

COMMENTS ON A COMPARISON OF CFD SOFTWARE FOR MICROFLUIDIC APPLICATIONS

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Introduction

A recent effort to compare the performance of four commercial computational fluid dynamics (CFD) software packages for microfluidic applications (T. Glatzel, 2008) was recently brought to the attention of the staff at Flow Science, Inc. The paper reported simulation results from the four CFD packages for a set of flow problems typically encountered in microfluidics. The intent of the paper was to compare the quality of the solvers by removing differentiating features (meshing, special numerical algorithms, etc.) from the analysis. While we acknowledge the worthiness and difficulty of the task, we believe there are some significant limitations to the usefulness of the comparisons made in the paper.

To begin, the modeling restrictions employed prevented the individual software programs from making use of particular options they might have for obtaining better simulations of particular flow problems. A second point, at least in connection with our software product, **FLOW-3D**[®], we have noted numerous inaccuracies in the software's description, an incorrect use of boundary conditions and several other failures to operate the software properly. This note is intended to correct these deficiencies and omissions as well as to present a repetition of the computational examples, as near as possible, from data given in the original paper. It will be shown that **FLOW-3D**[®] performs all the comparison problems as well or better than other software tools included in the original study.

General Comments

The discussion of the Volume-of-Fluid (VOF) method presented by Glatzel et. al., which they say is used in all the software tools they studied, is unfortunately incomplete. The authors fail to note that all the software tools, except **FLOW-3D**[®], must employ a two-fluid model in which it is necessary to model the dynamics of both gas and liquid. In **FLOW-3D**[®] this is not necessary because it has an option for free-surface boundary conditions such that only liquid regions need to be modeled. This is important, for when this option can be used it greatly reduces the computational effort of a simulation and generally improves the accuracy of the free surface dynamics. The reasons for this are as follows. When air regions are included in the dynamics, time-step sizes must often be reduced because of large gas velocities and pressure-velocity iterations have more difficulty reaching convergence. Furthermore, the motion of fluid/gas interfaces can be adversely affected when there is a large tangential velocity gradient at the interface, because all the software tools use only one velocity field to describe both air and water. To compensate it is sometimes necessary to employ a much finer grid to resolve such gradients, which greatly increases the computational effort. With the free-surface option in **FLOW-3D**[®], it is often possible to obtain better results with a coarser grid that does not have to resolve large velocity gradients at interfaces.

In this connection, it should also be remarked that **FLOW-3D**[®] has several gas “bubble” models that allow gas regions to exhibit a pressure-volume dependence as well as include phase changes, while still not having to perform detailed gas dynamic computations. These models offer big computational time savers that have many uses in microfluidic applications.

Additionally, while there are variations of the VOF method that are being investigated, it is not clear whether these represent refinements, as the authors claim, or whether they are simply different approaches.

Another point of contention is that the authors seem to emphasize that **FLOW-3D**[®] uses a combination of finite-difference and finite-volume methods as distinguished from the other software programs. **FLOW-3D**[®] is based on a control volume method as are all the software programs studied. The distinction they draw is not clear. Additionally, it is stated that the pressure-velocity coupling is “generally accomplished by the SimpleC algorithm which was originally proposed by Vandoormaal and Raithby...” This is not true as this general pressure-velocity coupling method was initiated by the Los Alamos fluid dynamics Group T-3 in the Marker-and-Cell (MAC) method (and following software such as the SOLA programs) years before there was a “Simple” method. The T-3 originators found no need to give the method a special name because it was only one part of an overall solution technique.

Several other errors and omissions are worth noting. First, it is mentioned that CFD-ACE+ has an additional feature “to remove the so called flotsam and jetsam” associated with the VOF method. This capability has been available in **FLOW-3D**[®] for a considerable amount of time, but was omitted in the discussion of **FLOW-3D**[®]. It is also incorrectly stated that **FLOW-3D**[®] cannot use a fixed time-step size. This is false; the program has had this capability from its inception. Such comments suggest, at best, a lack of experience and effort that would likely result in a reduced ability to properly operate the program. Regrettably, the authors did not contact Flow Science for assistance or comment.

Test Simulations

The four test simulations presented in the original paper were reanalyzed using the latest version of **FLOW-3D**[®], version 10.0.1, as distribution of version 8.2.5 ended 2005 and is of limited relevance to the modern microfluidics engineer.

