an optimized design that fits within this geometric space. Topology optimization is typically employed early in the design process because there is more flexibility at this stage and thus more potential for performance improvements related to topological changes of the design layout. The closer a project gets to the production stage, the fewer design changes can be made, unless the designer is willing to spend more resources to revamp the design. With topology optimization, the designer can decide on an optimal design with good performance and then, as they get closer to the production stage, shift their focus to simulation accuracy. Though simulation accuracy is always important, it is especially relevant in the latter half of the design process, when designers are using the simulation to predict how the device will work once it becomes a physical prototype.

To better understand the design freedom of topology optimization, consider the following example of creating the structure of a drone. For this model, we input two load cases, the volume fraction, and a minimum length scale.

In this case, our goal is to maximize stiffness for a certain amount of material. The load cases are symmetric, which allows us to save time and computational resources by only modeling a quarter of the domain rather than the full drone. The model is then replicated during the results visualization step so we can see the full, optimized design at the end of the process (Figure 1).

When running this topology optimization example, the computation starts with only the drone battery at the center and the four motors at the corners. We see the quarter that was originally modeled mirrored in the rest of the design and watch as the software adds material to connect the motors to each other and the battery at the center. The stiffness-to-weight ratio of the material is then adjusted until the end result has a clear physical interpretation.

» SUITABILITY FOR MANUFACTURING

When it is time to produce a design, its complexity is a key factor in deciding which manufacturing process to use. The unique results of generative design and topology optimization are usually not suitable for traditional manufacturing and mass production. For this reason, designs created with these methods, or a hybrid technique, often go hand-in-hand with additive manufacturing. For instance, the drone model example is best suited for additive manufacturing.

However, this compatibility does not mean that additive manufacturing is the only option for bringing software-generated designs to life. Often, designers may want to use topology optimization to improve on their design ideas but also need to manufacture products at a lower cost or larger scale than what additive manufacturing usually permits. Preparing such a design for traditional manufacturing may mean, for example, that milling constraints need to be considered in the optimization process. Specialized functionality for topology optimization available in the COMSOL® simulation software can be used to account for such constraints.

Consider a scenario where a topology-optimized wheel rim design needs to be produced using subtractive manufacturing. Figure 2 shows such an example modeled with the COMSOL® software: A wheel rim design is generated with optimal stiffness, and milling constraints are added along its axis. However, adding milling constraints reduces the design freedom and thus the stiffness for a given mass constraint. In this case, adding milling constraints results in a design that is 30% less stiff than it would have been if generated with conventional topology optimization. This compromise is necessary in order to meet the manufacturing requirements.

If complete design freedom were allowed, the optimal design would generally have the same symmetry properties as the load cases. However, it can require many load cases to achieve symmetry — and a large number of load cases can result in a high computational cost. In this example, design symmetry is expected since our wheel needs to be able to rotate, but we face the challenge of not having symmetric load cases. For this reason, the entire wheel needs to be modeled in every optimization iteration in order to see how the load cases affect the design.

FIGURE 2 The displacement magnitude of a wheel rim model.

To achieve symmetry here, we can enforce sector symmetry of the design explicitly by optimizing one of the sectors and then copying the design over to the other sectors during the optimization. Similar to how using symmetry features aided in the design of the drone model, this makes the process computationally cheaper and more efficient.

In the end, we obtain an optimized design that has good performance and still meets the manufacturing requirements.

» SIMULATION HELPS CUSTOMIZE DESIGNS

Like generative design, topology optimization automates the design process, enabling designers to explore options more efficiently than with manual iteration. Both generative design and topology optimization can be leveraged with the COMSOL® software, which also provides features for customizing automated designs so that they are suitable for specific manufacturing methods. These capabilities are applicable to all fields of engineering and scientific research and for any physics area, including structural mechanics, fluid flow, heat transfer, and acoustics. For instance, the software's topology optimization capabilities are actively being used in the automotive industry for the design of electric motors. ◎

The University of Southern Mississippi, Mississippi, USA

TRAINING UNCREWED UNDERWATER VEHICLES FOR VISUALIZATION OF SUBSURFACE STRUCTURES

The University of Southern Mississippi builds and uses simulation apps to integrate machine learning models into the training of uncrewed underwater and surface vehicles.

by **JOSEPH CAREW**

FIGURE 1 The sensor platform that USM used to record the experimental data.

On a calm day along the coast of Mississippi, a small surface vessel is pulled methodically back and forth in a test area. This low magnetic signature sensor platform is hard at work scanning the seabed for ferromagnetic targets. These scans are just one part of an ambitious project conducted by the University of Southern Mississippi's (USM) Roger F. Wicker Center for Ocean Enterprise. Through a combination of modeling, simulation, and machine learning (ML), USM researchers are laying the groundwork for intelligent uncrewed underwater vehicles (UUVs) capable of autonomously and accurately revealing what lies beneath the waves.

» MODELING FERROMAGNETIC STRUCTURES ON THE OCEAN FLOOR

Resting on the bottom of most harbors (and the ocean floor more generally) are ferromagnetic materials such as anthropogenic structures and debris, and even unexploded ordnance. To keep harbor traffic from hitting these hazards, navigational charts need to accurately reflect their locations. One of the more effective methods for scanning for these underwater magnetic anomalies is by using UUVs with advanced sensor equipment. However, these vehicles come with certain challenges, as they are expensive to build, their physical scans are complex, and, due to significant platform noise and environmental noise (such as environmental clutter and wind and waves), they do not always paint an accurate picture. To further complicate matters, the nonuniqueness of certain seafloor signatures can cause scans of different subsurface configurations to look similar. A team at USM is researching how to overcome these challenges and pave the way for better UUV-based sensing and mapping.

"We do a lot of data-driven testing and evaluation of emerging uncrewed systems platforms — both undersea and at the surface (Figure 1) as well as advanced sensor integration," said Dr. Jason McKenna, a researcher at

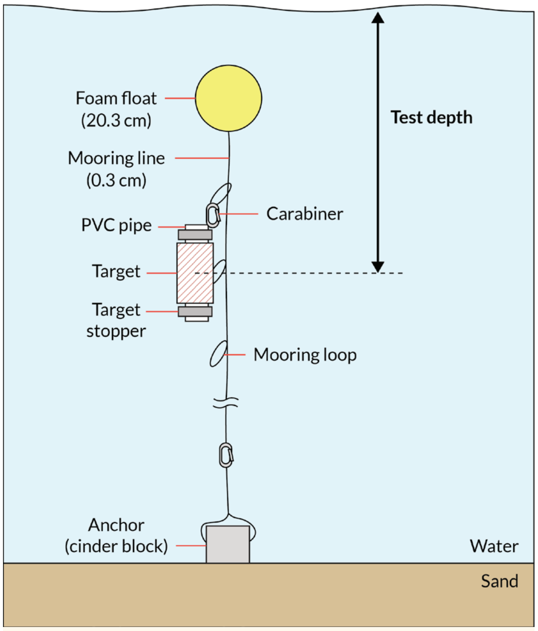

FIGURE 2 The 20.3-cm-long cylindrical magnet with a 2.5-cm diameter.

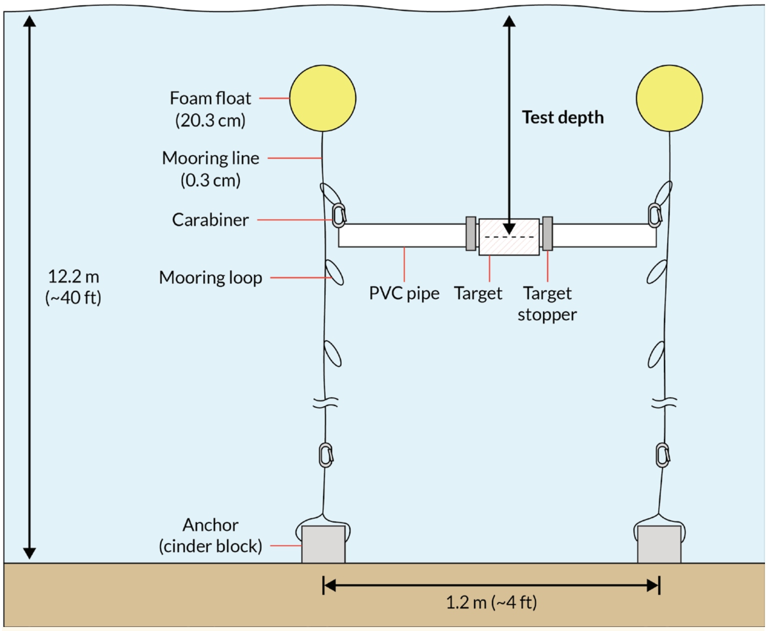

FIGURE 3 The horizontal 30.5-cm-long steel pipe with a 11.4-cm diameter.

USM. "In particular, we are studying the integration of magnetic sensors directly onto UUVs, where there is a lot of environmental and platform noise." The research team turned to modeling (validated through empirical data), simulation apps, and machine learning techniques to develop a computational system that can be integrated into a UUV for automatic target recognition (ATR) and improved accuracy of the magnetic and ultimately gravitational fields data that the vehicle is registering.

» NOT QUITE 20,000 LEAGUES UNDER THE SEA

Before creating models, the team had to obtain the real-world data that would be used to benchmark and validate the models. To do this, the team went to a controlled maritime environment with known targets that could be surveyed with high-precision gravity and magnetic sensors. The physical experiment took place near the Gulf of Mexico, where the team used a winch system to draw a sensor platform 70 meters between two points. Beneath the surface, the sensor platform scanned one of two different targets: a 20.3-cm-long cylindrical magnet that has a 2.5-cm diameter and is resting vertically (Figure 2) or a 30.5-cm-long steel pipe that has a 11.4-cm diameter and is resting horizontally (Figure 3). The team repeated this for several trials per target, with the canisters that held the magnet or pipe placed at depths of 1 meter, 3 meters, and 5 meters.

"The physics we are talking about here is governed one over r-cubed decay, so the magnetic field falls off very quickly," McKenna said. "If you want to observe anything, you have got to be close to the target. That is why when you are doing archeological surveys, generally speaking, you are towing the magnetometer so it is far enough away from the ship's signature, which is introducing noise, and you are flying it just a few meters off the seafloor."

McKenna explained that his team used a magnet that resulted in a stronger signature than what the sensor would likely encounter in the field. This was chosen purposefully.

"The data we use is never that clean but [this experiment] shows you that with the right approach, the right physics, and the right boundary conditions, you could start to approximate a lot of what you would experience in individual targets of interest," McKenna said. "Then you start adding all those targets together and introduce platform noise and use it to get very complicated results."

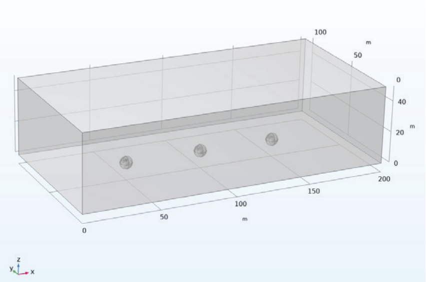

FIGURE 4 The geometry USM used for its modeling. The three interior spheres represent pipes that are 30.5, 70, and 91.4 cm (12, 24, and 36 inches) long, respectively.

