The Role of Computation in Continuum Transport Phenomena

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Status in 1967 when I started my career

  - 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 matrices (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.

**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 adjustment, automatic change of order if that was useful, and basically automatic solution of ordinary differential equations (IVP)

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

\[ c(y,t) = \sum_{i=1}^{N+2} a_i(t) P_i(y) \]

\[ \frac{\partial c}{\partial t} = D \frac{\partial^2 c}{\partial y^2} - \phi^2 R(c) \]

becomes

\[ \frac{dc_j}{dt} = \frac{D}{h^2} \sum_{i=1}^{N+2} B_{ji} c_i - \phi^2 R(c_j) \]
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).

\[ \varepsilon \frac{\partial c}{\partial t} = \frac{D}{r^2} \frac{\partial}{\partial r} (r^2 \frac{\partial c}{\partial r}) - kR(c,T) \]

\[ (\varepsilon \rho c_{ps} + (1-\varepsilon) \rho C_m) \frac{\partial T}{\partial t} = \frac{k}{r^2} \frac{\partial}{\partial r} (r^2 \frac{\partial T}{\partial r}) + (-\Delta H_{m\alpha}) kR(c,T) \]
Catalytic Converter

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

What is the importance of the shape of channel?
Model I-A is lumped
Model II-A is distributed, using orthogonal collocation on finite elements

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 $v$.

- $N_1 = (1 - u) (1 - v)$
- $N_2 = u (1 - v)$
- $N_3 = u v$
- $N_4 = (1 - u) v$
- For example:
  - $N_3(1,1) = 1; N_3(0,1) = N_3$

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

Constant interpolation with $32 \times 32 = 1024$ blocks.  
Bilinear interpolation with $4 \times 4 = 16$ blocks.
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

\[ \text{Re} v \cdot \nabla v = -\nabla p + \nabla \cdot \tau \]
\[ \nabla \cdot v = 0 \]

Newtonian Fluid:
\[ \tau = \eta d, \quad d = \nabla v + \nabla v^T \]

Maxwell Model ($\eta, \lambda$ constant), White-Metzner Model ($\eta, \lambda$ vary with shear rate):
\[ \tau + \lambda \left[ v \cdot \nabla \tau - \nabla v^T \cdot \tau - \tau \cdot \nabla v \right] = \eta d \]

Phan-Thien-Tanner Model:
\[ \tau + \lambda \left[ v \cdot \nabla \tau - \nabla v^T \cdot \tau - \tau \cdot \nabla v \right] + \frac{\lambda}{\eta} \tau \cdot \tau = \eta d \]

Stick Slip

\[ \text{fully developed viscoelastic flow} \]

Centerline

normal flow pressure
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)


Comparison to Experiment


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

<table>
<thead>
<tr>
<th>Table III. Coefficient $K$ for contractions and expansions for $Re$ negligibly small</th>
</tr>
</thead>
<tbody>
<tr>
<td>Picture</td>
</tr>
<tr>
<td>2:1 pipe/planar</td>
</tr>
<tr>
<td>3:1 pipe/planar</td>
</tr>
<tr>
<td>4:1 pipe/planar</td>
</tr>
<tr>
<td>45 degrees tapered, planar, 3:1</td>
</tr>
<tr>
<td>28.07 degrees tapered, planar, 3:1</td>
</tr>
<tr>
<td>3:1 square (quarter of the geometry)</td>
</tr>
</tbody>
</table>

\[
\frac{\Delta p x_c}{\eta v_s} = K
\]

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).


Streamlines and pressure profiles for \( \text{Re} = 0 \) (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


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)

\[
c_{\text{mixing cup}} = \frac{\int c \mathbf{u} \cdot dA}{\int \mathbf{u} \cdot dA}, \quad \text{variance} = \frac{\int (c - c_{\text{mixing cup}})^2 \mathbf{u} \cdot dA}{\int \mathbf{u} \cdot dA}
\]

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:

\[ \rho \frac{\partial \mathbf{v}}{\partial t} + \rho \mathbf{v} \cdot \nabla \mathbf{v} = -\nabla p + 2\eta \nabla \times \omega + (\eta + \zeta) \nabla^2 \mathbf{v} + \mu_0 \mathbf{M} \cdot \nabla \mathbf{H} \]

Conservation of internal angular momentum (spin equation):

\[ 0 = \mu_0 \mathbf{M} \times \mathbf{H} + 2 \nabla \times \mathbf{v} - 4 \omega + \eta \nabla^2 \omega \]

Magnetization (Shliomis, 1972):

\[ \frac{\partial \mathbf{M}}{\partial t} + \mathbf{v} \cdot \nabla \mathbf{M} = \omega \mathbf{M} - \frac{1}{\tau} \left( \mathbf{M} - \mathbf{M}_{eq} \right) \]

Maxwell’s Equations for non-conducting fluid:

\[ \nabla \cdot \mathbf{B} = 0, \quad \nabla \times \mathbf{H} = 0, \quad \mathbf{B} = \mu_0 (\mathbf{H} + \mathbf{M}) \]

\[ \mathbf{H} = \nabla \phi \quad \nabla^2 \phi = -\nabla \cdot \mathbf{M} \]
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


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

\[
\frac{Ra}{Ra_c} + \frac{N}{N_c} = 1, \quad Ra = \frac{\alpha \beta d^4 \rho C}{\nu k}, \quad N = \frac{\mu_0 K^2 \beta d \rho C}{\mu k(1 + \chi_c)}
\]


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Pressure drop of ferrofluid, Kris Schumacher

- **X** 158 Oe
- △ 316 Oe
- ▲ 474 Oe
- □ 948 Oe
- ○ 1264 Oe

Fractional pressure drop

\(Q\) (ml / min)
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
  - Microfluidics, 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.

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**Laser Evaporation of a Metal**

Westerberg, McClelland, and Finlayson

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![Image of Laser Evaporation Process](image-url)
Coating Problems, L. E. Scriven

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)
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.