Computation in Undergraduate Chemical Engineering Education

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ASEE-CACHE Award for Excellence in Computing in Chemical Engineering Education, 2008

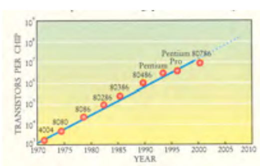
AIChE meeting, paper 19b, Nov. 17, 2008

Status in 1967 when I started my career

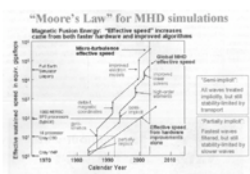
- Perry's Chemical Engineers' Handbook, 4th Ed. (1963) (nothing in earlier editions):
  - To solve ODEs: Euler, Adams, simple Runge-Kutta methods
  - To solve PDEs: diffusion/conduction steady problems in 2D (finite difference) or unsteady problems in 1D
  - None of this was reflected in Sections on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

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

Process Simulation: 1970s

- 1971-*Chemical Plant Simulation*, C. M. Crowe, A. E. Hamielec, T. W. Hoffman, A. I. Johnson, D. R. Woods - based on PACER, written at Purdue
- 1973 - *Computation for Process Engineers*, G. L. Wells, and P. M. Robson - wrote own code (in back)
- 1979 - *Process Flowsheeting*, A. W. Westerberg, H. P. Hutchison, R. L. Motard, P. Winter - discussed flowsheeting on computer, degrees of freedom, sequential solution, tearing
- ~1986 - ASCEND - A. W. Westerberg - simultaneous solution methods

1970s - Mass and Energy Balance Course

- As a young professor, eager to show students what marvelous things they could do on the computer, I taught them how to prepare a deck of cards, carry them to the computer center and solve the following energy balance:

$$\Delta H = \int_{T_1}^{T_2} C_p(T)\,dT\,,\quad C_p = \sum_{i=1}^{n} C_{pi}$$

$$C_{pi} = \alpha_i + \beta_i T + \chi_i T^2 + \delta_i T^3$$

CHESS Program
Rudy Motard, University of Houston

- Process simulator using card input, included short-cut distillation, thermodynamics using solubility parameters, but quite powerful within its area of application.
- 1973 - I volunteered to teach a one-credit course as an overload; the students would use the program to simulate a process.
- 1977 - expanded into a 3-credit course, now an elective and not an overload.
- 1982 - moved FLOWTRAN into the regular design course when older professors retired.

FLOWTRAN, Monsanto, in 1980s

- Monsanto agreed to let Universities use their process simulator, FLOWTRAN. This was the program being used in industry, and this gave a great impetus to the use of computers in chemical engineering education.
- FLOWTRAN formed the basis of AspenPlus.
- 1985 - I prepared the load module for FLOWTRAN when it was to run on CYBER computers; installed at 13 Universities

Textbooks for Process Design (sample)

- 1968 - Peters and Timmerhaus, 2nd Ed., Gives costs on graphs and includes a table of discount factors to calculate DCFROR
- 1983 - Valle-Riestra, still no computer use, but includes difference formulas so that students can derive discount factors
- 1985 - Coulson and Richardson, includes a FORTRAN program MASSBAL printed in the back of the book
- 1988 - Douglas, focused on design concepts, but includes FLOWTRAN input forms, line by line
- 1998, 2003 - Turton, Bailie, Whiting, Shaeiwitz, comes with a CD containing CAPCOST to allow efficient costing of a process, with automatic cash flow analyses; book oriented to process design using computer programs.
- 2003 - Product and Process Design Principles: Synthesis, Analysis, and Evaluation, Warren D. Seider, J. D. Seader, and Daniel R. Lewin

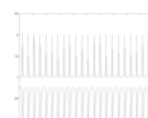
Things I've learned from process simulation

Early 1970s, 1-credit lab course using CHESS to model chemical processes. One student, GPA 2.1, was extremely creative when he had a computer to do the calculations for him. His grade problem had been that he lacked the skills to do the calculations fast; he certainly was creative. He learned by trying (inductive learning).