The first problem that was re-analyzed was the “Split and recombine mixer”. The simulation was run with the same mesh as used by Glatzel, et. al. and, as in the paper, it was run in two steps. First, the flow was run to a steady-state (approximately 1.655 seconds). Using these results a tracer was then advected through the domain in the fixed velocity field. This part of the simulation took approximately 300 seconds to reach a steady profile. These times are quite different from those reported by Glatzel, et. al., particularly the time documented for the advection of the tracer. The authors report that this part of the problem was run for 3.4 seconds. This does not make physical sense because the specified inlet velocity was 1 mm/s, so it would take at least 14 seconds for the fluid to travel the distance of 14 mm between the inlet and the outlet of the channel, not to mention reaching a steady-state.

Results for the split and recombine mixer simulation are shown below. It can be seen that they compare favorably to the results from the other CFD programs presented by Glatzel, et. al., with the pressure drop of 1.801 Pa, and lamination patterns very similar to those predicted by the other codes.

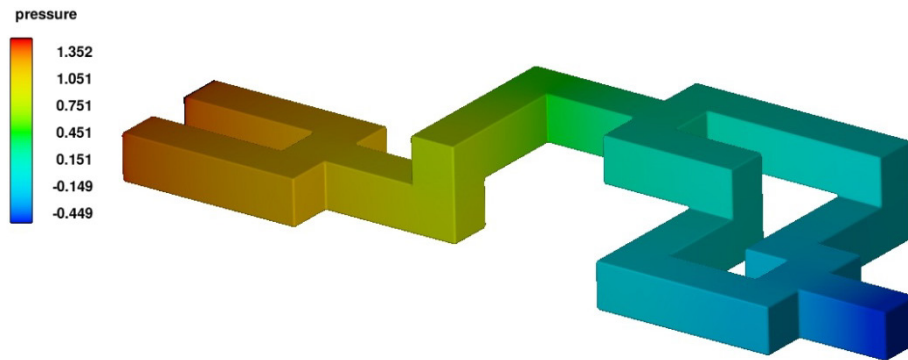


FIGURE 1: PREDICTED PRESSURE DROP

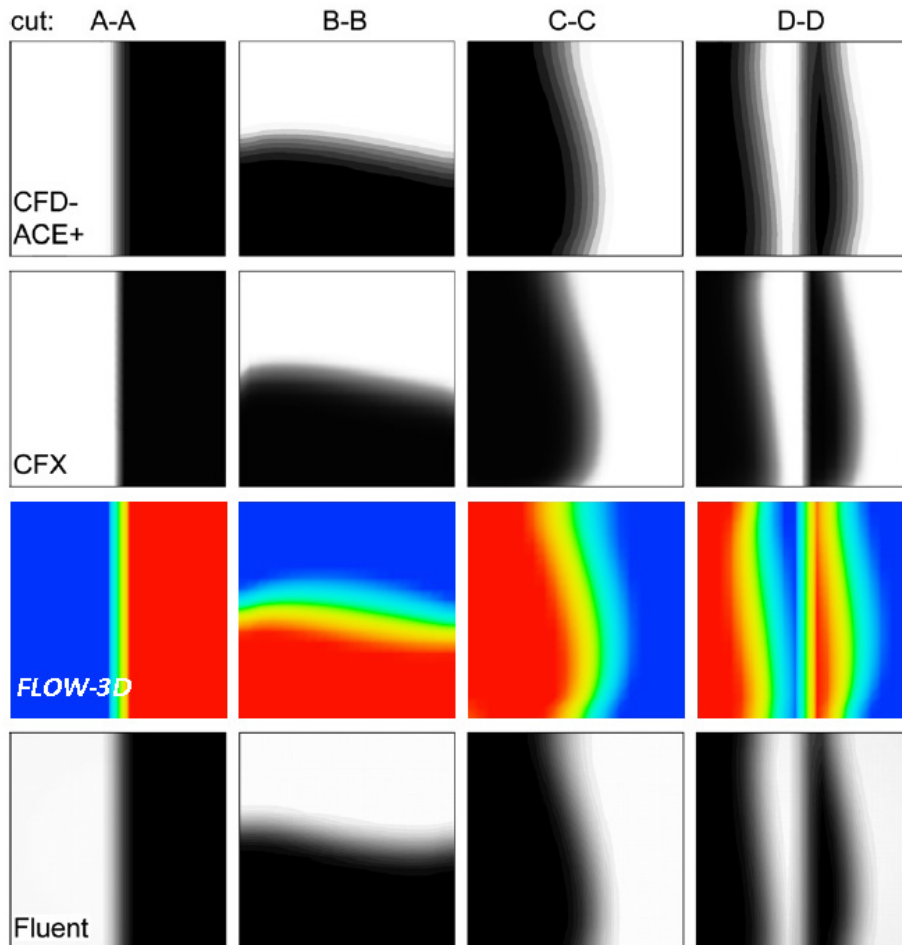


FIGURE 2: PREDICTED CROSS-SECTIONAL LAMINATION PATTERNS. THE PATTERNS FROM THE OTHER CFD PACKAGES ARE REPRINTED FROM GLATZEL, ET. AL.