» DEVELOPING MODELS FOR SYNTHETIC DATA PRODUCTION

Once the physical experimentation phase was complete, there were several steps the USM team had to take in order to obtain the algorithms they needed to enhance the UUV's performance. Ultimately, the process involved creating potential field models and performing uncertainty quantification (UQ) analyses; creating simulation apps based on the validated models that can generate data; and then, finally, using the generated data to train the ML models to help the UUVs detect objects of interest.

Potential Field Models

McKenna and his team used the COMSOL Multiphysics® simulation platform together with the AC/DC Module to build potential field models. These models can represent the interactions between magnetic, gravitational, or thermal fields and objects and are thus essential for quantifying the signatures of the seafloor and its objects.

He began by defining the target object's physical properties and generating a series of targets to create a test bed using the built-in *Magnetic Fields, No Current* interface in the software. He then introduced the spatial configuration with low (30.5 cm, or 12 inches), medium (70 cm, or 24 inches), and high (91.4 cm, or 36 inches) magnetic targets in the simulation space (Figure 4). Finally, he calculated the targets' interactions with the surrounding medium. The gravity and magnetic anomalies (the targets) were subsequently recorded from various UUV simulations, which provided a large dataset that captured the nuances of the potential field variations in different scenarios. To inform these UUV simulations, the research team used UQ analyses.

Scoping Out Variables with Uncertainty Quantification

UQ studies were integrated into the team's process in order to examine the role of uncertainty when modeling the operation of a UUV and to fill in the gaps for parameters that could not be replicated in a real-world experiment. Specifically, McKenna conducted a screening and sensitivity analysis using the Uncertainty Quantification Module, another add-on to COMSOL Multiphysics. The module acts as a general interface for characterizing uncertainties and propagating input uncertainties in models and statistically analyzing output quantities of interest.

> **"In a matter of minutes to an hour we can build up a rich and robust training set for the machine learning algorithms."**
>
> — DR. JASON MCKENNA, A RESEARCHER AT USM

"The model uncertainty quantification was fairly intuitive," McKenna said. "We wanted to try to do a screening analysis similar to what we would have done using a principal component analysis. It's a pretty elegant way to scope out the dependence of a lot of variables."

McKenna and his team were able to identify the expected ranges of the parameters of the ferromagnetic structures or devices they would be looking to measure with the scans. They were able to parameterize the targets by length, wall thickness, and magnetic susceptibility and then introduce the effects of Earth's magnetic fields (the party most responsible for inducing the signature in the metallic objects UUVs scan). The insight into the workable range of these parameters has allowed the potential field models to be easily recalibrated and solved, thus replicating various UUV runs that would normally take the team days on the water and come at a great expense computationally.

By varying the magnetic latitude, longitude, and strength of the force field, plus or minus x percent, the team was able to measure the effects of the alterations. "You could do a sensitivity analysis that way. You can use uncertainty quantification to find these value ranges and come up with some understanding and establish whether or not measurements are as you would expect," McKenna said. "In a matter of minutes to an hour we can build up a rich and robust training set for the machine learning algorithms."

From Validated Models to ML Training Apps

Once the uncertainty quantification studies were complete and the potential field models were established, McKenna was able to compare the results of the simulation with his real-life experiments (Figure 5). He created several simplistic models for the comparison and gained

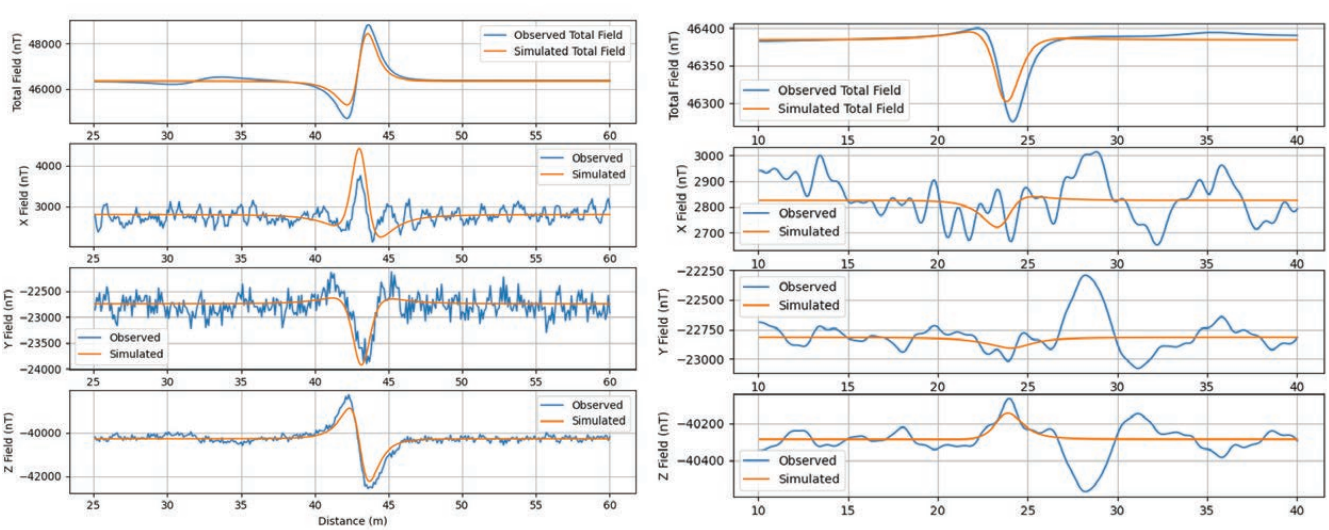

FIGURE 5 The comparison results of scanning and simulating the steel pipe (left) and cylindrical magnet (right).

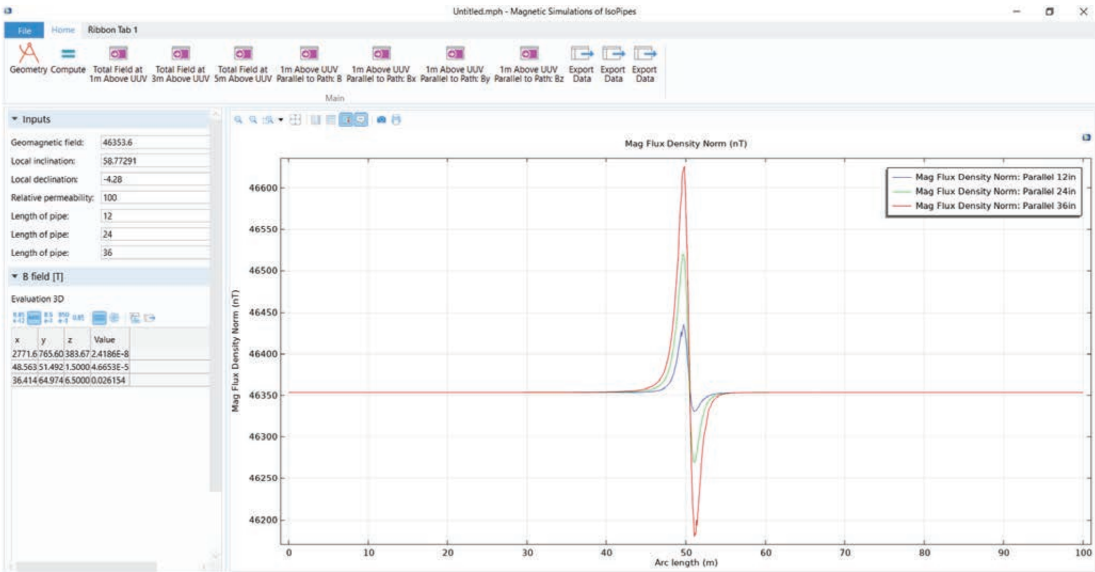

FIGURE 6 The user interface of USM's simulation app with input fields on the left and results on the right.

many meaningful results with close agreement.

The positive results led McKenna to use the validated models to create simulation apps (Figure 6) for the data science team, which requires access to a significant amount of training data for ML algorithms. McKenna used the Application Builder in COMSOL Multiphysics to create the apps, which are easily digestible and enable the scientists to generate ML training data.

"I was able to build the apps by following along with some examples, and, within a matter of an hour or two, get the apps up and running," McKenna said. "You can start to put in the different parameters, and if you change them, the field lines change, which is exactly what we wanted."

The data science team needs to ensure that the models are able to capture these data points, and with COMSOL®, it has been able to do that without having to constantly monitor the model. The data science team can vary the parameters and develop a variety of signatures that the UUVs are expected to encounter and scan. The simulation apps have provided USM with the quality and quantity of data the algorithms need in order to be properly trained.

With the apps, USM was able to divide the research work in a way that allowed each team to flex its expertise. "Everyone was able to be productive within their own spheres of knowledge," McKenna said. "It takes a team to do something like this."

» MACHINE LEARNING TECHNIQUES

The ML techniques the team used included long short-term memory (LSTM) network, regression, tree boosting, and deep neural network (DNN) models.

The LSTM models were used to assess how the predictive capabilities changed when running on simulated sensor sequence data. This assessment could further be used to determine if simulation could effectively be used in data augmentation for observational data. The regression, tree boosting, and DNN models were selected for confirmation of simulation data patterns.

These models were run exclusively on simulated data, and the LSTM models were run using an embedding sequence of 10 data points from a total of more than 500,000 data points. The models are compatible with sequence data, including time-series analysis, which makes them particularly useful for interpreting UUV integrated sensor data.

As explained in McKenna's paper for the COMSOL Conference (Ref. 1), "The synthetic datasets generated from our COMSOL models provide diverse training examples, allowing ML models to learn the complex temporal relationships and signature patterns associated with different target types."

» LOOKING AHEAD TO INTELLIGENT UUVS

Lying on the bottom of rivers, lakes, and waterways are ferromagnetic structures and devices that should be recorded for safety and navigational purposes. UUVs have a role to play in improving the navigational charts that can mark these potential hazards and improve the navigability of harbors. For instance, if a natural disaster were to sink ships and leave debris in unexpected places, smart UUVs would be able to quickly scan the seafloor and give insight into what lies below the waves.

The research team at USM is working at the confluence of simulation and machine learning to improve the predictive capabilities of UUVs. However, this project, which McKenna believes is a "blueprint for integrating simulation-driven ML into various geophysical and engineering domains," is just one step. His goal for the future is to add in more complexity to his models and emphasize phenomena that have yet to be factored in. This includes the self-demagnetization of larger ferromagnetic objects and incorporating physics such as acoustics and thermal phenomena. McKenna is also looking to deploy his apps internally for machine learning training through the app-management product COMSOL Server™, develop more realistic seafloor models, and further the use of uncertainty quantification optimization at USM. ◎

ACKNOWLEDGEMENT

This research was supported by a grant to USM from the Office of Naval Research.

iBMB Srls, Italy

SIMULATION APP INTRODUCES PERSONALIZED ONCOLOGY CARE

by **DIXITA PATEL**

To predict tumor progression for breast cancer, a spin-off company called initiatives for Bio-Materials Behavior (iBMB Srls) in Potenza, Italy, developed a simulation application to help healthcare professionals better monitor tumor lesion volumes and treatment effectiveness prior to neoadjuvant chemotherapy.

