Visions Realized: Using Comsol Multiphysics to Prepare Students for the Modern World

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The World is Flat: A Brief History of the Twenty-first Century
Thomas Friedman, NY Times

- After the fall of the Berlin Wall, and the economic development in Southeast Asia, there are potentially 3 billion more knowledge workers.
- The cost to transfer information is extremely low.
- New requirements: creativity and innovation.

My Journey

- Using a pre-2000 commercial code in classes proved to be too hard for students to use it on their own, and it took too much of my time. So I stopped trying to introduce finite element simulations of fluid flow and convective heat transfer to chemical engineering students.
- pde toolbox - pre-2000
- FEMLAB - 2D - 2001
- Comsol Multiphysics - 3D - 2002

Attractive Features to be Illustrated

- GUI
- Draw domain, internal boundaries
- Automatic mesh generation and refinement
- Solve equations one at a time, on different meshes
- Easy to add physics
- Easy to modify parameters, even those dependent upon the solution
- Parametric solver
- Post-processing capability to validate the solution

How I introduce students to Comsol Multiphysics

- a) Students solve a problem they have in their textbook - check their work against a known outcome
- b) Students solve a known problem with a slight extension - one that makes the problem intractable analytically, and that uses some of the FEMLAB features - this inspires the students to see what is possible.

Important Lesson:

How to check that your results are right!

Beginning problems

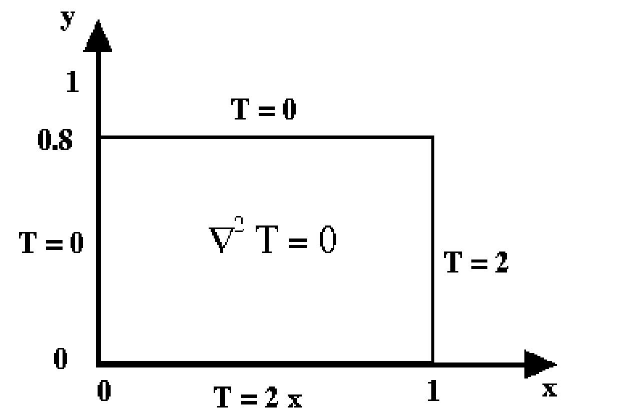
a) Flow in a pipe

Solve for fully developed flow in a pipe, with this inlet boundary condition:

$$u = u_0 \left[1 - \left(\frac{r}{R} \right)^2 \right]$$

and compare with the Hagen-Poiseuille law in your textbook.

b) Heat transfer in 2D



Put 2 * x into the BC window rather than a number.

Problem has a singularity at one corner.

Project Formulation

- Goal oriented, sometimes a model problem, solved in 10 week quarter
- Organized in 3-5 steps of increasing complexity
- Meet weekly, but I'm hands-off
- After 6 weeks, students are panicking
- I reassure them
- In weeks 7-8 they begin to get results and they are inspired - beautiful pictures, show my friends, Wow!, this is more than my textbooks cover!
- Then the innovation starts: What if…
- More complicated project goals the next quarter.

My Journey began with pdetool in MATLAB

Solved Poisson's equation in 2D

$$\nabla^2 u = f$$

Allowed one to adjust coefficients draw the domain (irregular), mesh automatically, refine the mesh on command, solve the problem, and plot the solution and its derivatives.

Ch. E. 475 - Tutorial for using Matlab/PDE Toolbox to solve elliptic boundary value problems

Open Matlab and give the command pdetool. (This only works if one has the professional version with pde toolbox. This is installed in BNS 125.)

Draw	click on the square icon and draw a rectangle
	for the inner rectangle, do again
	to make a hole, use R1 – R2
	double click on the object to set exact dimensions
boundary mode - choose ∂W icon	
	click on one boundary
	or shift click on all boundary segments with the same boundary condition
	double click on the last one, and set the boundary condition
Mesh	click once on triangle icon
	click on divided triangle icon to refine the mesh
Pde	choose specification - to check the differential equation
=	click on = to solve the problem
Plot	set parameters to choose the type of plot

• You can go back and refine the mesh (click the more refined mesh symbol) and resolve the problem. This gives you an indication of the accuracy of the solution.

• If you want detailed information about the solution, you must save the solution to the MATLAB command workspace (it is called u), and save the element information (it is called p e t).

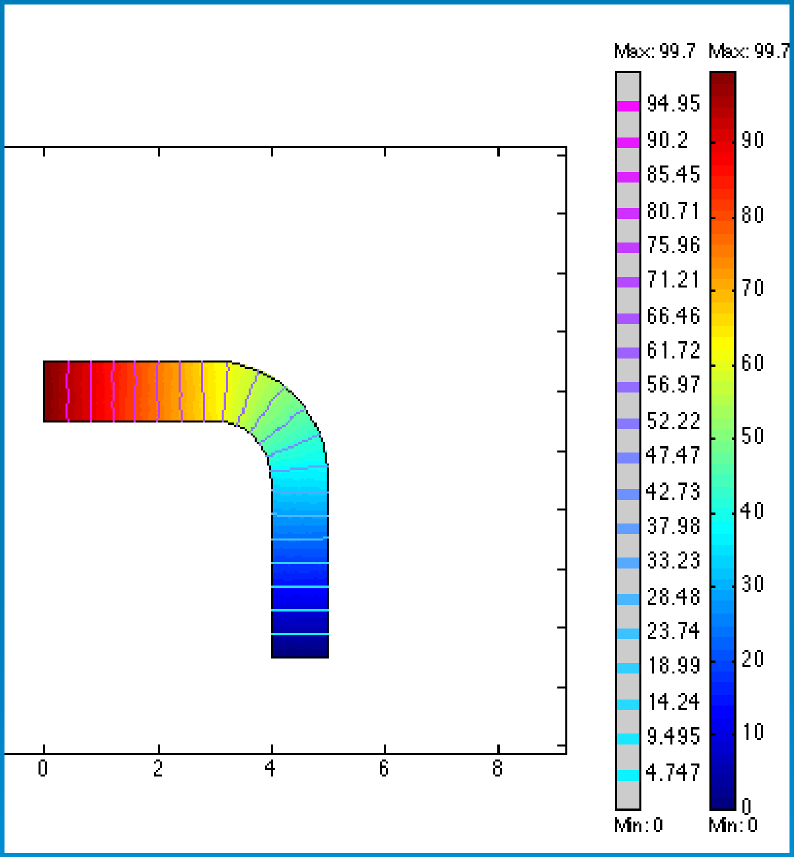
• Save your work frequently!

Wouldn't it be nice if someone did that for the Navier-Stokes equation?

Someone did!

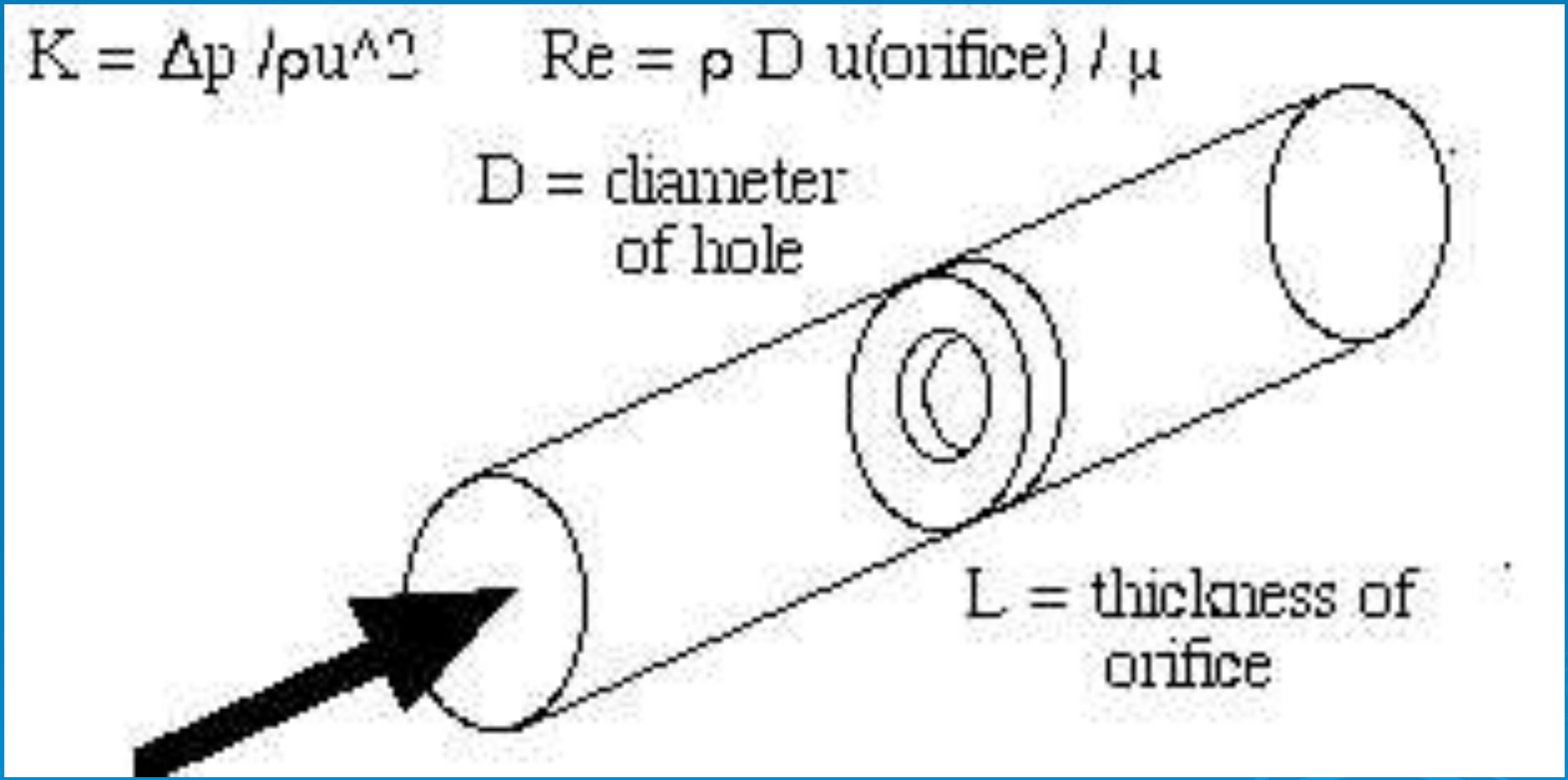
In March, 2001, Suwimol Kunaritipol, a junior Thai exchange student, asked me if she could do an undergraduate research project with me. I had not had much success with undergraduates, due to difficulty in getting a program to run correctly. But, I said, Comsol has just come out with a new program that will solve the Navier-Stokes equations in 2D. It won't be ready until half the quarter is over, but you can learn on pdetool until then. She accepted, and later in the quarter she came back with results and taught me something! That was when I decided to do more undergraduate projects.

What did she teach me?



In laminar flow, the pressure drop going around the bend depends only on the pathlength along the center.

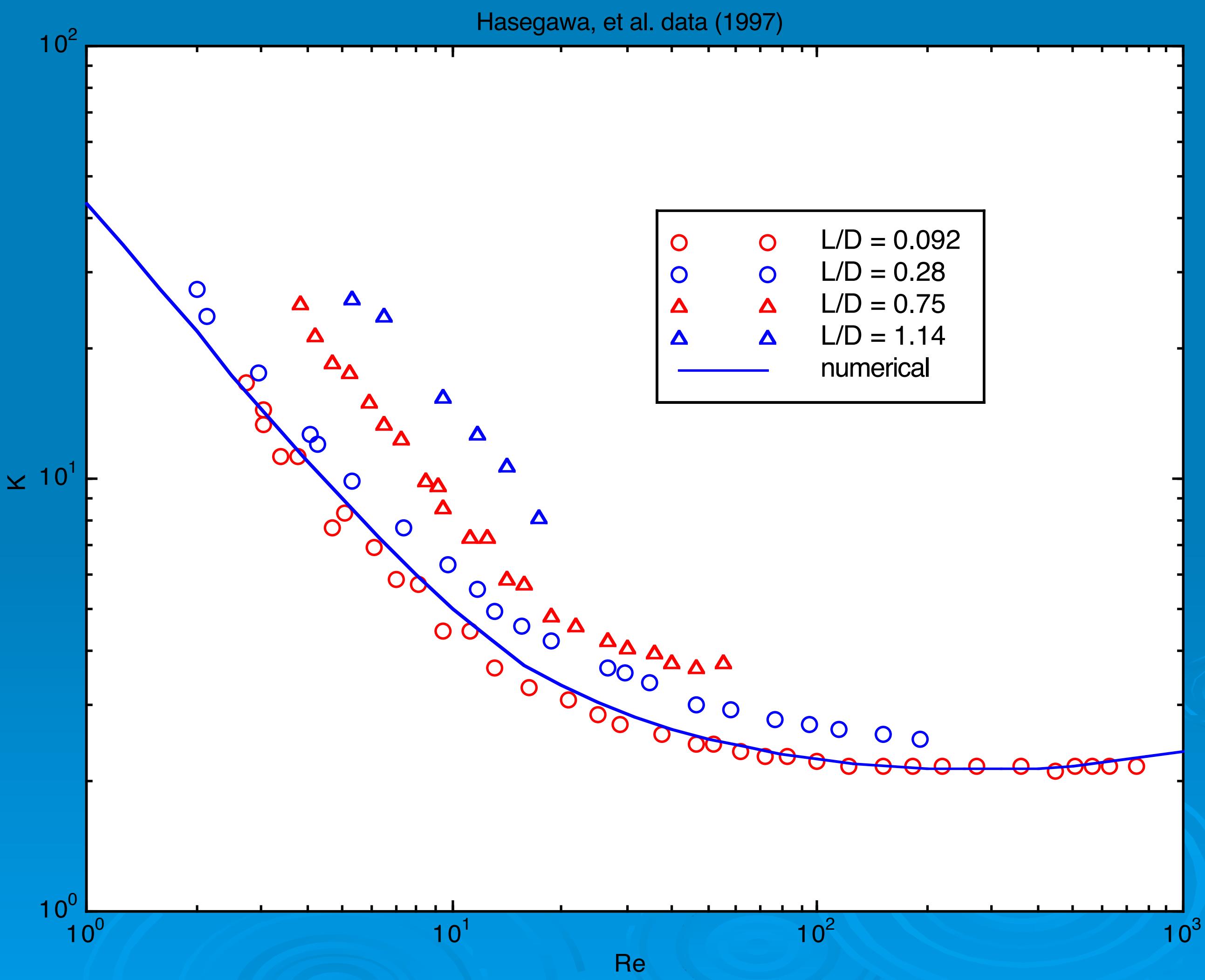
Pressure drop in orifice
Elissa Jacobsen and Febe Kusmanto