The second problem looks at mixing in a rotating, rectangular channel. The setup is identical to what was used in the paper except the boundary conditions correctly specify *static* pressure, instead of *stagnation* pressure, which was the cause of the erroneous results reported by Glatzel, et. al. The mixing patterns, shown below, are clearly in good agreement with those predicted by the other packages. Additionally, the predicted flow rate is 15.77 μ L/second, which is well within the predicted range from the other CFD packages as shown in Table 1.

TABLE 1: FLOW RATES IN THE ROTATING CHANNEL

Tool	Flow rate (μ L / sec.)
CFD-ACE+	16.30
CFX	15.65
FLOW-3D	15.77
Fluent	15.16

Furthermore, the pressure distribution along the centerline matches the expected pressure distribution quite well, with a minimum pressure of -120 Pascals and a zero pressure at both boundaries. The lower pressure at the boundaries reported by Glatzel, et. al. was the result of an erroneous user input specifying stagnation pressure at the boundaries and not static pressure.

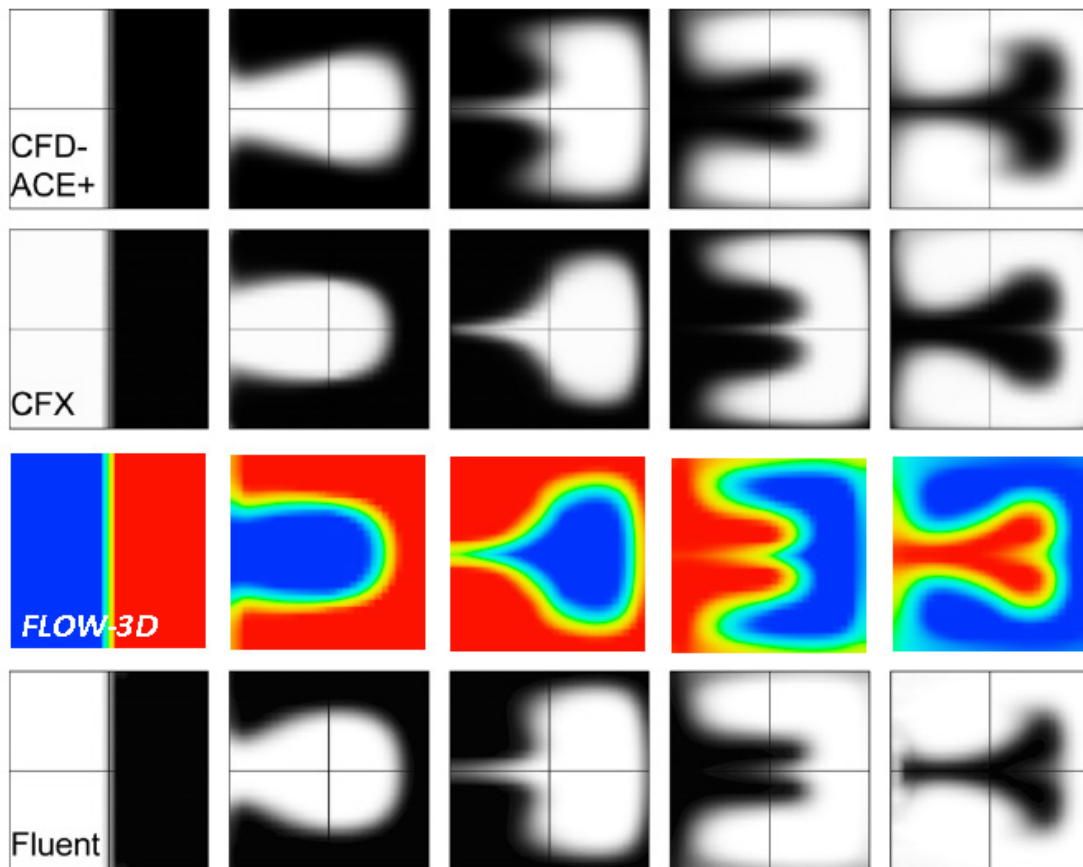


FIGURE 3: PREDICTED LAMINATION PATTERNS. THE RESULTS FROM THE OTHER CFD PACKAGES IS REPRINTED FROM GLATZEL, ET. AL.

