

COMSOL MULTIPHYSICS REVEALS UNKNOWN EFFECTS in process instrumentation



Modeling has become invaluable in MKS Instruments' development of first-class mass-flow controllers for the process industry. We have gained a detailed understanding of the complex gas dynamics in our instruments. With that knowledge we've achieved accuracy that clearly stands out as superior in the industry.

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FIGURE 1: The π -MFV Mass-Flow Verifier measures the rate of change of pressure in a fixed volume. COMSOL Multiphysics helped the designers verify the accuracy of a condensed set of Navier-Stokes equations that run in real time on an embedded processor in the device.

Rate-of-rise device

In new-product and technology development, the first step is to analyze and optimize a basic concept. When working with modeling software, we can quickly obtain initial results by reducing the problem to a 1D model, with which we can often understand a process' underlying physics. An attractive feature of COMSOL Multiphysics is its ability to solve 1D problems, which reduces the debug time to practically zero when we extend a model to 2D or 3D.

These techniques proved valuable in modeling a next-generation pressure rate-of-rise device (Figure 1). Often used in semiconductor manufacturing, such devices measure the rate of change of pressure in a fixed volume, and this parameter is related to the flow rate into the volume. Our latest product is the π -MFV (mass-flow verifier), a compact diagnostic instrument that provides *in-situ* verification of mass-flow controller (MFC) performance. This next-generation MFC includes technology improvements to help users in semiconductor and high-purity thin-film applications increase tool throughput. It features real-time accurate flow control that is insensitive to upstream and downstream pressure disturbances. Towards this goal, it runs advanced digital algorithms on an embedded processor and thereby achieves accuracy significantly improved over conventional PID-based digital MFCs.

Indeed, mass-flow verifiers traditionally have not considered the temperature rise of the gas inside the volume during a verification, so rate-of-rise devices can have as much as 10% error associated with them. Modeling and then creating a device that takes this effect into account involved solving the time-dependent compressible Navier-Stokes equations in 3D.

The ultimate goal of this project was to implement these equations in an embedded processor so they could run in real time on the π -MFV, a task we handled with Matlab® (see sidebar on page 7, “Navier-Stokes in real time”). We then needed to gain confidence that the numerics in the embedded code were accurate, so we compared results for the temperature dynamics in the volume from the real-time model, which uses the condensed equations, to the full 3D COMSOL Multiphysics model, which works with the full Navier-Stokes equations. A prerequisite step was to collect experimental data, which we did using the Matlab Data Acquisition Toolbox and PC-based digitizing hardware. By taking this approach, all the experimental data was immediately in Matlab format, so it was easy to plot pressure versus time in Matlab and superimpose a similar plot calculated in COMSOL Multiphysics. We were pleased to see that the agreement between the model and the experimental data was better than 99% for a wide range of

gases and flow rates. In other words, our real-time model now executes on the shipping instrument to achieve a flow reading accurate to 1% of setpoint for all gases.

In the process we also gained additional valuable knowledge. Specifically, when examining results from COMSOL Multiphysics simulations, we were surprised to see that pockets of gas inside the volume can heat up by as much as 100 °C at high flow rates (Figure 2). The simulation was instrumental in helping us understand how this temperature increase affects the reported flow rate.

Throttle valve for CVD

Another area in which we made great progress was in the design of a throttle valve used in chemical vapor deposition (CVD). CVD is a chemical process by which very thin layers of chemicals are deposited

on a given surface, called the substrate, which is usually a large single crystal of a material such as silicon or quartz. The substance to be deposited, called the precursor, enters a CVD chamber in a gaseous state. Often a precursor enters the chamber by means of a carrier gas that is not to be deposited.

Precursors are supplied with a carrier gas, which when at room temperature and pressure can often be liquid. Further, the precursor's vapor pressure at process temperatures can be as low as several torr (the torr is the standard measure of pressure in the semiconductor industry; 1 torr = 1 mm Hg, and 760 torr = 1 atmosphere = 101.325 kPa). The market is moving towards precursors that have lower vapor pressures, and this trend brings with it a new set of design challenges we could adequately evaluate and overcome with the help of modeling with COMSOL Multiphysics.

