Use of Comsol Multiphysics in Undergraduate Research Projects to Solve Real-life Problems

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Abstract

This paper shows how undergraduates are introduced to computational fluid dynamics (CFD) in research projects. The students first solve problems in their textbook, then solve extensions to them (i.e. they remove assumptions). Then they solve a simple version of their ultimate problem to learn how to verify their solution. Finally they solve the research problem.

Introduction

While transport phenomena textbooks are good at presenting the fundamentals, most of the problems are one-dimensional, since that is the limit of the mathematical ability of most undergraduates. Today's students are motivated by real-life examples, but they have limited time. With the advent of sophisticated software, however, it is possible for undergraduates to solve meaningful transport and flow problems in two and three dimensions. This talk presents the methods used to introduce undergraduates to Comsol Multiphysics and the problems they solve in a research project format.

The learning occurs in three stages. First, the students learn to solve problems in their textbooks and learn to validate the solution. This gives confidence that the computer program is solving the right equations. Next, they solve more complicated 2D problems, which go beyond their textbooks by removing assumptions. In this stage, students are confronted with the necessity of translating their problem into the notation of the computer program and proving they have solved the problem correctly even though there is no analytic solution. They learn how to check their data input to the program, look for artifacts in the solution, and use mesh refinement to estimate the numerical error. They explore the many ways to analyze and view the results, from streamlines, contour plots, integrals, etc. of the dependent variables as well as derived quantities (defined in terms of the dependent variables). For example, is the total flow in equal to the total flow out? – not a straightforward question when there are multiple inputs and outputs and the solution is numerical. The second step is illustrated in detail to show the breadth of analysis techniques.

The third stage in the learning process is to solve their research problem. Examples done during the past year (many suggested by research groups or companies) are shown in Table 1.

Valuable features of Comsol Multiphysics include the graphical user interface, the tools for creating the geometry and internal boundaries and domains, automatic mesh generation and refinement, the ability to solve different equations on different meshes (all in the same problem), the multi-physics capability which permits addition of equations to represent additional phenomena, the ability easily to make parameters depend upon the solution, the parametric solver, and the post-processing graphical features.

Table 1. Research Problems Tackled in 2006-7 by Undergraduate Chemical Engineering Students

Thermal field flow fractionation – the effect of entry effects;
Use of ferrofluid to remove arsenic from water supplies;
Flow of viscoelastic fluids in contractions;
Movement of nanoparticles in gels;
Mixing of pharmaceuticals in orbital mixers and injection/remove devices;
Mixing and flow in Swagelok and Circor Tech devices;
Flow in expansions – pressure drop and entry/recovery lengths;
Flow of water in porous media;
Perturbation method applied to the flow of a ferrofluid in an oscillating magnetic field;
Hole pressure problem – used to measure normal stresses in polymers;
Calculation of vortex viscosity of ferrofluids.

Organization of the Research Projects

The procedure for teaching students how to use CFD programs is described. An essential element of the process is to make the steps small and manageable, with the eventual goal clearly specified. The quarter is 10 weeks long. The first two weeks are spent introducing students to the program and having them solve the textbook problems, and extensions. Most of the students have already taken a computer course in which they have used the program some, but only in problems that were well defined. Weeks 3 and 4 are devoted to solving two-dimensional problems that are simplifications of their final project. The problems contain the essential features of the final project so that they have to address those features. For example, many three-dimensional problems have features that can be studied in two dimensional cases, too. Since the two-dimensional cases run much faster, they are used first when the students are learning. Then, when the three-dimensional real case is studied, fewer mistakes will be made and the project will run more smoothly. Weeks 5 to 9 are spent on the project. The project is defined in a broad context, as illustrated in Figure 1. The tenth week is devoted to finishing the work, preparing and giving the oral presentation, providing information for a project web page, and writing the final report. Sometimes the final report is finished after finals. During the quarter, the student meets with the instructor once per week to show their current work. In addition, the entire group of students meets together to discuss mutual problems and solutions. Progress reports are given, which is a motivating factor. One arrangement that works very well is to have several students working on similar and related projects. Then they can learn from each other and interact with each other. Progress made by one student is then a motivating factor for their partners. For example, in Autumn, 2007, correlations are being developed for pressure drop in flow devices: tees, ells, and devices with multiple input/output ports. Thus, each student is working on a different device, but they are all doing basically the same thing.

Hole Pressure for Newtonian Fluids
Spring, 2007, Ch.E. 499 Project for Stephanie Yuen

Project description: The project simulates the flow of a Newtonian fluid between flat plates. A hole is drilled in one of the plates and the pressure is measured at the bottom and across from the hole. That pressure can be related to polymer properties if the fluid is viscoelastic. This is a problem one of Prof. Finlayson's graduate students did in 2D when finite elements were just beginning. Can you believe we used only 28 elements? Now it is time to do it with more elements and in 3D and compare with published experimental results.

First steps:

- Do the problem in Table 10.1
- Read the paper by my students
- Meet with group on first two Tuesdays.
  - First week – I'll demonstrate Comsol Multiphysics
  - Second week – Have done the problem in Table 10.1; read the paper by my students; have read about your problem and have questions.

Milestones

Run the existing code, from the polymer paper by BAF
Change the dimensions and parameters to do the exact specs in the experiment
Prepare a 3D geometry
Solve the problem in 3D

At the end of the quarter you need to submit: written report, PowerPoint presentation, Comsol Multiphysics dataset, and suggested web page.

Here is the **checklist** for a proper submission of results.

1. Say what problem you are solving;
2. Give the shape and dimensions, number of elements, degrees of freedom;
3. Give the parameters in the equation and identify the boundary conditions;
4. Tell how you solved it;
5. Give checks to your answer (previous similar results, etc.);
6. Give your results, including pertinent plots and integrals;
7. Your report should have an Appendix with sample calculations.