In the late 1970s I took elements from CHESS and made an interactive program, DISTILL, which ran on computer terminals (now referred to as dumb terminals, with question/answer input). The user would specify the distillation problem and get the output and cost information. An inner loop allowed them to change the pressure, fraction of light and heavy key, and ratio of reflux to minimum reflux, and get another design, with all capital and operating costs displayed. Students would run case after case and learn about the economic effect of their decisions. That was when I learned that students can learn by repetition. A McCabe-Thiele diagram is still useful, but nothing beats rapid feedback about the cost of your decisions. Again, inductive learning. Copies made available for Mac and PC (they still work!)

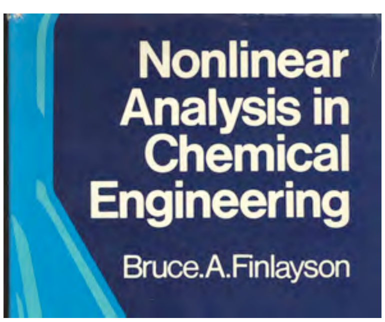
While this activity was going on in process simulation, numerical analysis was advancing, too. Stiffly-stable methods for ODEs

- 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 adjustment, 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.

$$\frac{dT_i}{dt} = \sum_{j=1}^{N+2} B_{ij} T_j$$

One eigenvalue is due to the problem (diffusion) and the other is due to the method.

$$As \;\; N \to \infty \;\; or \;\; \Delta x \to 0, \;\; \lambda_{largest} \;\; gets \;\; big.$$

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).

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

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

Catalytic Converter

Phenomena included:

Chemical reaction

Flow

Axial conduction of heat

Diffusion

Geometry

What is the importance of the shape of channel?

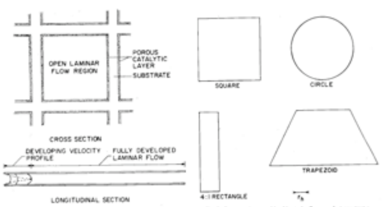


Fig. 1. Cross section and longitudinal section of the square cell.

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

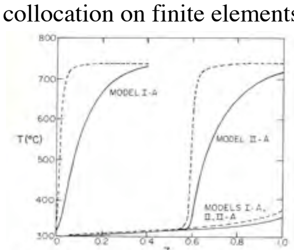
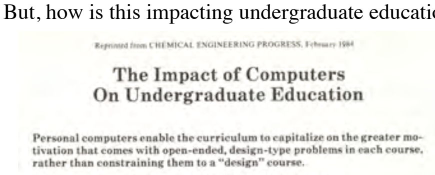


Fig. 8. Steady state model predictions for square geometry. Inlet T = 315°C, y_{CO} = 4%, $\hat{G}$ = 0.0151 m³/s, D^f_{CO}/D^e_{CO} = 70, ℓ = 0.0254 mm. - - - - - Solid temperature, ——— Fluid average temperature. P2 kinetics, model I-A: $Nu = Sh = 4.0$.

But, how is this impacting undergraduate education?



Reprinted from CHEMICAL ENGINEERING PROGRESS, February 1984

The Impact of Computers On Undergraduate Education

Personal computers enable the curriculum to capitalize on the greater motivation that comes with open-ended, design-type problems in each course, rather than constraining them to a "design" course.

Bruce A. Finlayson, Univ. of Washington, Seattle, Wash. 98195

- Article went on to discuss
  - Databases
  - Graphical capabilities
  - Spreadsheets (might be used for engineering calculation)
  - Word processing (enhances written communication)
  - Data acquisition
  - A new scheme Xerox developed: Windows

Changes brought about by the microcomputer

- Mechanize many tedious calculations
- Availability of software (more machines means bigger markets)
- User-friendly
- My 1984 article explained bit, byte, floppy diskette, networking
- For many years I edited a column in CACHE News in which computer programs provided by professors were reviewed for the chemical engineering education community.