One of the key parameters in a CVD process is the pressure in the reactor, which operators control with a throttle valve (Figure 3). The valve chokes off the flow so that a considerable pressure difference can exist on different sides of the valve—it can be as high as 10 torr in the process chamber upstream of the valve compared to only a fraction of a torr downstream. Such a dramatic pressure drop in a distance of just millimeters can lead to a significant drop in the temperature of the carrier gas. In addition, a vortex can form downstream of the valve because its opening is not exactly symmetric, so the flow area is larger on one side than the other. The vortex, in turn, leads to an increase in the local partial pressure of any precursor.

If the process does not use all the precursor, problems can potentially arise. In detail, the pressure drop and the vortex can both result in a drop in the temperature that causes the remaining precursor to condense. That condensate can cause process contamination and clog the valve over time. Before our study, engineers were unable to explain why the condensate was forming, but with the model we could see these effects and take appropriate countermeasures.

Using the Chemical Engineering Module we were able to draw these conclusions using three application modes: Non-Isothermal Flow, Convection and Conduction, and Convection and Diffusion. The most difficult part of the simulation was

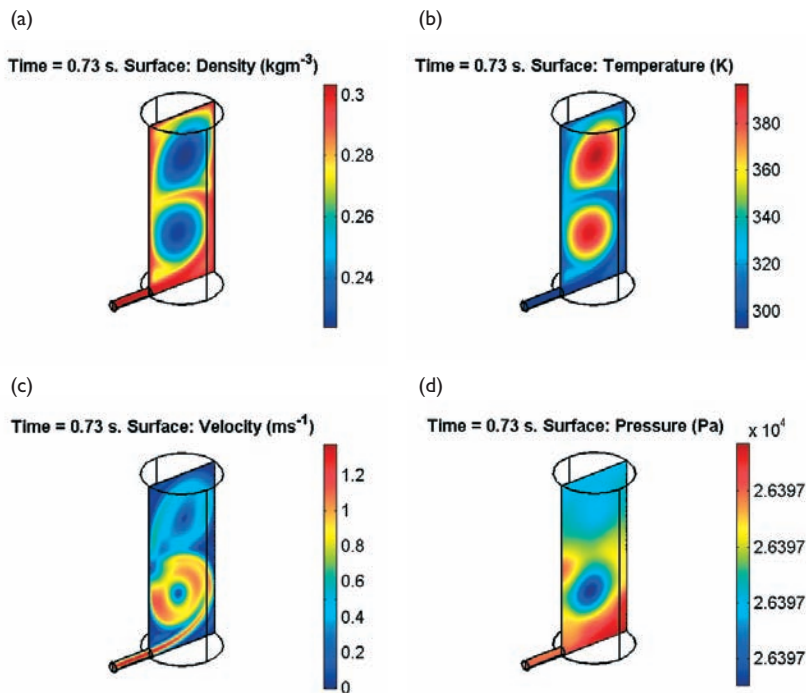
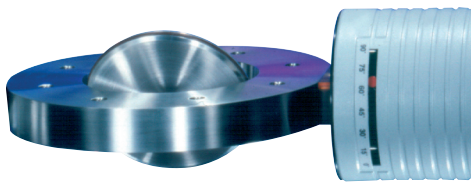
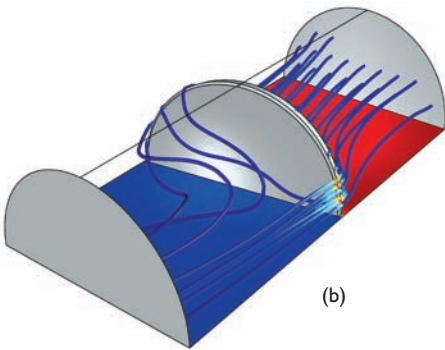


FIGURE 2: COMSOL Multiphysics plots of density (a), temperature (b), velocity (c), and pressure (d) inside the π -MFV rate-of rise instrument at a flow rate of 2000 standard centimeters cubed per minute of nitrogen. By capturing this temperature increase in real time, it is possible to substantially increase device accuracy.



(a)



(b)

FIGURE 3: In a simulation of a throttle valve (a), we plot the pressure (surface plot) and the velocity field (streamline and color) across the valve flapper (b). The sudden drop in pressure and resulting expansion of the gas leads to a drop in temperature and an increase in local partial pressure, leading to condensation.