Figure 1. Sample Statement of Goals

The Learning Process

Step One – Solve Problems with Known Solution

Shown in Figures 2 and 3 are two problems that are assigned. The student is to solve them, make plots of them, and report back to the instructor. This exercise gives the student confidence, since they are able to solve the problems, although maybe the comparison to their textbook is difficult the first time. It also gets them 'over the hump' on how to access the program, use it, save their results, print figures, etc. A printed copy of the mesh is always required, to emphasize the importance of mesh refinement. Figure 2 involves cylindrical geometry, and the student learns about inlet/outlet flow conditions. The pressure is set at the outlet and the velocity is set at the inlet. The solution gives the pressure drop in the device, which can be compared with the Hagen-Poiseuille law. The student also learns how to setup problems in cylindrical geometry. Figure 3 involves geometries that are not quite square, and boundary conditions that are not uniform. Thus, the student learns how to insert such boundary conditions into the computer code, and how to draw the boundaries.

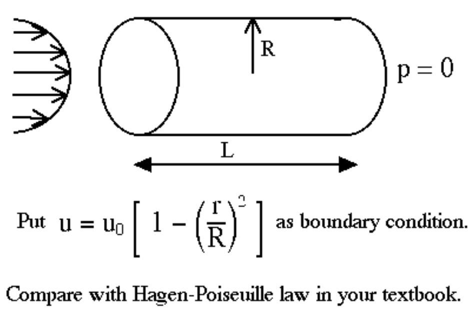


Figure 2. Flow in Pipe

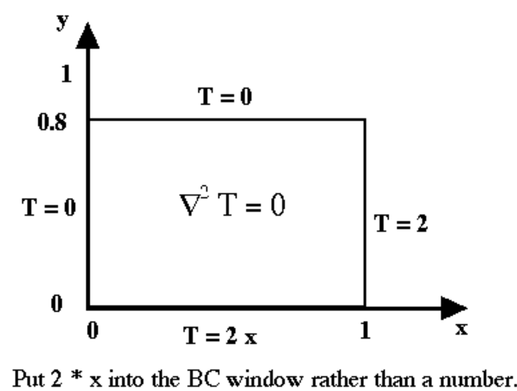


Figure 3. Heat Transfer Problem

The use of the computer program, Comsol Multiphysics®, is aided by reference to the book, *Introduction to Chemical Engineering Computing*, which has step by step instructions (1). Table 10.1 from that reference is shown in Figure 4. Reference (1) also has screen shots of the different steps: draw the domain, pick the equation and set the parameters, set the boundary conditions, create the mesh, solve the problem, and examine the solution. When drawing the domain, one learns how to resize objects, reproduce repeating patterns easily, create multiple domains with different properties. When setting the equations, one has complete flexibility including the Navier-Stokes equation, the convective diffusion equation, the energy equation, in two or three dimensions, as well as other modes, such as Nernst-Planck equation. The parameters can be functions of the solution: one merely needs to be able to type the function in a box. There are a variety of choices for boundary conditions; this is a good lesson because some combinations are physically realizable and some are not; thought is required! The mesh is created automatically to a scale which you set, and it can be refined automatically or adaptively or in regions the student specifies. If the mesh is not sufficiently fine, either the solution method does not converge (infrequently) or oscillations are observable. Thus, one must be alert. Postprocessing options are illustrated below.

Open FEMLAB (Note: FEMLAB with MATLAB® makes and reads .mat and .fl files. FEMLAB stand-alone only makes and reads .fl files.)

- Choose Axial Symmetry 2D
- Choose Chemical Engineering/Momentum/Incompressible Navier-Stokes and click OK

Draw
- Click on the square icon and draw a rectangle
- Double click on the object to set exact dimensions
- Use Option/Axis/Grid settings to set the plotting range on the screen

Physics/Subdomain Settings
- Select domain 1; set $\rho = 0$, $\eta = 1180$ (Newtonian), $F_x = F_y = 0$

Physics/Boundary Settings
- Click on a boundary number (1 through 4) (Note: the corresponding boundary is highlighted in red
- Set the boundary condition for each boundary segment
  1 – slip/symmetry; 2 – inflow/outflow, v = 0.02; 3 - Outflow/pressure; 4 - no slip

Mesh
- Click once on triangle icon or select mesh/initialize mesh
- Note how many elements are used (you should report this)
- Click on divided triangle icon to refine the mesh if desired
- To refine locally, click on the 'refine selection' icon, select some elements

Solve
- Click on '=' to solve the problem (click on  to re-start from the last solution)

Postprocessing
- Choose Domain Plot Parameters
- Select the desired quantities for contour plots and surface plots
- Or, click on the arrow plot icon, or streamline plot icon (flow plot)
- Choose Cross Section Plot Parameters to make line plots.
- Plot the v velocity along a line by selecting v velocity, put in the (r,z) coordinates of the beginning and ending points.

You can refine the mesh (click the more refined mesh symbol) and re-solve the problem. This gives you an indication of the accuracy of the solution. When you have a figure showing, you can export it in a figure format you choose such as jpeg. You always want a figure showing the mesh, as well as parts of the solution.

To document your work, show the domain and mesh, give the dimensions, identify the boundary conditions, give values of parameters you used in the subdomain options, list how many elements and degrees of freedom were used, and indicate how solutions with different number of elements compare. Then give the results and indicate why they are reasonable.

Table 10-1. Using FEMLAB to solve transport problems
(This example is for a 2D flow problem.)

Figure 4. Table 10.1 from *Introduction to Chemical Engineering Computing*

Step Two – Solve More Complicated Problems

The next lesson that must be learned is how to make the equations nondimensional, and how to report results that others can use. An important checklist is:

- What velocity is 1.0 in the computer?
- What distance is 1.0 in the computer?
- What boundary conditions did you use?
- What is the Reynolds number, and where did you use it (see below)?

