CM3110
Transport Processes and Unit Operations I

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Department of Chemical Engineering
Michigan Technological University

Numerical methods in transport phenomena/chemical engineering

www.chem.mtu.edu/~fmorriso/cm310/cm310.html

- Numerical integration (one-dimensional; trapezoidal rule)
- Optimization (Excel Solver)
- Iterative Problem Solving
- Numerical integration (two-dimensional; finite-element package Comsol)

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• Numerical integration (one-dimensional; trapezoidal rule)
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• Numerical integration (two-dimensional; finite-element package Comsol)

(easy on a calculator, but sometimes it is part of a larger calculation . . . . )

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An example from Rheology (Binding Analysis)

Calculate the following integral for known \( n \) and \( t \)

\[
I_{nt} = \left[ 2 - \left( \frac{3n + 1}{n} \right) \varphi^{\frac{n+1}{n}} \right]_{\varphi^{t+1/n}}^{t+1} \varphi \, d\varphi
\]

\[
I_{nt} = \int_{a}^{b} f(\varphi) \, d\varphi
\]

Use trapezoidal rule.

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Trapezoidal Rule

\[ I = \int_{a}^{b} f(x) \, dx \]

\[ dy = f(x) \]

\[ y(x) = I = \text{Area} = \sum \frac{1}{2} (b_1 + b_2) h \]

Trapezoidal rule integration

\[ I_{nt} = \int_{0}^{1} 2 - \left( \frac{3n + 1}{n} \right) \varphi^{\frac{1}{n}} \, d\varphi \]

\[ \text{area} = \frac{1}{2} (b_1 + b_2) h \]

<table>
<thead>
<tr>
<th>Trapezoidal rule integration</th>
<th>( \Delta \varphi ) (phi)</th>
<th>0.005 (phi)</th>
<th>areas</th>
</tr>
</thead>
<tbody>
<tr>
<td>PL_m= 6,682.50</td>
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<td>0.000000</td>
<td>0.005000</td>
</tr>
<tr>
<td>PL_m= 6,682.50</td>
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<td>0.005534</td>
</tr>
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<td>0.105000</td>
<td>0.1158618</td>
<td>0.006241</td>
</tr>
</tbody>
</table>

\[ \text{Integral=} \text{sum of areas column} \]

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Numerical methods in transport phenomena/chemical engineering

- Numerical integration (one-dimensional; trapezoidal rule)
- Optimization (Excel Solver)
- Iterative Problem Solving
- Numerical integration (two-dimensional; finite-element package Comsol)

Detailed handout is on the web

http://www.chem.mtu.edu/~fmorriso/cm4650/Using_Solver_in_Excel.pdf
Basic idea: minimize the error between the values predicted by a model and the data that you have.

\[
\text{Value to be minimized by Solver} = \sum_{\text{all data}} \frac{(\text{model} - \text{data})^2}{(\text{data})^2}
\]

The minimization is achieved by manipulating parameters of the model.

---

**Optimization with Excel Solver**

1. Office button
2. Excel Options
3. Add-ins, Excel add-ins, Go. (Solver installed; do once only)
4. Set up error cell (Target Cell)
5. Select: Data, Solver
6. Choose parameters that Solver manipulates (optimizes) to minimize the Target Cell
7. Select: Options, Use Automatic Scaling
8. Solve

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From measurements of entrance pressure loss versus flow rate, estimate the two parameters $t$ and $l$ in the elongational viscosity model. The two parameters $n$ and $m$ from the shear viscosity model are known.

Shear stress: \[ \tau_R = m \dot{\gamma}_R^n \]

Elongation viscosity: \[ \dot{\eta} = l \dot{\varepsilon}_o t^{-1} \]


\[ \Delta P_{ent} = \frac{2m(1+t)^2}{3t^2(1+n)^2} \left( \frac{l(t(3n+1)n^t I_{nt})}{m} \right) \frac{1}{2(l+1)} \hat{\gamma}_R^t \left( 1 - \hat{\alpha}^t \right) \]

\[ \hat{\gamma}_R = \frac{(3n+1)}{n \pi R_o^3} Q \]

\[ I_{nt} = \int_0^1 \left( 2 - \left( \frac{3n+1}{n} \right) \phi^{1+1/n} \right)^{t+1} \phi \, d\phi \]