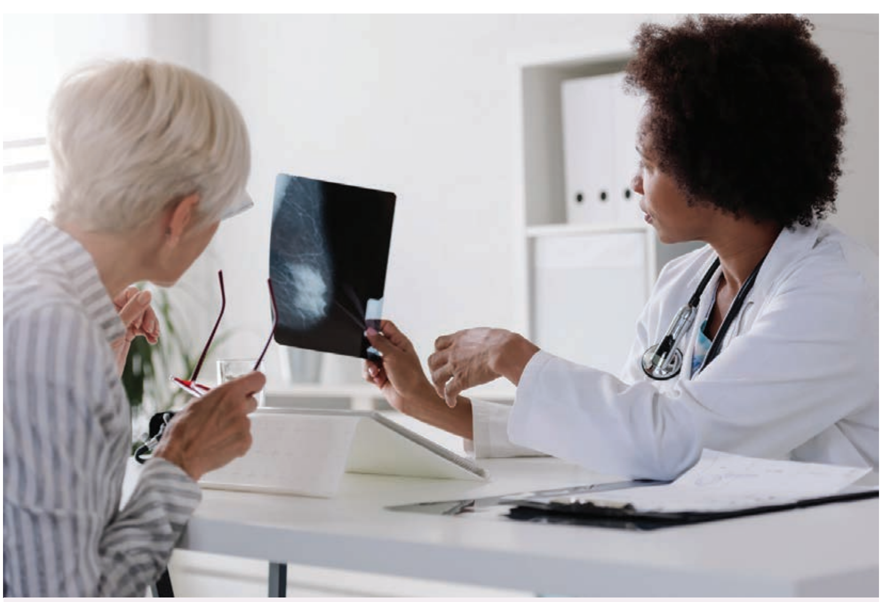

FIGURE 1 A traditional healthcare approach of reviewing patient scans.

Worldwide, one of the most common types of cancer among women is breast cancer, and while there have been improvements to the current available cancer treatments, determining an accurate prognosis for breast cancer remains a challenge. One approach that could help improve patient care is predictive oncology. This approach is a shift from traditional cancer treatments (Figure 1), instead taking patient-specific data into account in a more precise and personalized way so that oncologists can better understand how tumors will respond to specific treatments.

When combined with computational modeling (Figure 2), predictive oncology can be used to anticipate treatment outcomes for patients using algorithms and machine learning techniques. For instance, mathematical equations that describe the biological and physical

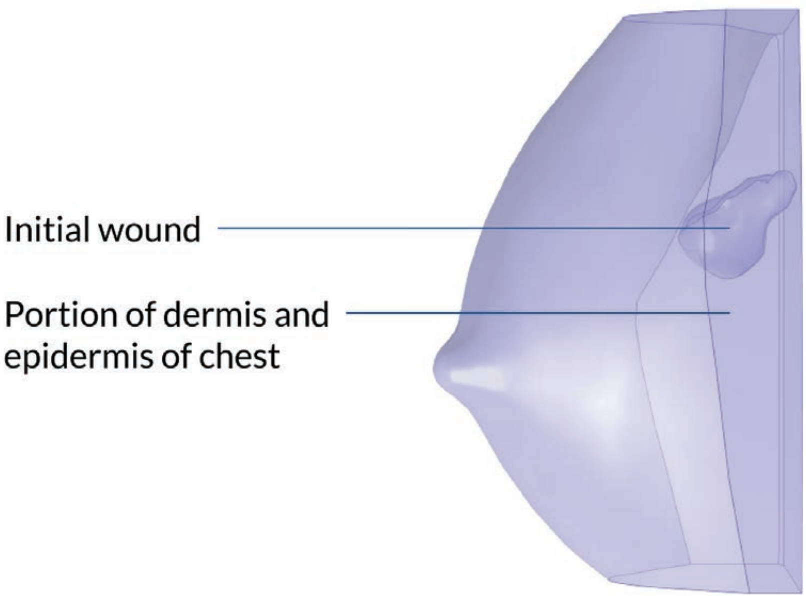

FIGURE 2 A 3D representation of a woman's breast, taken from a clinical Digital Imaging and Communications in Medicine (DICOM) image stack.

mechanisms behind cancer growth, as well as treatment responses, can be used to create deterministic models of tumor progression. One company that is using mathematical equations in this way is initiatives for Bio-Materials Behavior (iBMB Srls), a spin-off of the University of Basilicata. iBMB Srls used the COMSOL Multiphysics® software to create CancerMate, a simulation app that is based on a mathematical model that represents tumor behavior. Oncologists can use the app to better monitor and assess solid tumor progression for breast cancer, specifically nonmetastatic triple-negative breast cancer, treated with neoadjuvant LYNPARZA® therapy. With the results from the app, oncologists can adjust therapeutic strategies accordingly to help optimize therapy effectiveness and minimize adverse effects.

"The current treatments on the market lack personalization and precision," said Gianpaolo Ruocco, CEO of iBMB Srls. "CancerMate allows doctors to run virtual scenarios, reducing the burden on the patient and the cost of the treatment."

» DETERMINING TUMOR VOLUME VIA VIRTUAL BIOMARKERS

The intended focus of the CancerMate app is to quantify lesion volumes before a patient undergoes neoadjuvant chemotherapy to reduce tumor size. The Mark 1 version of CancerMate was validated against clinical data of patients with nonmetastatic triple-negative breast cancer, treated with the drug LYNPARZA® (olaparib). The clinical experiment involved a retrospective cohort of 17 patients, and the data from the experiment was used to test an *in silico* reactive-diffusive model (based on partial differential equations, or PDEs) to predict the metabolic response of breast cancer, virtualize tumor progression, and predict tumor dynamics in response to therapy for individual patients.

The clinical experiment helped the team identify key breast carcinoma biomarkers, which are necessary for predicting how a tumor will respond to treatment. In a clinical setting, biomarkers are indicators of a patient's health measured from bodily fluid, such as blood, and tissue tests. During the study, tumor-infiltrating lymphocytes (TILs), which describe immune response, and protein Ki67, which describes tumor aggressiveness, were closely monitored over time. In the CancerMate app, virtual biomarkers are integrated into models as digital or computational indicators that represent biological processes or disease characteristics, intended to supplement or predict traditional clinical biomarkers.

For the clinical experiment, the mathematical model incorporated the biomarkers for personalized malignancy (r_c) and personalized pharmacodynamic efficiency (ϵ_{PD}), which correlate to the traditional biomarkers Ki67 and TILs. The biomarkers helped to quantify the effectiveness of olaparib during the experiment. As explained in a research paper relating to the clinical experiment, "The model showed, without any preliminary assumption, the effective pharmacodynamic efficiency of olaparib was strongly dependent on basal TILs level and metric tumor volume V or metabolic tumor volume SUV_{max} growth rate. V or SUV_{max} were represented by a mathematical parameter that in our

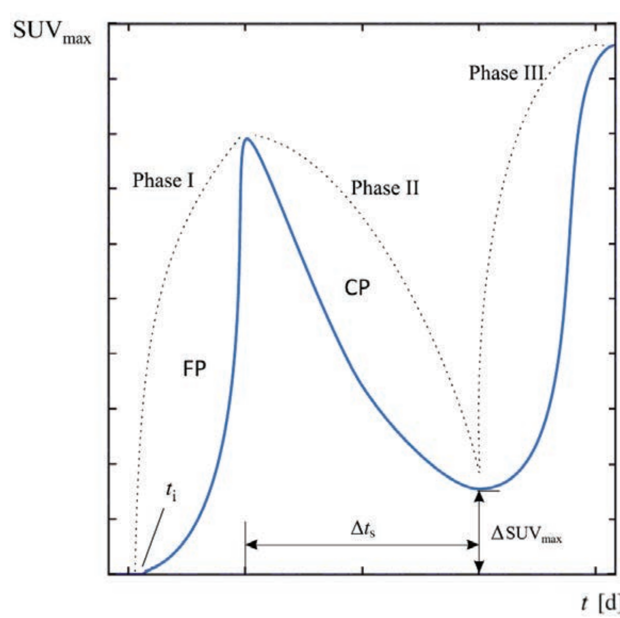

FIGURE 3 A representation of how a tumor progresses through the body. The proliferation phases I to III with metabolic tumor volume (SUV_{max}) versus time (t) are shown. Image taken from Ref. 1, CC BY 4.0.

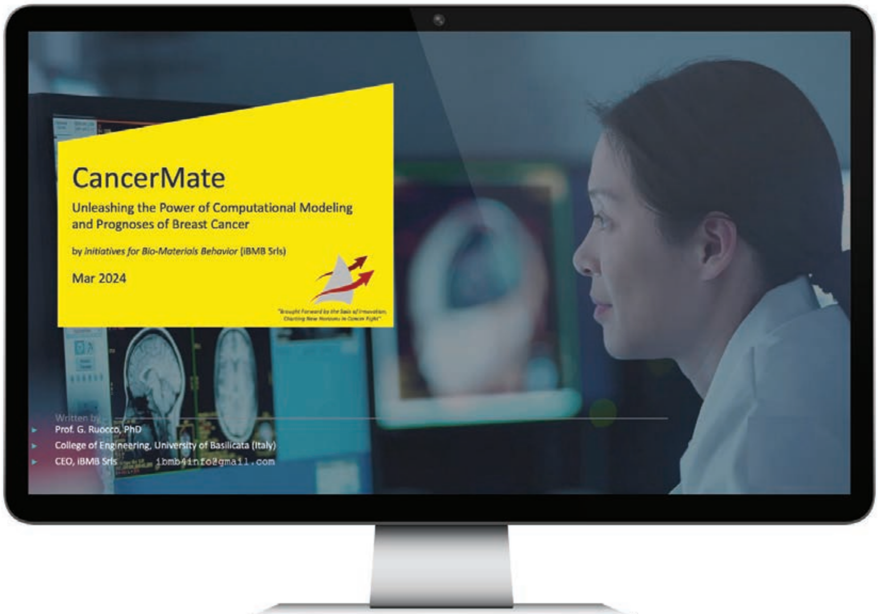

FIGURE 4 Splash screen that appears when opening the compiled CancerMate app.

case was directly dependent on Ki67 expression and TILs count." (Ref. 1)

To illustrate the mathematical model and visually compare the predicted and observed values from the experiment, the team at iBMB used a Gompertzian curve to model tumor growth, specifically during the phases before and after the administration of olaparib (Figure 3). The curve represents metric tumor volume V over time (t) over three different cancer growth phases. These three phases are free proliferation, challenged proliferation, and uncontrolled growth (denoted as "Phase I", "Phase II", and "Phase III", respectively, in Figure 3).

Phase I (free proliferation), begins at an unknown starting point (t_i) and continues until the diagnosis for the tumor is made ($t = 0$). At this point, a diagnostic image is performed and an oncologist will determine which therapy the patient needs. Following this, Phase II (challenged proliferation) represents the start of therapy and observes the partial regression of the tumor due to therapeutic intervention. Lastly, Phase III (uncontrolled growth) is an observation period to see if there is further tumor growth or an increase in metabolic activity after treatment has ended or resistance develops. This phase helps to highlight if further monitoring and additional treatments are needed. The validated mathematical model was integrated into CancerMate, where r_c and ϵ_{PD} are the two primary virtual biomarkers.

» CANCERMATE: A LEAP TOWARD PERSONALIZED ONCOLOGY

Ruocco and the team developed CancerMate using the equation-based modeling functionality in COMSOL Multiphysics. They integrated the PDEs (based on transport phenomena) that represent tumor growth and therapy responses and thus could be used to simulate the proliferation of cancer cells and the effects of neoadjuvant chemotherapy. The app was created with the Application Builder in COMSOL Multiphysics and turned into a standalone app with COMSOL Compiler™, an add-on product for compiling apps with the click of a button (Figure 4). By converting CancerMate into a standalone app, Ruocco is able to easily distribute the app to clinicians, enabling them to perform virtual scenarios and receive detailed information about cancer progression directly at their desktop.