The Navier-Stokes equation is

$$\rho \mathbf{u} \bullet \nabla \mathbf{u} = -\nabla p + \nabla \bullet [\eta(\nabla \mathbf{u} + \nabla \mathbf{u}^T)]$$

If one uses u_s, p_s, and x_s for the velocity, pressure, and distance standards, the dimensionless equations can be rewritten as

$$\mathbf{u'} \bullet \nabla' \mathbf{u'} = -\nabla p' + \frac{1}{Re} \nabla' \bullet [(\nabla' \mathbf{u'} + \nabla' \mathbf{u'}^T)] \text{ if } p_s = \rho u_s^2.$$

or as

$$Re\, \mathbf{u'} \bullet \nabla' \mathbf{u'} = -\nabla p'' + \nabla' \bullet [(\nabla' \mathbf{u'} + \nabla' \mathbf{u'}^T)] \text{ if } p_s = \eta u_s / x_s.$$

One must be careful to make sure the dimensions drawn for the problem are consistent with this non-dimensionalization. In both cases, the Reynolds number is given by $Re = \rho u_s x_s / \eta$. The first equation is used for high flow rates while the second one is used for low flow rates, since convergence is easier in those cases, respectively. In microfluidics, too, often the Reynolds number is low, and non-dimensional velocity solutions for all cases with Reynolds number less than one practically coincide. Thus, only one solution need be done for a range of Reynolds numbers.

In order to bring the lesson home, the students are asked to take a given non-dimensional solution along with specified standard velocity, density, size, and viscosity values (with dimensions) and provide the dimensional values derived from the non-dimensional solution. It is instructive to do this with both forms of Reynolds numbers to show that the velocities are the same (since the non-dimensional velocities are the same), and the dimensional pressure drops are the same even though the non-dimensional pressure drops differ in the two formats.

The solutions are found using the finite element method. While undergraduates are not expected to understand the details of the finite element method, it is possible to show them the essential features: dividing a region into smaller regions, approximating a function on each small region, having some means to determine the numerical values for the approximation, and seeing the effect of using more smaller finite elements. All of these steps are illustrated in a PowerPoint presentation; the one that is hard for undergraduates is the third one: determining the numerical values. This is done in the computer program by using the Galerkin method, which involves integrating by parts and some simple functional analysis. The undergraduates are not expected to understand these details, although the instructor is happy to discuss them, but it is essential that the students realize that an approximation is being made and the only way to test the accuracy of the approximation when the solution is not known is to examine solutions obtained on finer and finer meshes.

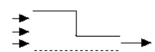
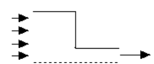
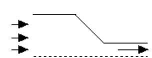
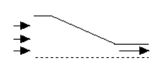
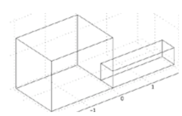
Once the solutions are found, they should be examined in great detail. Available in Comsol Multiphysics are a variety of tools. One can plot a variable as a contour plot, or a color plot, or in a line drawing across some part of a two- or three-dimensional domain. One can also integrate variables over boundary segments (or all of them) or over the domain (or parts of it if it is constructed that way). One can plot and integrate not only the variable itself, but variables defined as equations. For the problem of flow in a pipe, Figure 2, students are asked to calculate the flow rate in and the flow rate out; they should be the same (and they are to six or more significant figures). The pressure drop for a given length must be compared with the analytical solution, and this can be done in both dimensionless terms and dimensional terms. Two or more meshes should be tried, and the pressure drop compared. Streamlines can be plotted, and in this case they should be straight lines. Other complications involve different boundary conditions (slip or symmetry conditions on the axis in axi-symmetric geometry), no slip or velocity specified, specifying the pressure or velocity (but not both). When doing convective diffusion problems, if the Peclet number is large the mesh must be small, or a Petrov-Galerkin option should be used. These matters are discussed if the problems involve convection and diffusion.

Step Three – Solve Research Problem

The research problem obviously involves a problem whose solution that is not known. It is helpful, though, if the student can solve similar problems whose solution is known. This provides a check and is a confidence builder. As an example, suppose a student is going to determine a correlation for pressure drop in a flow element such as a tee (in laminar flow). At low Reynolds number (below 1.0) the form of the correlation is

$$\frac{\Delta p\, x_s}{\eta v_s} = K\,,$$

and one only needs to solve the flow problem to determine K. This has been done for other cases, which are illustrated in Table 2 (2). This table is part of a chapter in a book; it includes work done by ten prior undergraduate researchers.

Table III. Coefficient K_L for contractions and expansions for *Re* negligibly small	Picture	K_L
2:1 pipe/planar		7.3/3.1
3:1 pipe/planar		8.6/4.1
4:1 pipe/planar		9.0/4.5
45 degrees tapered, planar, 3:1		4.9
28.07 degrees tapered, planar, 3:1		10.8
3:1 square (quarter of the geometry)		8.1

v_s = average velocity, x_s = thickness or diameter, both in the small section

Table 2. Coefficient K for contractions and expansions at small Reynolds number (2)

Example Results

Case 1 - Flow in small orifices

When an orifice is used in a small device, the thickness of the orifice affects the pressure drop, particularly in laminar flow. Febe Kusmanto did simulations of this as shown in Figure 5. The dotted lines are an analytical solution due to Dagan, *et al.* (3) for Stokes flow. This work was published (4) and also corrects a misleading impression in the literature (5). Once a solution is obtained, it is possible to gain insight into the solution, by looking at the streamlines, as in Figure 6. Additional complications can also be considered, as shown in Table 3.