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Binding Analysis

Evaluation Procedure

1. Shear power-law parameter \( n \) must be known; must have data for \( \Delta p_{\text{ent}} \) versus \( Q \)
2. Guess \( t, \ l \)
3. Evaluate \( I_{nt} \) by numerical integration over \( f \)
4. Using Solver, find the best values of \( t \) and \( l \) that are consistent with the \( \Delta p_{\text{ent}} \) versus \( Q \) data

Binding Analysis (rheology)

Known: \( \alpha = \frac{R_o}{R_i}, n, m \)
Data for \( \Delta p_{\text{ent}}(Q) \)

\( \Delta p_{\text{ent}} = \left( \text{Ratio1} \right) \left( \text{Ratio2} \right) I_{nt} \)

\( \text{Ratio1} = \frac{2m(1 + t)^2}{3t^2(1 + n)^2} \)
\( \text{Ratio2} = \frac{lt(3n + 1)n'}{m} \)
\( myExp1 = t(n + 1)/(1 + t) \)
\( myExp2 = 1/(1 + t) \)

What are the best values of \( t \) and \( l \) so that the model is consistent with the \( \Delta p_{\text{ent}}(Q) \) data?

Need to repeatedly evaluate the integral as we optimize the values of \( t \) and \( l \).
Binding Analysis – using Excel Solver

Evaluate integral numerically

\[ \int_0^{1+1/n} \phi d\phi \]

\[ 2 - \frac{3n + 1}{n} \phi^{1+1/n} \]

<table>
<thead>
<tr>
<th>phi</th>
<th>f(phi)</th>
<th>areas</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.005</td>
<td>0.023748502</td>
<td>5.93663E-05</td>
</tr>
<tr>
<td>0.01</td>
<td>0.047492829</td>
<td>0.000178098</td>
</tr>
<tr>
<td>0.02</td>
<td>0.094962739</td>
<td>0.000415533</td>
</tr>
<tr>
<td>0.025</td>
<td>0.119724352</td>
<td>0.000534268</td>
</tr>
<tr>
<td>0.03</td>
<td>0.142461832</td>
<td>0.000652965</td>
</tr>
<tr>
<td>0.035</td>
<td>0.166193303</td>
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<tr>
<td>0.04</td>
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<td>0.045</td>
<td>0.213628991</td>
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<tr>
<td>0.05</td>
<td>0.237327345</td>
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<tr>
<td>0.065</td>
<td>0.308304107</td>
<td>0.001482433</td>
</tr>
</tbody>
</table>

\[ \text{area} = \frac{1}{2} (b_1 + b_2) h \]

\[ \text{int} = 1.36055 \]

Summing:

By varying these cells:

\[ (\text{predicted} - \text{actual})^2 \]

\[ (\text{actual})^2 \]

\[ \text{target cell} = 5.57E-02 \]

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---

Binding Analysis – using Excel Solver

Optimize \( t, l \) using Solver

\[ \text{Minimize this cell} \]

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It is much easier to proof-read the formula if you use this method.

Good Excel Habits:

• Break formulas into chunks that are easier to check
• Name cells so that the names appear in the formulas (easier to check)
• Do unit conversions explicitly rather than hidden in formulas
• Numerical integration (one-dimensional; trapezoidal rule)
• Optimization (Excel Solver)
• **Iterative Problem Solving**
  • Numerical integration (two-dimensional; finite-element package Comsol)

---

**Iterative Problem Solving with Excel 2007**

1. Office button
2. Excel Options
3. Formulas
4. Calculation Options
5. Select: *Manual recalculation*
6. Select: *Enable Iterative Calculation; Maximum iterations = 1*
7. Set a circular reference
8. Use F9 to recalculate one step at a time

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Example: Calculate flow rate in a pipe from a known pressure drop

\[ \frac{1}{2} \text{” nominal Schedule 40 pipe (smooth)} \]

\[
\text{Length}=55\text{ft}
\]