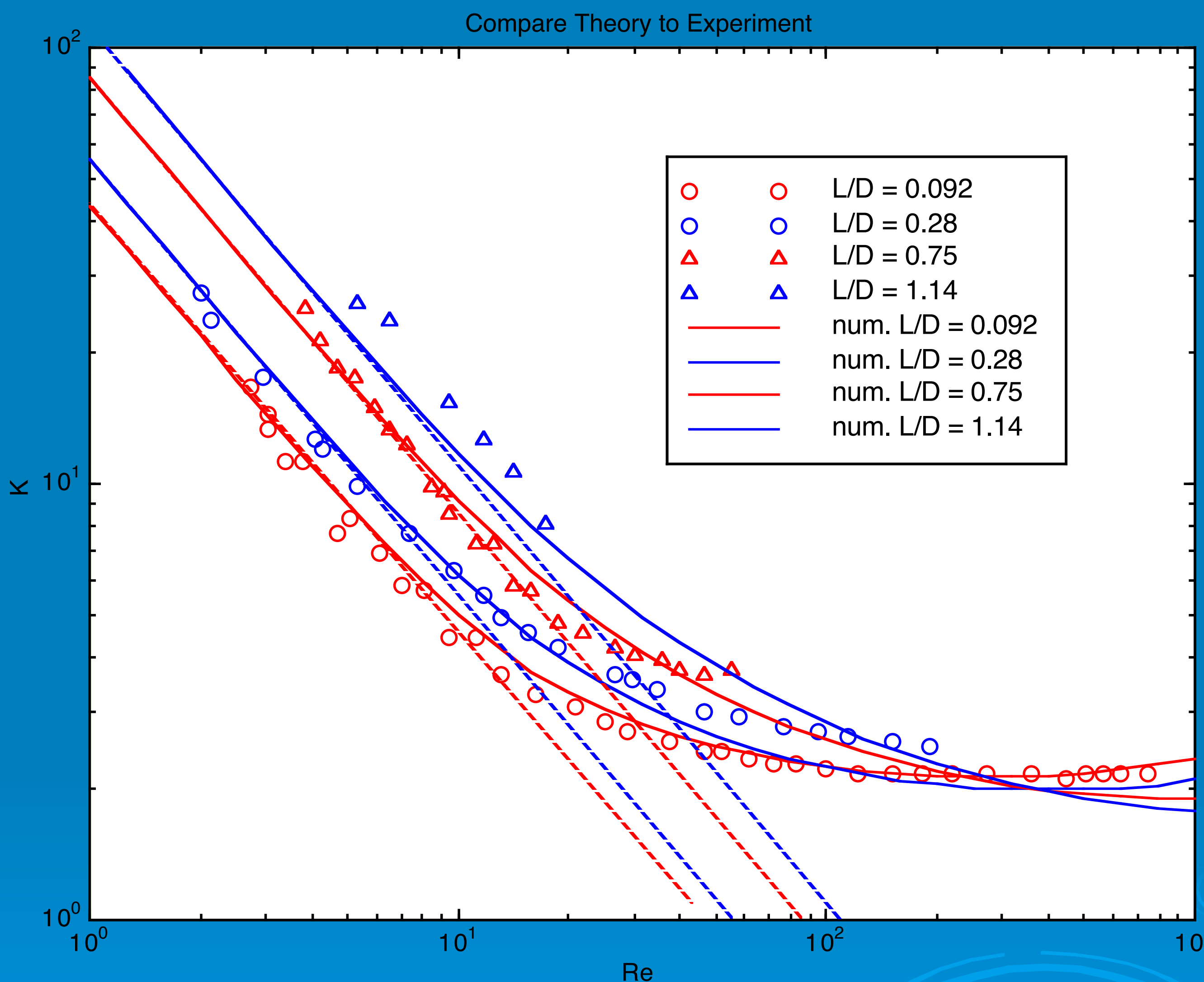
Orifice diameters as small as 8 microns

Hasegawa, et al., Physics of Fluids,1997 says: 'this data cannot be predicted using classical fluid mechanics'

If continuum mechanics does not hold in orifice of 8 microns, how small is small?

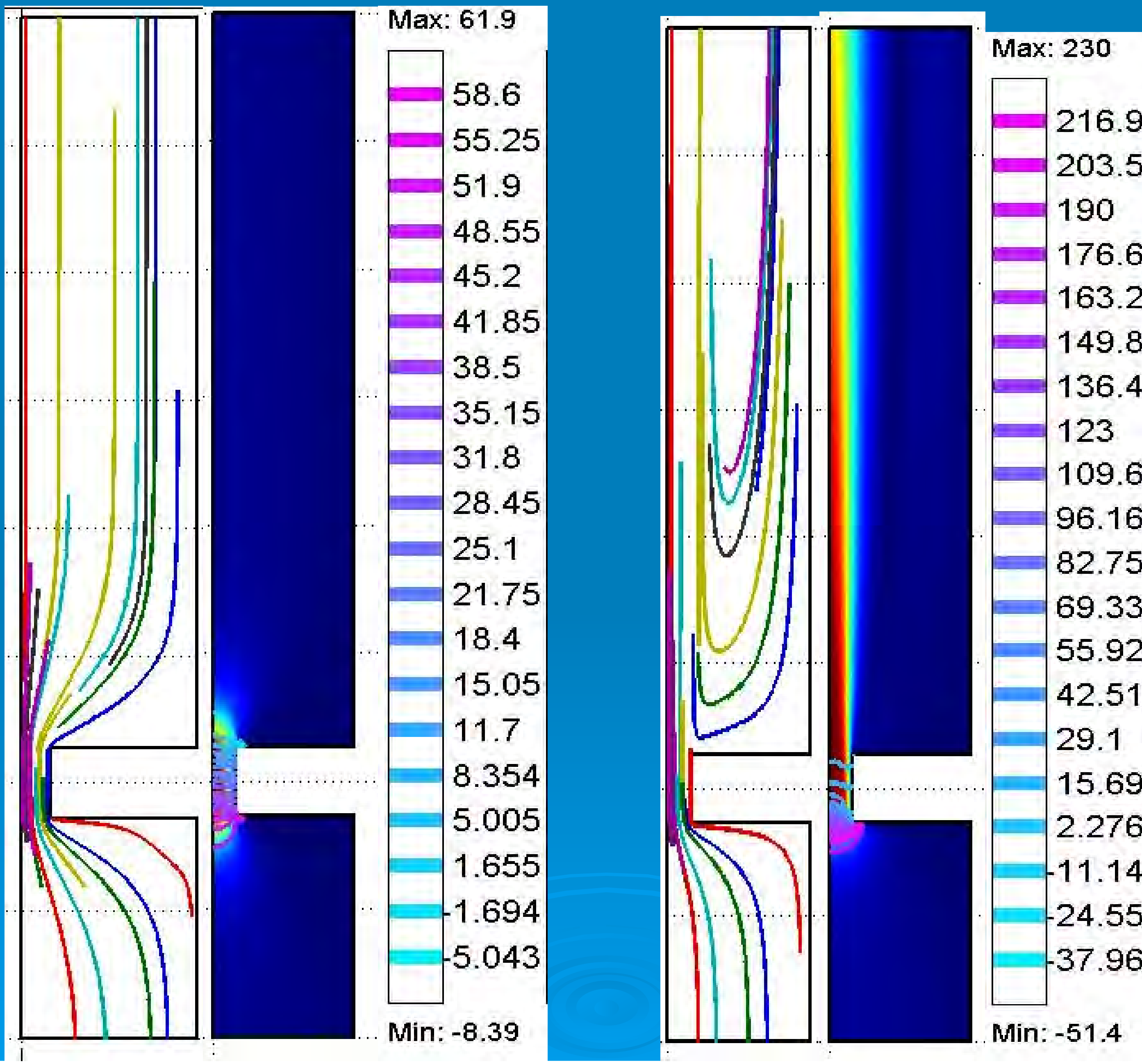


Continuum mechanics can in fact explain data in devices as small as 8 microns.



Dagan, et al., J. Fluid Mechanics, 1982, solved the Stokes problem analytically (straight lines). Our finite element simulations for Reynolds number = 0 agree with their solutions. The rest of the curve is numerical, solved for a range of parameters using the parametric solver with Re = 10^x, x=0:0.1:3.

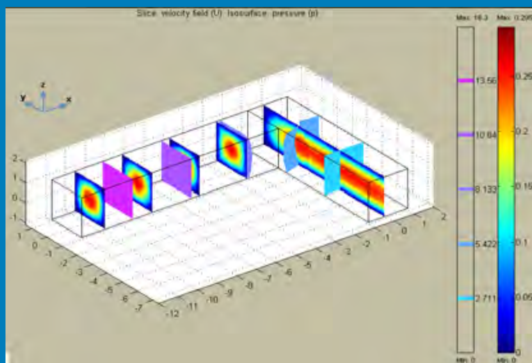
Pressure Profile at Re = 0 and 316

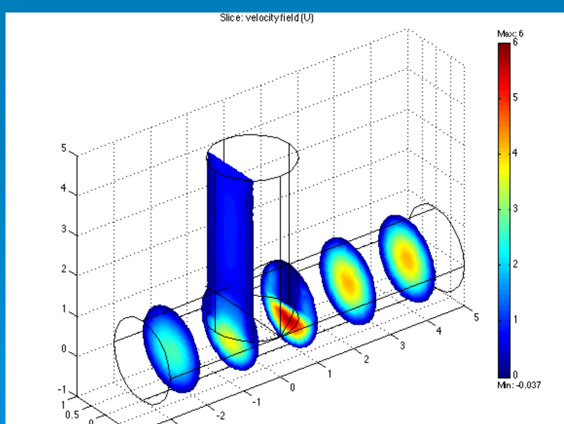


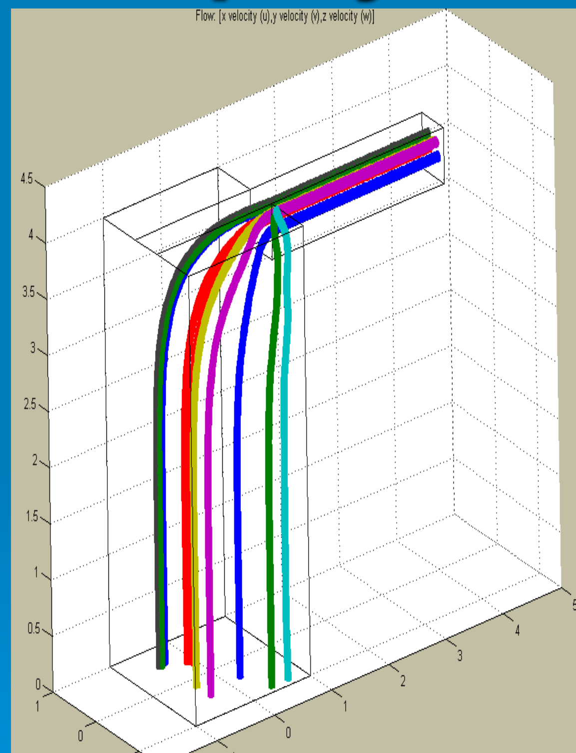
Additional insights using Comsol Multiphysics

- Does the temperature rise enough to cause the viscosity to change?
- Solve the energy equation, too, with the viscous dissipation included using FEMLAB's ability to put in equations.
- Found the temperature rise was less than one degree for an adiabatic channel.
- Work done with Yuli Tan

That fall, Marlina Lukman and Albert Witarsa, from Indonesia, began a series of projects

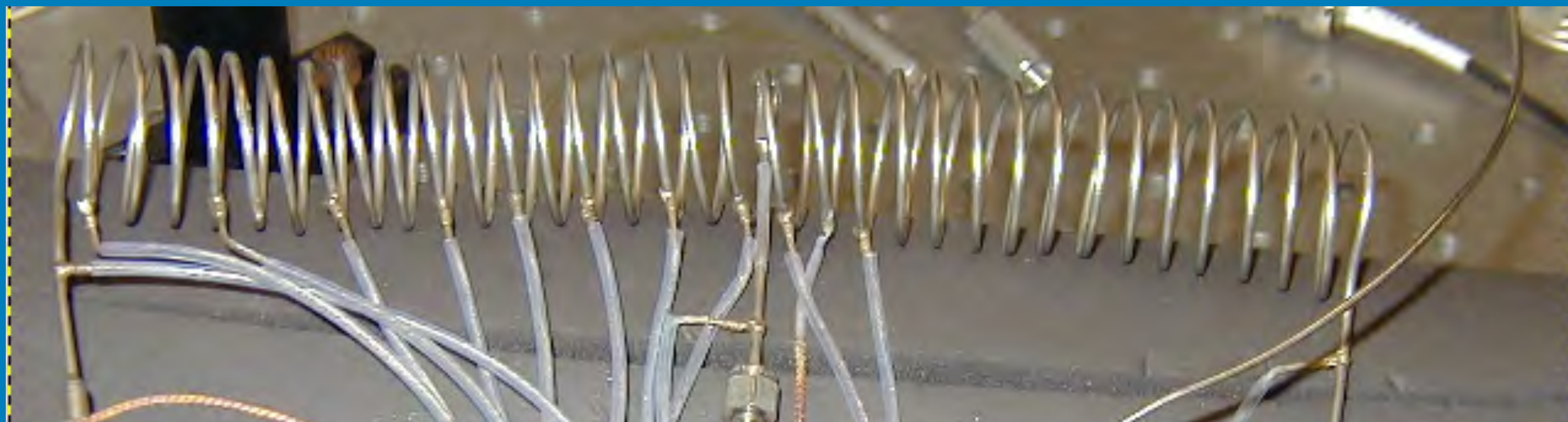






- Pressure drop in contractions, depend upon geometry and flow rate. Correlations exist for turbulent flow, but not for laminar flow.
- Mixing in microfluidic devices