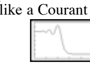
Learn by induction, CACHE News, Fall, 1987

- Graduate students were given a program CDEQN (available through CACHE at the time) to solve the diffusion equation. We had worked out the stability limitation on the time step size for the finite difference method, and I asked them to deduce the limit for the finite element method. The program used a GUI, solved and plotted the solution; by choosing several dx and dt they found it was 1/3 that of the finite difference method.

$$\frac{\partial c}{\partial t} = D\frac{\partial^2 c}{\partial x^2} \qquad D\frac{\Delta t}{\Delta x^2} \le \frac{1}{6}$$

- Then I asked them to do the same thing for the problem with convection. Many of them determined there was something like a Courant number limit.

$$\frac{\partial c}{\partial t} + u\frac{\partial c}{\partial x} = D\frac{\partial^2 c}{\partial x^2} \qquad u\frac{\Delta t}{\Delta x} \le 1$$



- Finally, one student persisted and said - there are two stability limits: one says it is stable the other unstable. What he had found was the difference between a von Neumann analysis (does the disturbance continue growing?) and the eigenvalue analysis (does the solution at a point eventually reach a steady state?). There are articles in the engineering literature discussing this difference, derived using lots of trigonometry and linear algebra, but the student deduced it by trial and error.

Chemical Reactor Design Tool (CRDT) - 1992

- Models CSTR, Plug-flow reactors, reactors with axial dispersion, reactors with radial dispersion.
- User supplies only a FORTRAN reaction rate expression.
- Allows up to 20 components plus temperature.
- Won the Martin Award, 1994, ASEE, ChE

$Cl_2 + C_3H_6 \rightarrow CH_2{=}CHCH_2Cl + HCl$
allyl chloride

$Cl_2 + CH_2{=}CHCH_2Cl \rightarrow CHCl{=}CHCH_2Cl + HCl$
allyl chloride 1,3–dichloropropene

$Cl_2 + C_3H_6 \rightarrow CH_2ClCHClCH_3$
1,2–dichloropropane

$$r_1 = A_1 \exp\left(-\frac{15{,}840}{RT}\right) C_{Cl_2} C_{C_3H_6}$$
$$r_2 = A_2 \exp\left(-\frac{23{,}760}{RT}\right) C_{Cl_2} C_{allyl\ chloride}$$
$$r_3 = A_3 \exp\left(-\frac{7920}{RT}\right) C_{Cl_2} C_{C_3H_6}$$

$$\frac{dF_i}{dV} = Da_i RA_i,\ F_i = F_{i0} \text{ at } V = 0$$
$$\sum_{j=1}^{NC} F_j C_{pj}\frac{dT}{dV} = Da_{III} RT - St\,(T - T_c)$$
$$T = T_{in} \text{ at } V = 0$$
$$St = \frac{UA}{F_s C_{ps}}, \text{ where } F_s \text{ and } C_{ps} \text{ are standard}$$

$$\frac{\partial F_i}{\partial V} = \alpha_i \nabla^2 C_i + Da_i RA_i$$
$$\sum_{j=1}^{NC} F_j C_{pj}\frac{\partial T}{\partial V} = \alpha_T \nabla^2 T + Da_{III} RT$$
$$-\frac{\partial T}{\partial r} = Bi_w\,(T - T_c) \text{ at } r = 1$$

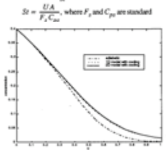


Figure 13. Average Concentration of Chlorine

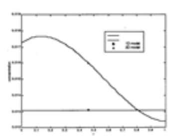


Figure 15. Chlorine Concentration at Exit

B. M. Rosendall and B. A. Finlayson, "Reactor/Transport Models for Design: How to Teach Students & Practitioners to Use the Computer Wisely," FOCAPD, 1999, AIChE Symposium Series No. 323, 96 176-191 (2000).

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.

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

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.

Hole Pressure Problem, Nancy Jackson

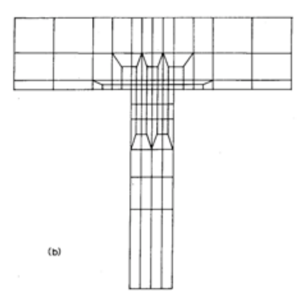
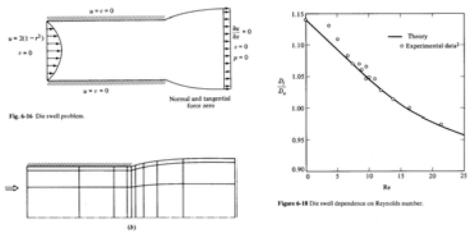
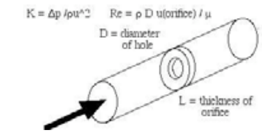


Fig. 3. Finite element mesh: (a) 29 elements; (b) 110 elements.

