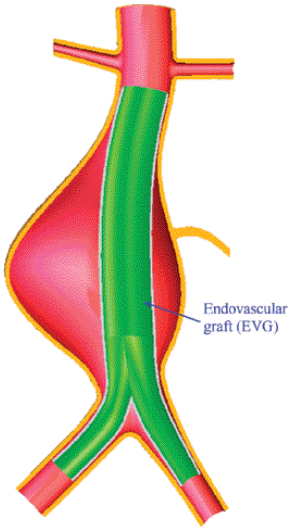
# CFD Software Streamlines Product Development

An increase in computational fluid dynamics software's ease-of-use and capacity to simulate complex models are boosting its popularity in the medical and pharmaceutical fields. This rise is leading to the displacement of physical prototypes by virtual models.

Pharmaceutical and medical companies are coming under increased regulatory and financial pressure to accelerate and improve the results of their R&D efforts. As a result, they are expanding their use of computational fluid dynamics (CFD) software to build virtual biological models to predict a product's performance before spending the time and money to build it.

Researchers use CFD software to divide the biological areas they are studying into three-dimensional finite element-type grids, or meshes, and use partial differential equations to describe the fluid flow through each mesh element to determine different variables, such as temperature, pressure, and velocity. CFD solutions can take minutes or hours to solve, depending on the size and complexity of the model being simulated. However, with the speed and capacity of computers increasing, these run times continue to improve. An added benefit is CFD software's present capacity to operate on most common platforms, such as Linux, UNIX, and Windows.




**ANSYS's CFX software is used by North Carolina State Univ.'s biomechanical engineering research group to represent a cross-section of an aortic artery aneurysm (bulge on left) between the renal artery (to the kidneys, top) and the iliac bifurcation (to the legs).**

## The new market high-flyers

"The medical, bioengineering, and pharmaceutical industries have long been an area where modeling has been absent," says Tim Niu, marketing manager at COMSOL, Inc., Burlington, Mass. This was due to the nature of the phenomena studied by these researchers, which was too complex to be adequately represented by the CFD software that was available then. However, with enhanced numerical methods and computers, "even highly specialized multi-physics modeling is being handled at the desktop," says Niu. As these industries continue to enjoy the advantages of CFD tools, they are becoming "the new high-flyers" for venture capitalists.

To rapidly gain an insight into the new technologies emerging in these fields, mathematical modeling is key. Providing such a modeling solution is COMSOL's FEMLAB 3.0, which integrates with MATLAB, offering more flexibility to its user. One such user is Steven Conrad, a professor in the department of emergency medicine at the Louisiana State Univ. Health Sciences Center, Shreveport. Conrad applies FEMLAB to examine the fluid and solute flux in hollow fiber membranes that are used for hemofiltration in critically ill individuals with fluid overload or renal failure. The goal is to discover the factors that affect the solutes' and fluid's transfer across the membranes to acquire a greater understanding of these membranes' limitations.

The advantage for Conrad in using FEMLAB lies in the software's ability to "model with almost microscopic spatial resolution." This sharply contrasts with earlier solute transfer models, which employed coarser models of hemofilters.

Due to this microscopic resolution, proteins—which do not cross the membrane—were revealed as the possible greatest contributors to the limitation of the fluid transfer at elevated filtration rates. At these rates, "the protein concentration near the membrane resulted in sufficient elevation in osmotic gradient to account for all of the fluid limitation," says Conrad.

## Airflow modeling

Improvements in computer speed are also driving pharmaceutical and medical researchers to reap the benefits of CFD simulation tools by Fluent, Inc., Lebanon, N.H. This CFD use is expected to benefit from the software's increasing relevance to the needs of these industries. As a result, "many in the future will find even more ways to take advantage of flow modeling software," says Ahmad Haidari, global business industry director at Fluent.

The company's line of CFD software includes FLUENT 6.1, whose applications range from modeling physiological

flows in the respiratory, circulatory, and digestive systems, to medical instruments and drug manufacturing. In the study of drug delivery systems, for instance, this software is used to examine the differences between the respiratory tract of laboratory animals and people, to determine the inhaled medication's airflow. This ability to complement animal experimental techniques is useful, since "these experiments take a long time to perform, are expensive, and in certain cases, may involve risk to both animal and/or human subjects," says Haidari.