Mixing in the Dow reactor, Zach Tyree



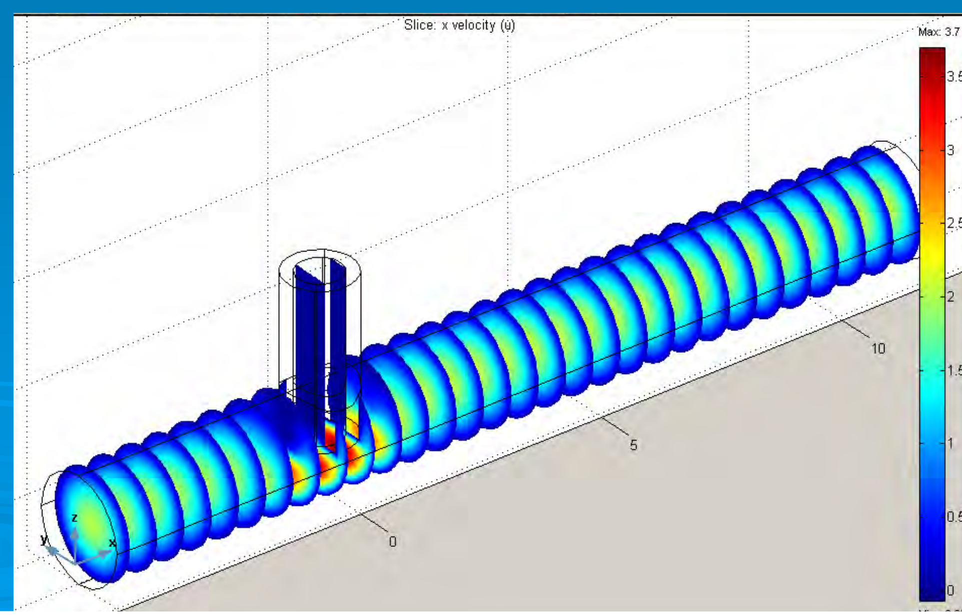
Entrance of Liquid A

Entrance of Liquid B

Exit

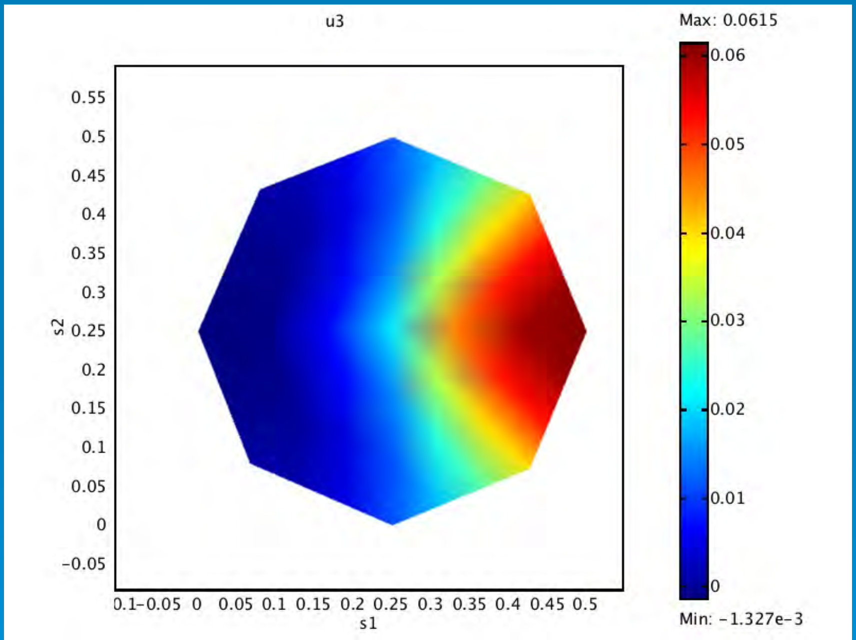
Need geometry and flow rates, viscosity, but density is not very important at low Re.

Relatively easy at low Reynolds numbers.

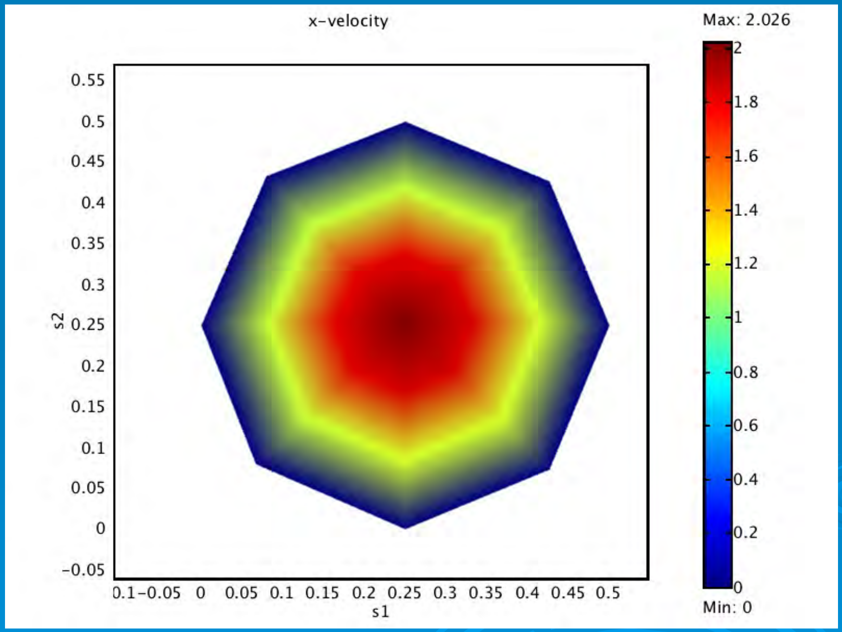


Good mixing won't occur in laminar flow.

The concentration distribution at the exit is very different from the velocity distribution and is quite irregular.

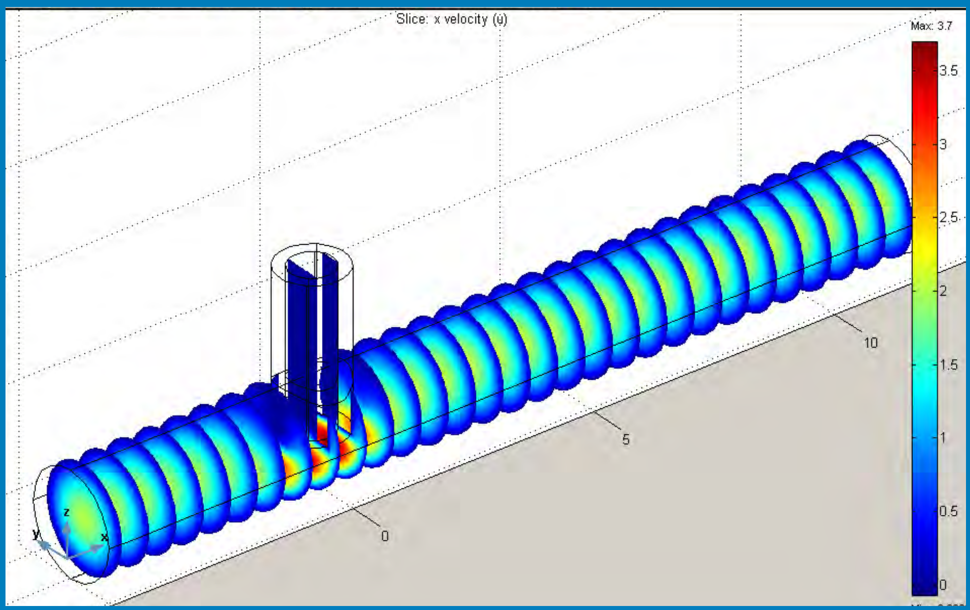


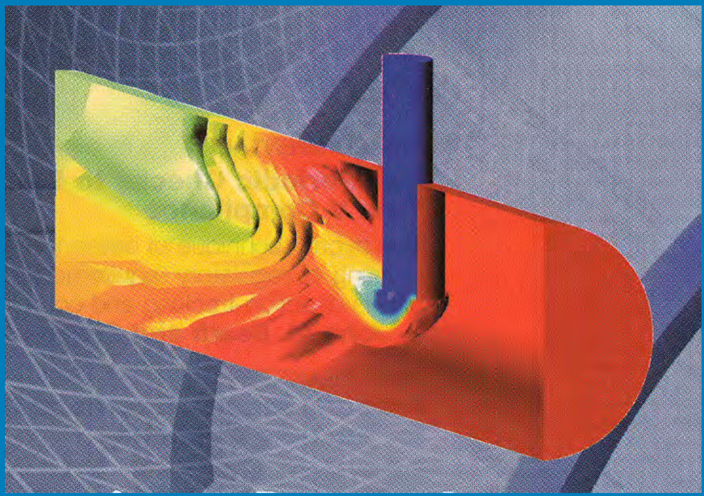
Product concentration



Axial velocity

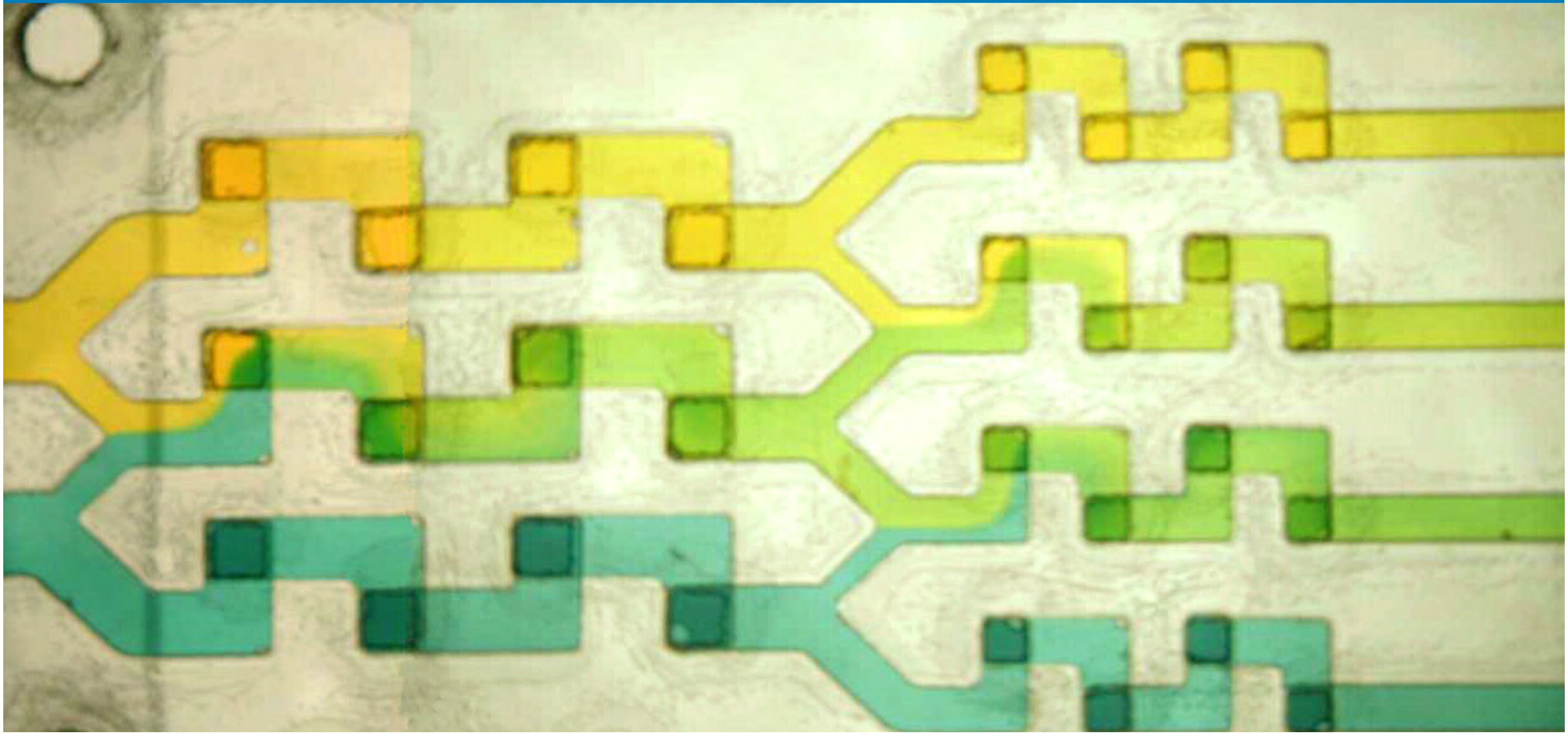
Our model became one of the icons



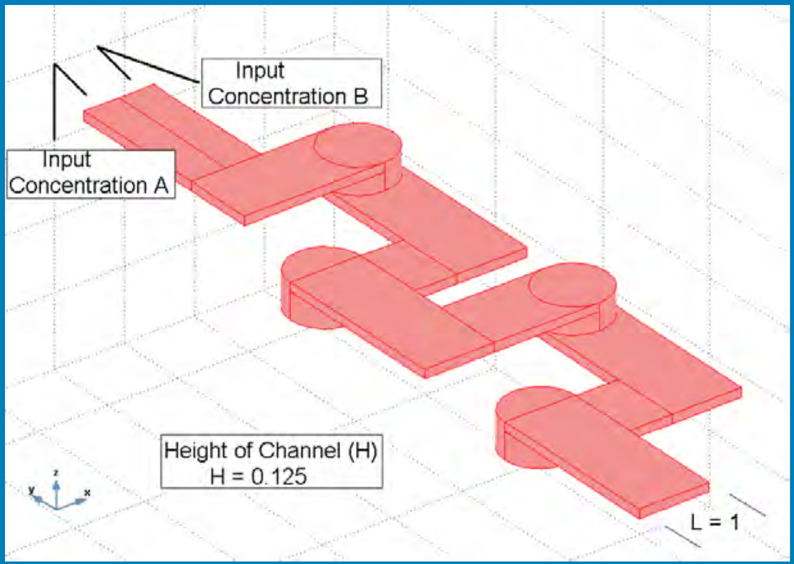


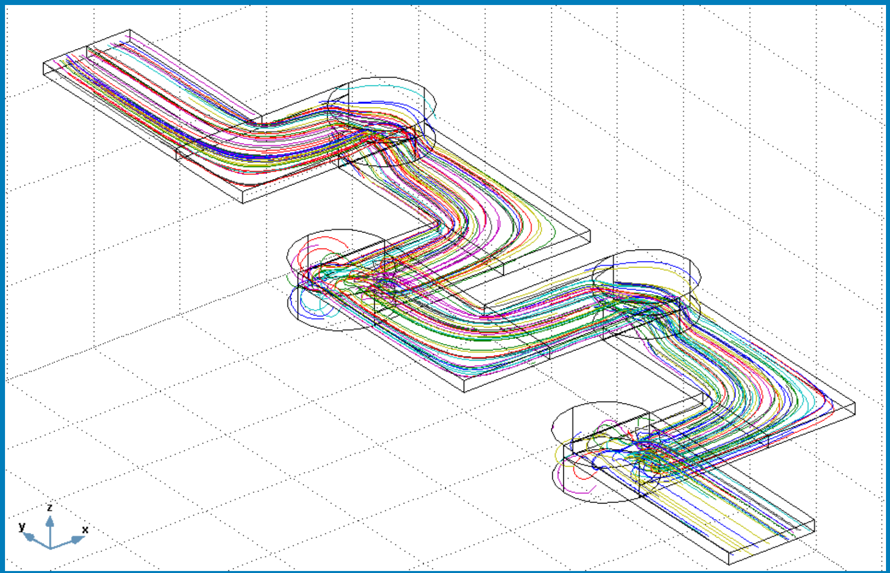
You see this icon in the Chemical Engineering module.