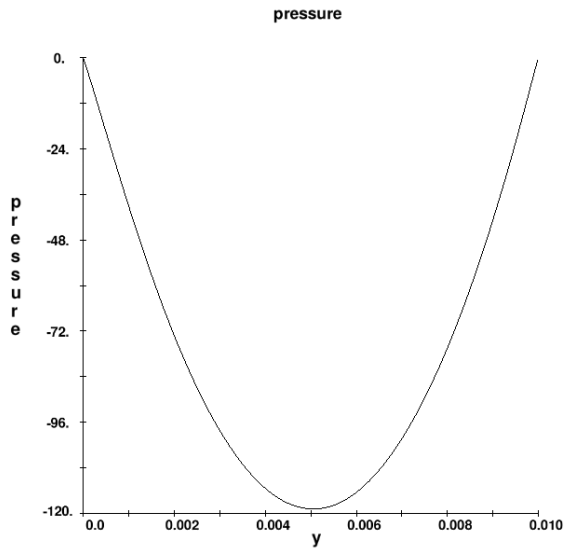


FIGURE 4: THE PREDICTED PRESSURE DISTRIBUTION ALONG THE CHANNEL CENTERLINE.

The third problem was a design study looking at the motion of a gas bubble in a microchannel. The model setup was similar to that used by Glatzel, et. al., but the mesh could not be replicated because of an uncertainty in the mesh design reported in the paper. As such, each model used 45000 total cells with approximately 35000 active, open cells. Each model was run for 30ms to ensure the results had stabilized to a steady value. Depending on the case, the simulation results could be approximated as steady between 8ms and 12ms. The results, shown in Figure 5, are clearly very similar to the results predicted by both CFD-ACE+ and Fluent. The main difference was the use of a fluid fraction cleanup function that removed some unimportant small fluid fraction droplets, tidying up the surface tension calculations.