A “noise-free” laboratory

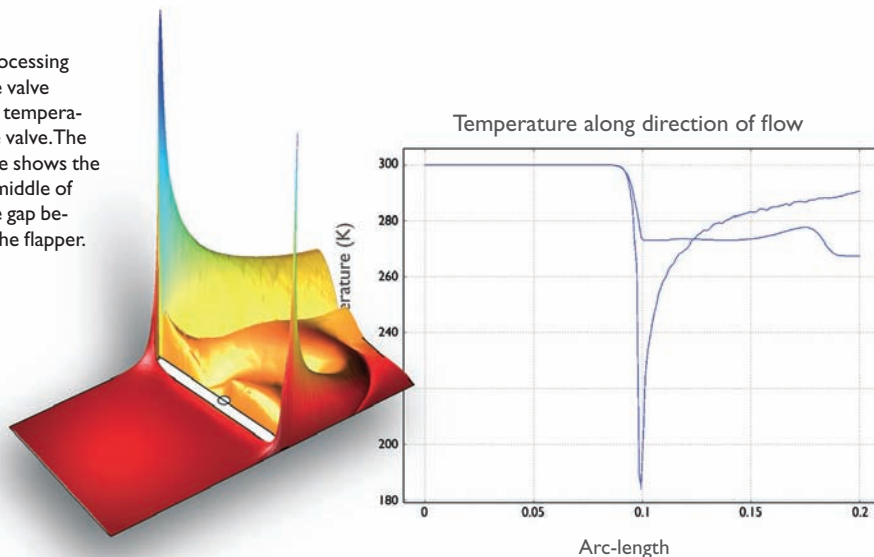
We will continue to simulate and debug our designs. The ability to solve 1D problems and quickly evaluate a concept, freely manipulate the PDEs, and specify ODEs as boundary conditions give COMSOL Multiphysics a huge advantage compared to other FEA packages. We have been able to discover the cause of unwanted effects. Many of our competitors don't have this level of modeling expertise and release products to the market without knowing all of the details of what is going on inside them.

In addition, once we have determined that a model agrees with experimental data, we can use it as a “noise-free” laboratory to further refine our designs. Field measurements and experiments by their very nature always involve some amount of noise and uncertainty, but in the simulation we can eliminate these effects and better study the basics behind new control algorithms and systems. Moving forward, the ability to solve large-displacement fluid/structure interaction problems with the ALE method in the latest version allows us to simulate the dynamics of many existing and future products. ■

resolving the shock downstream of the valve blade. Streamline diffusion and a high mesh density were necessary to accurately resolve the shock and thus observe the large temperature drop (Figure 4).

The simulations clearly showed that heating the blade was not sufficient to prevent the gas condensation, which results from the expansion of the carrier gas. Given this information, our engineers developed a novel way of eliminating the problem, a method we are now testing and plan to incorporate into future designs.

FIGURE 4: A postprocessing image of the throttle valve reveals the dramatic temperature drop across the valve. The cross-sectional figure shows the temperature in the middle of the device and in the gap between the wall and the flapper.



ABOUT MKS INSTRUMENTS

MKS Instruments Inc (www.mksinst.com), with headquarters in Wilmington, Massachusetts, is a leading worldwide provider of process-control solutions for advanced manufacturing processes such as semiconductor device manufacturing; thin-film manufacturing for flat-panel displays, optical storage media, architectural glass, and electro-optical products; it also supplies technology for medical imaging equipment. The firm's instruments, components, and subsystems incorporate sophisticated technologies to power, measure, control, and monitor increasingly complex gas-related manufacturing processes, thereby enhancing customers' uptime, yield and throughput, and improving their productivity and return on invested capital.

NAVIER-STOKES IN REAL TIME

To run the Navier-Stokes equations on the MFV's embedded processor, we had to write them in C code. Here Matlab played a major role. We first developed the conceptual model using “back-of-the-envelope” calculations, then we wrote a Matlab script to implement and debug the control algorithm based on the equations. Next we condensed them into a simplified form to create a real-time model, and using Matlab we converted it into C code that fits into the instrument processor's memory. Before committing the code to production models of the instrument, we validated the COMSOL Multiphysics model with experimental data.