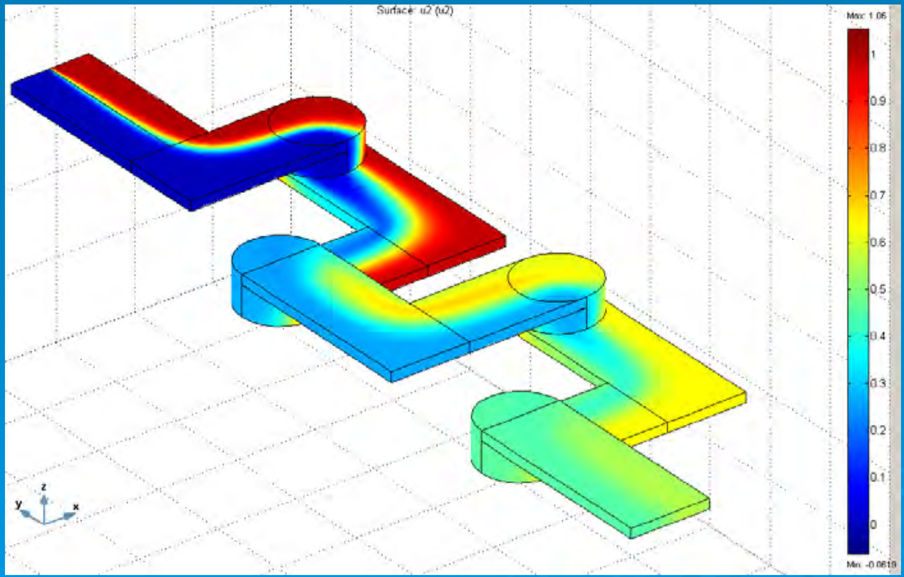
Serpentine mixer is used to create good mixing in laminar flow in a short distance. Work with Chris Niels and Prof. Albert Folch



Serpentine mixer, Zach Tyree

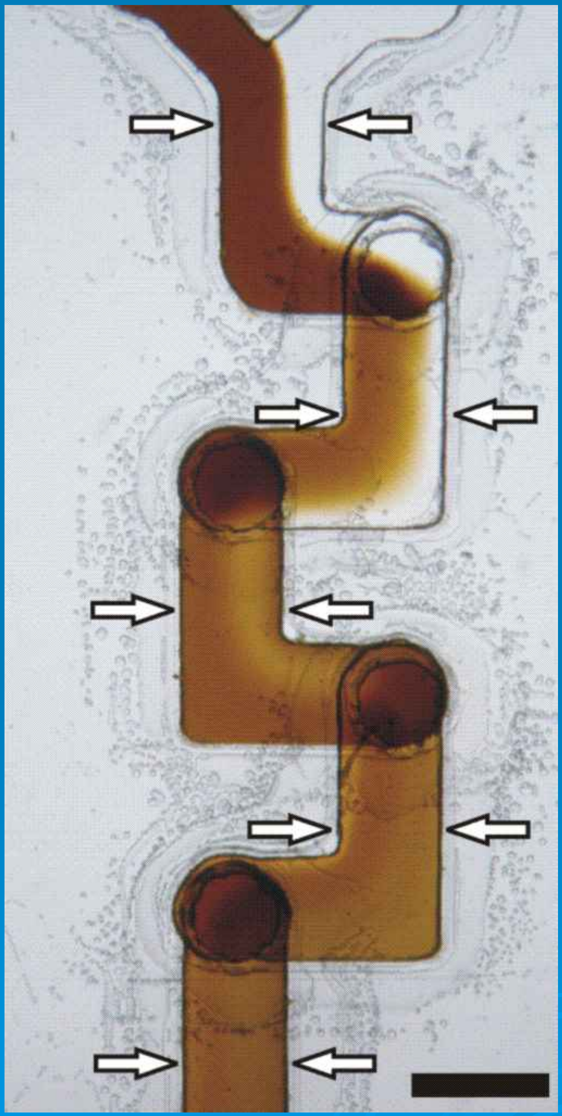


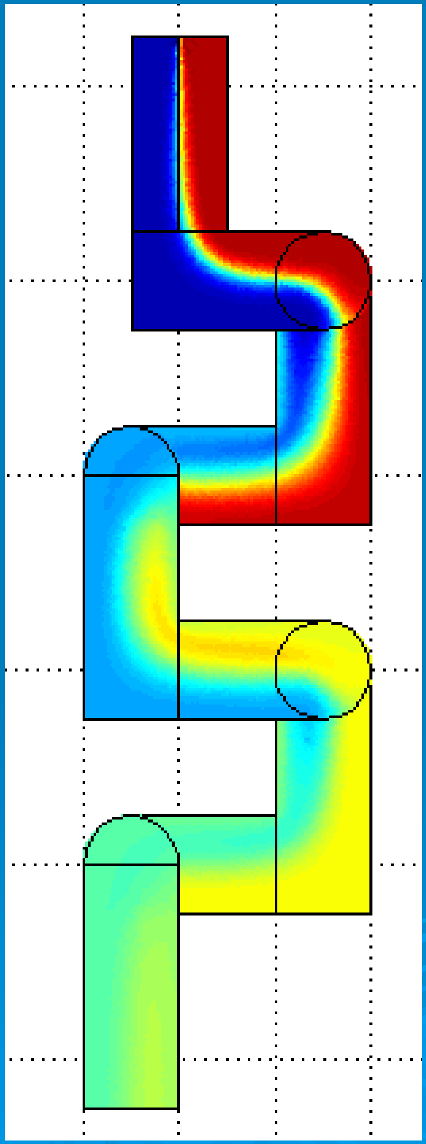




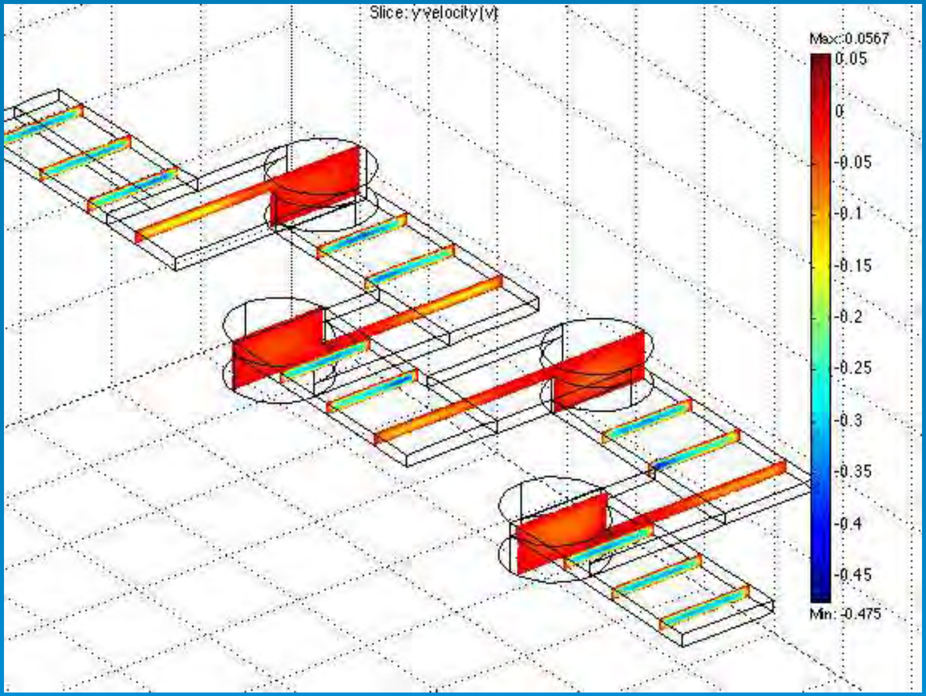
Used Comsol Multiphysics' ability to solve the convective diffusion equation after the Navier-Stokes equation is solved, and on a different mesh, needed for Peclet number = 2200, 280,000 dof