The interface of the app includes the ability to input patient data, display numerical results, and visualize the graphical progress of predicted lesion volume and integrated drug concentration over time (Figure 5). The input fields for the patient-specific biomarkers are the starting points for the oncological predictions, where the first input field is an estimation of the start time of the tumor lesion. The other input fields include the total observation period (which depends on the therapy that will be used), patient mass, body surface area, and the baseline Ki67 and TILs values. Additionally, input fields for the dosage and baseline creatinine indicators are included, which directly relate to the pharmacodynamics (how the drug fights the tumor) and the pharmacokinetics (how the body disposes the drug by bodily functions).

The app uses the mathematical model to integrate clinical data that includes baseline measurements such as SUV_{max}, TILs, and Ki67. The virtual biomarkers, r_c and ϵ_{PD}, inform the model's predictions, and then the app will apply these biomarkers to a set of equations that describe tumor growth and response to treatment over time. After computing, the numerical result for the predicted clinical lesion value at $t = 0$ and $t = \Delta t_s$ are displayed, and a graphic shows the progress of the predicted cancer lesion volume and the integrated drug concentration. By utilizing the built-in functionality in COMSOL Multiphysics for solving complex PDEs, CancerMate provides clinicians with an efficient way to monitor a patient's response to therapy.

» THE FUTURE OF CANCERMATE AND VIRTUAL HUMAN TWINS IN ONCOLOGY

CancerMate's user-friendliness and simulation capabilities make it valuable in personalized cancer treatment for oncologists and pharmaceutical researchers. The current version of CancerMate is ready for implementation in a clinical setting, specifically for the treatment of triple-negative breast cancer and LYNPARZA® therapy. Ruocco said that upon further dataset availability, the underlying model could be trained to cover more couplings between different breast cancer subtypes and therapies. Moreover, while the app is currently focused on breast cancer, the team at

"The current version of CancerMate is ready for implementation in a clinical setting, specifically for the treatment of triple-negative breast cancer and LYNPARZA® therapy."

— GIANPAOLO RUOCCO, CEO OF IBMB SRLS

iBMB plans to extend the underlying technology of the app to also focus on other types of cancer and drug products.

In addition to extending the use of the app, iBMB intends to promote CancerMate as a tool that can be used alongside technology for creating virtual human twins (VHTs), with the intent of creating twins that represent a cancerous disease state. VHTs are significant because they have the potential to improve precision and advance customized cancer care. Ruocco said that one possibility for VHTs is to project them via a head-mounted display that surgeons could wear. With such a headset, the surgeon would be immersed in a virtual reality where they could see, for instance, if a lesion in a breast was too close to the bone and, depending on the results, adjust treatment plans as needed. "VHTs are a way of approaching medicine in a personalized and precise way, which is a change of paradigms," said Ruocco.

As predictive oncology evolves, tools like CancerMate can shape personalized medicine by helping clinicians assess and monitor tumor lesion volumes. As explained by Ruocco, "Patients are often treated longer than necessary, but this can be modified with *in silico* tools." ◎

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1. F. Schettini et al., "*Computational Reactive–Diffusive Modeling for Stratification and Prognosis Determination of Patients with Breast Cancer Receiving Olaparib*," *Scientific Reports*, July 2023; https://doi.org/10.1038/s41598-023-38760-z

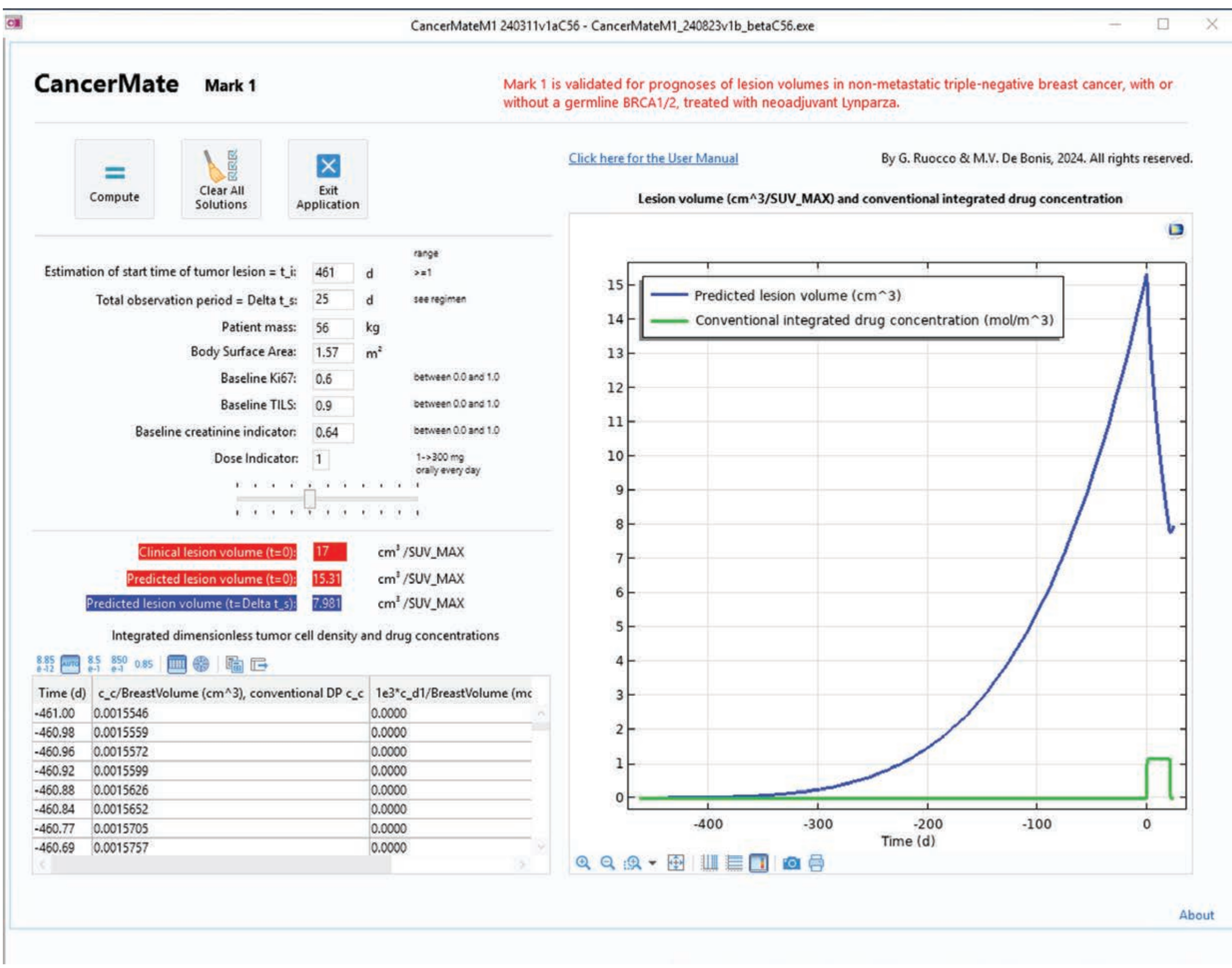


FIGURE 5 The user interface for the CancerMate Mark 1 app showing the input options and an example of computed results based on the underlying COMSOL model.

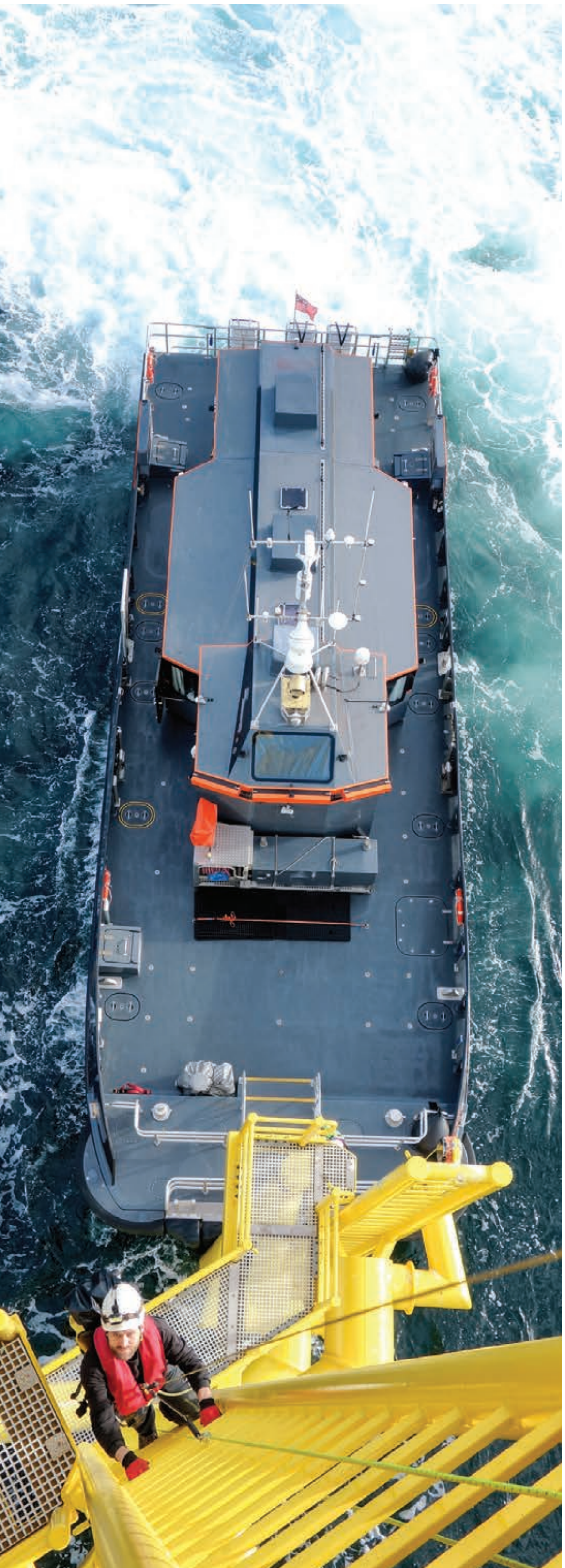


FIGURE 1 A vessel landing at a wind turbine terminal.

Wood Thilsted, Denmark

UNDOCKING BETTER BOAT LANDING DESIGNS FOR OFFSHORE WIND TURBINES

Structural analysis helps an offshore engineering company design boat landings that withstand interactions with rough waters and 200-tonne vessels.

by **JOSEPH CAREW**

The sea churns, and a vessel is heaved back and forth as maintenance personnel approach an offshore wind turbine. The craft is pressed against the structure's specially designed boat landing, and the crew members begin to disembark (Figure 1). As they move from boat to turbine, a wave rolls the vessel away and then back toward crew members still on the lower section of the landing. Fortunately, disaster is averted as the steel fenders absorb the impact and the transfer proceeds safely.

Due to the relentless force of the sea, the vulnerability of personnel being transferred, and frequent interactions with weighty vessels, it is a given that boat landings have to be strong. Building up strength could involve adding steel, but without the right information to guide decisions, design engineers may end up adding material to pieces that do not actually need it, unnecessarily running up the final bill. Therefore, designing boat landings with an eye toward not only safety and strength but also an efficient use of materials is crucial to making offshore wind turbines operational.