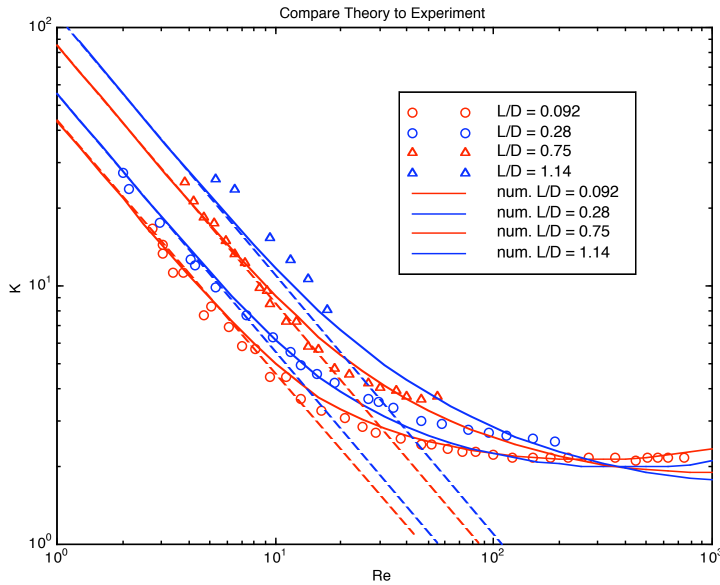


Figure 5. Excess pressure for orifices with a non-negligible thickness

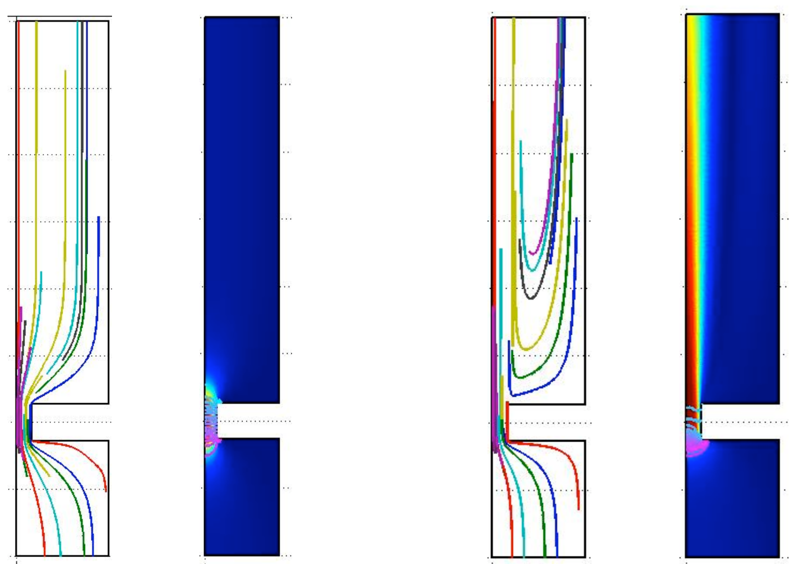


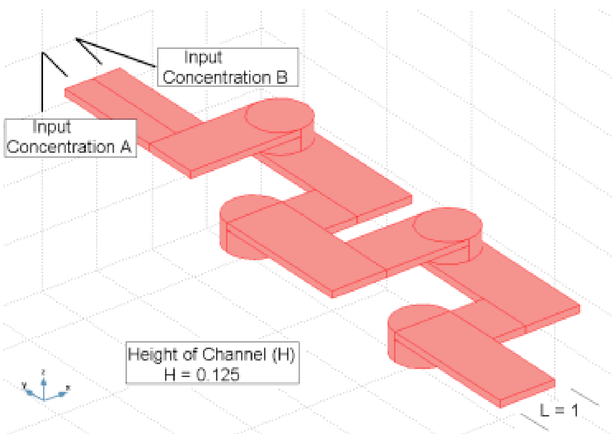
Figure 6. Streamlines and pressure profiles for Re = 0 (left) and 316 (right)

Table 3. Extensions to Orifice Problem

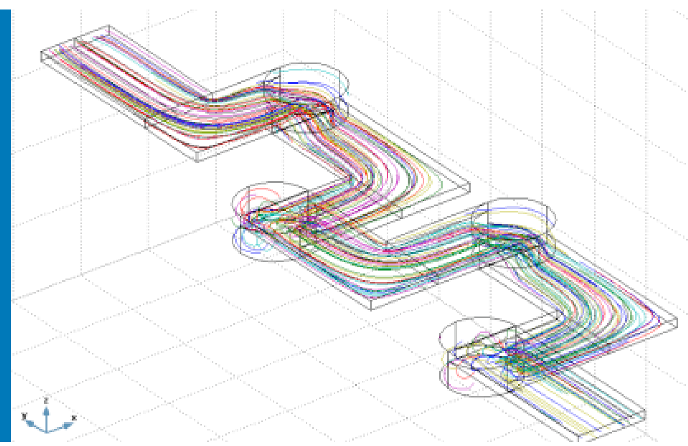
Does the temperature rise enough to affect the solution?
Just add in the temperature equation.
An adiabatic situation shows a temperature rise of less than one degree at the highest Reynolds number.
Work done by Yuli Tan.

Case2 – Mixing in a Serpentine Microfluidic Mixer

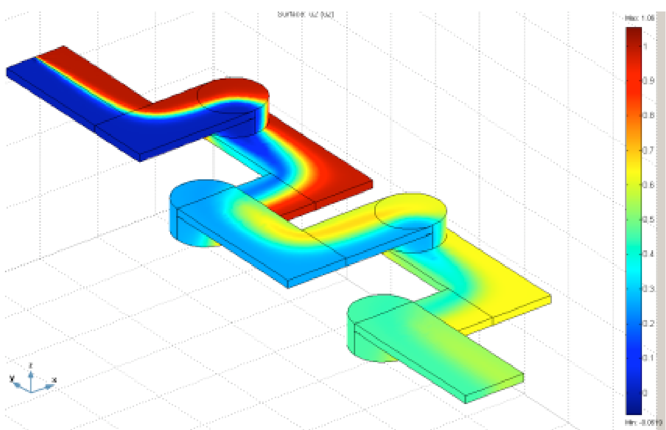
In microfluidic applications, mixing is slow because it is done mostly by diffusion unless the flow geometry causes the fluid paths to mix. The serpentine mixer shown in Figure 7(a) has been designed to mix better in a smaller total length. This problem was solved by Zachery Tyree; first the Navier-Stokes equation was solved, and the streamlines are shown in Figure 7(b). Then the convective diffusion equation was solved, as shown in Figure 7(c). Since the Peclet number is large (2200) it was necessary to refine the mesh for the convective diffusion equation. Thus, the finite element problem is being solved on two meshes, one sufficient for the flow and the other sufficient for the convective diffusion equation. Furthermore, the convection-diffusion problem is solved after the flow is solved. This flexibility in Comsol Multiphysics makes the solution much faster than it would be if all equations had to be solved simultaneously on the same mesh. Figure 8 shows the comparison with experiment (6) and Figure 9 shows the concentration distribution internal to the device, which shows how the mixing actually takes place.



