

Tips: Getting started with CFD

What computational fluid dynamics can (and can't) do for you

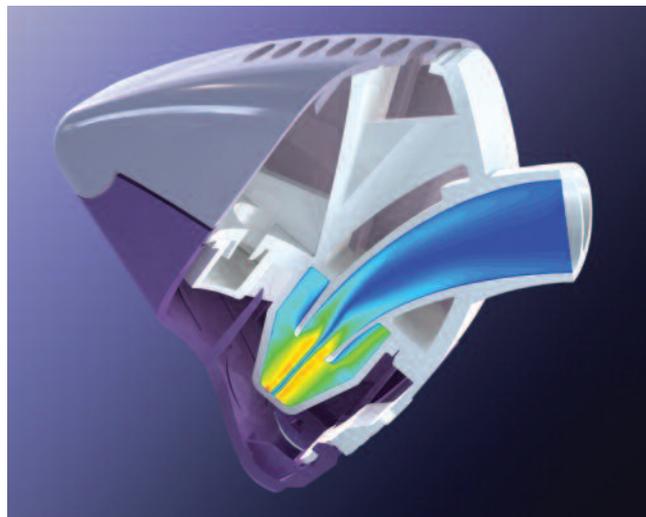
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With so much recent interest in the use of computational fluid dynamics (CFD) for developing inhalation and nasal products – an entire afternoon at RDD 2008 was devoted to papers on the topic – you may be wondering how to get started using CFD yourself. The benefits are pretty obvious; why spend months tweaking device designs and performing experiments in the laboratory when you can hit a button on your laptop computer and find out within minutes how a change in a design dimension will affect retention time? Before you rush out to buy a software package with CFD capabilities, however, make sure that you take the time to understand its (and your) limitations.

Availability

In the early nineties, when experimenting with CFD for computerized modeling became mainstream at universities, users generally wrote all of the code themselves. All of the interfaces were text based, and models were validated against only a few applications. Besides universities, only large blue chip engineering firms had sufficient resources to use CFD regularly in their design approaches. Today, several companies offer computer aided engineering (CAE) packages that include CFD programs bundled with computer aided design (CAD) software.

You can buy the software package, install it on your PC, and all you have to do is to click on the CFD button on the screen. Once your CAD design is complete, the program will simply ask what you would like to know about the device. If you select one of the options offered, maybe flow or pressure drop, and press “go,” you can come back 20 minutes later and see wonderful pictures, very impressive, very believable pictures showing the fluid dynamics within your device. If you make a design decision based on those pictures without fully understanding the concepts involved, however, you may find yourself in trouble. CFD isn't likely to save you any time if you spend



weeks working on a design before realizing that your experimental data don't match the computer model.

It's a little like using the GPS unit in your car to guide you to a new location. The simplest to use versions don't adapt for changes in route necessitated by road construction or accidents. If you know the city well, you just ignore the voice telling you to make a right turn onto a barricaded road, and you find another route that will get you back in sync with the GPS device. On the other hand, if you are unfamiliar with the streets or with how the system works, you may follow directions that lead you in the wrong direction or leave you stranded. If you are new to CFD, chances are you don't know your way around well enough to know if you are headed in the wrong direction or to make adjustments if you hit a dead end.

Limitations

The first thing to remember is that for most CFD codes, the default options presented to you in your CAE package were initially designed to replace wind tunnel testing for large industrial equipment. That code may work for the design of a combustion chamber for the latest jet engine, but that does not mean that it will give the correct results for an inhaler. The simple models that allow designers to model flow separation in an industrial pipeline will probably not produce similarly accurate results for flow in the lower airways of the lung. CFD models designed to calculate evaporation time for 1-2 mm water droplets will not give you the correct answer for evaporation of the 1-2 μm propellant droplets emitted by an MDI because the physics involved are significantly different.

Using CFD for turbulence calculations can be particularly tricky for beginners. Most CAE programs use the k-epsilon turbulence model, which is often referred to as the “industrial standard model.” The k-epsilon model has been validated against a number of applications such as flow separation in a pipe or over a step, but many designers go wrong by using it for things it hasn’t been validated for, like a cyclonic chamber. The wrong answer the model produces shows the flow going around and around as it should, but the gradients, peak velocity, and location of the peak velocity will likely be wrong because very simple models like this make very gross approximations.

The k-epsilon model assumes that the magnitude of turbulence is the same in all three dimensions and therefore causes the same distortions in the velocity fields in all directions. An experienced CFD user will know to avoid the use of this model in this case and to use the Reynolds Stress Model, which solves for turbulence in all three dimensions, instead, but a beginner may not know that the option exists, much less how to locate it in the program.

The ability to model and understand a drug-particle-laden air flows path through a device and how and where drug can build up within it is a key factor in the design of a high performance delivery system. Although almost all commercially available codes offer models for deposition in one guise or another, using a number of different simulation techniques, these CFD models tend to solve deposition problems like this very poorly, if at all. One of the most widely used models performs a method of particle tracking in which the fluid flow interacts with discrete particles to influence the particles’ paths. A separate mathematical model that shifts the particle slightly off track in a randomized direction dependent on the level of turbulence accounts for the effects of small eddies within the flow.

The problem with using simple models for deposition is that turbulence models all overpredict the turbulence very close to the wall; so as particle gets close to the wall, the model says that the increased turbulence causes increased deposition by throwing the particles into the walls. In one design project for a DPI, even a more sophisticated CFD turbulence model overpredicted deposition by as much as 400%. The computer predicted 40% deposition of the drug within the device, but experiments showed only 10% deposition. No matter how the users manipulated the CFD model, it failed to give answers in line with experiments.

Where to start

So what can you do with CFD that doesn’t require getting a Ph.D. in mathematics first? All CFD models

Suggested reading:

Turbulence Modeling for CFD by David C. Wilcox provides good basic information on CFD in language that beginners can understand.

NAFEMS is a not-for-profit association dedicated to computer modeling technology. The following publications produced by the NAFEMS CFD working group are available at www.nafems.org:

- How to Understand Computational Fluid Dynamics Jargon
- How to Plan a CFD Analysis
- Why Do Computational Fluid Dynamics?
- How to Get Started with Computational Fluid Dynamics

prove good at design problems that resemble those for which the models were designed. A CFD model designed to predict pressure drop in a pipe will do a pretty decent job of predicting pressure drop or velocity in the throat, in a ventilator tube, or in an MDI spacer. You can probably also obtain good results for peak velocity, residence time history, particle acceleration history, and particle strain history as well. In the case of a simple swirl chamber based on a reverse flow cyclone that generates the forces required to efficiently de-agglomerate a drug powder and separate it from any carrier particles, using CFD with the Reynolds Stress Model produced very good agreement with the experimental data.

Make sure to get some training if you want to use CFD, starting with the 1 to 4 day commercial training courses provided by the software vendors. Learning to use the programs by reading the software manuals is usually hard work for most people unless they have a working knowledge of really hardcore mathematics. Several excellent texts written in plain English are available (see sidebar), and taking the time to read those books can help you to evaluate the vendor’s claims for what you can and can’t do with the software. When the vendor creates a benchmark model for you to demonstrate the package’s capabilities, you will need to understand how well that model matches your needs. If your CFD package won’t provide you with the answers you need even after this training, you can always find a consultant with CFD expertise to solve your problem.

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