Computation in Undergraduate Chemical Engineering Education

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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. Hutchinson, 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:

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

\[ C_{pi} = \alpha_i T + \beta_i T^2 + \gamma_i T^3 \]

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 ICFORR
- 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.

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

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

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

$$c(y,t) = \sum_{i=1}^{N} a_i(t)P_i(y)$$

$$\frac{dc}{dt} = D \frac{\partial^2 c}{\partial y^2} - \phi^T \vec{R}(c)$$ becomes

$$\frac{dc}{dt} = D \sum_{i=1}^{N} \sum_{j=1}^{K} B_{ij} c_j - \phi^T \vec{R}(c)$$

1980 - orthogonal collocation, finite difference, finite element, with programs (still available at www.ravennapark.com)
Stiff methods essential for partial differential equations

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

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

As \( N \to \infty \) or \( \Delta x \to 0 \), \( \lambda_{\text{arg min}} \) 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)."

\[ \frac{\partial}{\partial \tau} \left( \rho C_p \frac{\partial}{\partial \tau} \right) + \frac{k}{\rho C_p} \frac{\partial}{\partial \tau} \left( \rho C_p \frac{\partial}{\partial \tau} \right) \]

Catalytic Converter

Phenomena included:
- Chemical reaction
- Flow
- Axial conduction of heat
- Diffusion
- Geometry

What is the importance of the shape of channel?

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

But, how is this impacting undergraduate education?

- 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.

\[ \frac{\partial c}{\partial t} + \frac{u}{\Delta x} \frac{\partial c}{\partial x} = \frac{D}{\Delta x^2} \frac{\partial^2 c}{\partial x^2} \]
\[ \frac{\partial^2 c}{\partial x^2} \leq \frac{1}{6} \]

- 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.

\[ \frac{\partial c}{\partial t} + \frac{u}{\Delta x} \frac{\partial c}{\partial x} \leq \frac{D}{\Delta x^2} \leq 1 \]

- 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

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

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

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

Mixing in a Serpentine Microfluidic Mixer
Published in Neils, Tyree, Finlayson, Folch, Lab-on-a-Chip 4 342 (2004)

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)

- 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

Problem Centered Course n Numerical Methods

- 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.

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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

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.

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

- First assignment using Aspen asked them to design a once-through process (not for making allyl chloride). They were asked to calculate the cost of the utilities only. Part of the discussion the next week was about the cost of the utilities. How the form of them affected the process, how the price dropped precipitously when lead was phased out of gasoline.
- Second week they added a recycle stream and solved 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.

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.

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

\[ \Delta \frac{P_s}{\nu_s} = K \]

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

Steps in Solution

- 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.)

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)

\[ \text{Variance} = \frac{\int (c - c\text{mixing cup})^2 \cdot u \cdot dA}{\int u \cdot dA} \]

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

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.