60 psig \hspace{1cm} 0 psig

What is the flow rate?

\[ \frac{16}{\text{Re}} \]

Data correlation for friction factor (ΔP) versus Re (flow rate) in a pipe

(Moody Chart)

(Geankoplis, 1993, p88)

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Data are organized in terms of two **dimensionless** parameters:

### Reynolds Number

\[
Re = \frac{\rho \langle v_z \rangle D}{\mu}
\]

- \(\rho\) – density
- \(\langle v_z \rangle\) – average velocity
- \(D\) – pipe diameter
- \(\mu\) – viscosity
- \(P_0 - P_L\) – pressure drop
- \(L\) – pipe length

### Fanning Friction Factor

\[
f = \frac{1}{4} \left( \frac{P_0 - P_L}{L} \right) \left( \frac{1}{D} \right) \left( \frac{1}{2} \rho \langle v_z \rangle^2 \right)
\]

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**Data Correlations for \(f(Re)\)**

For \(Q\) known, calculate \(f\) directly.

For \(f\) known, requires iterative calculation of \(Re\).

For \(Re > 4000\), turbulent flow:

<table>
<thead>
<tr>
<th>Correlation</th>
<th>Equation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Prandtl (smooth pipes)</td>
<td>(\frac{1}{\sqrt{f}} = 4\log\left(Re \sqrt{f}\right) - 0.40)</td>
</tr>
<tr>
<td>Colebrook (rough pipes)</td>
<td>(\frac{1}{\sqrt{f}} = -4\log\left(\frac{\varepsilon}{D} + \frac{4.67}{Re \sqrt{f}}\right) + 2.28)</td>
</tr>
</tbody>
</table>

(Prandtl and Colebrook are equivalent for \(\varepsilon=0\))

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implemented in excel

given

<table>
<thead>
<tr>
<th>Step</th>
<th>Flow rate (guess)</th>
<th>Flow rate</th>
<th>velocity</th>
<th>Re</th>
<th>guess f</th>
<th>RHS Prandtl</th>
<th>error</th>
<th>new f</th>
<th>velocity second</th>
<th>Q_new</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>4.60 gpm</td>
<td>0.0102 ft^3/s</td>
<td>4.8559 ft/s</td>
<td>26,092</td>
<td>0.00607</td>
<td>12.83</td>
<td>0.0000%</td>
<td>0.00607</td>
<td>4.86 ft/s</td>
<td>0.0102 ft^3/s</td>
</tr>
<tr>
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<td></td>
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<tr>
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<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

alternative (but more complex) correlation; no iteration on f required (F. A. Morrison, 2011)

flow in smooth pipes: (all Reynolds numbers)

\[ f = \left( \frac{0.0076 \left( \frac{3170}{\text{Re}} \right)^{0.165}}{1 + \left( \frac{3170}{\text{Re}} \right)^{7.0}} \right) + \frac{16}{\text{Re}} \]

(would still need to iterate on Q if used in our problem)
Numerical methods in transport phenomena/chemical engineering

- Numerical integration (one-dimensional; trapezoidal rule)
- Optimization (Excel Solver)
- Iterative Problem Solving
- Numerical integration (two-dimensional; finite-element package Comsol)

Analytical Integration of Differential Equations

Solve for \( y(x) \):

\[
\frac{dy}{dx} + 2xy = 3x^2 + 1
\]

Analytical solution (integrating factor):

\[
u = 2x
\]

\[
\int u \, du = \int 2x \, dx = x^2
\]

\[
e^{\int u \, du} = e^{x^2}
\]

\[
e^{x^2} \frac{dy}{dx} + e^{x^2} 2xy = e^{x^2} (3x^2 + 1)
\]

\[
\frac{d}{dx} (e^{x^2} y) = e^{x^2} (3x^2 + 1)
\]

\[
e^{x^2} y = \int e^{x^2} (3x^2 + 1) \, dx + C
\]

Carry out integral here to obtain final solution for \( y(x) \).
Numerical Integration of Differential Equations

Solve for $y(x)$:

$$\frac{dy}{dx} + 2xy = 3x^2 + 1$$

Before, we were calculating:

$$\frac{dy}{dx} = f(x)$$

$$I = \int_a^b f(x) \, dx$$

and $f(x)$ was known. In the current calculation, our integration is not explicitly $dy/dx = f(x)$

In the trapezoidal rule integration, we discretized $x$, evaluated $f(x)$, and summed areas.