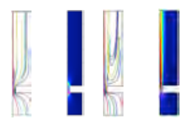
Extrudate Swell, Tom Patten, 1977

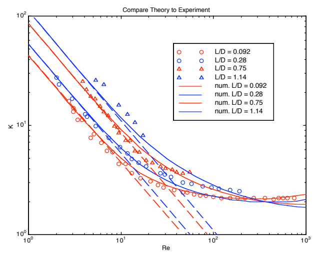




Later, undergraduates could solve harder problems using Comsol Multiphysics (FEMLAB).

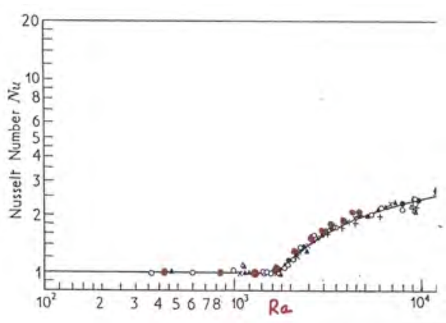
Kusmanto, Jacobsen, and Finlayson, Phys. Fluids **16** 4129 (2004)



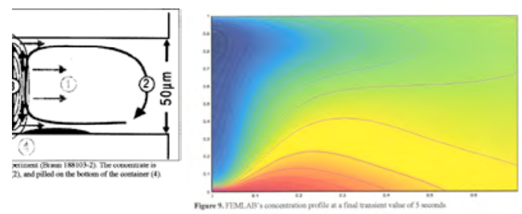


Convective Instability, Michael Harrison

Heat transfer between flat plates, heated from below

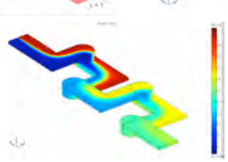


Thermal diffusion, Pawel Drapala



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

Mixing in a Serpentine Microfluidic Mixer



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

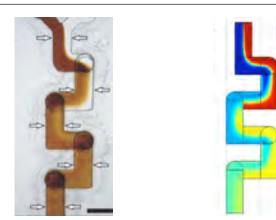


Figure 8. Comparison with experiment (6)

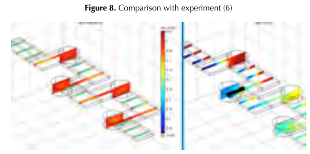
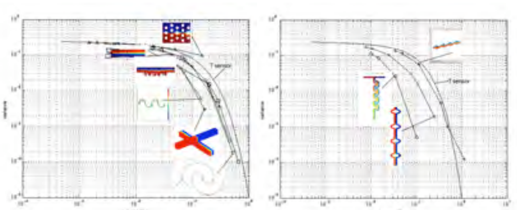


Figure 9. Velocity profiles and concentration profiles inside serpentine mixer

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 Microfluidic Devices
(11 undergraduate projects)



Problem Centered Course n Numerical Methods

- Created model of catalytic converter in summer of 1995.
- While doing so, realized that every type of equation that was covered in my numerical analysis class was in the model somewhere.
- Reorganized the course to be a problem-centered course - everything had to do with catalytic converters.

• Write short theme in first week.
• Solve succession of numerical problems.
• Work in a team to design a catalytic converter for the 'two minute problem'.
• Prepare a web lesson about their work, one suitable for high-school seniors, one for undergraduate chemical engineering students.
• Won Award from DOE in 1996 for Undergraduate Computational Science and Engineering

In successive years:

- Catalytic converter
- Plastic garbage bags from natural gas
- Membrane Separation
- Microreactors
- Fuel cells
- This was the course in which students taught me that the computer can differentiate!

But, it also led me to a new paradigm for teaching, and my next book.

