Ongoing advances have helped to make Computational Fluid Dynamics (CFD) modeling faster and easier to use than ever before. This is helping users to cost-effectively streamline product design and to optimize operations.

Providing powerful design *and operational insight*

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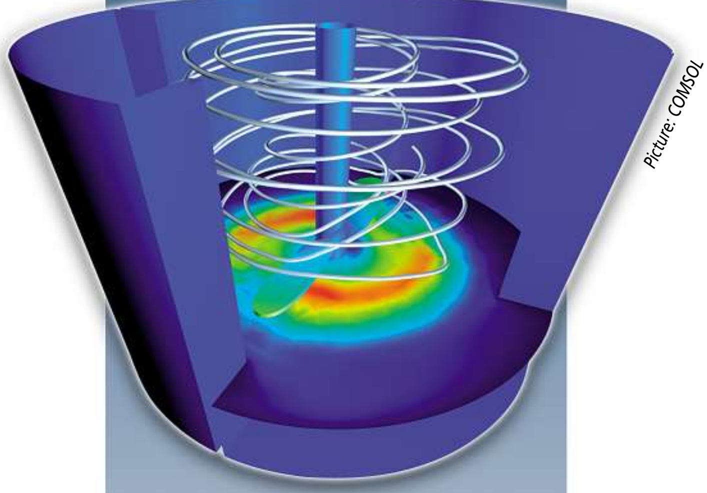
Computational fluid dynamics (CFD) software enables the rapid numerical solution of the physics-based equations (otherwise known as the Navier-Stokes equations) that govern the conservation of mass, momentum and energy, fluid motion, heat transfer and other phenomena. By solving these equations at several thousand discrete points on a computational grid (called the "mesh") that is set up to approximate the geometry of the equipment component or system being modeled, CFD programs are able to effectively simulate such critical process phenomena as fluid flow behavior, temperature distribution and chemical reactions.

Today, CFD modeling provides a powerful way for engineers, researchers and other technical professionals to visualize what's going on inside most types of chemical process equipment, such as mixers, reactors, pumps, combustion systems, material-handling equipment, pollution-control systems, pipelines and other types of complex process vessels. And, when CFD modeling is combined with other types of modeling software (discussed below), users are able to not only understand fluid behavior in the system, but to analyze and predict structural response, fatigue and vibration characteristics in the machinery, as well, in order to better predict equipment performance.



The velocity field in a baffled mixer. Seen is the magnitude of the velocity on the blades of the propeller and in the slice plot. The velocity vector field is described by the streamline plot.

Picture: COMSOL

When CFD modeling was first developed several decades ago, it was mainly used by researchers and academics who had the specific background and training that was needed to work with such specialized software. More recently, aspects of CFD modeling – including upfront mesh generation, the CFD solver itself, and downstream post-processing capabilities – have been improved, so today, off-the-shelf programs are faster, more powerful, more intuitive, and easier to use than ever before. This has vastly increased the adoption of this powerful modeling technique throughout the global chemical process industries.

For equipment designers, CFD modeling is now widely used to streamline the equipment-design process. For instance, by carrying out CFD analyses, equipment designers are able to envision and evaluate next-generation machine designs, modify or eliminate inefficient approaches, and validate winning strategies – before costly physical prototypes are ever manufactured to test each case. This helps to reduce the design cycle, speed the time-to-market for the product, and trim manufacturing expenses by reducing the need for extensive prototype development and physical testing.

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Meanwhile, for process operators, CFD modeling is being used to fine-tune operating parameters and evaluate alternating operating scenarios and potential adjustments to operating parameters, in order to troubleshoot and optimize operations, reduce emissions, address vibration problems, increase throughput rates and product yields, and more.

Whether it's used during design or operations-improvement efforts, CFD provides a cost-effective way to support engineering creativity in the virtual realm, and allow users to pursue innovative design modifications and operational adjustments that may not otherwise be intuitively obvious. And these efforts are paying off, in terms of demonstrable benefits to users, in terms of improved operations and savings.