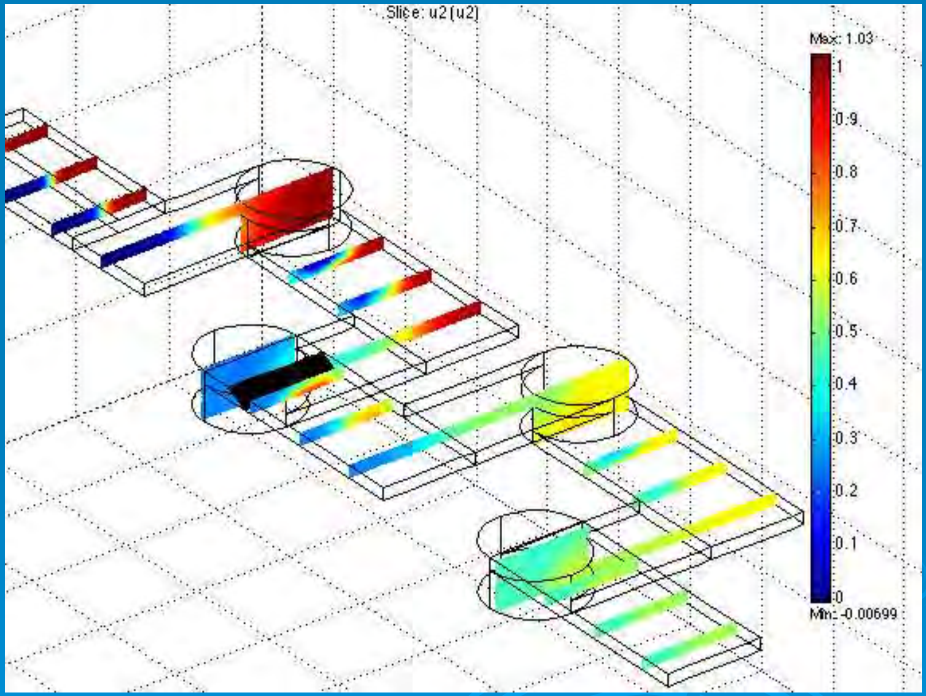
Comparison with experiment



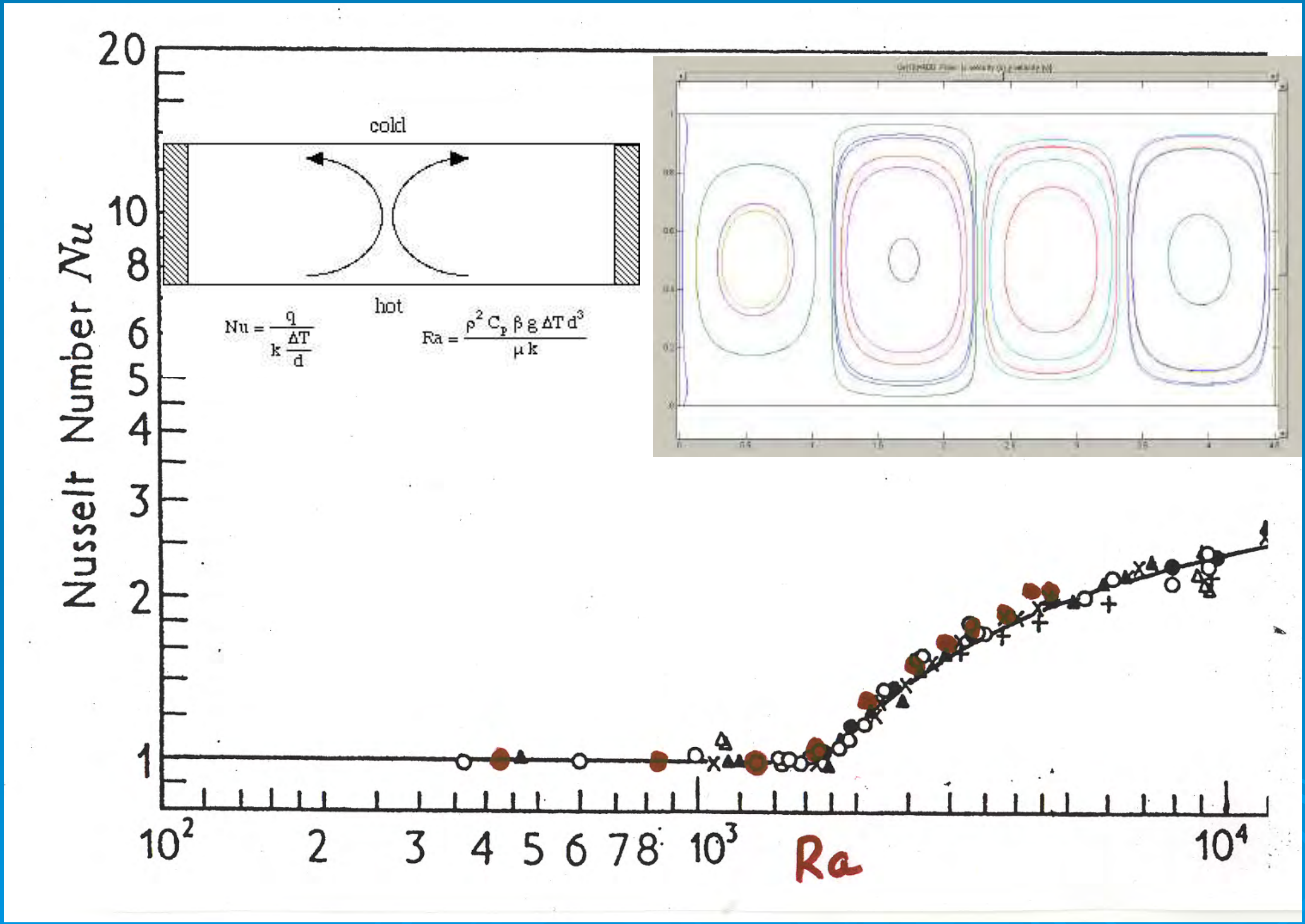


Internal view of velocity and concentration - post processing leads to insight

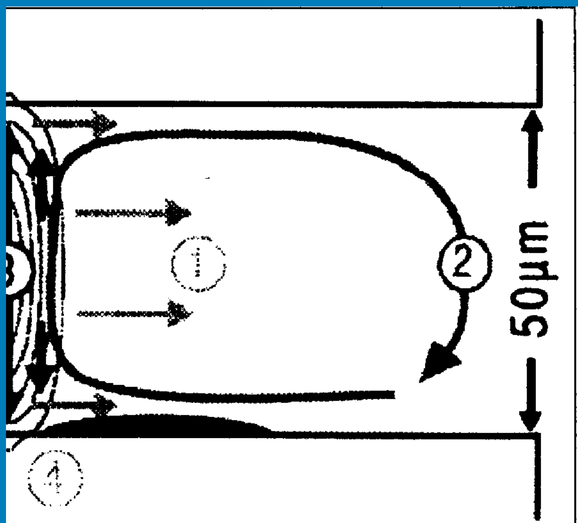




Convective Instability, Michael Harrison



Thermal diffusion, Pawel Drapala



periment (Braun 188103-2). The concentrate is
(2), and pilled on the bottom of the container (4).

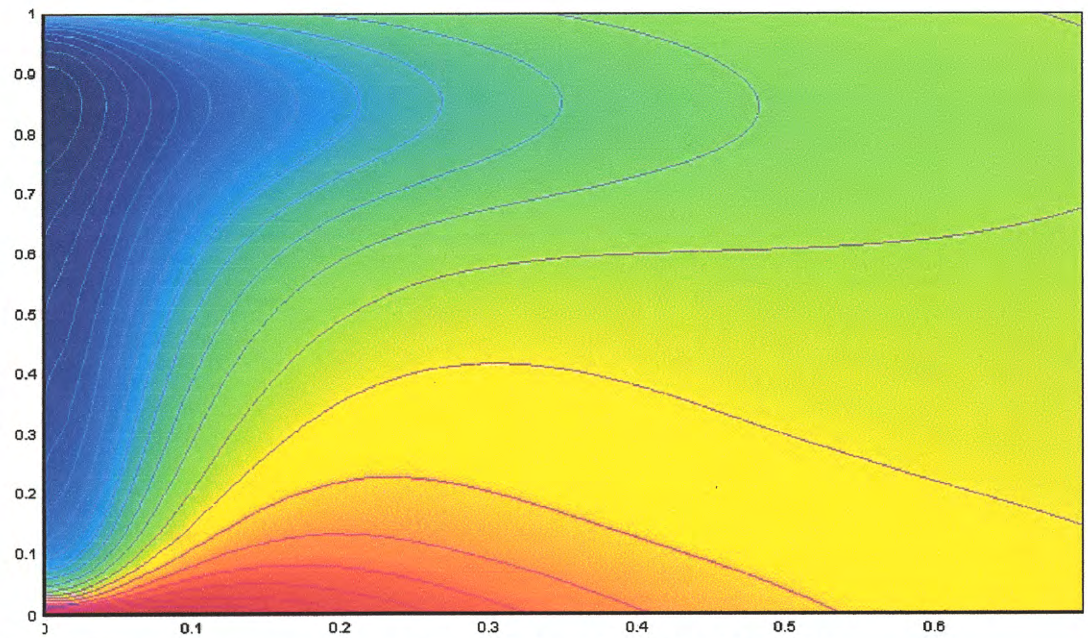
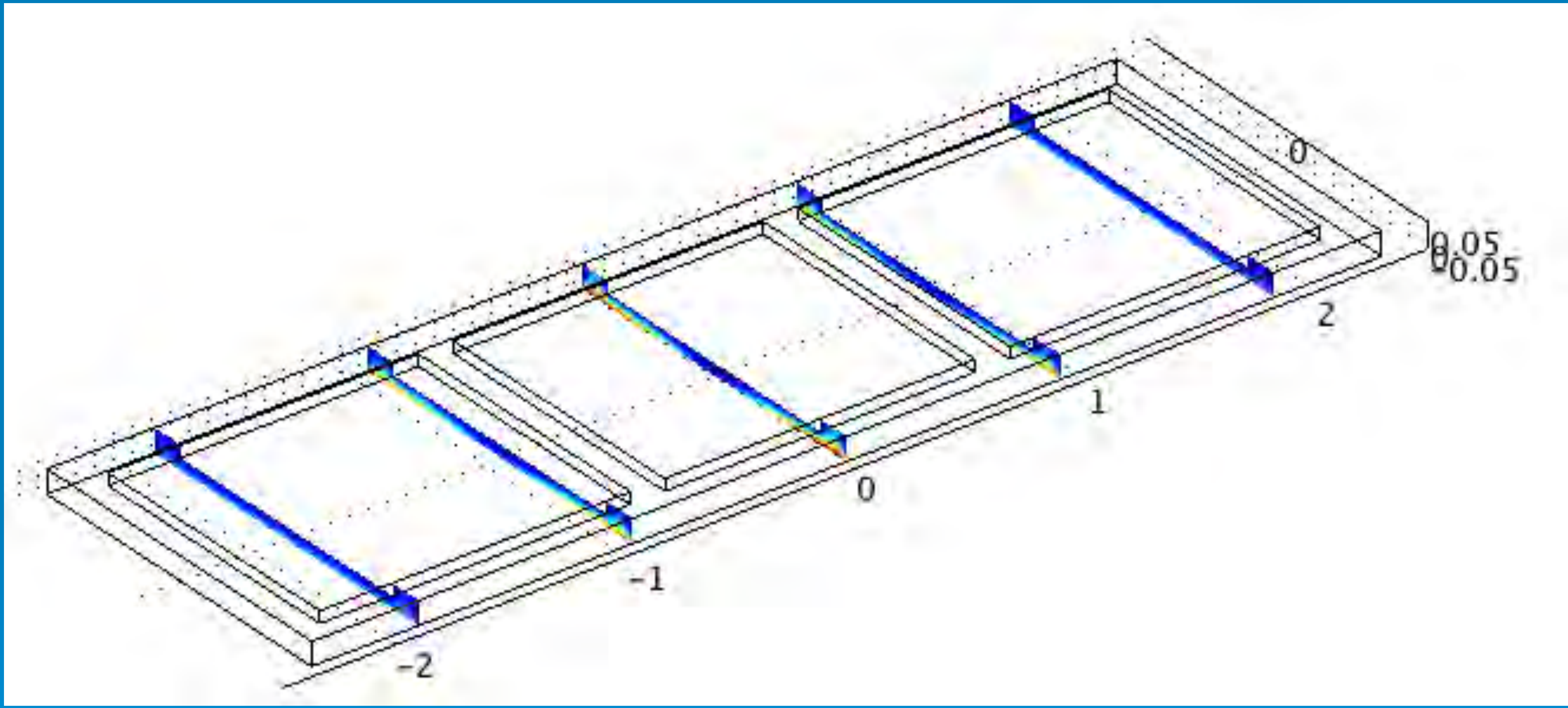


Figure 9. FEMLAB's concentration profile at a final transient value of 5 seconds.

Mimicking the concentration of DNA by thermal gradients, experiments by Braun and Libchaber, Phys. Rev. Lett., 2002

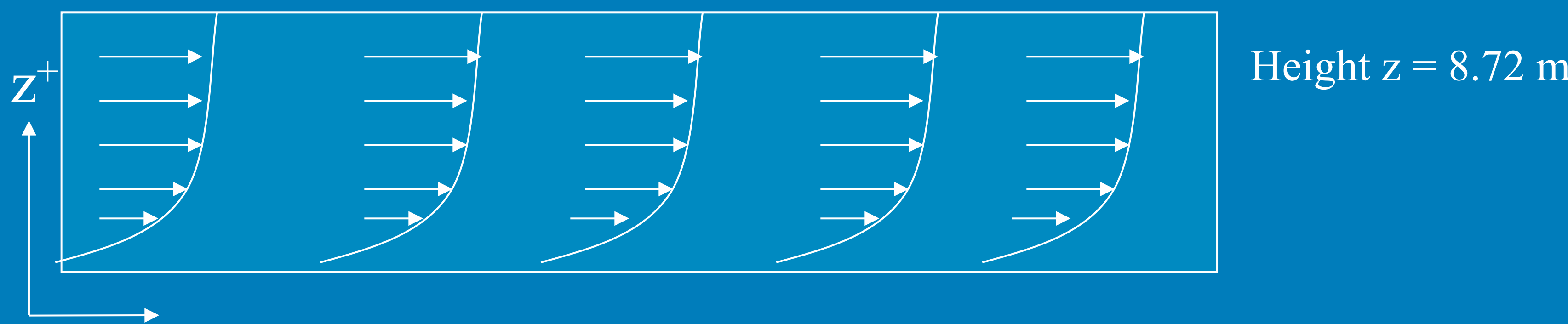
Flow in an Aluminum Cell
Zudtky Wisecarver

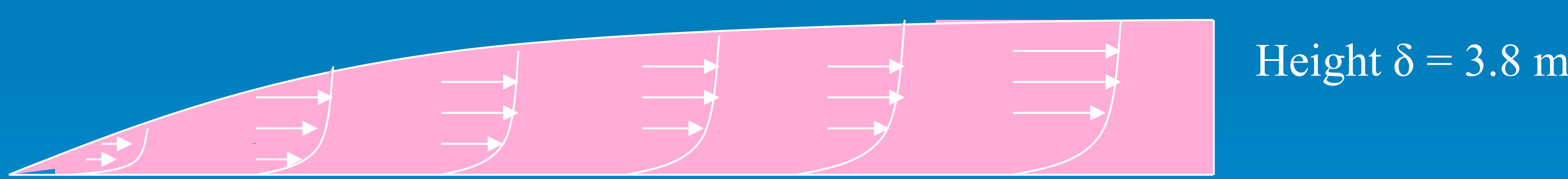


Use Comsol Multiphysics' ability to draw the geometry, and solve the problem in 3D.

Chemical Spills - Megan McMauley

Turbulent theory/FEMLAB = Nearly constant velocity profile





Flow past flat plate = variable velocity profile

Equations

- Governing equation
  - Convection and diffusion
  - Steady-state

$$u^+ \frac{\partial \theta}{\partial x^+} = \frac{1}{Sc} \frac{\partial}{\partial z^+} \left(1 + Sc \frac{\in_m}{\nu} \right) \frac{\partial \theta}{\partial z^+}$$

- Eddy-diffusivity

$$0 < z^+ < 45: \quad \frac{\in_m}{\nu} = \frac{0.00090 z^{+3}}{\left[1 + 0.0067 z^{+2}\right]^{/2}}$$

$$z^+ \geq 45: \quad \frac{\in_m}{\nu} = 0.4 z^+$$

- u^+ is x-velocity

$$z^+ < 10: \quad u^+ = z^+$$

$$z^+ \geq 10: \quad u^+ = 5.1 + 2.5 \ln\left(z^+\right)$$

Used Comsol Multiphysics to validate a published solution and determine that the evaporation rate predicted is highly dependent upon the assumption of flow geometry.

Mixing of polymer solution to make sludge flocculate

A polymer solution is added to digested sludge in order to cause it to flocculate. The sludge is then sent to a centrifuge to separate the water from the sludge, which is used for fertilizer. This project began as a study of the incomplete mixing of the polymer. The goal of the Renton Wastewater Treatment Plant is to reduce the cost of the polymer by achieving good mixing with less polymer.