Programs

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

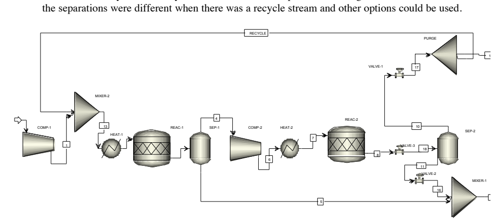
➢Philosophy - students can be good chemical engineers without understanding the details of the numerical analysis.
➢By using modern programs with good GUIs, the most important thing is to check your results.
➢Instead of teaching a small fraction of the class numerical methods, I now teach all the class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

Introduction to Chemical Engineering Computing, process applications

➢Cubic equations of state
➢Vapor-liquid equilibria
➢Chemical reaction equilibria
➢Mass balances with recycle, vapor-liquid equilibria, and chemical reaction equilibria
➢Process simulation, including proper choice of thermodynamic model and use of Aspen Plus

Computing Class - one objective: how do you check your work?
http://courses.washington.edu/checomp

- First assignment using Aspen asked them just to design a once-through process (given) for making ethyl chloride. They were asked to calculate the cost of the utilities (only). Part of the discussion the next week was about the cost of raw materials, how the form of them affected the process, how the cost of utilities could be reduced, how the price dropped precipitously when lead was phased out of gasoline.
- Second week they added a recycle stream and redid the problem, leading to different results because the separations were different when there was a recycle stream and other options could be used.



Class was asked: when you are the supervisor and one of your employees brings a simulation to you, what questions will you ask?

- Do the results seem reasonable?
- What assumptions did you make?
- What equations or models did you use and why?
- How do the answers compare to other simulations?
- Have you done an error analysis? Shows?
- Where or how did you get your data?
- What is the biggest source of uncertainty?
- Compare trends to literature values.

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
  - adsorbtion
- 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

Checklist for Transport Problems

- 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;
- Your report should have an Appendix with sample calculations.

- Some of these steps verify what choices they made in the program to verify that they are solving the right problem.
- Some of them verify the accuracy of the solution.
- If they use complicated expressions (like kinetic expressions) they must do a hand calculation to verify that they typed it correctly.

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.)

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

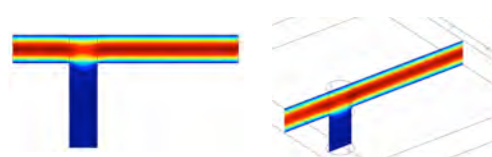
v_s = average velocity, x_s = thickness or diameter, both in the small section

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.

Three-dimensional hole pressure

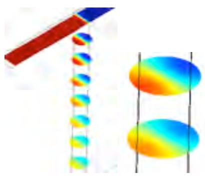
(work done by junior Stephanie Yuen)

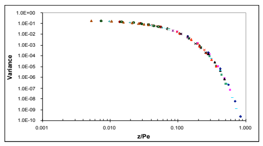
Comparing 2D and 3D calculations. Hole pressure is used in rheology to measure the first normal stress difference.



Mixing in a Three-dimensional T
(work done by junior Daniel Kress)

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



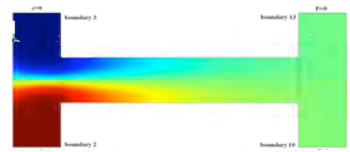


Variance as a function of length in the outlet leg

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

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

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



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

Another approach: FLOWLAB, Jennifer Curtiss, University of Florida

- A special, academic version of FLUENT has been made by the company. It can only solve specific problems, but students can use it to explore the details of fluid flow.
- Problems:
  - Turbulent entry flow into a pipe
  - Boundary layer flow past a flat plate
  - Heat transfer to a fluid in a pipe
  - Drag with flow past a cylinder
  - Flow through an orifice
  - Flow in a sudden expansion
- Limited geometries
- Usually turbulent

New CACHE-CFD Taskforce is developing model problems to use in chemical engineering curriculum.

Conclusions

- Computer usage in chemical engineering education has advanced from non-existent to the solution of very complicated problems.
- The emphasis now is more on how to solve chemical engineering problems (and verify that) than on writing the computer code.
- The computer programs are powerful enough that they permit inductive learning.
- Comsol Multiphysics is so powerful it can be mis-used.
- Introduction in a step-by-step way helps undergraduates learn to solve the problem and show they have solved the problem correctly.
- The 2D and 3D nature of the problems provides motivation beyond the simplified problems solved in textbooks.