To meet these challenges, Wood Thilsted, a leader in offshore engineering, developed a way to create, test, and validate boat landing designs cost effectively and efficiently — with both sea and safety in mind. Specifically, the team used the COMSOL Multiphysics® simulation software to reduce workload, minimize potential errors, and automate many of its design processes.

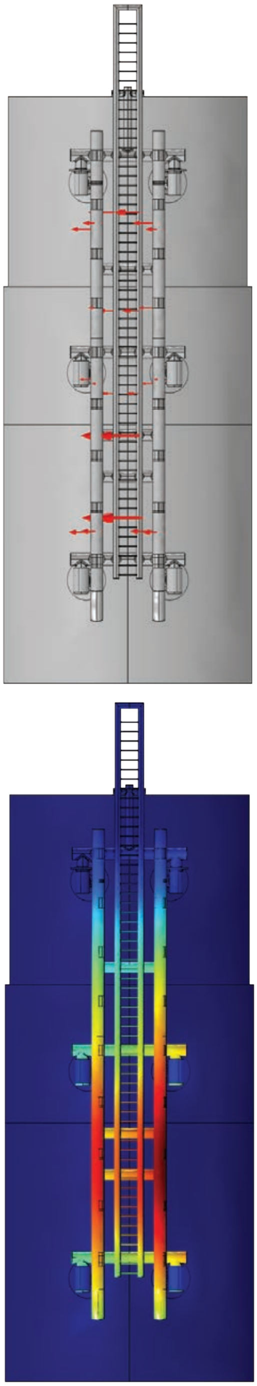


FIGURE 2 Models visualizing the forces acting on the boat landing designs while at sea. Top: Red arrows show lateral forces. Bottom: A surface plot highlights important points of strain in the design.

» THE CHALLENGES OF DOCKING

On a typical project, the team at Wood Thilsted will spend just one to two months designing a new boat landing that can withstand interactions with rough waters and 200-tonne vessels and last for 30 years. Louise Bendtsen, senior structural engineer at Wood Thilsted, said that when reduced to their most basic concept, these landings can seem misleadingly simple to create. Bendtsen recalled: "Someone once said: 'It is just tubes! It is not that difficult.' But it really is challenging." The demanding real-life requirements make offshore boat landings a daunting design prospect.

"The challenge with the design is that we have a set of requirements with different load cases, and these are contradicting. I can spend a lot of time optimizing one aspect of the design and then figure out that it does not work for another design case," said Bendtsen. "[As a designer, this means that you] need to have a broader perspective on the design as a whole and you cannot spend too much time focusing on one small detail, because it just will not work."

The need for maintenance personnel to safely transition from their vessel to the wind turbine using the boat landing adds to the complexity of its design. During this process, the bow of a specially designed, 200-tonne vessel is pressed against the fenders of the boat landing while the personnel transfer to the ladder on the structure and climb to safety. A boat landing needs to be able to withstand these impacts as well as the forces that waves will subject it to over the course of the projected 30-year lifespan. Engineers must also design for accident cases, such as unintended collisions, in addition to meeting the overarching load case requirements.

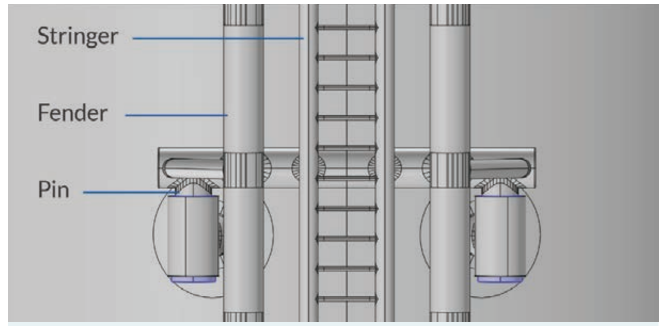


FIGURE 3 The relevant design components for a boat landing.

Finding the Ultimate Limit State and Fatigue Limit State

To best understand the capabilities of various designs, the team at Wood Thilsted needs a simulation software platform capable of modeling an ultimate limit state (ULS) wave as well as a fatigue limit state (FLS) wave, and, for this, it has turned to the COMSOL Multiphysics® software. The ULS wave represents the maximum peak forces that a boat landing is expected to experience throughout its projected lifespan, while the FLS wave stands for the cumulative impact of 30 years of waves and transfers on the structure (Figure 2). The ULS and FLS waves are the governing load cases for any potential design solution for safe offshore wind turbine access.

As boat landings include ladders, fenders, pins, and many components (Figure 3), the Wood Thilsted team also needs to be able to test a variety of different designs to ensure user safety. However, altering each part individually and building the entire geometry again is time intensive. By using the COMSOL® software's streamlined environment, the team quickly adjusts, tests, and optimizes key measurements, including the distance between rungs, the width of the ladder, the space between fenders, and the step-over distance.

» LANDING ON A DESIGN

Wood Thilsted's designs for boat landings rely on steel and feature three sets of horizontal ladder supports that are welded to the transition piece of the wind turbine, where the turbine meets the water. The top support is a pin welded to a flange, which acts as the vertical restraint for the boat landing. The two lower supports are pins covered in vulcanized neoprene inside buckets. The neoprene ensures that there is no coating damage to the support system. Altogether, this design approach makes it possible to easily remove the boat landing in the unlikely event of a replacement being required before the end of its expected lifespan.

Automation with Simulation Software

In an effort to prevent having to perform repetitive analyses, an inefficient approach with regard to time and resources, the Wood Thilsted team has chosen to automate the simulations.

"We are using COMSOL to quickly and easily calculate what the stress concentration factors (SCFs) of our boat landings

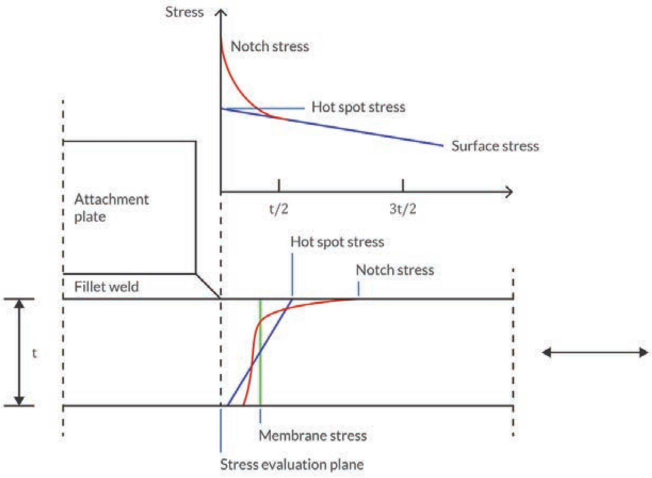


FIGURE 4 While deployed, the structure contends with stress-specific hotspots.

are and keep track of that throughout a project," said Bendtsen. To further validate potential designs, her team collaborates with Wood Thilsted's Primary Steel team for feedback on the SCFs and the limits of the materials being used (Figure 4).

The Wood Thilsted team uses LiveLink™ *for* MATLAB®, an add-on product to COMSOL Multiphysics®, to automate processes such as applying loads, setting material properties, and choosing the analysis type — thereby ensuring consistency and high quality.

"By using COMSOL Multiphysics®, we get the stresses automatically, and then we connect this data to MATLAB® using LiveLink™ *for* MATLAB®," said Bendtsen. "This allows us to write our own scripts that extract stresses and strains and perform all the results evaluations for the different load cases, freeing up time for us to improve the design and focus on its challenging parts."

These load cases include simulating normal wave loads as well as unexpected vessel impacts. All of this can be optimized and automated in COMSOL® by building up and storing information on particular parts. "There is a lot of opportunity for automation in the software, and that is really beneficial for us because we have all of these load cases that are similar but different," said Bendtsen.

Part Library and Parameters

Part of what allows Wood Thilsted to be efficient in its design approach is its geometry part library. Within COMSOL Multiphysics®, users can create designs and store them, as well as reproduce and parameterize their complex geometries. Using this functionality, Bendtsen and the team build their boat landing designs piece by piece, mapping out each part individually and saving its parameters so that they can swap out one design portion for another. This approach gives them the ability to alter multiple similar parts simultaneously by making changes to the corresponding governing global geometry parameter, allowing them to easily measure a design against previous iterations.

Specifically, Wood Thilsted has everything including the fender support, bucket support, fenders, and ladders in its geometry part library (Figure 5), and it is able to plug parts into a model as it needs. "That means I can combine these different geometry parts to build up my total boat landing design," said Bendtsen. "We also have multiple configurations in our parts, so I can change joint types and angles, making different configurations possible."

Bendtsen finds this particularly helpful when working with various fabricators after their designs have been modeled and simulated. Working with different fabricators leads to encounters with individualized preferences for actually building a boat landing. "We have a lot of different configurations, so we have created a part library that really allows us to configure our boat landing in many ways, and it is easy to adapt," said Bendtsen.

On top of that, Wood Thilsted's 3D COMSOL model allows the designer to easily perform a visual check of a potential design to verify that everything looks right. With structural mechanics simulation, the Wood Thilsted team is able to accurately model its boat landing designs and simulate the dramatic impact the environment and vessels can have on them.

» SETTING THE STAGE FOR BETTER BOAT LANDINGS

More than an assortment of tubes, boat landings need to be designed efficiently and with safety in mind. With so much at stake in terms of both costs and risks, modeling and simulation has helped remove guesswork from the process. Furthermore, Wood Thilsted has been able to automate parts of its processes and hone its wind turbine boat landing designs. "Clients continue to come to us to design boat landings because our designs have a track record and have been proven to work," said Bendtsen. This sentiment goes hand in hand with Wood Thilsted's motto to execute designs with speed and flexibility; as Bendtsen puts it: "Our project teams are agile and fast. We can handle design changes in hours instead of weeks, producing the most steel-efficient designs at fast speeds." ◎

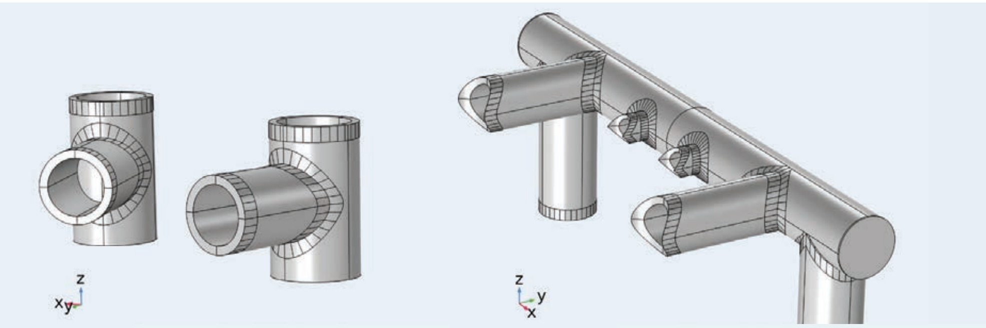


FIGURE 5 A combination of custom saved parts and parts from the COMSOL Part Library. Left: bucket support assembly parts. Right: fender support assembly parts.