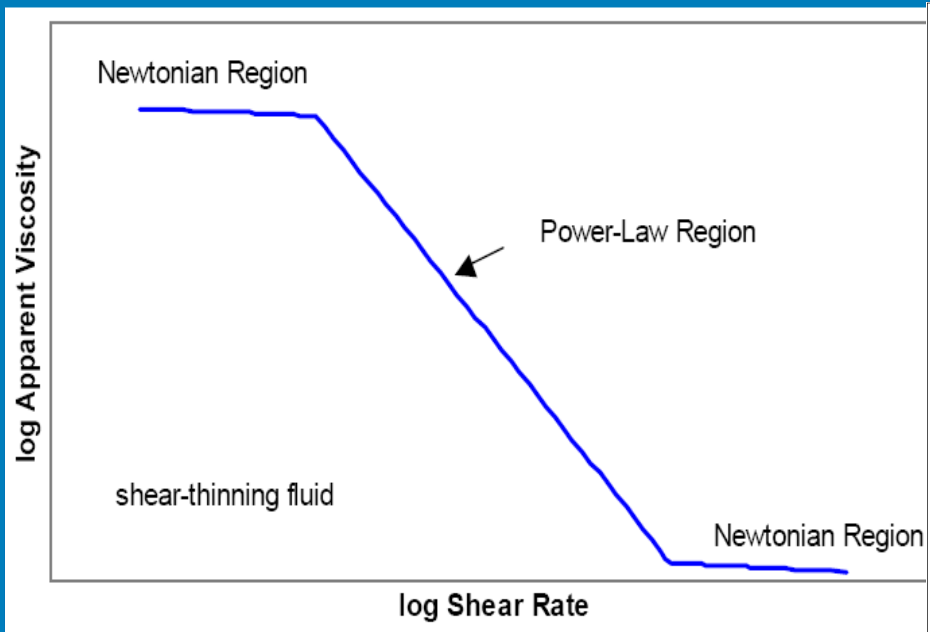
Problem posed by Sharpe Mixers and the Renton Wastewater Treatment Plant: Is it in laminar flow?

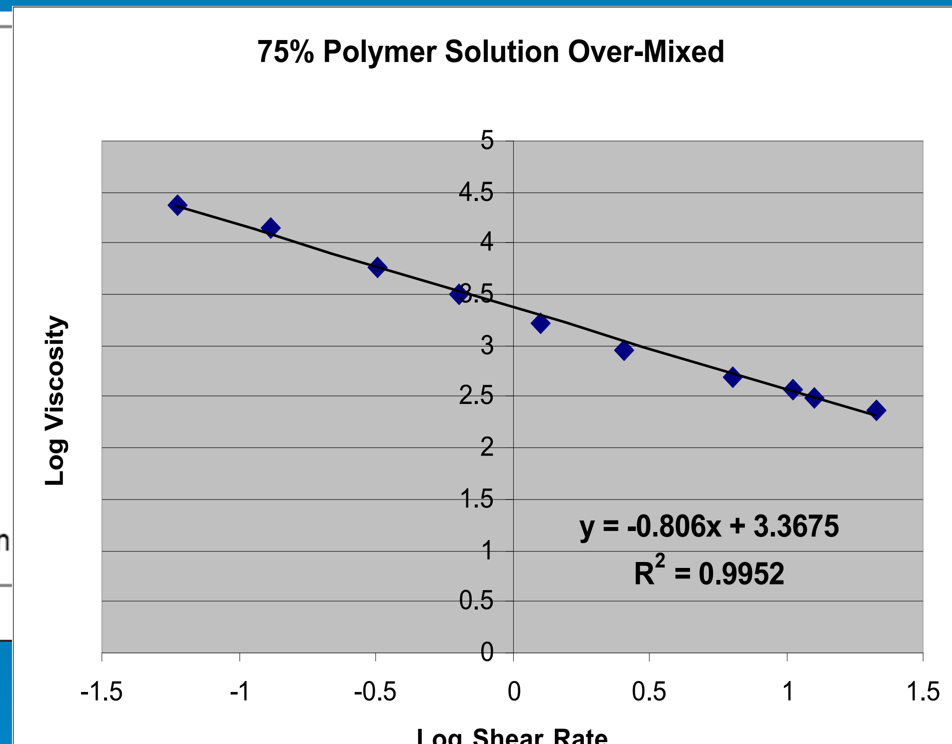
Designed a project for 11 students

- measure the viscosity as a function of concentration
- solve the flow problem with two pipes leading to one pipe
- use the static mixer in the Comsol library
- make the static mixer rotate

Students went through the standard introduction to Comsol Multiphysics and then began work.

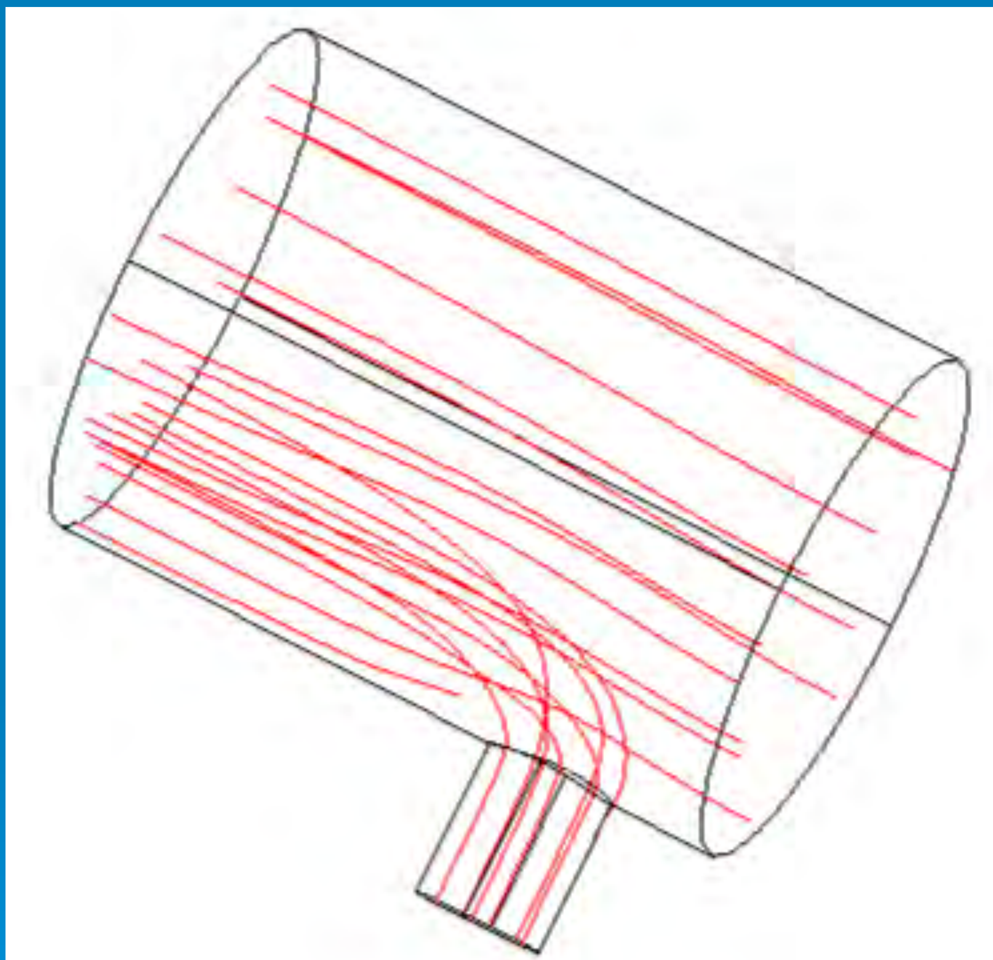
Viscosity

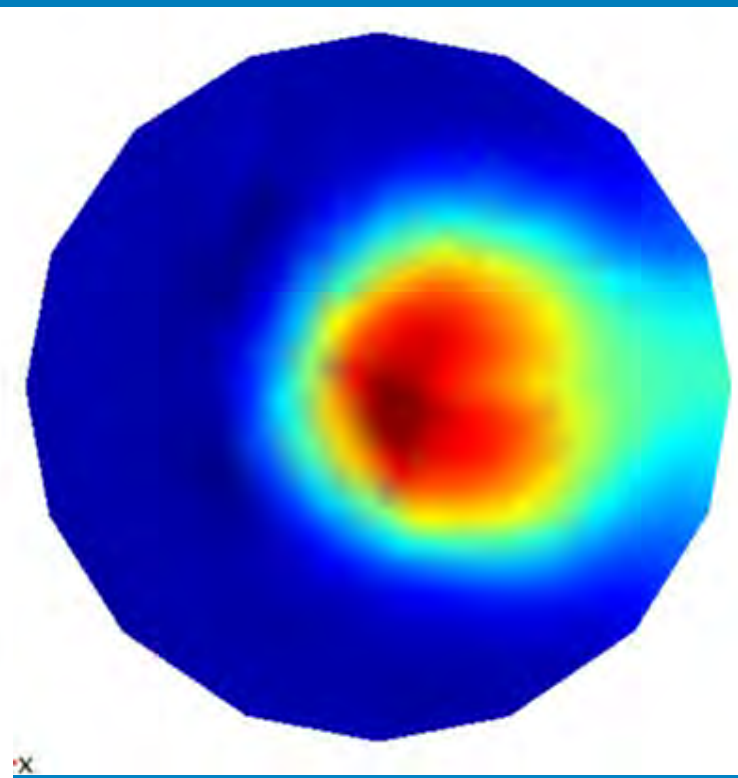




Solution	Power law index
Polymer	0.319
Sludge	0.251
Over-Mixed	0.055

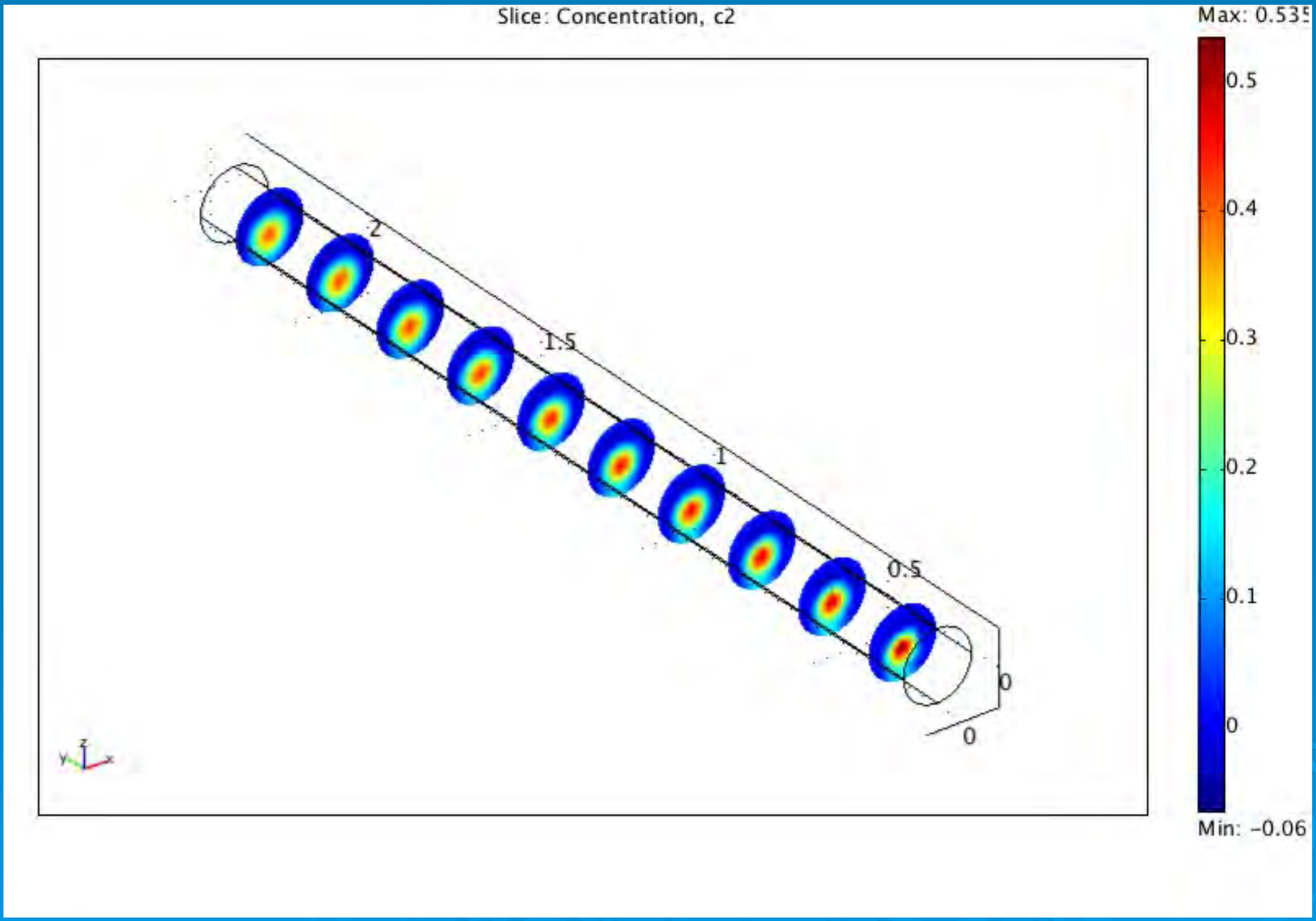
Mixing with power law fluid



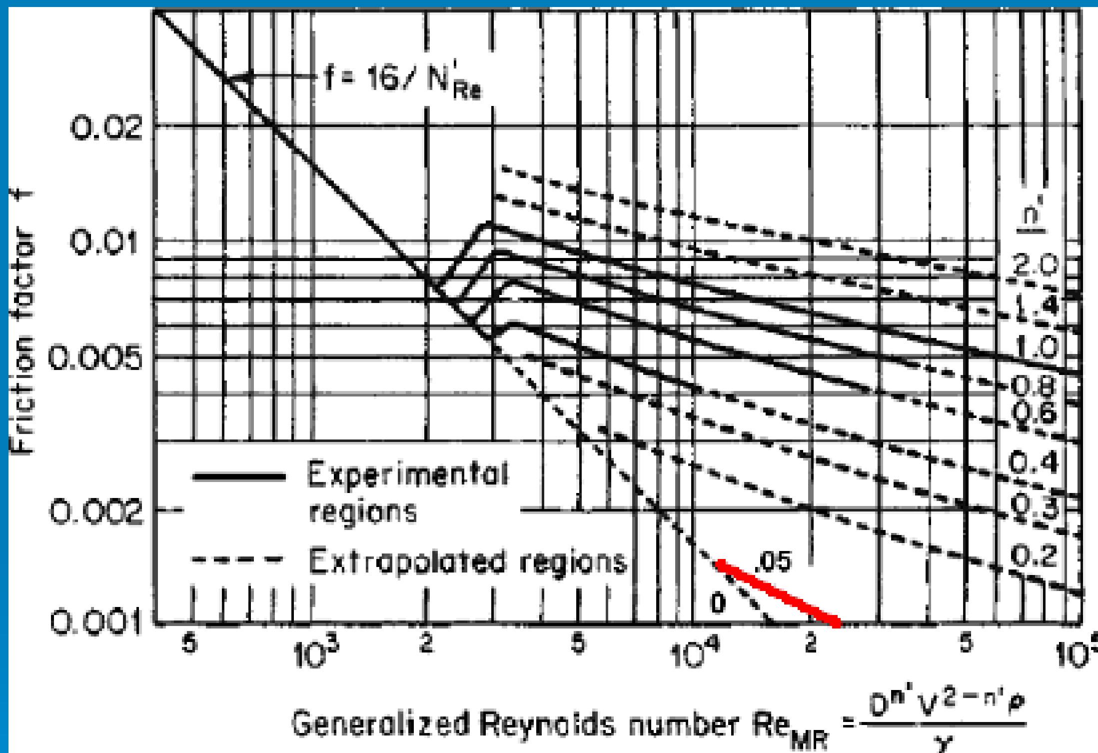


I was willing to settle for a Newtonian solution; students wanted a full power-law model and succeeded.

