The Role of Computation in Continuum Transport Phenomena

Bruce A. Finlayson
Professor Emeritus
Department of Chemical Engineering
University of Washington

Session 308, Perspectives on Transport Phenomena (TH014)
AIChE meeting, paper 308c, Nov. 18, 2008

Status in 1967 when I started my career

- Perry's Chemical Engineers' Handbook, 4th Ed. (1963) (nothing in earlier editions):
  - To solve ODEs: Euler, Adams, simple Runge-Kutta methods
  - To solve PDEs: diffusion/conduction steady problems in 2D (finite difference) or unsteady problems in 1D
  - None of this was reflected in Sections on Fluid Flow or Heat Transmission
- Luther, Carnahan and Wilkes, Applied Numerical Methods (1969)
  - Detailed treatment of numerical analysis, but only explicit techniques with specified time steps

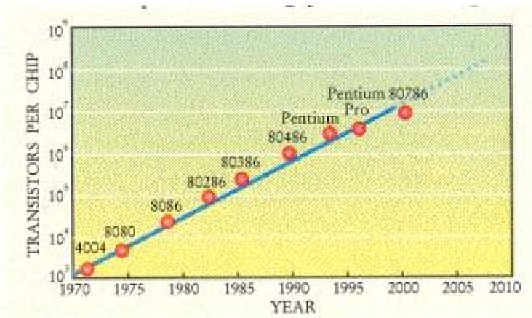
Changes in Perry's Handbook

- 5th edition, 1973
  - For PDEs added alternating direction method and Thomas algorithm for solving tri-diagonal matrics (essential for finite difference methods)
- 6th edition, 1984
  - 2/3 page on finite element method, plus fast Fourier transform, splines, least squares, nonlinear regression, multiple regression
  - In fluid flow section, gave contraction losses, laminar entry flow, vortex shedding
  - In heat transmission and mass transfer, still graphical and algebraic

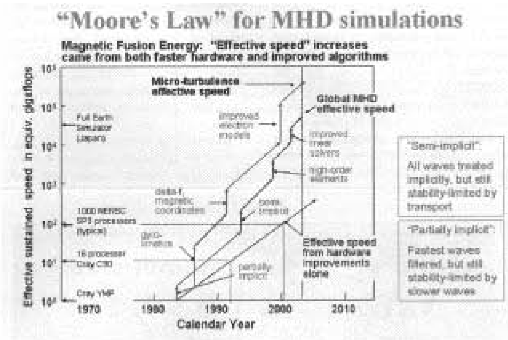
- 7th edition, 1997
  - Better methods for ODEs, errors, implicit
  - Added boundary value problems (BVP), finite difference, finite element, orthogonal collocation, shooting methods
  - In fluid flow section, more recognition of numerical results: laminar entry flow, sudden contraction, vortex shedding, k-epsilon turbulent models, LES, DNS
  - In heat and mass transfer, nothing
- 8th edition, 2008
  - Stiffness for ODEs
  - Molecular dynamics
  - BVP using spreadsheets and the finite difference method
  - Finite volume methods for PDEs
  - In fluid flow section, mention of numerical results for power law fluids (1978 papers) and viscoelastic fluids (1987 papers)
  - In heat and mass transfer, some linear algebra in radiation section

Numerical Analysis is now used to solve problems ranging from the orientation of nanoparticles to predicting global climate change.

It wasn't always that way.



Physics Today, Jan. 2000, p. 40

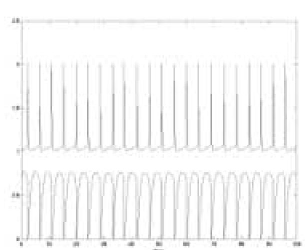


Algorithms help, too! MHD Simulations, faster hardware and improved algorithms, SIAM Newsletter

Numerical Methods for Stiff ODEs

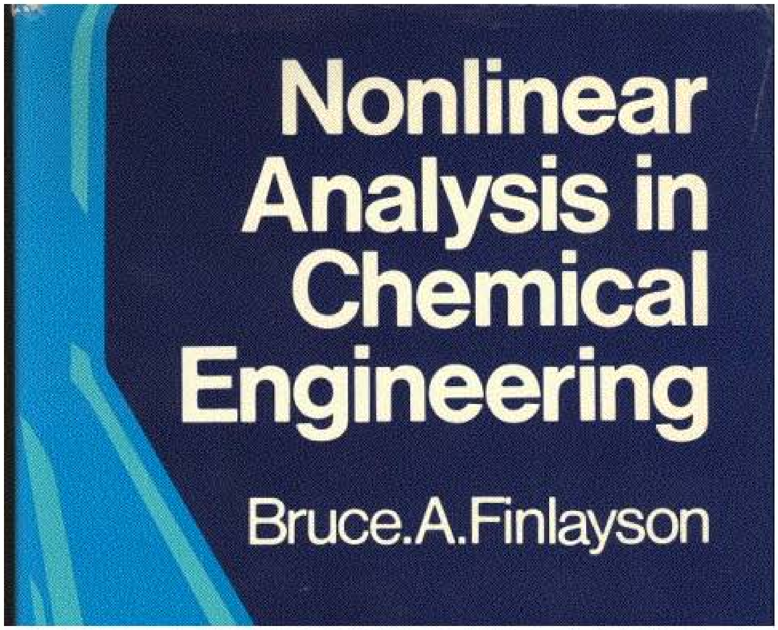
- Runge-Kutta methods existed with error control and automatic step-size adjustment.
- Most engineers used Crank-Nicolson methods, but had to guess a stable step size.

- Gear, 1971; Hindmarsh, 1975, GEARB, later LSODE
  - –When different time constants are important - you want to resolve something occurring on a fast time scale but need to do so over a long time - explicit (RK) methods take a long time.
  - –Implicit methods can be 1000 times faster.
  - –Gear's method allowed for automatic step size adjusment, automatic change of order if that was useful, and basically automatic solution of ordinary differential equations (IVP)



Stirred tank reactor example with a limit cycle

But, the methods are useful for partial differential equations, too!



1980 - orthogonal collocation, finite difference, finite element, with programs (still available at www.ravennapark.com)

Orthogonal Collocation - a good idea

Lanczo, 1938 - collocation method with orthogonal polynomials

Villadsen and Stewart, 1967 - solved in terms of value at collocation nodes rather than coefficients - the programming is much simpler

$$c(y,t) = \sum_{i=1}^{N+2} a_i(t) P_{i-1}(y)$$

$$\frac{\partial c}{\partial t} = D \frac{\partial^2 c}{\partial y^2} - \phi^2 R(c) \quad \text{becomes} \quad \frac{dc_j}{dt} = \frac{D}{h^2} \sum_{i=1}^{N+2} B_{ji} c_i - \phi^2 R(c_j)$$

Stiff methods essential for partial differential equations

Depends upon the eigenvalues of the matrix of the Jacobian.

$$\frac{dc_j}{dt} = \frac{D}{h^2} \sum_{i=1}^{N+2} B_{ji} c_i - \phi^2 R(c_j), \quad \left| \frac{D}{h^2} B_{ji} - \phi^2 \frac{\partial R(c_j)}{\partial c_i} - \lambda \delta_{ji} \right| = 0$$

For a diffusion problem, one eigenvalue is due to the problem (is small) and the other is due to the method (and is big).

$As\ N \to \infty\ or\ h \to 0$, the largest $|\lambda|$ gets bigger.

The more accurate your model, the stiffer the problem.