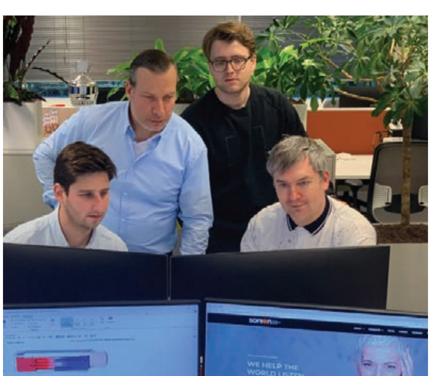
Sonion, Netherlands

HELPING THE WORLD LISTEN WITH HEARING AID TECHNOLOGY

Sonion uses vibroacoustic modeling and experimental tests to develop components for hearing instruments and professional audio. Michele Colloca of Sonion spoke with COMSOL about his team's work and the future of hearing aid technology.

by JOSEPH CAREW

Audio monitors, earphones, headphones, hearing aids, and other popular audio technologies often feature the name of a single brand, but most of these products incorporate parts designed and made by a variety of companies. For example, five of the world's six largest hearing aid companies feature transducer components developed by Sonion, a global company that designs and manufactures advanced miniature components — such as balanced armature receivers, high-end microphones, voice pick up sensors, and other electromechanical components — for manufacturers of hearing instruments and professional audio. The engineers at Sonion support their customers at each stage of product development, from initial concept through design refinement and mass production. "Our goal is to become partners with our customers and codevelop with them, rather than just being their suppliers," said Michele Colloca, head of receiver & RIC development at Sonion.



The modeling and simulation team at Sonion. Clockwise from top left: Michele Colloca, Justin den Heijer, Oleg Antoniuk, and Bas Haayen.

In his work, Colloca can be found leading teams of simulation engineers in the Netherlands and Vietnam, providing different R&D departments at Sonion and their customers with modeling support for existing products and new concepts, validating models with experiments, and explaining the mechanisms behind Sonion's transducers. "We see modeling as a place of mutual enrichment, where we can exchange information and solve problems. Our models are a place where we and our customers can join together to improve the end users' experience," said Colloca.

As captured in the following Q&A, we connected with Colloca to learn about the main challenges in designing hearing instruments, how modeling and simulation helps accelerate R&D, and how Sonion is moving hearing aid technology forward.

Q What trends and consumer demands are driving new developments in hearing aid technology?

MC: The main goal of hearing aids is to help people hear better in any environment. This involves improving the audio quality of these devices, particularly their speech understanding in noisy environments. Additionally, it entails enhancing the robustness of hearing aids and improving their visual appearance by making them smaller and less visible, so people want to wear them. Finally, it involves making hearing care more accessible and affordable, so more people are able to make use of hearing aids.

Q When it comes to designing components for hearing aids, what are the main challenges?

MC: At Sonion, we design and develop balanced armature receivers for a wide range of hearing aid power levels and applications, in both single and dual configurations; hybrid and electrostatic receivers for specialized and professional use cases; ready-made steel or plastic-based receiver-in-canal (RIC) systems for hearing aids; and miniature electret and MEMS microphones for high-performance and low-power hearing aids (Figure 1).

Therefore, we need to deal with multiple key tradeoffs. For instance, our transducers must be small enough to fit in a hearing aid while performing with low power consumption, minimal distortion, and, in the case of balanced armature receivers, reduced interference from mechanical vibrations, magnetic feedback, and acoustic feedback. In addition, our MEMS microphones need to be highly sensitive to sound but not to vibrations. Further, our components must be reliable and robust against temperature, humidity, and contamination via earwax and dust.

From a modeling perspective, our devices are inherently multiphysics and characterized by strong nonlinearities. For example, optimizing a model's electrical domain can have a negative impact on its acoustical domain and vice versa. Finding the right balance is always a challenging yet fascinating task.

FIGURE 1 Sonion's balanced armature receivers (top), ready-made steel RIC system (middle), and miniature electret and MEMS microphones (bottom).

Q Considering the stakes in this work, what are the consequences of getting a design wrong?

MC: When an optimal design is not achieved, it can result in the need for multiple design iterations, leading to long development times and higher R&D costs; delays in market and product launches for original equipment manufacturers (OEMs); and missing out on design-win opportunities in bid phases.

Q Why does Sonion turn to modeling and simulation to help develop hearing aid components?

MC: Our modeling and simulation work allows us to spend time and resources more efficiently before starting the prototyping phase. Building virtual prototypes in the COMSOL Multiphysics® software also allows us to achieve faster iterations on design concepts. In addition, with the finite element analysis (FEA) techniques offered in the software, we are able to thoroughly study the behaviors of our products that would otherwise be difficult to measure or observe clearly in a lab.

Q Can you share an example where you found modeling and simulation especially important?

MC: In many applications, a balanced armature (BA) receiver can get close to a strong external magnet. For example, this can happen when a hearing instrument, such as an earbud, is placed in the charging case. The charging case can contain magnets to guide the inserted device into position. This can have negative consequences because the external magnet's field can penetrate high permeability components of the BA receiver and interfere with its magnetic operation. As a result, the hearing aid or earbud may malfunction, as the interaction between the external and internal magnetic fields — from the charging case and BA receiver, respectively — will impede the BA receiver's ability to produce sound, or the sound may have high distortion (Figure 2).

To analyze this interaction, we created a model in COMSOL® to analyze the interference of the magnetic flux due to the external magnets with the magnetic flux generated by the BA receiver used to displace the armature. The simulation results showed that when an additional magnetic flux is added by the external magnet to the magnetic path inside a receiver, the flux changes the magnetic reluctances of the entire magnetic circuit and causes the receiver magnets to demagnetize.

Q Can you share a second example where you found the use of modeling and simulation useful?

MC: In professional audio and hearing aid technology, lumped element models are often used as a quick and convenient tool to predict the behavior of audio transducers, such as MEMS microphones. To increase the accuracy of these models, end corrections for a spout or sound inlet need to be included on the acoustic channel length. These end corrections describe how an acoustic channel is open to the outside environment, such as a channel with an open end or a channel that ends with an opening in the infinite plane, called a *baffle*. The coefficients that reflect the end correction to the acoustic mass of the spout or inlet are well known. The end correction coefficient for the real part of the acoustic impedance, which corresponds to the channel's acoustic resistance, is typically assumed to be the same as that for acoustic mass.

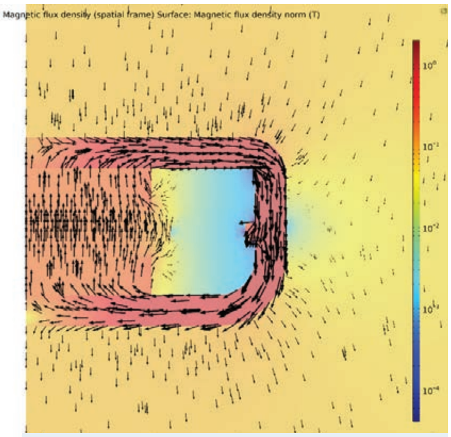


FIGURE 2 Magnetic flux density created by both external magnets in the charging case and internal magnets in the balanced armature receiver.

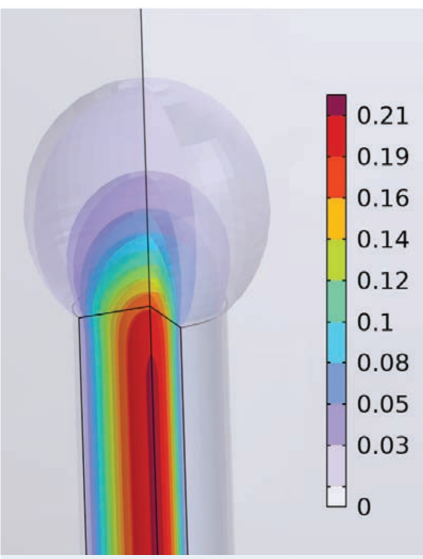


FIGURE 3 A simulation illustrating the particle *z*-direction velocity profile of the acoustic channel open to the outside with thermoviscous effects included. This simulation allowed Sonion to accurately quantify the end correction due to acoustic radiation to the open environment.

In our study, we used thermoviscous acoustics in COMSOL to introduce and quantify the end correction for acoustic resistance. By doing so, we found that the end correction for acoustic mass can be different from that used for acoustic resistance (Figure 3).

Q Why are lumped element models important for audio and hearing technology R&D?

MC: The key receiver performance indicators, such as electrical impedance, sound pressure levels, and vibration, strongly depend on the design of the transducer itself as well as the acoustic load connected to it. In this case, the acoustic load represents the human ear and the connecting sound channel. The typical device used to model the average human ear is the ear simulator, known as the *711 coupler*. However, when considering the entire volume and special features of this ear simulator, as well as the structure of acoustic tubing needed to connect the receiver to the ear simulator, we end up with a very large fully coupled FEA model that is computationally expensive.

We adopted an approach to simulating the acoustic tubing and 711 coupler as a two-port network instead of a fully coupled FEA model. Such an approach can offer significant gain in computational time. We validated the transfer matrix method with the COMSOL Multiphysics software against a complete FEA of a transducer, tubing, and a coupler. Setting up a lumped representation of tubing and a coupler by adopting a transfer matrix implementation reduced model complexity and computational time dramatically. In the end, we were able to test different concepts and quickly select the virtual prototype to develop into a physical one for testing in the lab.

Q How has simulation improved product development at Sonion?

MC: A virtual prototype cannot replace a real prototype, we will always need to build a physical prototype, measure, and validate the model. But once the model is validated, the virtual prototype will be robust enough to be used for selecting the right design concept. To further illustrate this point, let's consider an example of a prototyping process: When testing a singular design concept, you need one virtual prototype, which takes roughly seven hours to build. However, without a virtual prototype, you would need to build at least 5 samples, test them, and measure them for each concept, which takes 40 hours on average. Therefore, simulation reduces the time required for testing one design concept by a factor of at least 5.7. In this scenario, the number of learning processes per euro invested increased exponentially by adopting virtual prototyping.

Q How are your products helping to move hearing aid technology forward?

MC: Sonion products address the key trends in the hearing aid market. We strive to improve the performance of our products and make their audio quality better. New products must adhere to rigorous quality standards, and we continuously push the limits of our products' reliability to enable better and more robust hearing aids. Our product designs take the full hearing aid into consideration, which helps enable manufacturers to make even smaller hearing aids. Finally, we always design cost-effective solutions so that we can support more affordable hearing care.

In the future, we plan to further develop our multiphysics models, increase the accuracy of our virtual prototypes by adding variations of component size, drastically reduce our computational times, and improve the parameter vectors for lumped-element-model-based circuits via FEA investigations.

Q What role does simulation play in the future of hearing aid technology?

MC: Virtual prototypes will be more accurate, and the gap between them and physical prototypes will be minimized. And thanks to the increase in computer processing speed, the transition from design to testing and from testing to product launch will be rapid.

As for the future of hearing aid technology in general, I believe it will involve advanced signal processing features that improve speech intelligibility in different environments, connectivity, sound quality, robustness, and size reduction. The new hearing aid platforms will include more and more AI for enhancing speech recognition in noise, with a tradeoff on power consumption. ◎

NASA Ames Research Center, California, USA

DESIGNING NEXT-GENERATION CARBON DIOXIDE REMOVAL TECHNOLOGY FOR BETTER LIFE IN SPACE

NASA combines thermal modeling and experimental testing to find the best compressor design for the system that keeps the air breathable at the International Space Station.

by **FANNY GRIESMER**

The International Space Station (ISS) is made livable in great part thanks to a system that captures and removes CO_2 from the air. The workhorse inside that system is a compressor, which fulfills its CO_2-capture duties, but at a cost: it is noisy and requires frequent maintenance. Engineers at NASA used modeling and simulation with experimental testing to analyze the next generation of compressor designs that get the job done more quietly, with fewer maintenance needs, and at lower fabrication cost.