Little mixing, even in 8 feet



Discovered that the flow is laminar



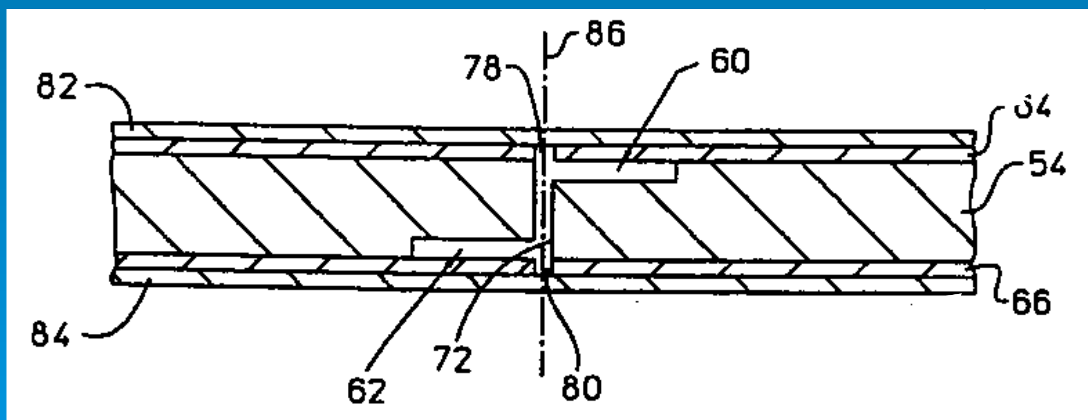
A longer pipe won't help much. This was news to the polymer manufacturer.

Used Comsol Multiphysics with patents in graduate fluid mechanics class - 2002

Optical Detection

(Janine Buseman-Williams, Jon Ladd, Jamie Wilson)

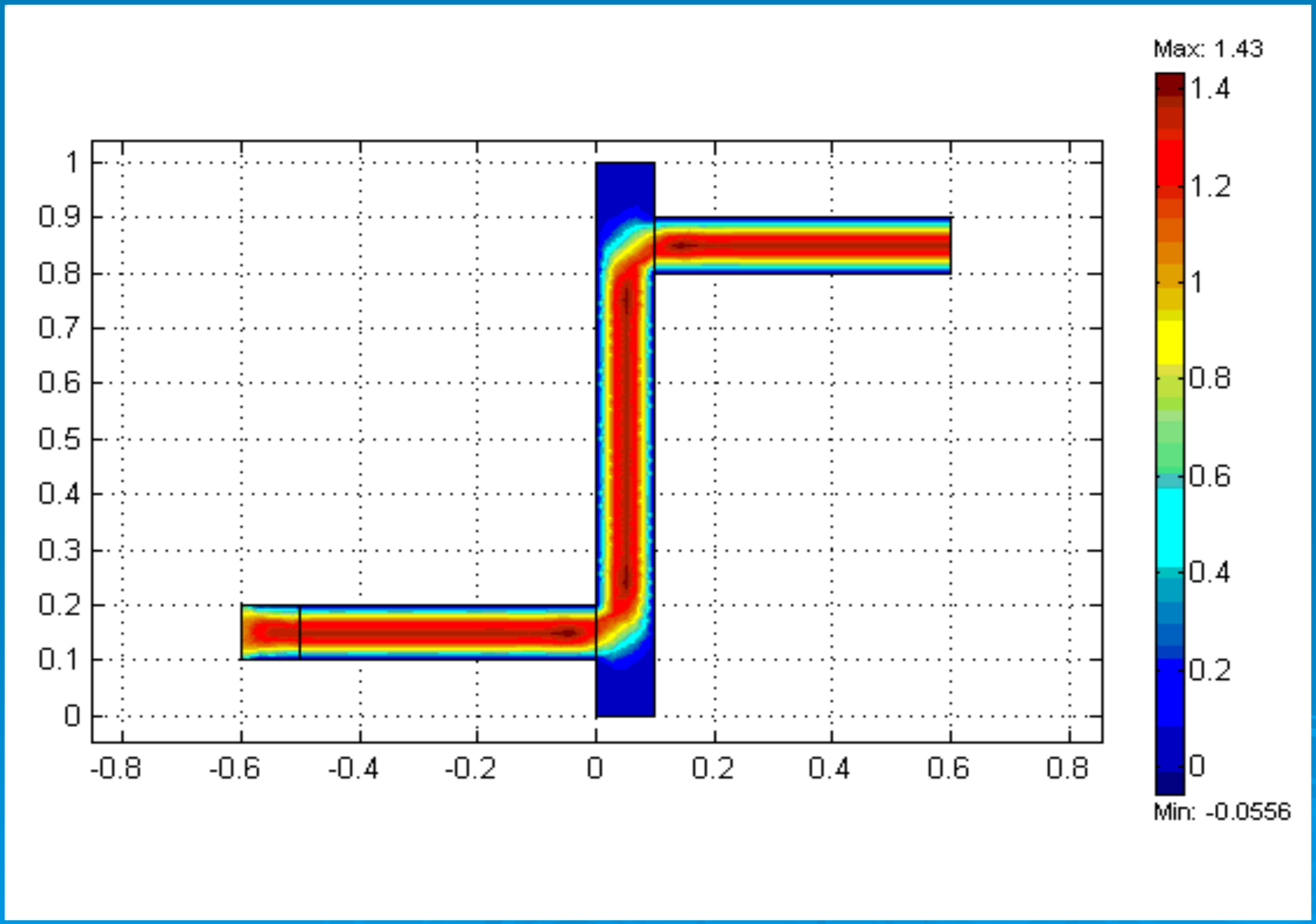
- Analytes pass through column and are carried along optical detection pathlength
- Beer's Law: $A = \varepsilon * b * C$
- Extended Pathlength of up to 1 mm



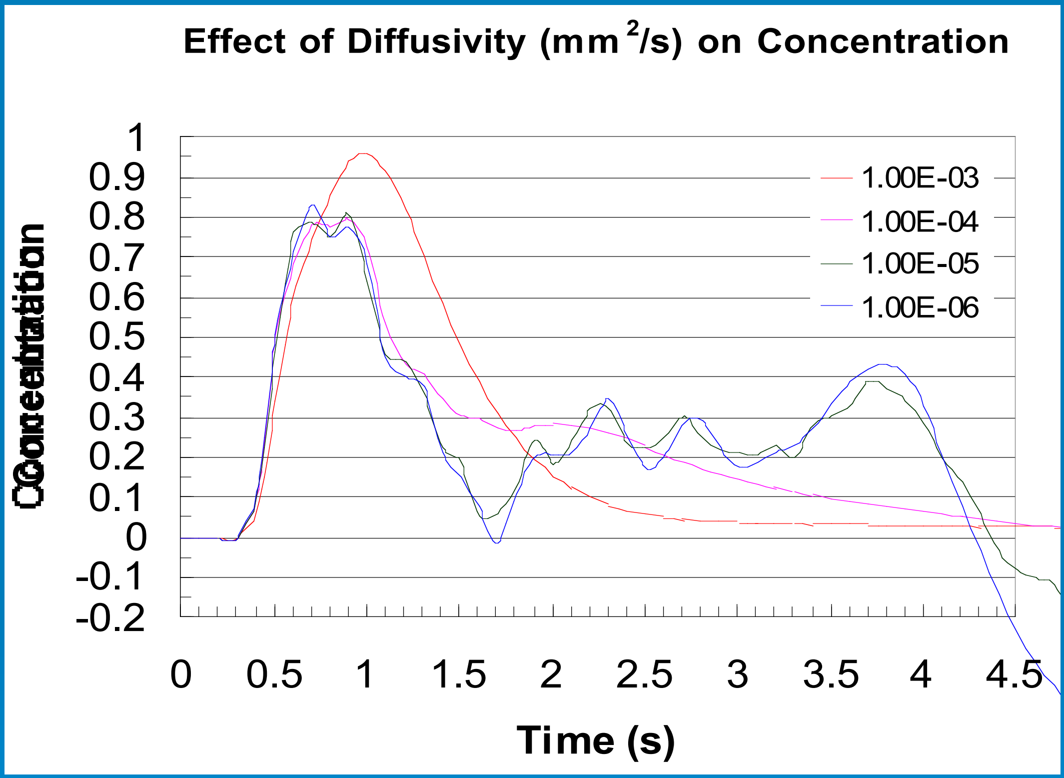
Optically Transparent

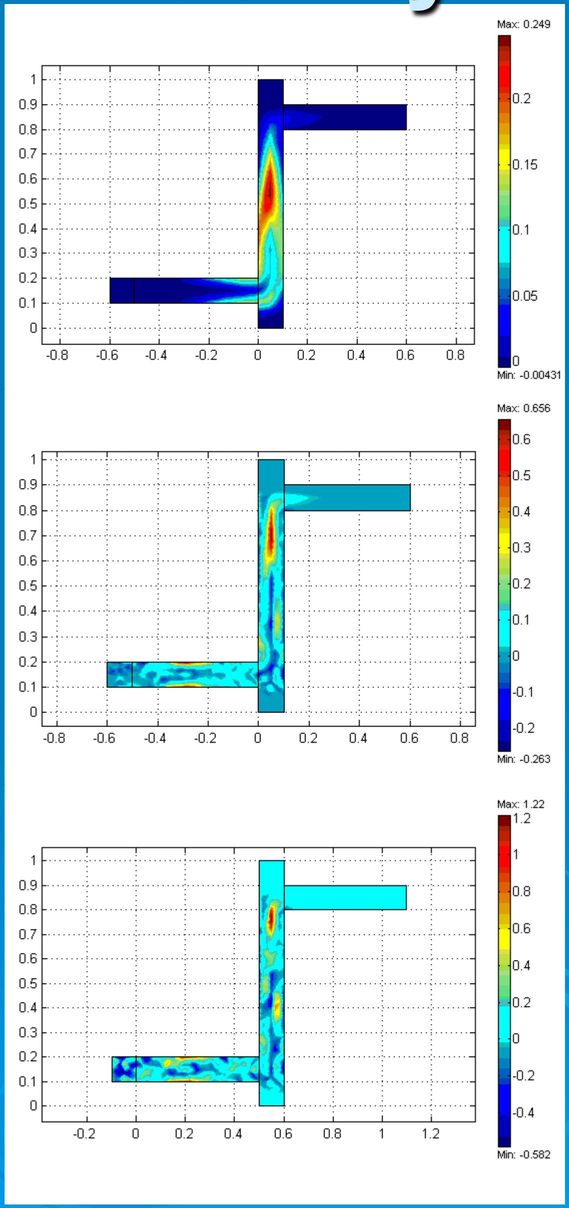
Optically Transparent

Velocity Profile and Device Geometry



FEMLAB Choices: Diffusivity





The students also made movies of the slug of material passing through the device.

Comsol multiphysics made it easy for students to innovate - they did much more than was required.

The next year the class size doubled.