Application to catalytic converter

Involves unsteady heat and mass transport with a complicated rate expression, perhaps eased by occurring in a thin layer of catalyst. The problem may be only one-dimensional, but it must be solved thousands of times in a simulation, even if in steady state. The solid heat capacity makes the time scales very different. Orthogonal collocation models were "4 to 40 times faster (Chem. Eng. J. **1**, 327 (1970).

$$\varepsilon \frac{\partial c}{\partial t} = \frac{D_e}{r^2} \frac{\partial}{\partial r}(r^2 \frac{\partial c}{\partial r}) - kR(c,T)$$

$$\left(\varepsilon \rho C_{pf} + (1-\varepsilon)\rho_s C_{ps} \right) \frac{\partial T}{\partial t} = \frac{k_e}{r^2} \frac{\partial}{\partial r}(r^2 \frac{\partial T}{\partial r}) + (-\Delta H_{rxn}) kR(c,T)$$

Catalytic Converter

Phenomena included:

Chemical reaction

Flow

Axial conduction of heat

Diffusion

Geometry

What is the importance of the shape of channel?

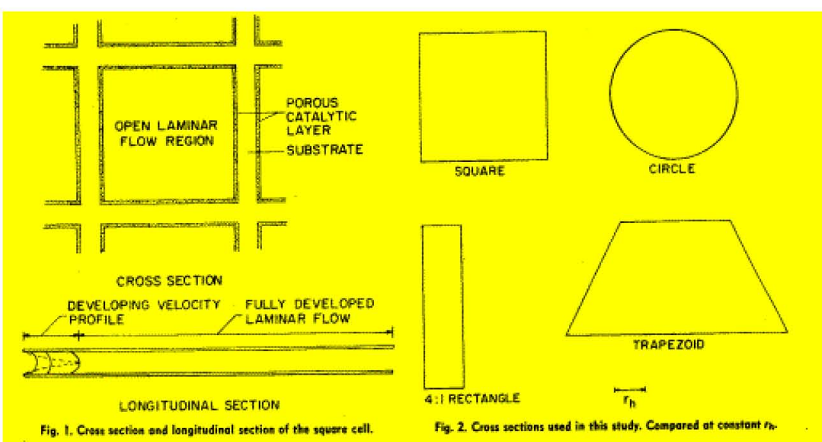


Fig. 1. Cross section and longitudinal section of the square cell.

Fig. 2. Cross sections used in this study. Compared at constant r_h.

Page 344 March, 1976 AIChE Journal (Vol. 22, No. 2)

Model I-A is lumped
Model II-A is distributed, using orthogonal collocation on finite elements

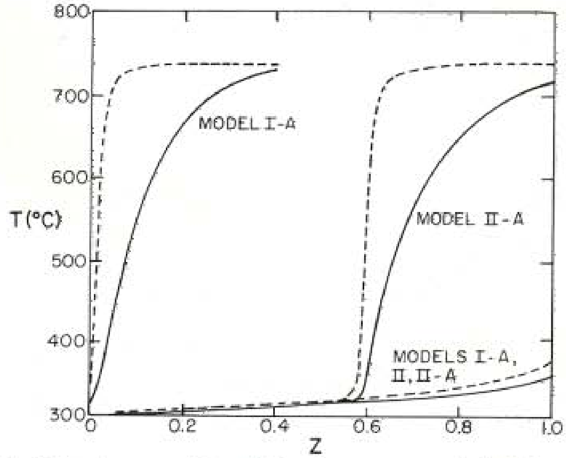


Fig. 8. Steady state model predictions for square geometry. Inlet T = 315°C, y_{CO} = 4%, $\hat{G}$ = 0.0151 m³/s, D^f_{CO}/D^s_{CO} = 70, ζ = 0.0254 mm. - - - - - Solid temperature, ——— Fluid average temperature. P2 kinetics, model I-A: $Nu = Sh = 4.0$.

Finite Element Method

Began in Civil Engineering for structural problems. The finite elements were beams and rods. It solved the same kind of problems done in Physics 101, except in more complicated structures. Then it was expanded to differential equations.

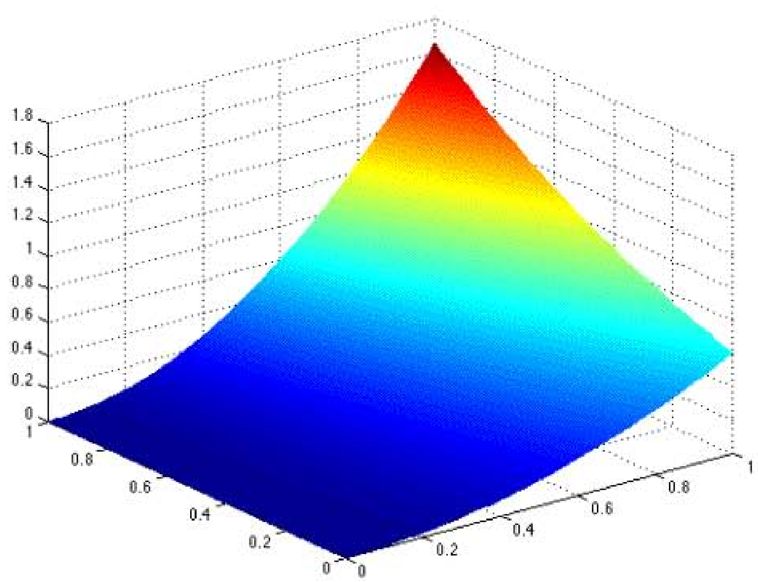
The dependent variable was expanded in known functions.

$$c(x) = \sum_{i=1}^{N+2} a_i P_{i-1}(x)$$

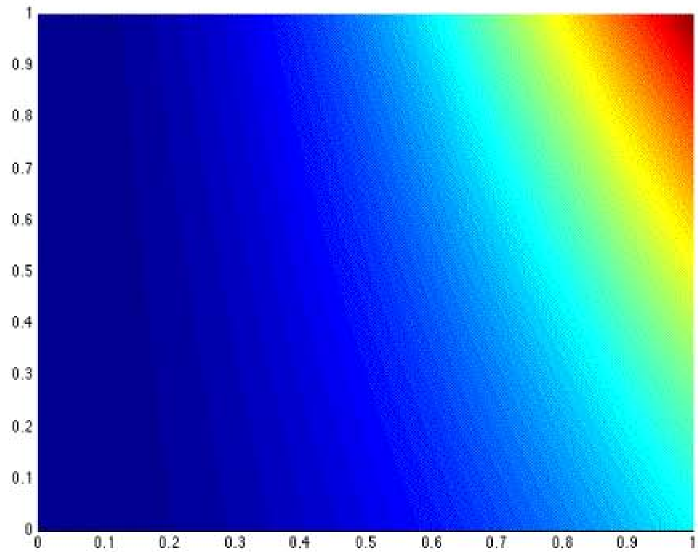
Key ideas in Finite Element Method

- Cover domain with small triangles or rectangles, or their 3D equivalents.
- Approximate the solution on that triangle using low order polynomials.
- Use Galerkin method to find solution at nodal points.
- Can use higher order polynomials.
- Requires lots of memory, fast computers.