» CONTAMINANT REMOVAL TECHNOLOGY

Astronauts signing up to live and work on the ISS put a lot of trust in the engineers behind the contaminant removal technology that rids the cabin of CO_2 (Figure 1). "Currently, there is a system called the Carbon Dioxide Removal Assembly (CDRA)," explained Dr. Hannah Alpert, an aerospace systems engineer at NASA Ames Research Center.

"The CDRA absorbs CO_2 to remove it from the cabin. Then, that CO_2 is sent to a Sabatier reactor where it is combined with hydrogen from the oxygen generation system to produce water." That water is supplied to the astronauts for drinking. (Figure 2) "We have this closed-loop system to keep the astronauts alive, but in order for the CO_2 to work with the Sabatier reactor, it has to be at a higher pressure than what it is absorbed at, so we have a compressor in between the CDRA and the Sabatier reactor," said Dr. Alpert. The CDRA is currently being upgraded to a new four-bed molecular steam system: the four-bed, CO_2 scrubber, or 4BCO2.

FIGURE 1 Astronauts working on the CDRA. Image by NASA and in the public domain via Wikimedia Commons.

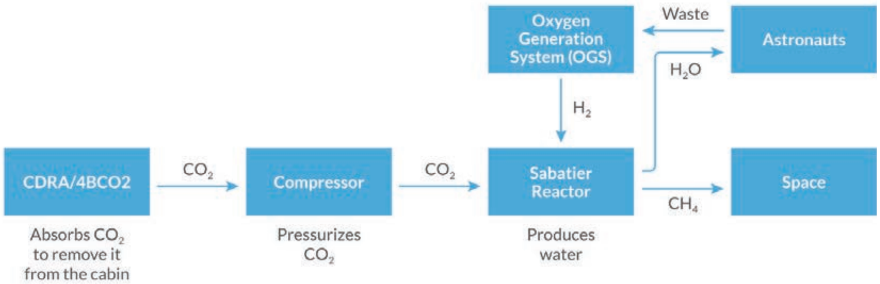


FIGURE 2 The contaminant removal system process.

Dr. Alpert explained that the new system is meant to improve reliability and performance over the CDRA, which means that they are making various changes. For starters, the sorbent they were using for the CO_2 capture needs to be replaced. Additionally, they have redesigned some of the components. "They switched from a rectangular to cylindrical bed, redesigned the heater core to better distribute the sorbent and eliminate the void spaces, and they are adding a filter to capture dust and new valves for longer operating lifetimes," outlined Dr. Alpert. That said, the basic functionality as far as how the 4BCO2 integrates with the compressor that Dr. Alpert's team is working on is essentially the same as the current system.

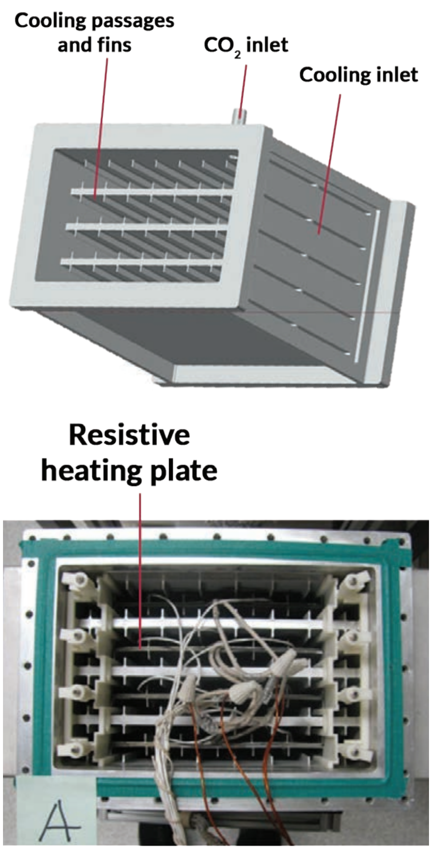
» REDESIGNING THE COMPRESSOR

The current system features a mechanical compressor that is high mass and power, resulting in a lot of noise. The many mechanical rotating parts require frequent maintenance, and it is expensive to manufacture and run. "So, we are looking at some alternative technologies, and one of our leading options is called an air-cooled temperature swing adsorption compressor (AC-TSAC)," said Dr. Alpert. "The AC-TSAC has lower mass and power requirements; it is less noisy; there are no rotating parts, so that will hopefully reduce the frequency of needing to replace parts; and then it is lower fabrication cost and easier to make."

The AC-TSAC is a bed filled with minerals that capture CO_2, called zeolite pellets, and it adsorbs CO_2 more efficiently at room temperature. After pressurizing the CO_2, it is delivered to the Sabatier reactor. To ensure that CO_2 is constantly being supplied to the Sabatier reactor, the AC-TSAC is split into two beds. The team has developed one version of the AC-TSAC, and now they are using thermal modeling to further improve on their designs.

» THERMAL MODELING INFORMS DESIGN CHOICES

Dr. Alpert turned to the COMSOL Multiphysics® software to build models of the current AC-TSAC design. "We have found COMSOL® extremely useful over the past few years. One of the first projects I worked on when I joined NASA was modeling a heat flux gauge that flew on the Mars 2020 heat shield, and



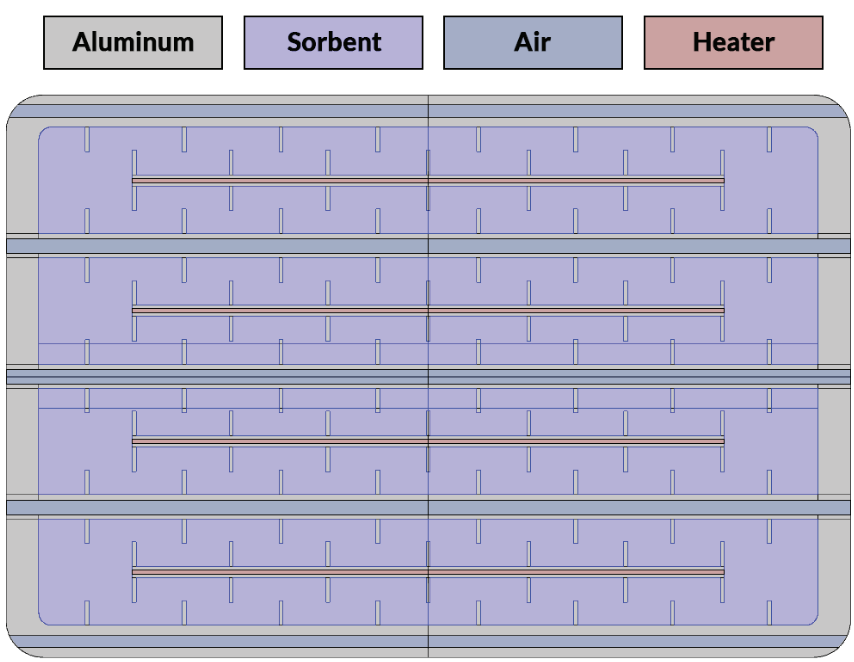


FIGURE 3. The actual compressor and models representing it.

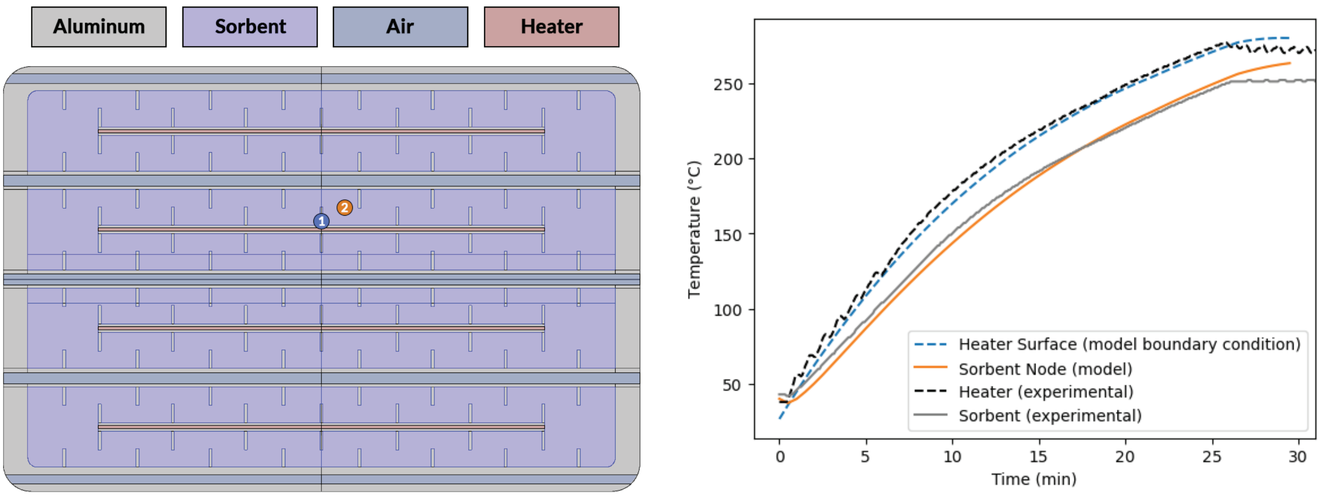


FIGURE 4 Experimental results from the two-bed test and model show good agreement.

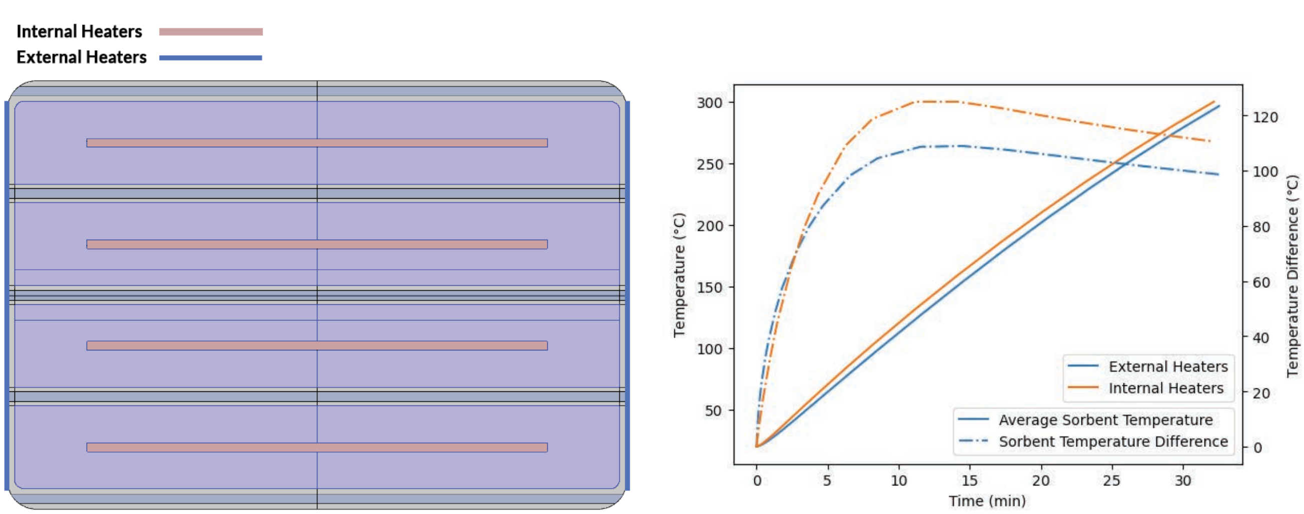


FIGURE 5 Thermal modeling shows that external heaters (blue) perform similar to internal heaters (orange).

lately, I have been using the Optimization Module to reconstruct the surface heat flux on a heat shield," Dr. Alpert said.