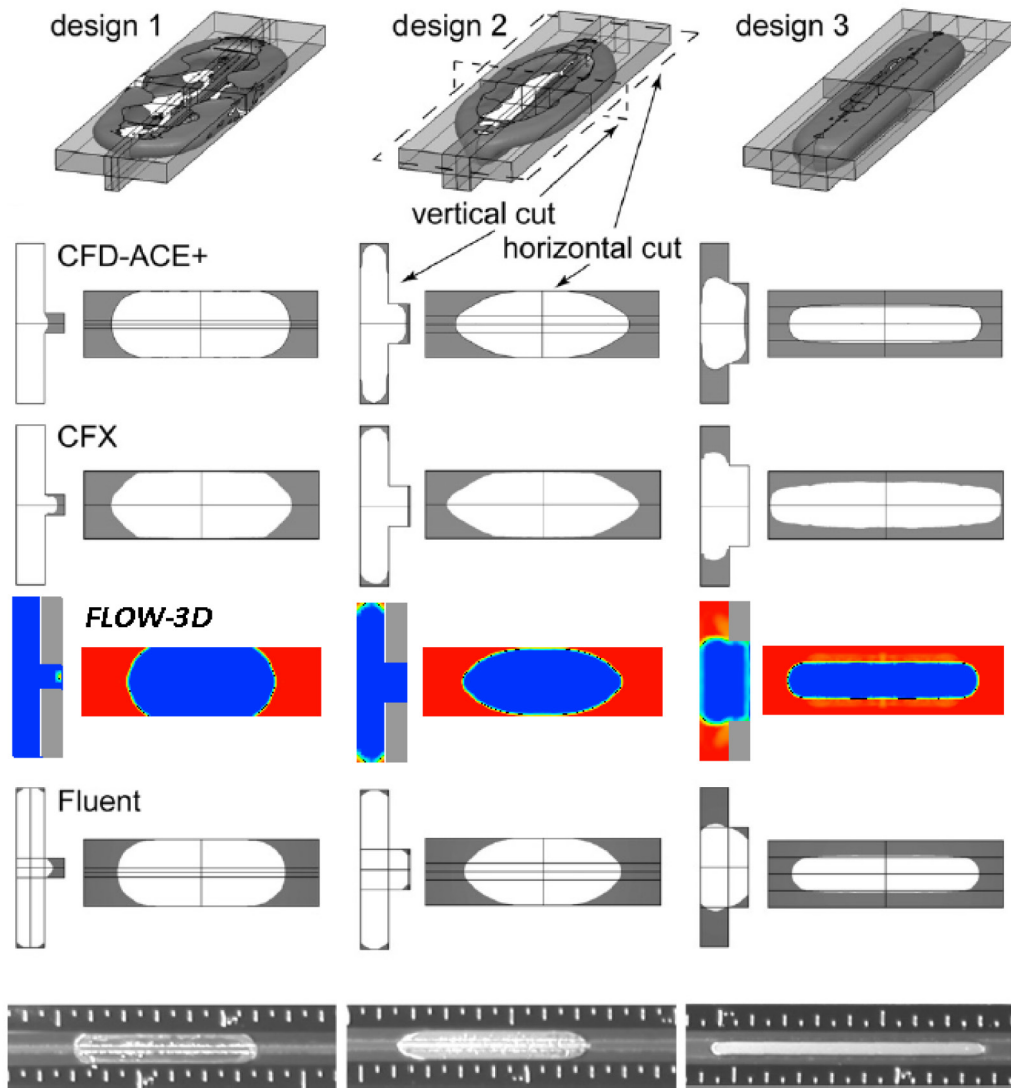


FIGURE 5: PREDICTED BUBBLE SHAPES IN A T-SHAPED CHANNEL. THE RESULTS FOR THE OTHER CFD PROGRAMS AND THE EXPERIMENTAL RESULTS ARE FROM GLATZEL, ET. AL.

The fourth and final problem is an analysis of the TopSpot® printhead. The parameters of interest for this simulation were the droplet separation time and the droplet volume for a given inlet pressure. The geometry was relatively easy to recreate, but there was not enough information to recreate the mesh used in the paper. A simple axisymmetric mesh comprised of uniform 5µm cells was chosen as the replacement mesh. The standard angle of symmetry used for the mesh was two degrees, though larger angles were investigated. The fluid used was water, and the input pressure was digitized using the key points and is shown below.

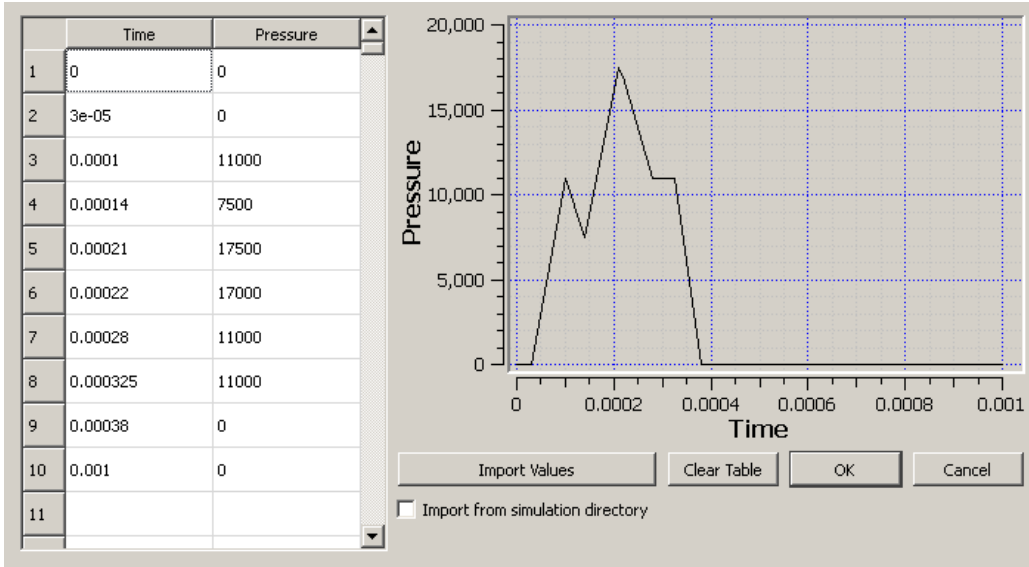


FIGURE 6: INPUT PRESSURE PROFILE

It can be seen that the droplet separation time is predicted to be just before 400µs rather than the 450µs reported by the experiment. Some of this difference can be attributed to the approximation of the pressure profile, as the separation time was observed to vary by ±10µs depending on the mesh angle in the azimuthal direction and convergence criteria. An additional ±10µs variation appeared if the input pressure profile was adjusted by ±5% of the peak pressure, as was done by Glatzel, et al. Interestingly, if the viscosity was increased (by up to 50% of the true viscosity) to simulate a method used by CFD-ACE+ to damp capillary waves the droplet separation time could be delayed by up to 25µs.