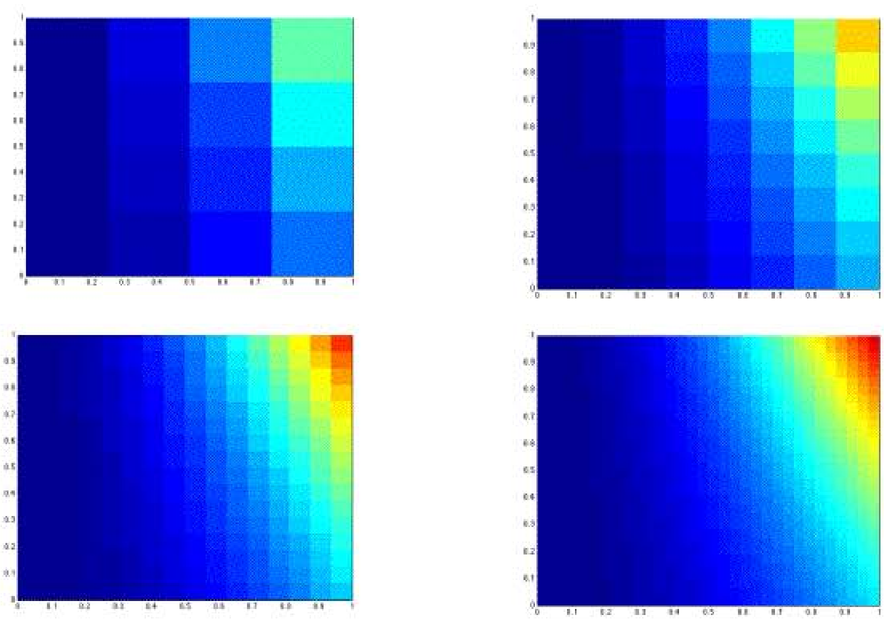
The function x^2 exp(y-0.5) looks like this when plotted:



Here is what we expect in a contour plot of the function:

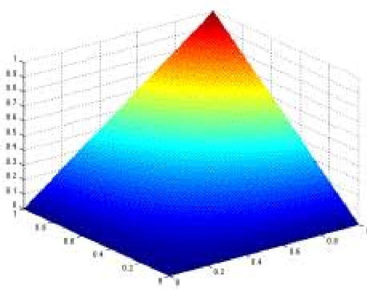


With square elements with one value: N = 4, 8, 16, and 32:

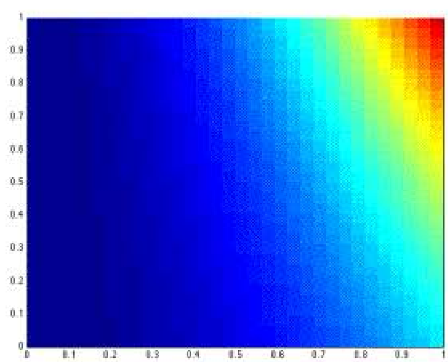


Let functions in the block be bilinear functions of u and v.

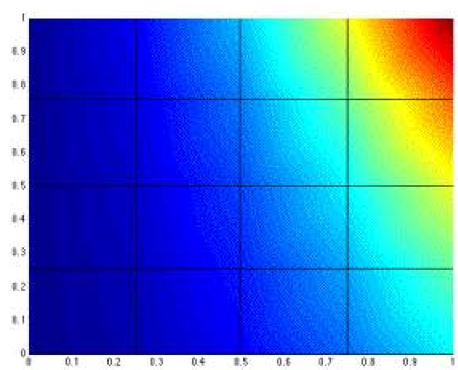
- $N1 = (1 - u)(1 - v)$
- $N2 = u(1 - v)$
- $N3 = u v$
- $N4 = (1 - u) v$
- For example:
- $N3(1,1) = 1$; $N3(0,1) = N3$



Compare constant interpolation on finite elements with bilinear interpolation on finite elements.



Constant interpolation with 32x32 = 1024 blocks.



Bilinear interpolation with 4x4 = 16 blocks.

Hole Pressure Problem, Nancy Jackson, 1982

Examined hole pressure for viscoelastic fluids and learned that all four assumptions made by Lodge to relate to the first normal stress difference were wrong, but they all averaged out.

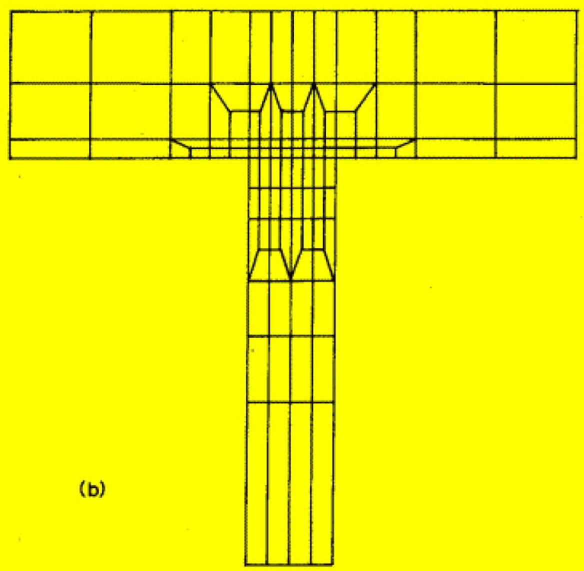
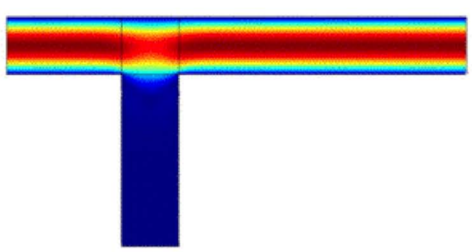


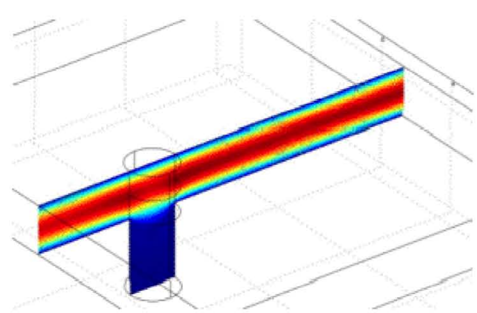
Fig. 3. Finite element mesh: (a) 29 elements; (b) 110 elements.

J. Non-Newt. Fluid Mech. **10** 71 (1982).

Three-dimensional hole pressure
(work done by junior Stephanie Yuen, 2007)

Comparing 2D and 3D calculations. Hole pressure is used in rheology to measure the first normal stress difference.





Equations for Viscoelastic Fluid

$$Re\,\mathbf{v} \bullet \nabla \mathbf{v} = -\nabla p + \nabla \bullet \tau$$

$$\nabla \bullet \mathbf{v} = 0$$

Newtonian Fluid:

$$\boldsymbol{\tau} = \eta\, \mathbf{d}, \;\; \mathbf{d} \equiv \nabla \mathbf{v} + \nabla \mathbf{v}^T$$

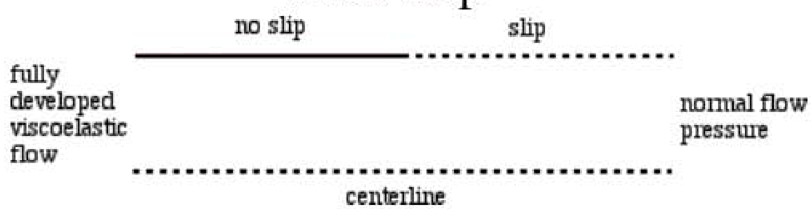
Maxwell Model (η, λ constant), White-Metzner Model (η, λ vary with shear rate) :