For the compressor project, she built both 3D and 2D versions of the model and, after concluding that both produced the same results for her purposes, she moved forward with the 2D model, since it took less time to run. Inside the AC-TSAC there are three shelves in the middle and zeolite pellets packed into the open spaces (Figure 3). Between each of the shelves are resistive heating plates to heat up the bed. The cooling channels allow air to flow through during the cooling stage.

» VALIDATING THE MODEL

To validate the model, the team used temperature and power readings from two test campaigns that were done on the AC-TSAC. "The first one was a two-bed test for functionality at NASA Marshall. Then, we did a more focused test campaign at NASA Ames, where we used one bed to isolate the exact properties more," said Dr. Alpert.

During the NASA Marshall test, they placed resistance temperature detectors on the heater surface to measure the temperature. From there, they used the measured temperature as one of the boundary conditions of the model and ran the model to check if the modeled temperature matched the experimental data (Figure 4).

Next, the team performed the focused test at NASA Ames, which tested a single bed and collected experimental data from the heater surface and sorbent node. In this case, they used the measured power as input to their model and then they measured the temperatures at the heater node and sorbent node in the model. When they compared the model to the test results, they saw good overlap between the data.

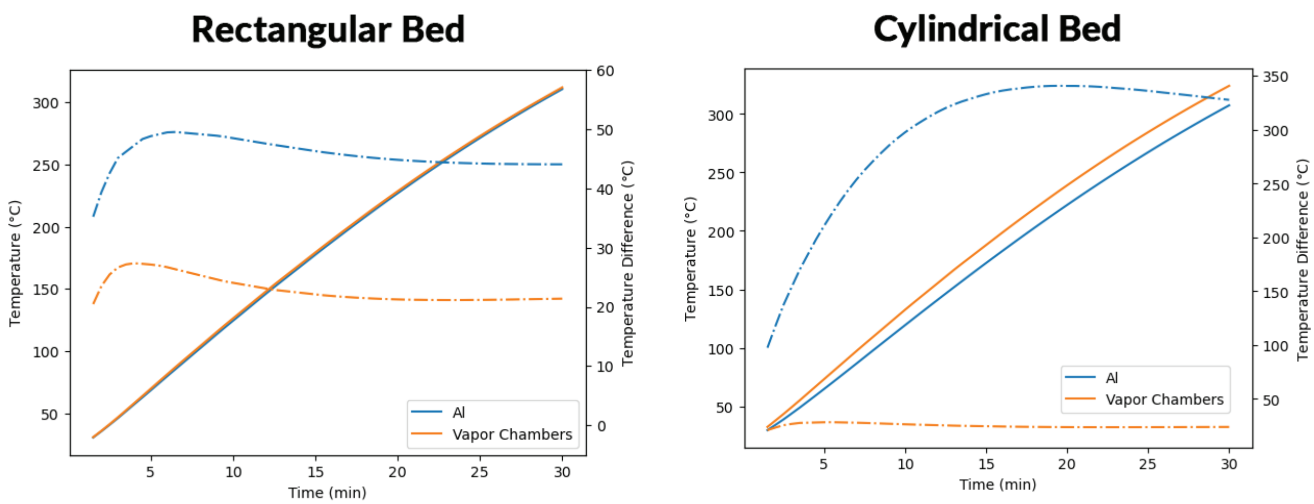


FIGURE 6 Average sorbent temperature (solid lines) is largely unchanged, but uniformity (dashed lines) is much better for the vapor chambers.

Validated model in hand, Dr. Alpert and her team were ready to analyze how different design changes would affect the heating and heating rate of the compressor.

» DESIGN TRADE STUDIES

As part of their search for the best new design, the team looked at specific design trade studies, including, but not limited to: internal vs. external heaters and aluminum bed vs. vapor chambers. The goal was to reach high temperature quickly and for the temperature to be uniform throughout the bed during ramp-up.

"The first design trade that we looked at was switching from internal heaters. Right now, there are internal heaters that are in the middle of the beds, and these are a potential point of failure. There are a lot of wires going into the bed, and it is just a complex, messy bundle of wires and heaters," said Dr. Alpert. This led the team to wonder if it would be possible to move those heaters and if doing so would still heat up the sorbent quickly and uniformly. Using Dr. Alpert's model, they applied power to the internal and external heaters to compare the heating rate and uniformity (Figure 5). "Switching from internal to external heaters did not have a very big impact, which means that using external heaters rather than internal has the potential to improve or at least have the same amount of temperature uniformity of the sorbent while also reducing the complexity of the system."

In another study, the team analyzed the effect of switching from an aluminum bed to using vapor chambers (Figure 6). NASA works with external partners that manufacture and test the vapor chambers and perform high-fidelity modeling. The team modeled the vapor chambers using the material properties of aluminum, but at a much higher thermal conductivity, to get an idea of what the effects would be. Dr. Alpert noted that their main takeaway "is that when we switch to a vapor chamber bed instead of an aluminum bed, while the average sorbent temperature remains pretty much the same, using vapor chambers has the potential to improve the temperature uniformity of the sorbent."

» PERFORMANCE SENSITIVITY ANALYSES

The NASA team also sought to increase the thermal conductivity of the sorbent itself. In the thermal model of the original AC-TSAC design, the team saw that increasing the thermal conductivity of the sorbent did not have much of an effect on the average sorbent temperature, but it did improve the temperature uniformity to a large degree. "That tells us that we are definitely going in the right direction and [as a result are] focusing a lot of our development efforts on that," said Dr. Alpert.

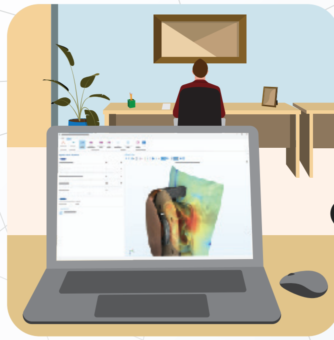
Similarly, when the team increased the thermal conductivity in their model of a cylindrical bed with vapor chamber, the simulation results showed a large improvement in the temperature uniformity of the sorbent throughout the bed.

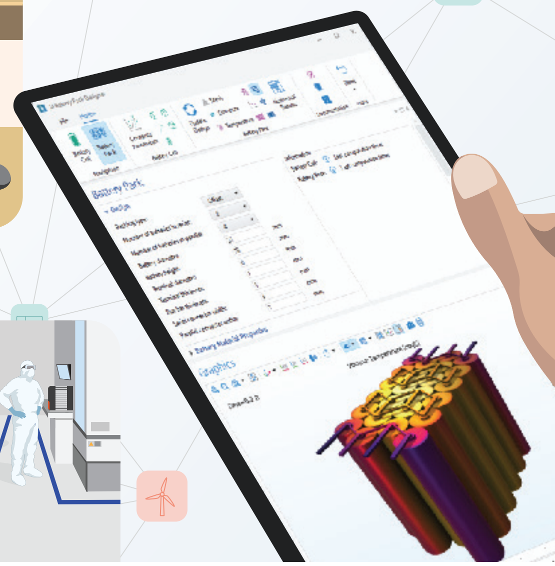
» COMBINING SIMULATION WITH EXPERIMENTAL TESTING TO FIND BETTER DESIGNS

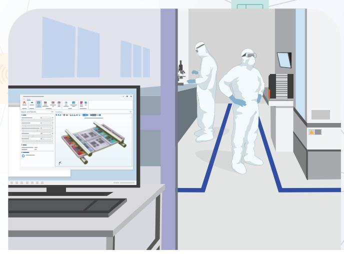
Dr. Alpert and her team successfully created a thermal model of the existing AC-TSAC and validated it against test data. Using the validated model, they were then able to determine which design parameters to change in order to get the desired results. Through simulation the team learned that external heaters reduce the system complexity and failure potential, vapor chambers have higher thermal conductivity and thereby improve the temperature uniformity of the sorbent, and they should continue to focus on increasing the sorbent thermal conductivity. The team will continue to validate the thermal model with experimental data and account for mechanisms like heat loss. ◎

This is an abridged version of the article published at https://www.comsol.com/story/designing-next-generation-co2-removal-technology-for-better-life-in-space-131721

Figures 2–6: Original images courtesy of NASA, modified by COMSOL.







Press Fast Forward on Development with Simulation Apps

by **FANNY GRIESMER**

Time and again, engineers from all types of industries demonstrate that by using modeling and simulation, they can iterate on designs much faster, enhance their understanding, and plan R&D projects more effectively. A selection of such success stories are in this very magazine. It is worth noting, though, that using simulation in the more traditional sense requires specific expertise and training on how to use the software of choice. As a result, modeling and simulation is most useful to those engineers who have learned the necessary skills to build computational models and the benefits reaped by the organization are more limited than they could be. What if the use of simulation was extended beyond the R&D department? Simulation-based decision making could greatly benefit colleagues and customers working in the field, factory, and lab, with broader impacts for the business at large as a result.

For instance, technicians, sales staff, and customers in the field could make simulation-guided decisions on site using real-time inputs such as weather data, customer-provided details, and other situational information. Colleagues working on the factory floor could optimize production processes based on facility conditions and validate on-the-spot design changes, ultimately leading to better manufacturing outcomes for the company. Researchers in the lab could combine experimental testing with simulation right then and there to enhance their understanding of the results and make faster predictions based on what they learn.

We already know that modeling and simulation is effective at giving a preview of the real-world outcome before you commit to a project plan or design, and coupled with experimental data, it creates a more comprehensive understanding of results. One roadblock in the way of expanding on its use is that colleagues and customers in the field, factory, and lab need answers on the spot, in the moment, and cannot afford a back-and-forth with the simulation engineer working in a completely different location. So, what's next?

Instead of accepting that there are some places simulation cannot go, consider building your own custom apps that are based on your computational models but with a select subset of input fields and faster results. Building and distributing your own simulation apps is like putting a personal simulation expert into the pockets of your employees and colleagues, one they could consult in the exact moment when they need answers, no matter where they are located. The real-world data gathered through the apps can also be sent back to the design and simulation engineers working in the office, helping them validate their models and improve on them.

The tools to build and edit simulation apps from your models are included in the COMSOL Multiphysics software. There is built-in functionality to quickly customize your app's user interface, but you can also write your own code if that is your preference. For apps that display results with lightning speed, you can take advantage of machine learning capabilities. In terms of getting your simulation apps out to those who need them, there are two main ways to go about it: compile them into standalone files that anyone can run anywhere in the world or host them in your own COMSOL Server environment with managed access via web browser. There are different advantages to each method, so the choice is entirely yours.

Simulation apps do serve a purpose within the general R&D workflow as well, of course, bringing productivity gains by enabling engineers to test design iterations very quickly and improving collective knowledge retention within the broader organization. Sometimes the app author is also the app user; by building a streamlined user interface for a model, you can save yourself time, too. The possibilities are endless and customizable — by you! — to fit nearly any given context. COMSOL does not build or control the apps for you; we put that power into your hands.

Organizations that build and distribute their own apps are able to extend the benefits of simulation-based decision making to more collaborators within the R&D workflow and even to colleagues and customers far removed from it. What follows is effective collaboration and accelerated innovation. ◎