## Fluid-structure interaction

The rising relevance of CFD software to the biomedical and pharmaceutical sectors is complemented by its enhanced geometric capabilities. "CFD has come a long way. Geometric flexibility has increased to the point where there are now few geometries too complex to be represented accurately," says Ian Jones, CFX consultancy manager at the European site of ANSYS, Inc., Canonsburg, Pa. With the challenges of modeling geometrically intricate configurations surmounted, "one of the future directions of CFD, and in particular ANSYS, is integration in areas such as fluid-structure interaction."

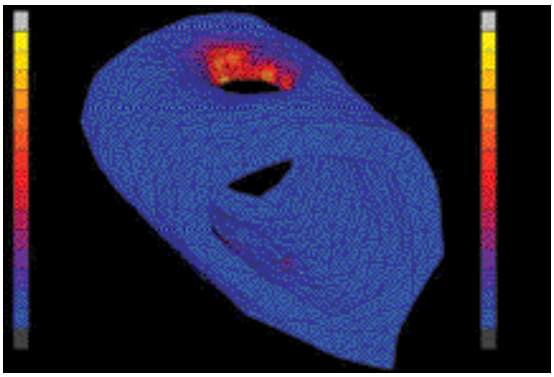
This integration is manifested in the work being conducted by a team of researchers led by Clement Kleinstreuer, director of the biomechanical engineering research group (BERG) at North Carolina State Univ., Raleigh. Using a predecessor of ANSYS's CFX-5.7, which was launched this year and runs on all standard platforms, the team applied the software to study the use of stent-grafts in the repair of abdominal aortic aneurysms (AAA). Such a repair typically involves propping the stent-grafts, which are tubular wire mesh stents interlaced with synthetic graft material, open in the aorta to provide support.

The problem is that these grafts occasionally get dislodged, re-exposing the weakened artery wall to the high pressure of the pulsating blood flow. This endangers the patient's life due to the increased risk of an AAA-rupture, which is generally fatal. To find a possible solution to this migration, the BERG team used CFD, along with computational structure analysis, to examine an aorta both before and after the surgical introduction of a stent-graft.

The work showed that the risk of an aneurysm rupture is minimized with the surgical insertion of stent-grafts. It also "helps us with design optimization of stent-grafts and secure stent-graft placements," says Kleinstreuer.

## Design and analysis consolidation

Another software that is being applied in research involving stents is the CFD software by CFD Research Corp., Huntsville, Ala., which was recently acquired by ESI Group, Paris, France. The application involves the examination of drug elution from polymer-coated stents to forecast drug uptake in and around the stented area. Such simulations are facilitated by the company's CFD-CAD*alyzer*, which consolidates design and analysis in one operation. This consolidation "addresses the trend toward integration that eliminates the need to specify a design twice, once in computer-aided design (CAD), then again in the analysis software," says Mike Nieburg, strategic marketing manager at ESI Group's American division. This ability to work directly on the CAD model eliminates the problems encountered when translating between varying geometry depictions.



**MSC.Software allows users to study the forces acting on dental implants and bone, gaining insight into the complex processes occurring with the modification of the bone.**

CFD-CAD*alyzer* targets non-CFD experts, who rely on CAD early in the design stage of product development. This is useful since "global competitive pressure and squeezed margins are driving companies to invest where they have high leverage—early in the design process," says Nieburg. Delivering results in a few minutes to a few hours, the software allows parallel CFD simulations to determine the potential performance of numerous designs. It also uses OpenHSF, an interface commonly used to easily proceed through all the stages of a product life cycle.

Additionally, CFD-CAD*alyzer* provides the operator with all of the multi-physics capabilities and features of the company's CFD-ACE+, which was used by Altea Therapeutics, Tucker, Ga., to develop the PassPort patch. Comprised of a porator—a planar array of metallic filaments linked to a reservoir filled with a drug—the PassPort patch continuously releases therapeutic macromolecules through the skin. When a specific amount of electrical energy is delivered to the porator through a portable activator, the skin cells in contact are ablated. The generated micropores are then used to locally deliver the drug into the body.