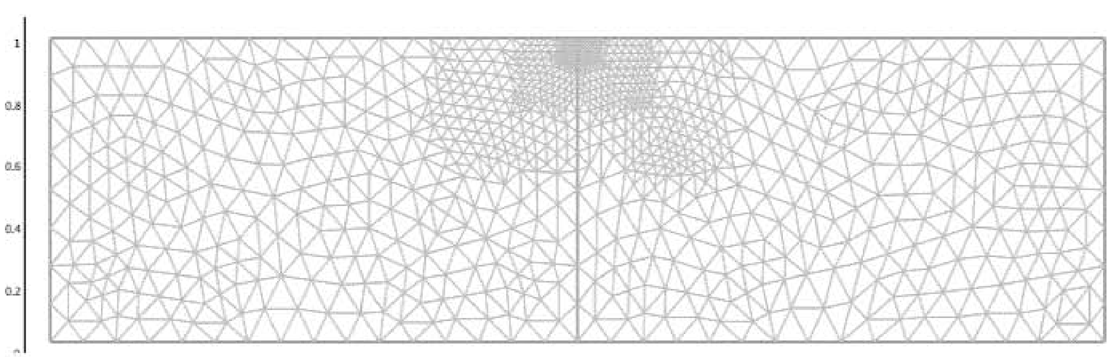
$$\boldsymbol{\tau} + \lambda\left[\mathbf{v} \bullet \nabla \boldsymbol{\tau} - \nabla \mathbf{v}^T \bullet \boldsymbol{\tau} - \boldsymbol{\tau} \bullet \nabla \mathbf{v}\right] = \eta\, \mathbf{d}$$

Phan-Thien-Tanner Model:

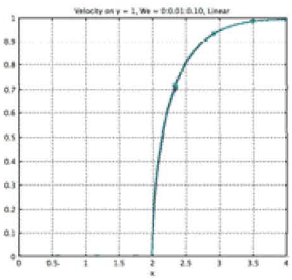
$$\boldsymbol{\tau} + \lambda\left[\mathbf{v} \bullet \nabla \boldsymbol{\tau} - \nabla \mathbf{v}^T \bullet \boldsymbol{\tau} - \boldsymbol{\tau} \bullet \nabla \mathbf{v}\right] + \varepsilon \frac{\lambda}{\eta} tr(\boldsymbol{\tau})\boldsymbol{\tau} = \eta\, \mathbf{d}$$

Stick Slip

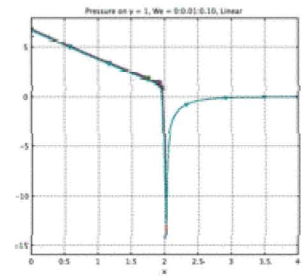




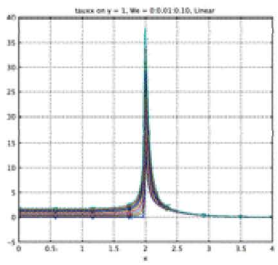
Stick Slip, Standard Method, We = 0:0.01:0.1



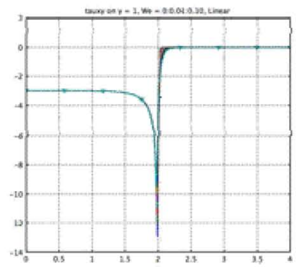
velocity



pressure

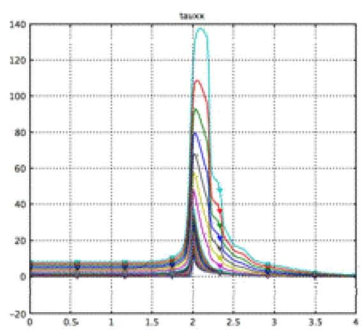


xx stress



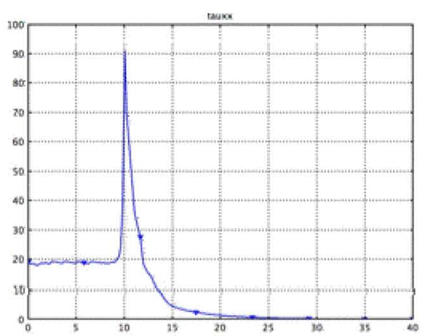
xy shear stress

Stick Slip with DEVSS Method



Maxwell fluid,

We = 0:0.05:0.45



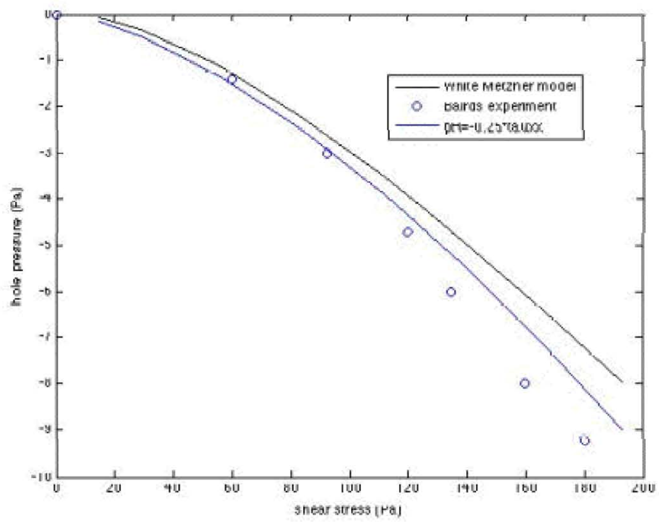
PTT fluid, We = 5

Differential-Elastic-Viscous-Split-Stress (DEVSS)

Guenette, R. and M. Fortin, *J. Non-Newtonian Fluid Mech.* **60** 27 (1995)

R. G. Owens and T. N. Phillips, *Computational Rheology*, Imperial College Press (2002)

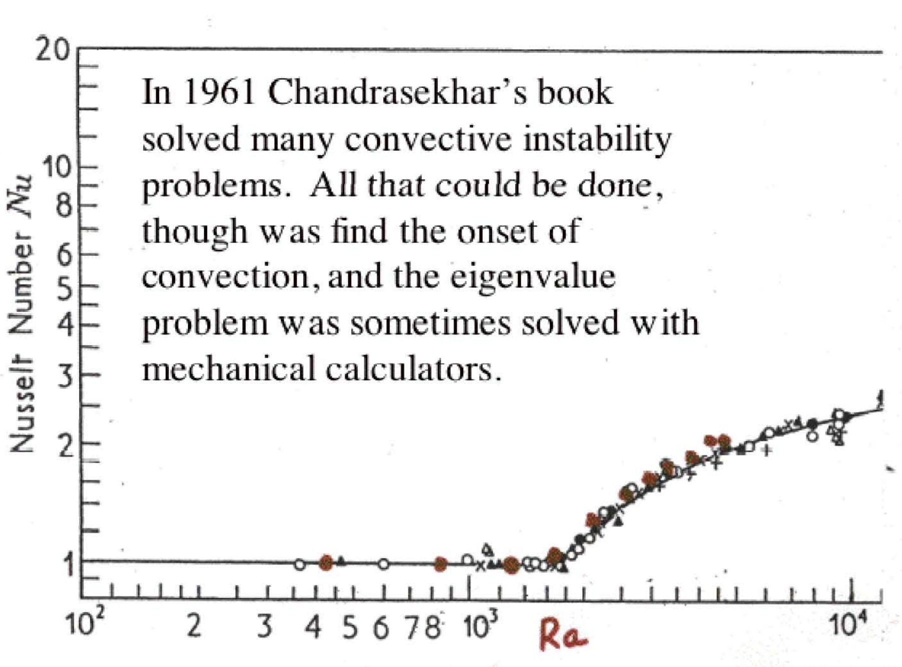
Comparison to Experiment



Ref: D. G. Baird, *J. Appl. Poly. Sci.* **20** 3155 (1976)

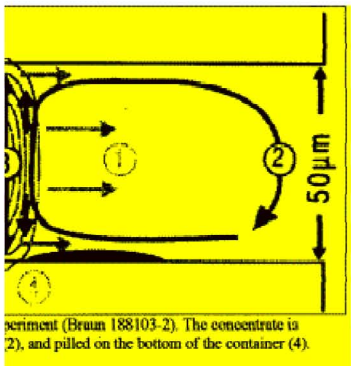
N. R. Jackson and B. A. Finlayson, *J. Non-Newt. Fluid Mech.* **10** 71 (1982)

Convective Instability, Michael Harrison (2003)
Heat transfer between flat plates, heated from below



In 1961 Chandrasekhar's book solved many convective instability problems. All that could be done, though was find the onset of convection, and the eigenvalue problem was sometimes solved with mechanical calculators.