(a)



(b)



(c)

Figure 7. Serpentine mixer

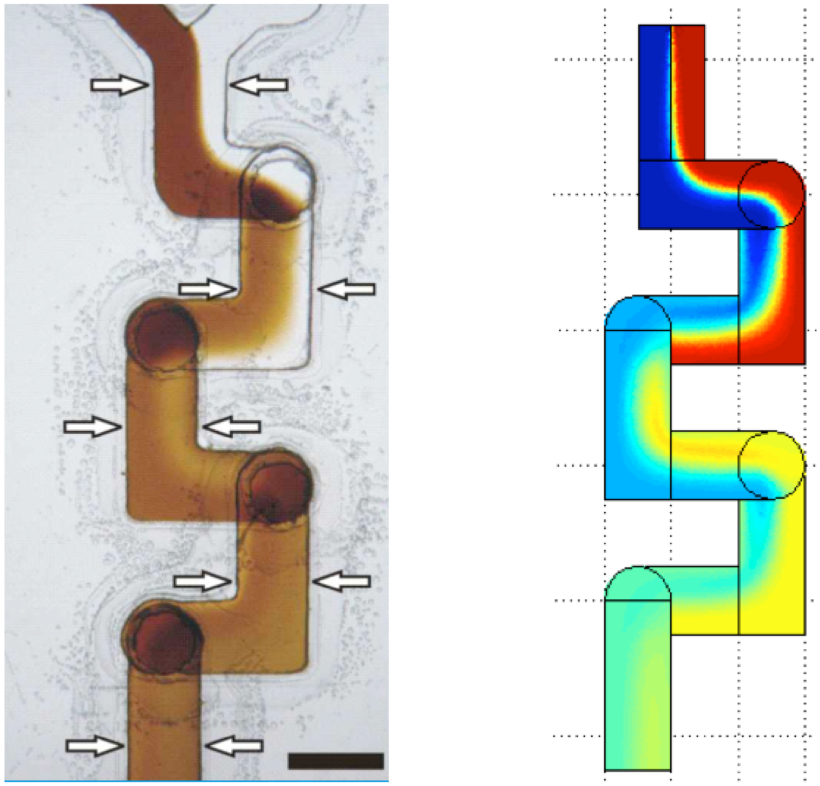


Figure 8. Comparison with experiment (6)

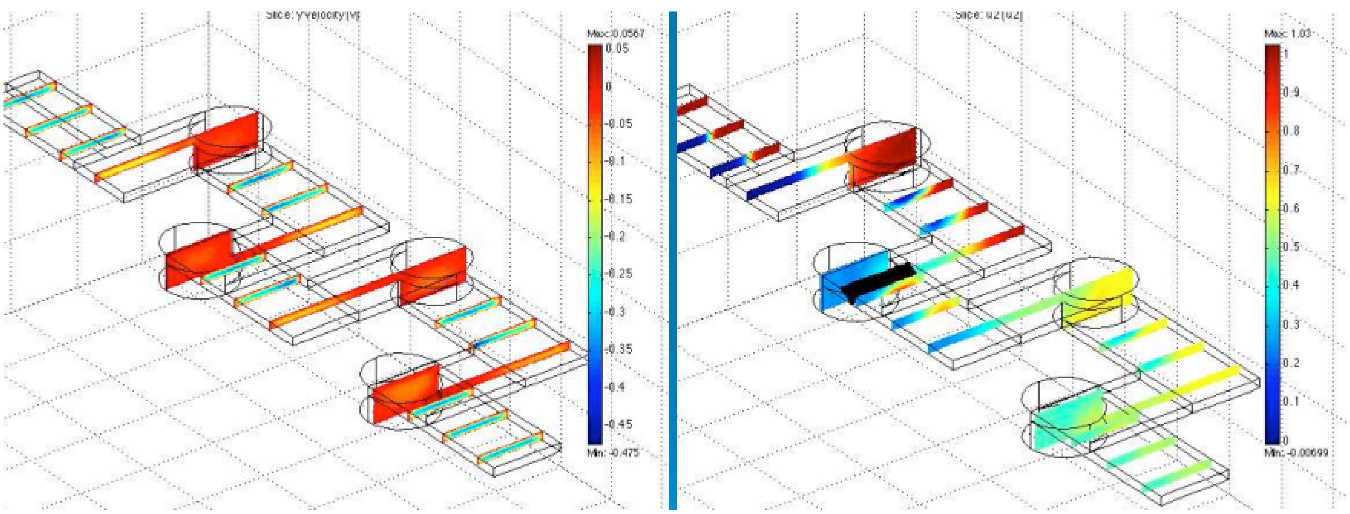


Figure 9. Velocity profiles and concentration profiles inside serpentine mixer

Case3 – Mixing in a Pharmaceutical Device

One method of mixing chemicals for analysis is to use a process which injects one chemical into a solution and then removes part of the solution (aspiration). Nick Cox studied such a device based on suggestions from Dr. Mark Petrich, Rosetta Inpharmatics, Inc. The talk will show a movie of the mixing that takes place.