Elena Garcia/Prof. Paul Yager

- Medical devices on a chip
- Interdiffusion-based enzyme inhibition assay
- Dissolution from cavity as a way of delivering drugs on demand

Surface binding of antigen
Jennifer Foley/ Prof. Paul Yager

1) Solve N-S

   Velocity profile

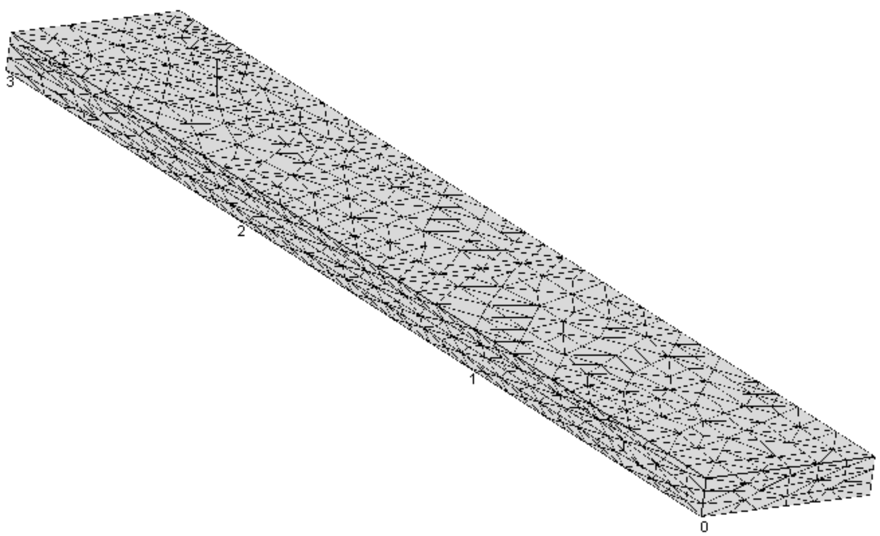
   ~10,000 elements

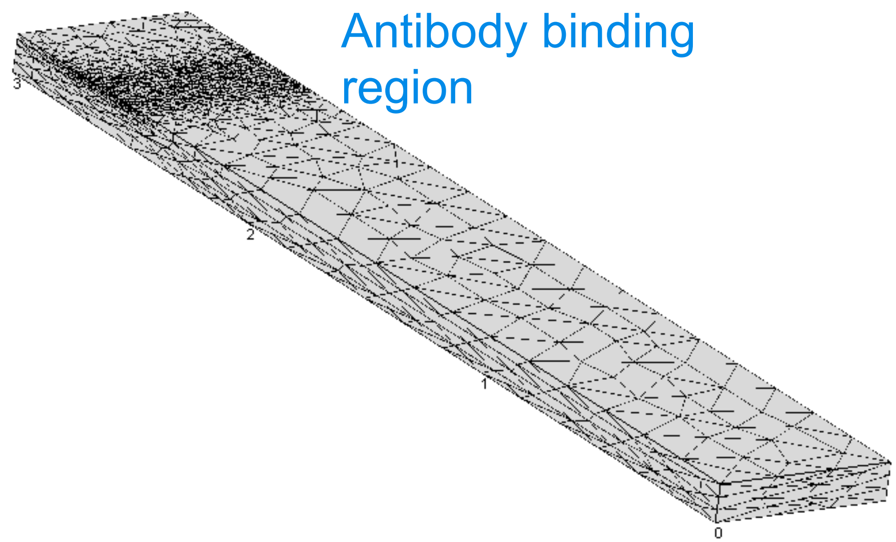
   ~200 seconds to solve

2) Solve C-D/Surface Rxn

   ~13,000 elements

   ~45 minutes to solve





Surface Equations

Weak Boundary Mode

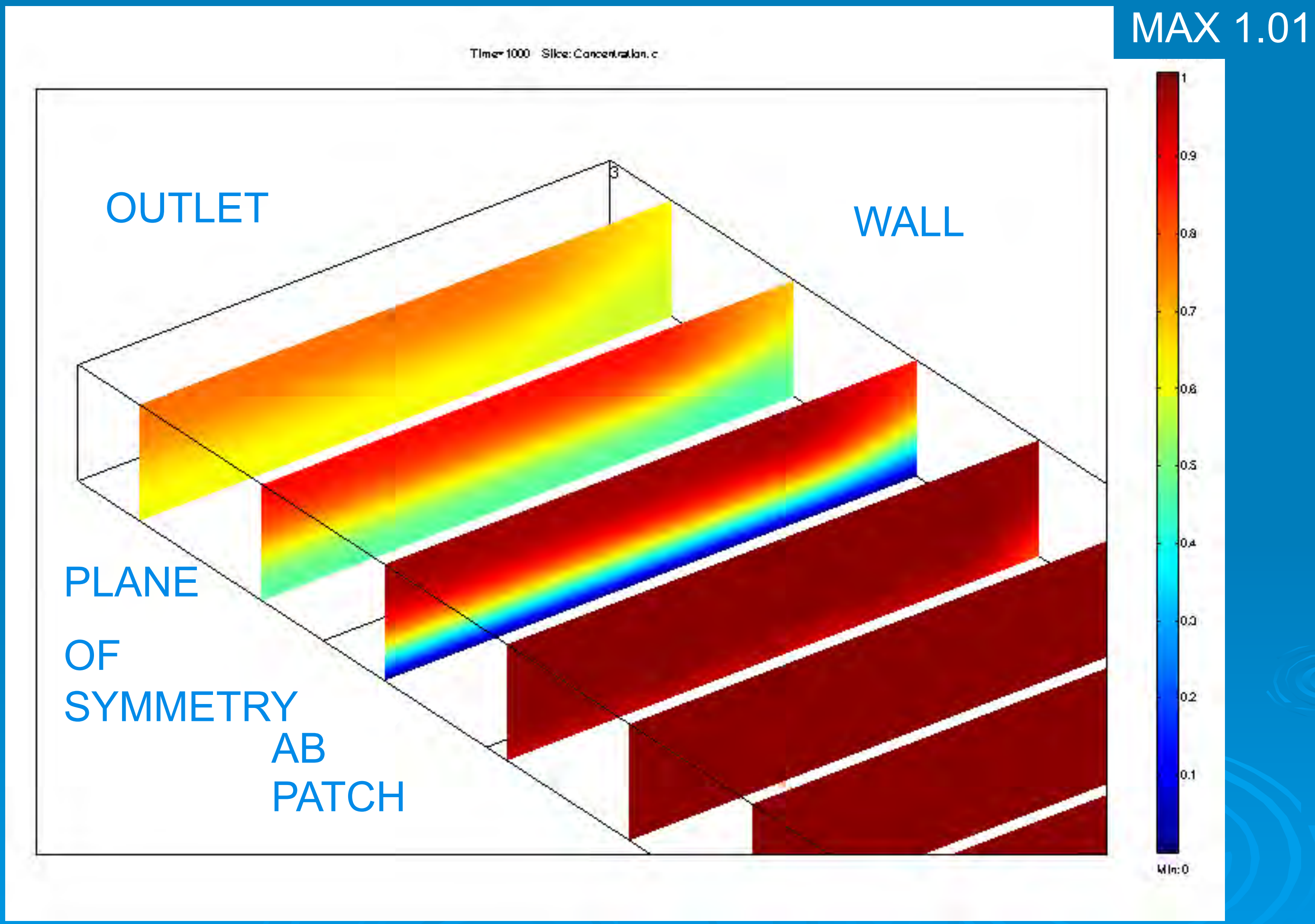
$$c + \theta \underset{k_{des}}{\overset{k_{ads}}{\Leftrightarrow}} c_s$$

$$\frac{\partial c_s}{\partial t} + \nabla \cdot \left(D_s \nabla c_s\right) = k_{ads} c \underbrace{\left(\theta_0 - c_s\right)}_{\text{Theta (\# of available binding sites/area)}} - k_{des} c_{ads}$$

C – bulk antigen concentration

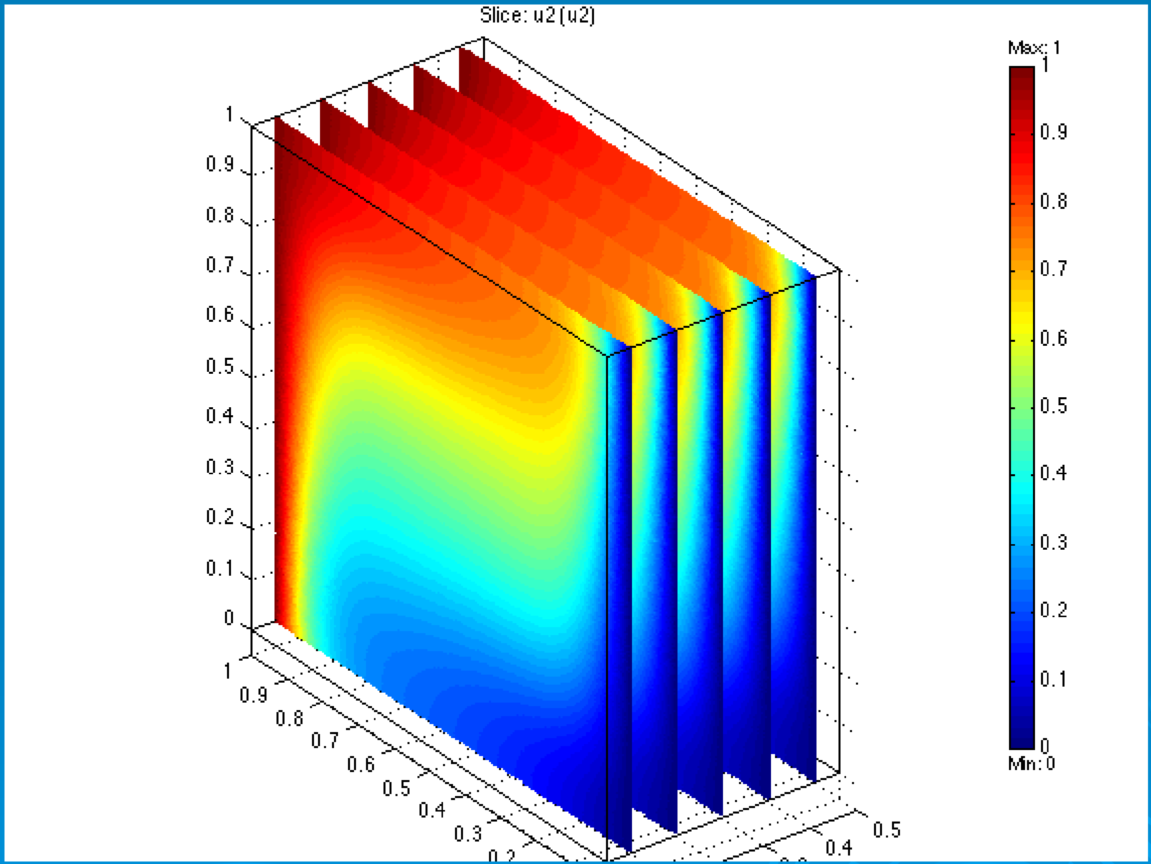
C_s – surface bound antigen concentration

Concentration further depleted with lower flow rate



Heat Transfer to Ferrofluid
Suzanne Snyder

Comsol Multiphysics made it possible to easily solve using a user-specified body force, and do it easily in 3D.



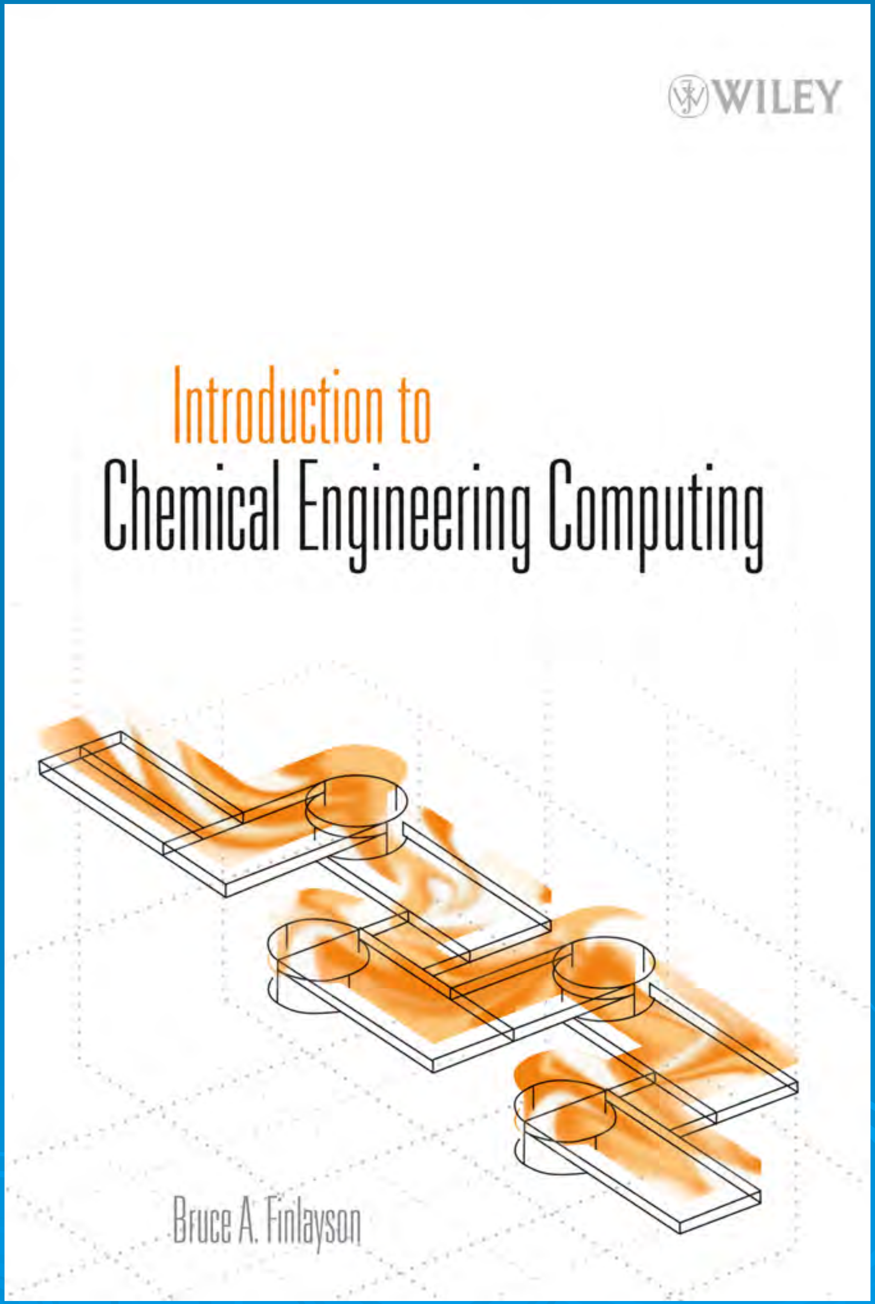
Introduction to Chemical Engineering Computing

- Philosophy - students can be good chemical engineers without understanding the details of the numerical analysis.
- By using modern programs with good GUIs, the most important thing is to check your results.
- Instead of teaching a small fraction of the class numerical methods, I now teach all the class to use the computer wisely.

Programs

- Microsoft Excel ®
- MATLAB®
- Aspen Plus ®
- FEMLAB ®

Available, Dec., 2005



- Chemical reactor models with radial dispersion, axial dispersion
- Catalytic reaction and diffusion
- One-dimensional transport problems in fluid mechanics, heat and mass transfer
  - Newtonian and non-Newtonian
  - Pipe flow, steady and start-up
  - adsorbtion
- Two- and three-dimensional transport problems in fluid mechanics, heat and mass transfer
  - Entry flow
  - Laminar and turbulent
  - Microfludics, high Peclet number
  - Temperature effects (viscous dissipation)
  - Proper boundary conditions

Conclusions

- Comsol Multiphysics is your problem-solving partner.
- It helped me grow my vision, one student at a time.
- It provides simulation for the flat world generation.
- It provides and promotes:

  Motivation - Responsibility - Innovation and Creativity.