Trapping of DNA using thermal diffusion, Pawel Drapala (2004)



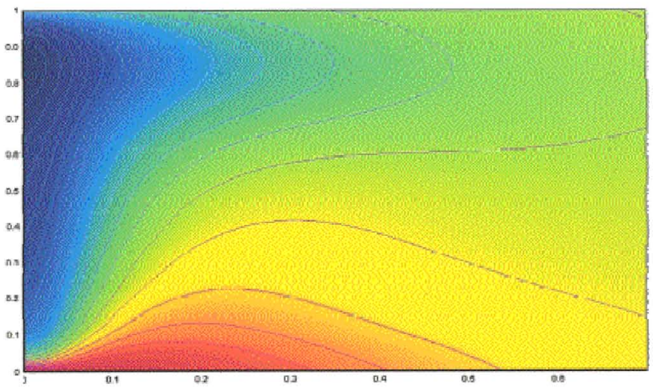
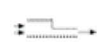
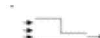
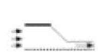


Figure 9. FEMLAB's concentration profile at a final transient value of 5 seconds.

Patterned after experiments by Braun and Libchaber, *Phy. Rev. Letters* **89** 188103 (2002).

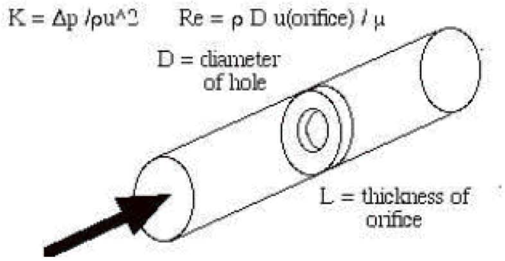
Determine Pressure Drop Coefficients for Slow Flow (to mimic those available for turbulent flow)

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

Table III. Coefficient K_L for contractions and expansions for Re negligbily 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

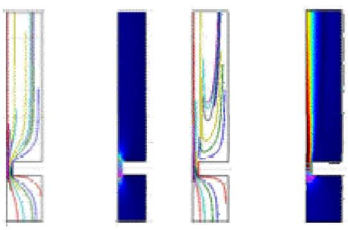
v_s = average velocity, x_s = thickness or diameter, both in the small section

Table in Ch. 8, "Micro-component flow characterization," Koch, Vanden Bussche, Chrisman (ed), Wiley (2007). The chapter has 11 authors, 10 UW undergraduates plus Finlayson.

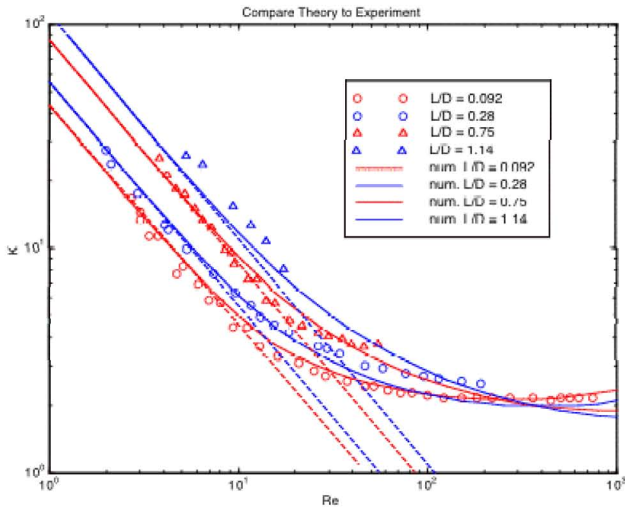


Later, undergraduates could solve harder problems using Comsol Multiphysics (FEMLAB).

Kusmanto, Jacobsen, and Finlayson, Phys. Fluids **16** 4129 (2004)

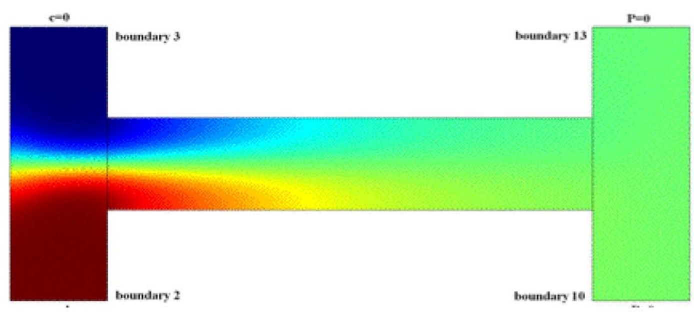


Streamlines and pressure profiles for Re = 0 (left) and 316 (right)

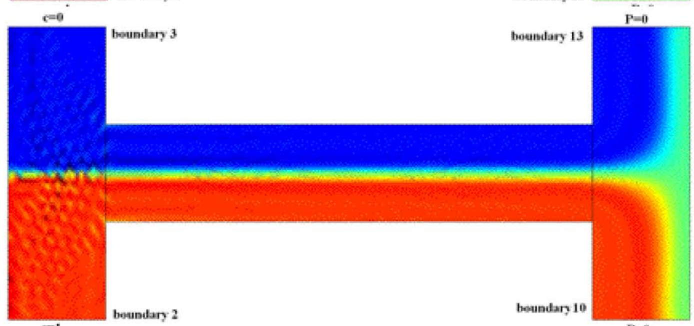


H-sensor - used to separate chemicals by diffusion (solutions by Krassen Ratchev, 2008)

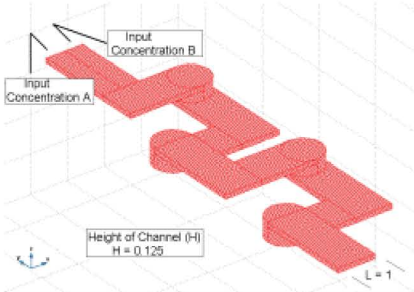
$D = 10^{-9}\ m^2 / s$

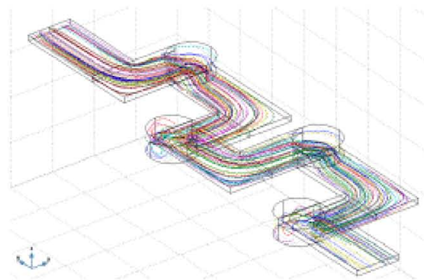


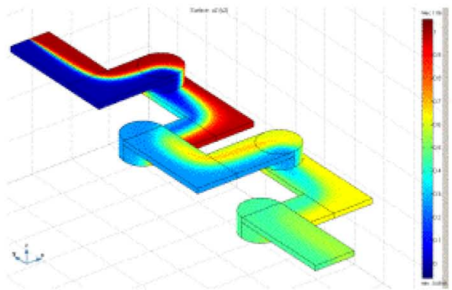
$D = 10^{-11}\ m^2 / s$



Mixing in a Serpentine Microfluidic Mixer







Published in Neils, Tyree, Finlayson, Folch, *Lab-on-a-Chip* **4** 342 (2004)