The creation of the proprietary PassPort patch involved 3-D numerical models and analyses to examine skin ablation by a rapidly-heated tiny filament, taking into consideration gas escape and the vaporization of volatile skin components. Numerical analyses of the generated model were used to forecast the shape of the micropore, as well as the interface dynamics during its formation. "The model demonstrated the existence and importance of convection in the gas phase caused by the heated vapor escaping from the micropore to the outside environment," says Vadim Yuzhakov, principal engineer at Altea Therapeutics. It also showed that the vapor escape changes over time, leading to undulations in the micropore's morphology.

## Customized solutions

The reduction in design time is also being addressed by MSC.Software, Santa Ana, Calif. Previously in the R&D medical sector, "manufacturers relied upon time and cost-intensive physical testing, or building and breaking multiple prototypes, before releasing a design for clinical trials and regulatory approvals," says Leslie Mackin, biomedical business development manager at MSC.Software. But, with today's focus on reducing cost, a software that predicts a product's performance before it is fabricated is essential.

To help medical device manufacturers in this quest is a variety of MSC.Software customized simulation software packages. These packages can be used by an individual on a laptop or numerous users with cluster connectivity. They target specific manufacturers in different fields, ranging from dental, and ocular, to orthopedics. Among these packages is MSC.Patran, applied for the modeling of complex medical devices, and MSC.Marc, which simulates complex interactions, including nitinol materials.

The simulation of the interaction between medical devices and complex human tissue is "truly revolutionary in that these types of devices, materials, and contacts could not have been simulated even two or three years ago," says Mackin. Conducting such work is Centerpulse, Zurich, Switzerland, which used MSC.Patran to model and assess the function and impact of a joint implant on bone. With this software, researchers were able to apply inverse kinematics, muscle forces from *in vivo* measurements, and set material properties as in real bones. In the end, this virtual testing enabled Centerpulse to gain insight into the various kinds of implants that can be introduced into the same bone without damaging it.

Operating on a laptop and desktop is also the ACUITIV CFD Visualization Software by ACUITIV Software, Batavia, Ill. ACUITIV's strength lies in its ability to integrate with immersive environments. The integration enables users to alter viewpoints or parameters in real-time, without having to exit the 3-D environment. This is due to the software's architecture, which uses virtual reality Juggler and OpenGL libraries.

ACUITIV software is used by Richard Calabrese at the Univ. of Maryland, College Park, to perform simulations of a high shear mixer, which pumps chemicals together to make emulsions and dispersions. "Today, most medicines are purified by crystallizations and high shear mixing helps control the crystals," says Calabrese. These simulations allow the visualization and understanding of the flow fields, enabling the researcher to refine the process.

## Upfront CFD

Maximizing the throughput of non-CFD specialists is also on the agenda at Blue Ridge Numerics, Inc., Charlottesville, Va. Its recently launched CFdesign v7.0 "was developed for multi-tasking product development personnel—people who do not have the time or ability to master traditional commercial CFD applications," says Len Whitehead, CFdesign product manager.

An extra advantage of this software is its ability to fully simulate and optimize translating and rotating machinery, depicting the interaction with its surrounding stationary objects. This is crucial because "most rotating frame implementations are suited only for analyzing a single blade passage, and provide no provision for neighboring stationary objects," says Whitehead.

Applications of earlier versions of this software have included the flow of liquid in sterilization tools, and the cooling flow for electronic medical apparatus, such as ultrasound machines.

*–Danielle Sidawi*

### >> Resources

ACUITIV Software, 630-845-4500, www.acuitiv.com
Altea Therapeutics, 678-495-3100, www.alteatherapeutics.com
ANSYS, Inc., 724-746-3304, www.ansys.com
Blue Ridge Numerics, Inc., 434-977-2764, www.cfdesign.com
Centerpulse, 41-1-306-96-96, www.centerpulse.com
CFD Research Corp., 256-726-4800, www.cfdrc.com
COMSOL, Inc., 781-273-3322, www.comsol.com
ESI Group, 33-1-53-65-14-14, www.esi-group.com
Fluent Inc., 603-643-2600, www.fluent.com
Louisiana State Univ. Health Sciences Center, 318-675-5000, www.lsuhsc.edu
MSC.Software Corp., 714-540-8900, www.mscsoftware.com
North Carolina State Univ., 919-515-2011, www.ncsu.edu
Univ. of Maryland, 301-405-1000, www.umd.edu