Bringing CFD to the people

In addition to ongoing improvements in the algorithms that are at the heart of any CFD program – enabling more-complex modeling challenges to be addressed by the average user – the user interfaces included in today's CFD packages have been continuously refined over the years. For instance, today, they routinely include a range of prompts, wizards and other embedded tools that provide step-by-step instructions to guide users through the process. These include intuitive features such as pull-down and pop-up menus, intuitive templates, and built-in and user-programmable functions, which prompt users through the model setup and execution.

Users also benefit from the automatic error-checking functionality that is included in most of today's CFD programs. These can spot inconsistencies during data input and model setup, and alert users before they move on to the next step. Similarly, "geometry healing" features help many of today's CFD solvers to automatically reconcile "non-optimal" geometry characteristics, such as small gaps, non-matching edges and very small surfaces, in a way that improves both the consistency of the underlying geometry, and the accuracy of the modeled results.

Similarly, orders-of-magnitude improvements in the speed and memory capabilities of today's computers have opened the door for larger and more complex equipment components and chemical process systems (which are typically characterized by inherently unsteady flow fields and involve large, unsteady datasets) to be reliably modeled using standard desktop and even laptop computers – not the supercomputers that were once required for CFD modeling – in a matter of days or even hours, by users who have not particular specialized training in CFD.

Mesh generation

To simplify the complex calculations that are carried out during CFD modeling, the geometry of the system or device to be modeled must first be divided into a mesh of tiny cells – essentially a "virtual prototype" that approximates the intricate geometry of the component being modeled. Then, the underlying equations are solved at each cell.

The number of mesh cells required to accurately convey the complex geometry that is being modeled can number from the hundreds of thousands of cells to millions of cells.

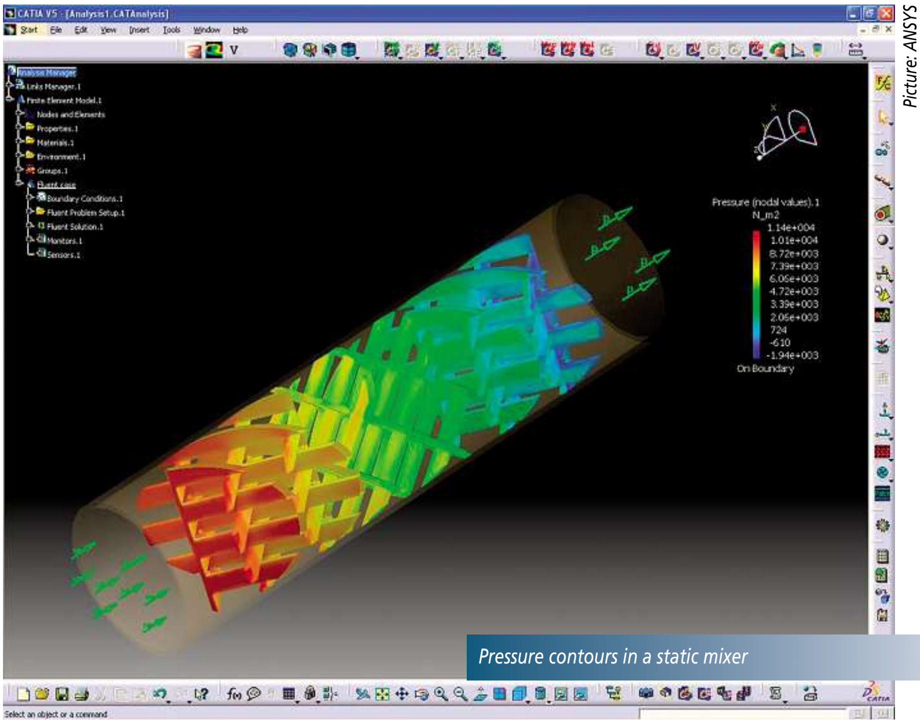
Contemporary mesh-generation programs use a variety of predefined building blocks and standard mesh-style templates based on a variety of geometric elements, such as hexahedral, tetrahedral and polyhedral elements, pyramids, wedges, prisms (or any combination of these). Compared to the conventional tetrahedral meshes, the newer polyhedral meshes have fewer cells, so convergence during modeling is faster, thereby accelerating the simulation. And, these advanced meshing techniques also allow the geometry of virtually any complex component to be accurately represented, even those