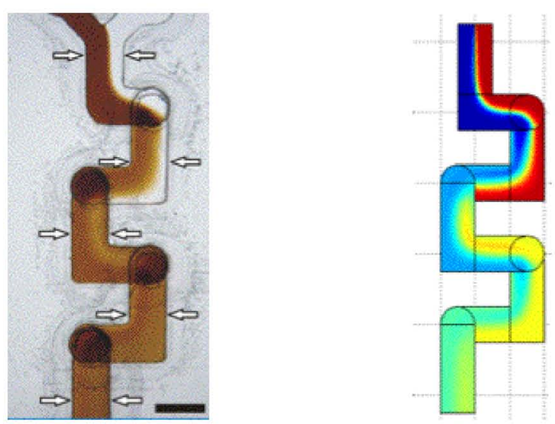


Figure 8. Comparison with experiment (6)

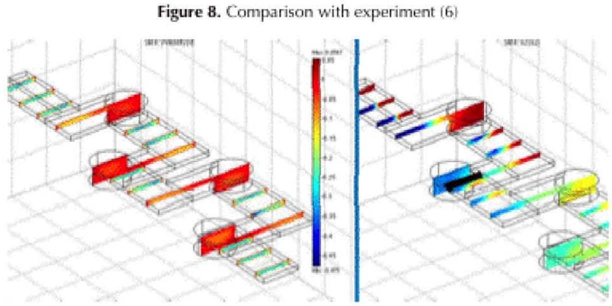


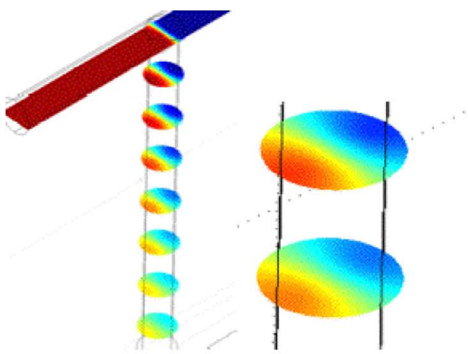
Figure 9. Velocity profiles and concentration profiles inside serpentine mixer

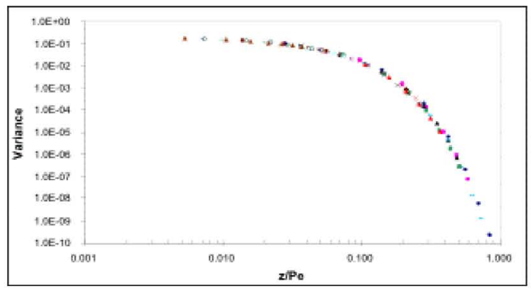
For Re = 1 or so, the flow problem is easy. But, the Peclet number can be large (2000). Then the mesh for the concentration problem has to be refined significantly. Comsol allows solution of the flow problem and the convective diffusion problem on different meshes, thus speeding up the solution time.

Mixing in a Three-dimensional T

(work done by junior Daniel Kress)

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



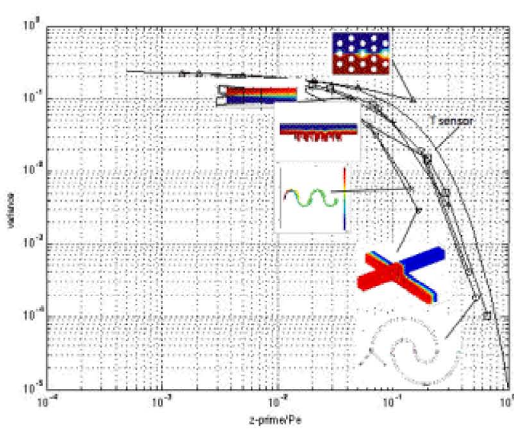


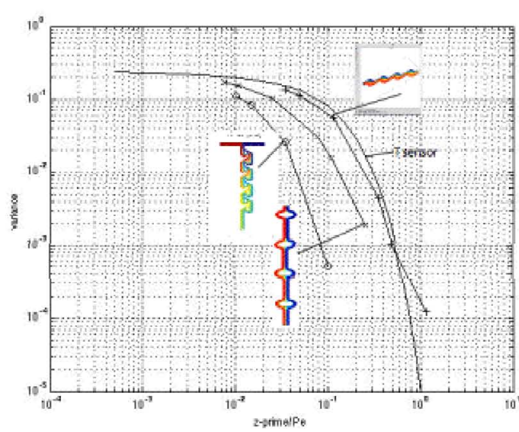
Variance as a function of length in the outlet leg

The work showed that the 3D case followed the same curve as the 2D case (T-sensor).

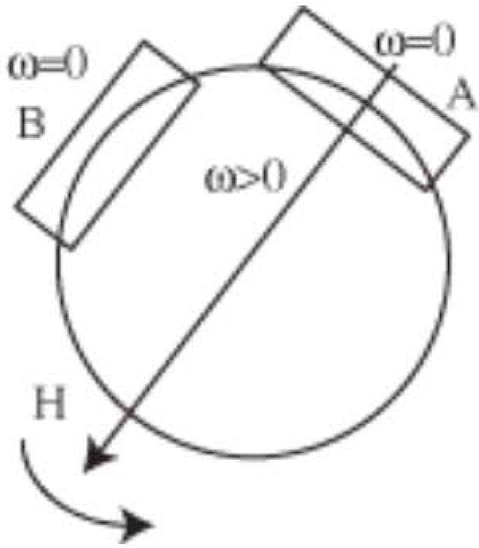
Mixing in Microfluidic Devices

(11 undergraduate projects)





Spin-up of ferrofluid



Governing Equations

due to Rosensweig (1985)

Extended Navier-Stokes Equation:

$$\rho \frac{\partial \mathbf{v}}{\partial t} + \rho \mathbf{v} \bullet \nabla \mathbf{v} = -\nabla \mathbf{p} + 2\varsigma \nabla \times \boldsymbol{\omega} + (\eta + \varsigma)\nabla^2 \mathbf{v} + \mu_0 \mathbf{M} \bullet \nabla \mathbf{H}$$

Conservation of internal angular momentum (spin equation):

$$0 = \mu_0 \mathbf{M} \times \mathbf{H} + 2\nabla \times \mathbf{v} - 4\boldsymbol{\omega} + \eta' \nabla^2 \boldsymbol{\omega}$$

Magnetization (Shliomis, 1972):

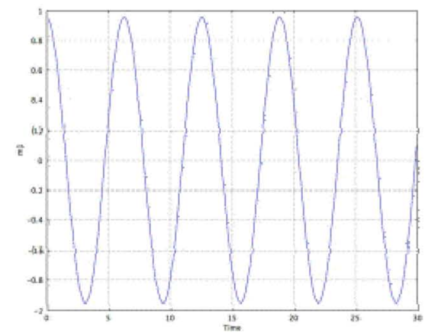
$$\frac{\partial \mathbf{M}}{\partial t} + \mathbf{v} \bullet \nabla \mathbf{M} = \boldsymbol{\omega} \times \mathbf{M} - \frac{1}{\tau}\left(\mathbf{M} - \mathbf{M_{eq}}\right)$$

Maxwell's Equations for non-conducting fluid:

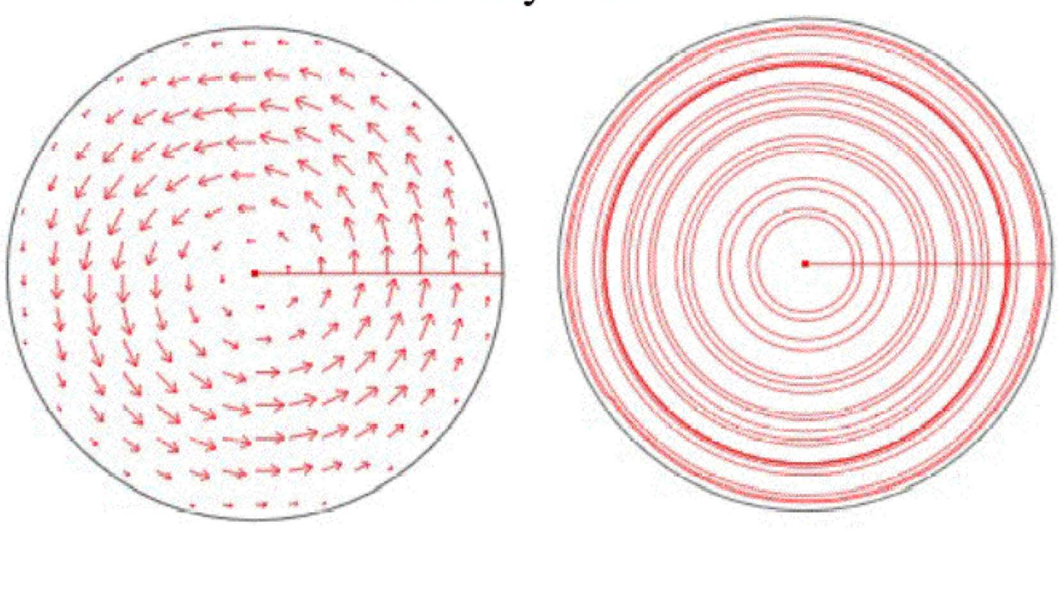
$$\nabla \bullet \mathbf{B} = \mathbf{0}, \ \nabla \times \mathbf{H} = 0, \ \mathbf{B} = \mu_0(\mathbf{H} + \mathbf{M})$$

$$\mathbf{H} = \nabla \phi \qquad \nabla^2 \phi = -\nabla \bullet \mathbf{M}$$

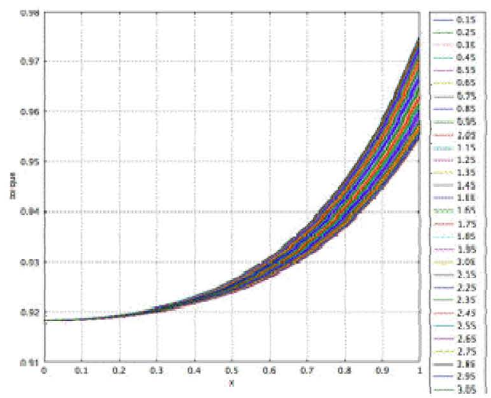
Rotating H and Magnetization

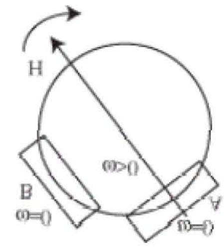


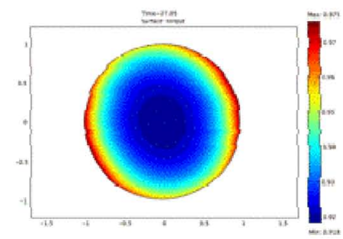
Velocity Field



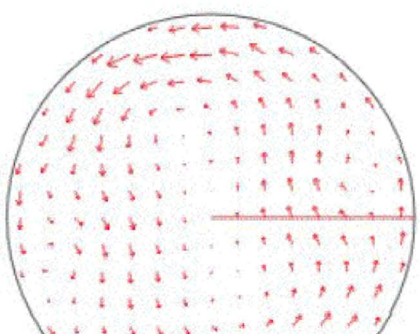
Torque along y = 0



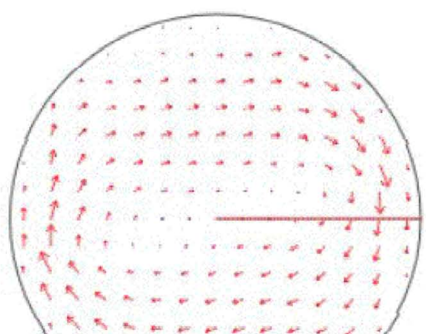




Flow reversal at large H (relative H = 32)



Spin viscosity 10x higher



Relative spin viscosity = 1

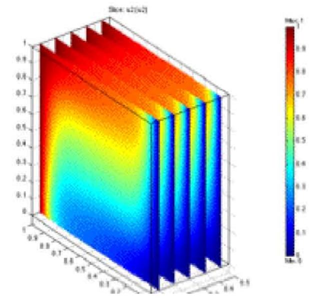
Heat Transfer to Ferrofluids

Convective instability of ferromagnetic fluids

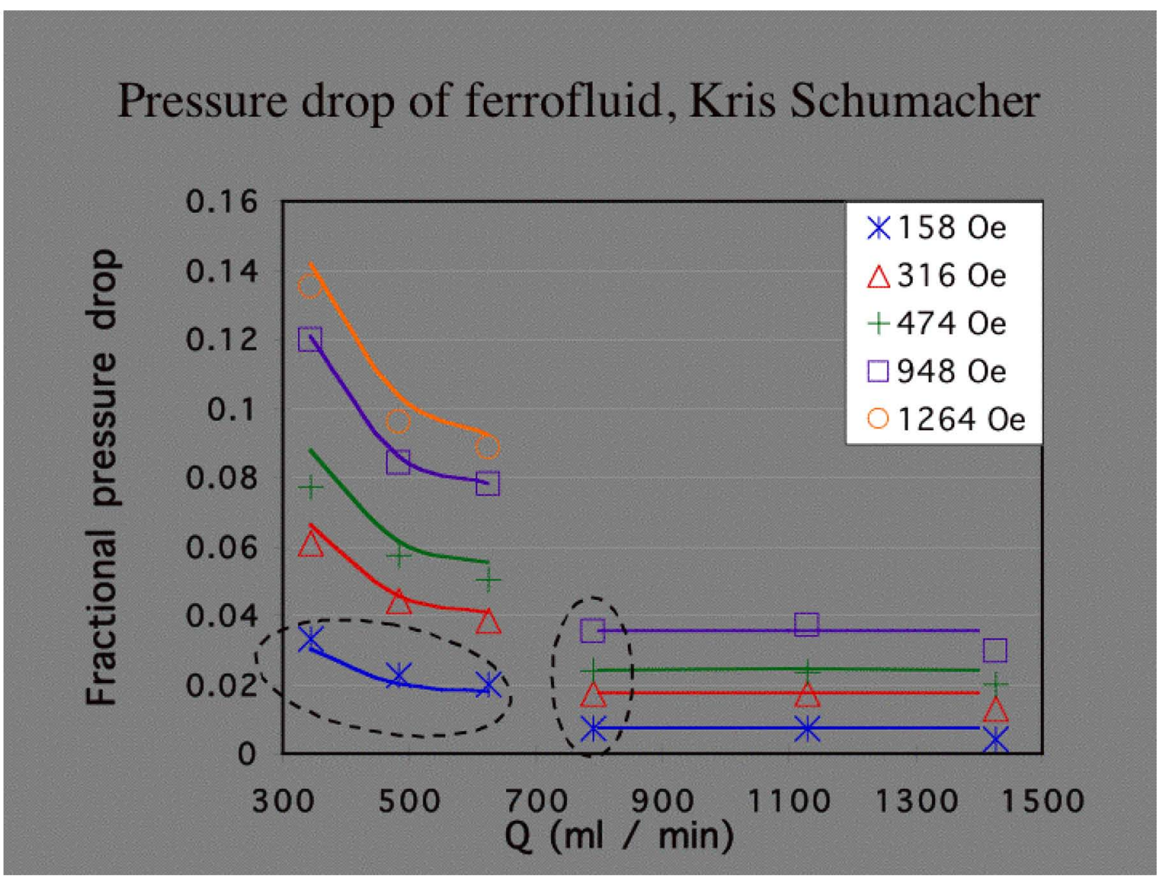
B. A. Finlayson, *J. Fluid Mech.* **40** 753 (1970)