Droplet volumes were predicted to be approximately 1nL and vary by ±0.1nL depending on the pressure profile, mesh angle, and convergence criteria. This is larger than the experimental value of 0.68nL but between the values presented by Glatzel et. al. for CFD-ACE+ (0.66nL) and CFX (1.4nL). Again, simulating the method used by CFD-ACE+ to damp capillary waves by increasing the viscosity resulted in decreasing the droplet volume by up to 0.1nL.

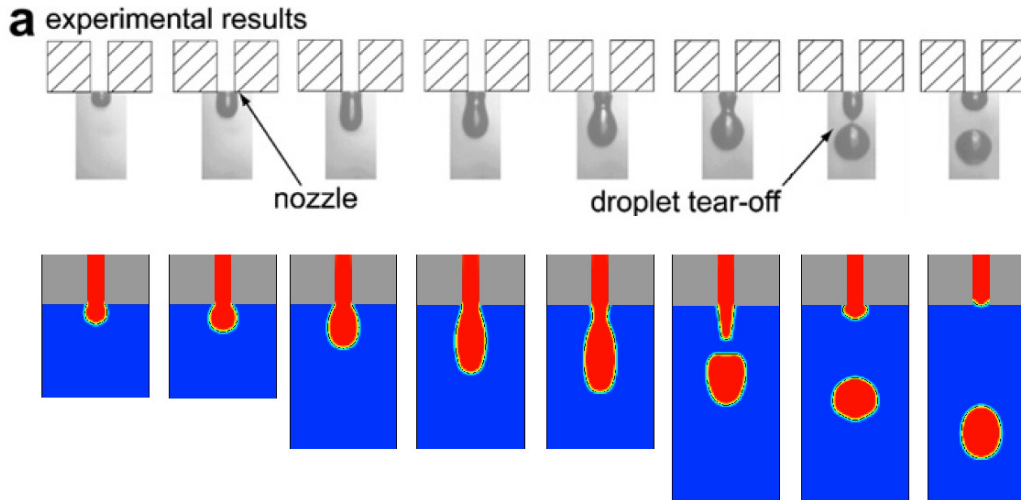


FIGURE 7: PREDICTED DROPLET SIZE AND SEPARATION TIMING. EXPERIMENTAL RESULTS ARE REPRINTED FROM GLATZEL, ET. AL.

Run times were quite manageable, with simulations taking approximately 78 CPU seconds on a typical desktop machine with 8Gb of memory and a 2.8GHz Intel Core i7 930 CPU. The associated wall clock time was 19 seconds. Admittedly, this is not a fair comparison to either the machine or the mesh used to create the original paper, but it is representative of the actual time it would take for **FLOW-3D**[®] to generate a solution to this problem. In this case, a 148,956 cell mesh was not necessary because of the design of **FLOW-3D**[®].

Concluding Remarks

Thoughtful comparison studies can be useful for helping guide decisions, but one must always approach these studies with a critical eye because of the potential for error or unintentional biases. The paper that is the topic of this rebuttal is a fine example of this point. The user failed to use the software properly for any of the problems and erroneously determined that the program was to blame for the poor results.

Furthermore, it is insufficient to consider a single part of a CFD package, because one cannot mix and match the best of each program. Instead, one must typically choose a single program that best meets their overall needs. **FLOW-3D**[®], for example, includes fully integrated models for dielectrophoresis, conducting fluids with free-charge densities and Joule heating, phase change, Marangoni forces associated with non-constant surface tension, temperature-dependent material properties, general moving solid objects (e.g., valves, pistons, etc.) and more. A comprehensive evaluation should be done by each prospective user in terms of his or her particular needs. For this purpose, it is generally best to contact the suppliers of a software package and to ask some tough questions.

References

1. Thomas Glatzel, Christian Litterst, Claudio Cupelli, Timo Lindemann, Christian Moosmann, Remigus Niekrawietz, Wolfgang Streule, Roland Zengerle, and Peter Koltay. "Computational fluid dynamics (CFD) software tools for microfluidic applications - A case study." *Computers and Fluids* 37, 218-235. 2008.