Case4 – Examination of magnetic field for removal of arsenic from water

Jonathan Lundt, an undergraduate physics student, studied the problem of removing arsenic from water. The method is to add a magnetic material on which the arsenic absorbs and then to remove the magnetic material (7,8). The removal is achieved by passing the magnetic solution through a bed (or steel wool) that is in an applied magnetic field. The magnetic particles then adhere to the steel wool. His role was to find a geometry that would give the maximum magnetic force. One geometry, and its force magnitude, is illustrated in Figure 10.

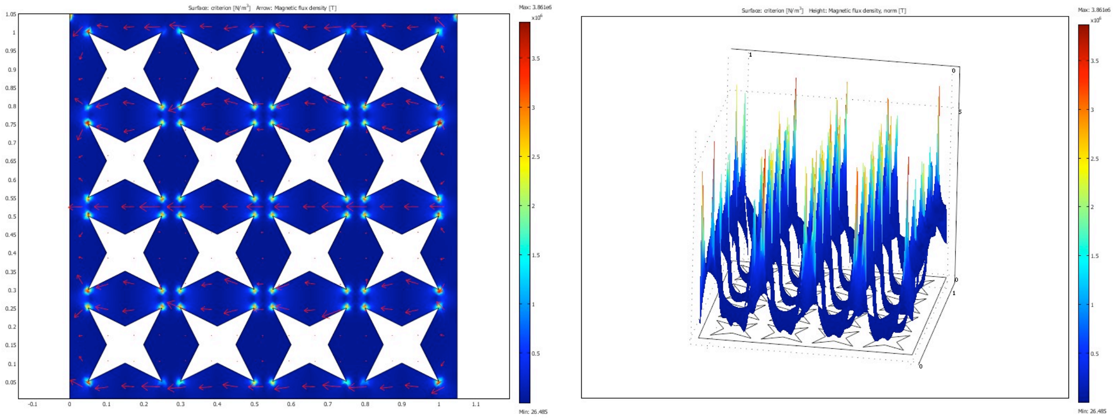


Figure 10. Geometry of packing and magnetic force field for removal of arsenic-coated magnetic particles

Case 5 – Polymer mixing

In the Renton Wastewater Treatment plant near Seattle, a polymer is added to a solution of sludge to encourage it to flocculate. Then the stream goes to a centrifuge where the sludge is removed and sent over the Cascade mountains for fertilizer in Eastern Washington. To enhance the mixing, a mixer was installed, but the mixing was still insufficient. Sharpe Mixers helped develop a project that eleven students worked on. Shown in Figure 11 are the streamlines for a simulation when a polymer is injected into the main stream. The interesting feature discovered by the students is that the power-law index of the polymer solution is very low (by measurements) and turbulent flow only occurs at a higher Reynolds number for low power-law indices. Thus, the flow was in a regime which could have been laminar. Figure 11 shows that the polymer solution is not well mixed, and other simulations over eight feet show it still isn't well mixed, when the flow is laminar. In this case, the instructor was willing to settle for a Newtonian flow, since the problem is so complicated, but the students proceeded to use a non-Newtonian model, not knowing it might be hard. But they succeeded!

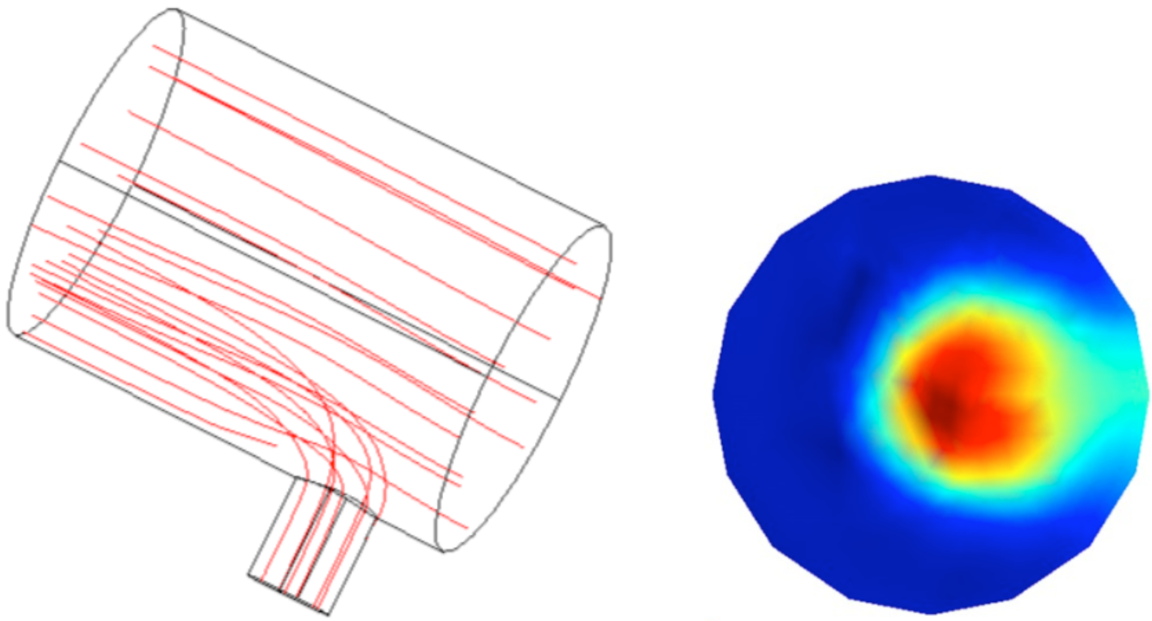


Figure 11. Streamlines and polymer concentration at the exit

Case 6 – Transport Effects in Thermal Flow Field Fractionation

This case is treated in another presentation, paper 304c, with co-authors Nick Cox and Pawel Drapala.