---

Numerical Integration of Differential Equations

We can discretize the current differential equation as well:

$$\frac{dy_i}{dx_i} + 2x_i y_i = 3x_i^2 + 1$$

$$y_i = \frac{1}{2x_i} \left( 3x_i^2 + 1 - \frac{dy_i}{dx_i} \right)$$

where to get this at each step?

Strategy: Develop efficient and accurate algorithms that allow us to calculate $y(x)$ and its derivatives at a location $(i+1)$ from knowledge of $y(x)$ at neighboring locations $(i)$, $(i-1)$, etc.
Numerical Integration of Differential Equations

In two dimensions (or three), the discretization system is called the mesh.

Algorithms:
- Finite difference
- Finite elements
- Finite volumes
- Etc.

Different algorithms use different logic to estimate the values of $y$ and derivatives of $y$ at different locations.

Reference:

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A group of female “Computers” at Aberdeen Proving Ground (US Army) doing ballistics calculations (numerical integration) during WW2.
Meshes for Numerical Integration of Differential Equations

The discretization (mesh) is chosen to minimize the effect of numerical errors and modeling approximations on the final results.

Issues affecting accuracy of solutions of flow problems using the Navier-Stokes equation

Analytical Solutions are affected by BOTH Numerical Solutions are affected by

- Continuum hypothesis
- Symmetry assumptions
- Approximate geometry
- Approximate boundary conditions
- Steady state assumption
- Incompressible fluid
- Newtonian fluid
- Isothermal, single-phase flow
- Finite domain size

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**Issues affecting accuracy of solutions of flow problems using the Navier-Stokes equation**

<table>
<thead>
<tr>
<th>Analytical Solutions are affected by</th>
<th>Numerical Solutions are affected by</th>
</tr>
</thead>
<tbody>
<tr>
<td>Neglect inconvenient terms</td>
<td>Discretization of flow domain</td>
</tr>
<tr>
<td>Linearization and other approximate analytical solution methods</td>
<td>Derivative approximations</td>
</tr>
<tr>
<td>Final solution series truncation error</td>
<td>Round-off error</td>
</tr>
<tr>
<td></td>
<td>Interpolation error in final engineering quantities</td>
</tr>
<tr>
<td></td>
<td>Numerical instability induced by accumulation of error</td>
</tr>
<tr>
<td></td>
<td>Inappropriate implementation of commercial code</td>
</tr>
</tbody>
</table>

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**Numerical PDE Solving with Comsol 4.2**

www.comsol.com

Finite-element numerical differential equation solver. Applications include fluid mechanics and heat transfer.

1. Choose the physics (2D, 2D axisymmetric, laminar, steady/unsteady, etc.)
2. Choose flow geometry and fluid (shape of the flow domain)
3. Define boundary conditions
4. Design and generate mesh
5. Solve the problem
6. Calculate and plot engineering quantities of interest.

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Comsol Multiphysics 4.2

Launch the program

Comsol Multiphysics 4.2

Choose the physics

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Choose flow geometry and fluid

Define boundary conditions
Comsol Multiphysics 4.2

Design and generate mesh

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Comsol Multiphysics 4.2

Solve the problem

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Comsol Multiphysics 4.2

View the solution

Comsol Multiphysics 4.2

Calculate engineering problems of interest

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**SUMMARY: Numerical methods in transport phenomena/chemical engineering**

- Numerical integration (one-dimensional; trapezoidal rule)
- Optimization (Excel Solver)
- Iterative Problem Solving
- Numerical integration (two-dimensional; finite-element package Comsol)

Calculators can do numerical integration of the problem is a once-and-done sort.

Optimization (Excel Solver) is great for model fitting.

Iterative Problem Solving can do iterative calculations if it is a once-and-done sort.

Numerical integration (two-dimensional; finite-element package Comsol) is state of the art for complex geometries in many fields.

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