Using linear stability theory to show when a fluid layer, heated from below, would become unstable.

$$\frac{Ra}{Ra_c}+\frac{N}{N_c}=1,\quad Ra=\frac{\alpha g\beta d^4\rho C}{\upsilon k},\quad N=\frac{\mu_0 K^2\beta^2 d^4\rho C}{\mu k(1+\chi_0)}$$



Heat Transfer to Ferrofluid, Suzanne Snyder, *J. Mag. Mag. Mat.* **262** 269 (2003)



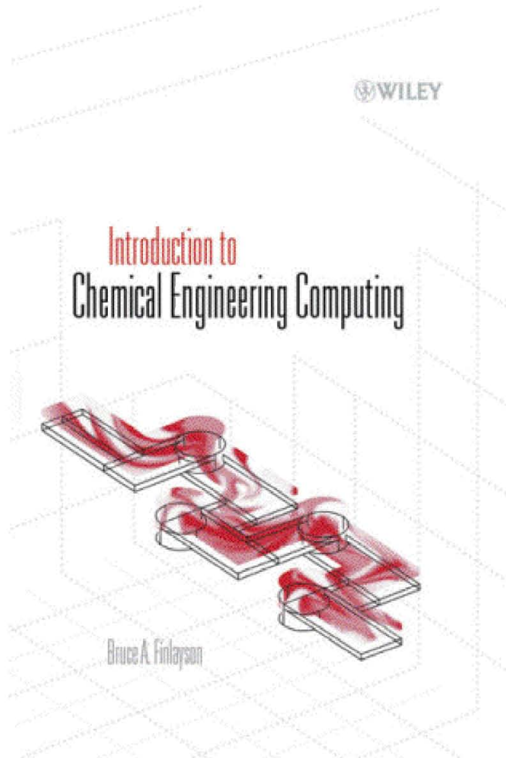
Programs

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

➢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.



Introduction to Chemical Engineering Computing, transport applications

➢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
- adsorption

➢Two- and three-dimensional transport problems in fluid mechanics, heat and mass transfer - focused on microfluidics and laminar flow

- Entry flow
- Laminar and turbulent
- Microfludics, high Peclet number
- Temperature effects (viscous dissipation)
- Proper boundary conditions

Steps in Solution

from *Introduction to Chemical Engineering Computing*, Bruce A. Finlayson, Wiley (2006)

- Open Comsol Multiphysics
- Draw domain
- Physics/Subdomain Settings
- Physics/Boundary Settings
- Mesh (Need to solve one problem on at least three meshes, each more refined than the last, to give information about the accuracy.)
- Solve (Can solve multiple equations together or sequentially; can use parametric solver to enhance convergence of difficult non-linear problems.)
- Post-processing (Plot solution, gradients, calculate averages, calculate or plot any expressions you've defined.

Laser Evaporation of a Metal

Westerberg, McClelland, and Finlayson
Int. J. Num. Methods Fluids **26** 637 (1998)

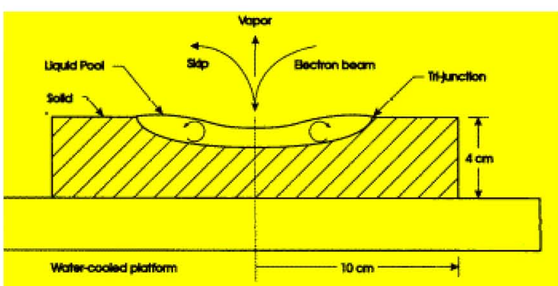
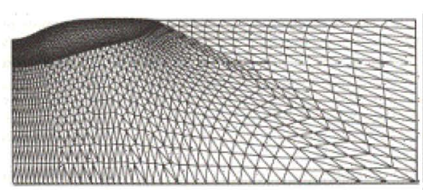
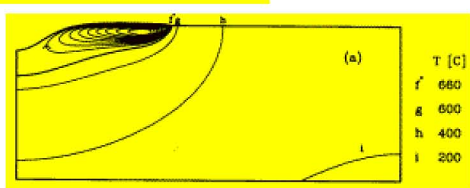
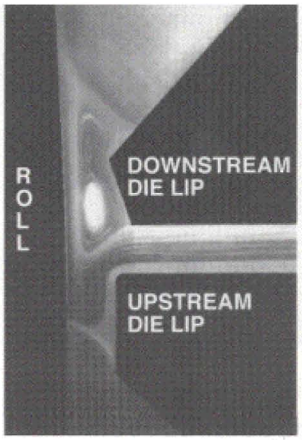


Figure 1. Evaporation of aluminum from a plate on a water-cooled platform.



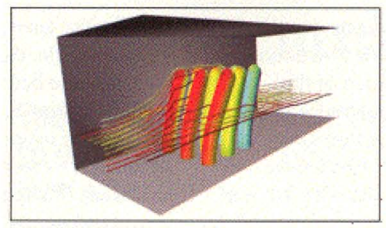


Coating Problems, L. E. Scriven



Microvortex made visible with fluorescent dye and hydrogen bubbles in 250-μm-wide gap between coating die lip and substrate moving about 1 m/s. Luigi Sartor and Wieslaw Suszynski.

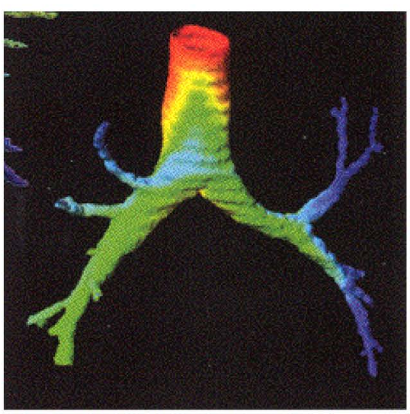
Fluid-Solid Interaction, Comsol



Flow field, pressure, and structural deformation of a set of micro-pillars in a protein sensor calculated using FSI-simulations. The deformation of the pillars depends on the flow field and the amount of adsorbed material. Source: Comsol.

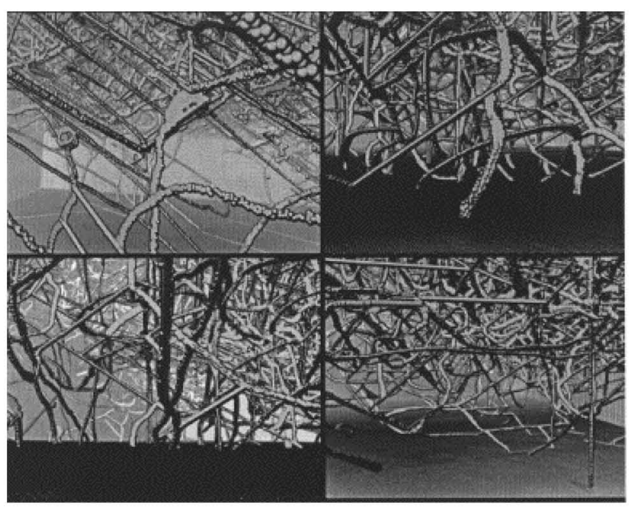
CEP **103** 12 (2007)

Particles in lung



CFX Update, No. 23, p. 26 (2003)

Defects in Materials, Simulations with billions of atoms and fast computers



Abraham, et al., *Proc. NAS* **99** 5783 (2002)

Conclusions

- Computer usage in chemical engineering has advanced from non-existent to the solution of very complicated problems.
- Continuum transport problems are being solved routinely using desktop computers, sometimes with commercial software.
- Current tools enable even undergraduates to solve problems in 2D and 3D that were not solvable in 1960.