Industry examples

CFD is widely used to model a wide variety of mixing applications, including impeller-based mixers for low-shear applications, rotor-stator mixers for high-shear applications, or static mixers. The goal of such modeling is to optimize blending times and mixing conditions, ensure the desired product uniformity, reduce power draw, and reduce wear and tear on the machine.

Similarly, CFD has also proven to be a useful tool for modeling all types of burners and combustion systems, particularly those used in as turbines to produce power and generate electricity. For instance, when CFD is used to characterize fluid flow, combustion-related reactions and temperature distributions at any given cross-section, users are able to evaluate the potential impact of competing burner designs and arrays inside the combustor, optimize inlet air temperatures, maximize combustion efficiency, minimize the overheating of turbine blades, vibration and fatigue-related failures, and improve overall turbine performance and efficiency.

When it comes to managing the particular challenges associated with converting wind power into electricity, today's advanced CFD programs are well-suited to model such complexities. As a result, many in the wind-energy community are turning to CFD to better understand the performance of both existing and future wind turbine designs, and to design state-of-the-art advances in wind blade designs that are both strong and lightweight, in order to maximize wind capture and reduce the cost of wind-based power. They are also using the tool to model site-to-site, and site-specific variations, at various locations, in order to locate wind turbines in the most advantageous locations and arrangements.



Pressure contours in a static mixer

Picture: ANSYS

with complex features such as fuel nozzles and intricate holes and passageways.

Meanwhile, to speed and automate the meshing process, most of today's mesh-generation software programs are also able to accept computer-aided design (CAD) drawings of the component from virtually any commercial CAD program, and to use this as the starting input for the mesh-generation process.

Post-processing software to manage the modeled results

CFD modeling produces vast volumes of data. Without proper data management, the sheer volume of excessive data produced by any CFD simulation can overwhelm the user and slow down the overall computational speed required to resolve the questions at hand.

Today, sophisticated post-processing software (including both software that is embedded in many off-the-shelf CFD programs, and software that is available as standalone programs) is helping investigators to more effectively interrogate large, unsteady datasets, and to visualize critical aspects of complex simulations more meaningfully. Post-processing tools help the user to produce high-resolution color graphics and animations that represent such things a velocity vectors, contours of pressures, and lines of constant flow-field properties.

Partnering CFD with other modeling techniques

These days, CFD modeling is increasingly being coupled with other types of engineering software, to integrate fluid-flow modeling with other types of physics-based modeling and simulation (such as Finite Element Analysis, or FEA, software, and Discrete Element Modeling, or DEM), to allow users to carry out more complex fluid-structure interaction (FSI) analyses.

Using FSI analysis, users can perform detailed thermal and stress analyses of the solid components – not just the flowing streams – and more accurately model the complex interactions. For instance, when CFD is combined with FEA, users are able to model how the flow of high-temperature gases impact the structural components, they can then implement strategic design or operational changes to improve overall equipment performance and minimize the risk of problems related to such things as erosion, vibration and fatigue.

Similarly, when CFD is combined with DEM, the potential impact that fluids with entrained particle may have on pipelines can be accurately modeled (for instance, to enable redesigns that minimize erosion at pipe elbows).

Final thoughts

Most often, the cost of implementing simulation software is justified based on the direct payback that such modeling provides, in terms of reductions in expenses and improvements in operational efficiency. With CFD-related engineering simulation becoming so widespread, the big question now for equipment designers and process operators is not whether to use the technology, but how best to take advantage of the many opportunities it provides. ■