Case 7 – Three-dimensional hole pressure problem

Stephanie Yuen solved the two- and three-dimensional hole pressure problem for a Newtonian fluid. This geometry can be used with polymers to deduce the first normal stress difference. Shown in Figure 12 are the velocity magnitudes for the two-dimensional problem and for the center of the three-dimensional problem. As can be seen, the two results are very similar.

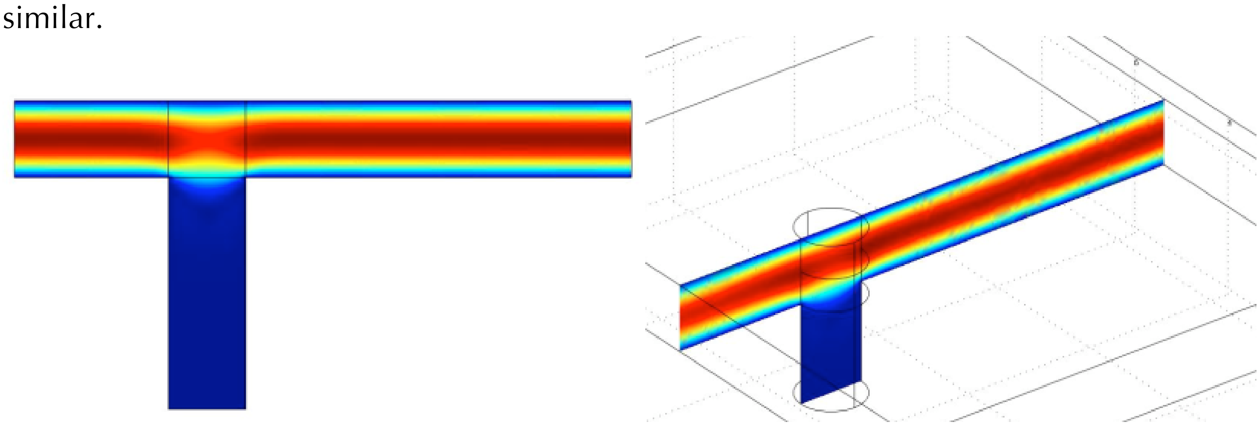


Figure 12. Flow profiles in the hole pressure problem

Case 8 – Mixing in a Three-dimensional T

It has long been recognized that in a two-dimensional T-sensor the mixing of two fluids is entirely by diffusion. Previous students have solved the problem and measured the mixing using a mixing cup concentration and a variance defined below.

$$c_{\text{mixing cup}} = \frac{\int_A c\,\mathbf{u} \bullet d\mathbf{A}}{\int_A \mathbf{u} \bullet d\mathbf{A}}, \quad variance = \frac{\int_A (c - c_{\text{mixing cup}})^2\,\mathbf{u} \bullet d\mathbf{A}}{\int_A \mathbf{u} \bullet d\mathbf{A}}$$

Daniel Kress studied the same situation but in a three dimensional case with two circular channels coming together and forming a T with a third channel as the outlet. There was no problem creating the geometry because Comsol Multiphysics handles the complications of two circular pipes joining in sideways to another circular pipe. The inherent three-dimensional nature of the problem is illustrated in Figure 13, where it is seen that regions near the walls have more time to diffuse sideways because their velocity is smaller. Figure 14 shows variance for a variety of conditions. Plotted there are two-dimensional variances for Peclet numbers from 14 to 288 as well as three-dimensional variances. Figure 14 shows that there is a universal mixing curve that can be determined even from a two-dimensional simulation.

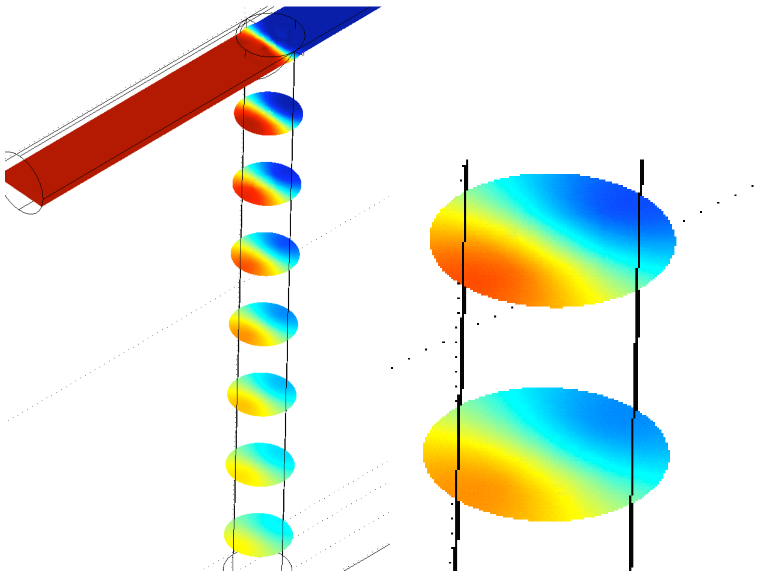


Figure 13. Concentration profiles in mixing device

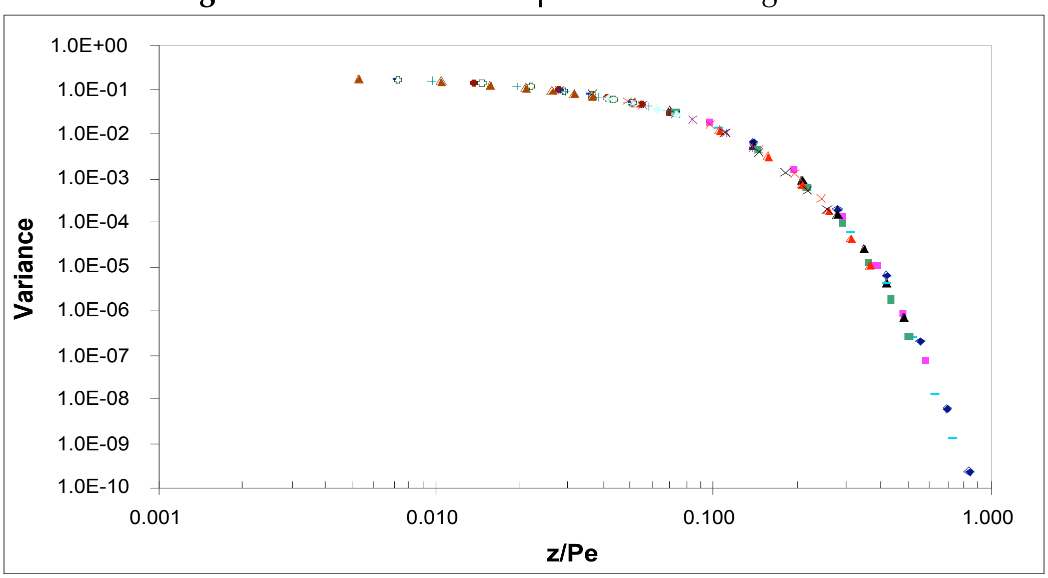


Figure 14. Variance as a function of length in the outlet leg

Case 9 – Flow of Water in Partially Saturated Soils

Comsol Multiphysics also has equations for flow through porous media. Anna Moon solved a one-dimensional case in which water flowed under pressure through a series of four different soils. The pressure profiles are shown in Figure 15. This problem was one the author originally tackled when studying the flow of water in dry soils, as in the Hanford Atomic Energy Complex. Once the one-dimensional problem was solved, it was easy to extend it to two dimensions, as shown in Figure 16.

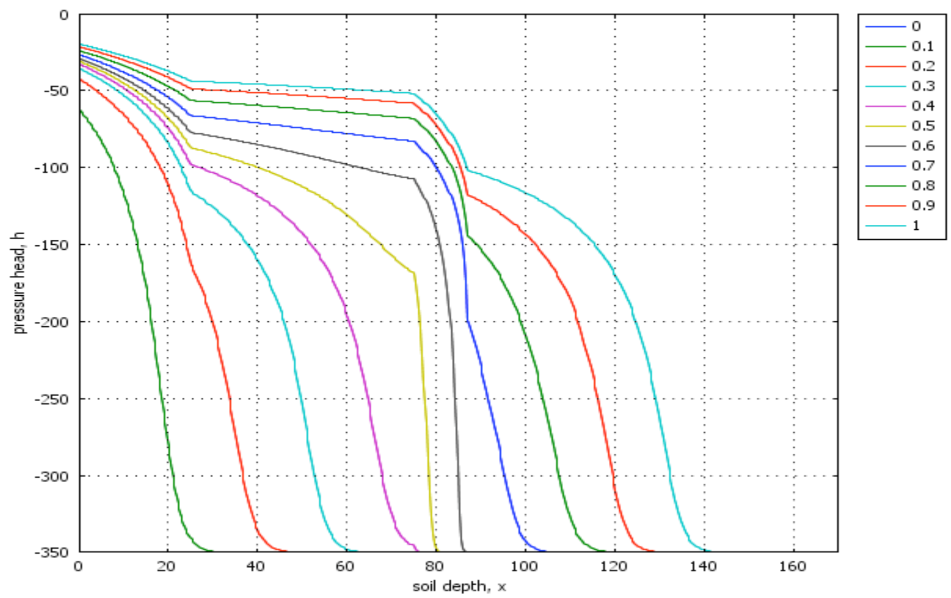


Figure 15. Pressure change when water flows through different soils

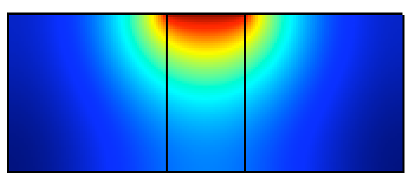


Figure 16. Two-dimensional injection into a porous media

Conclusions

The program Comsol Multiphysics is relatively easy to use for quite complicated problems. This allows undergraduates to perform meaningful simulations that go beyond their textbook examples, challenge their creativity, and improve their problem-solving skills. Results of prior quarters are described on the web site:

http://courses.washington.edu/microflo/

Acknowlegement

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References

1. Finlayson, B. A., *Introduction to Chemical Engineering Computing*, Wiley (2006).
2. Bruce A. Finlayson, Pawel W. Drapala, Matt Gebhardt, Michael D. Harrison, Bryan Johnson, Marlina Lukman, Suwimol Kunaridtipol, Trevor Plaisted, Zachary Tyree, Jeremy VanBuren, Albert Witarsa, "Micro-component flow characterization," Ch. 8 in Micro-Instrumentation, (M. Koch, K.Vanden Bussche, R. Chrisman (ed.), Wiley, 2007).
3. Dagan, Z., Weinbaum, S. and R. Pfeffer, "An infinite-series solution for the creeping motion through an orifice of finite length," J. Fluid Mech. **115** 505 (1982).
4. Febe Kusmanto, Elissa L. Jacobsen, Bruce A. Finlayson "Applicability of Continuum Mechanics to Pressure Drop in Small Orifices", Phys. Fluids **16** 4129-4134 (2004).
5. Hasegawa, T., Suganuma, M., and H. Watanabe, "Anomaly of Excess pressure drops of the flow through very small orifices," Phys. Fluids **9** 1 (1997).
6. Christopher Neils, Zachary Tyree, Bruce Finlayson, Albert Folch, "Combinatorial mixing of microfluidic streams", Lab-on-a-Chip **4** 342-350 (2004).
7. Yavuz, C. T., *et al.* "Low-Field Magnetic Separation of Monodisperse Fe3O4 Nanocrystals," *Science* **314** 964-967 (2006).
8. Halford, Bethany. "Cleaning Water with 'Nanorust.'" *Chemical & Engineering News,* **84(46),** p.12, November 13, 2006