Use of *Mathematica* as a Teaching Tool for (Computational) Fluid Dynamics and Transport Phenomena

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Outline

• **Mixing**
  – Importance of dimensionless groups
  – Experimental study of mixing of viscous materials

• **Numerical solution to flow in a rectangular duct**
  – *Mathematica* used to show finite difference vs finite element

• **Mathematica notebooks on computational fluid flow and heat transfer problems**
  – Boundary-layer flow, Falkner-Skan problem
  – Natural convection thermal boundary layer

• **Mathematica notebooks for other fluid flow problems**
  – Creeping flow past a sphere
  – Introduction to multiphase flows

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Dimensionless groups

- A big theme throughout the Junior-Level Fluid Dynamics course is the importance of comparing competing or cooperating effects and how dimensionless groups inherently do this.
- To make the point we did a laboratory exercise on mixing and combined with dimensional analysis.
Mixing Experiment

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Coloring Liquid Soap

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Toothpaste and Karo Syrup

http://www.nd.edu/~chegdept
They can be mixed
Mixing questions using Dimensional analysis

Mixing

Homework due 9/5. (There will be other questions.)

We would now like to do dimensional analysis of the mixing of two liquids. You can go to the learning center and check out some mixing instruments and some substances that can be mixed. These will be different fluids that require different levels of effort and different mechanical actions to mix well.

1. Once you have gained some feel for mixing from the experiments, choose the variables that seem to be most important to mixing for say, two liquids that will be mixed in a cylindrical tank with a single agitator.

2. Now do dimensional analysis, perhaps patterned after the work done above, to find the dimensionless groups that will be important for this mixing problem.

3. Now consider that you have to design a flowing process in a 500 gallon tank to mix the same substances. Can you convince me it will work?

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Mixing Answers

• Viscous mixing

\[ \frac{\mu_1}{\mu_2}, \quad \frac{L}{R}, \quad \frac{P}{L^3 \mu \omega^2} \]
Dimensionless groups do not need to be on technical subjects

\[ Cr \equiv \frac{\text{How Smart You Are}}{\text{How Smart You Think You Are}} \]
Dimensionless

Confucius Proverb

• He who knows not and knows he knows not is a child, teach him, $Cr \sim 1$
• He who knows not and knows not he knows not is a fool, shun him, $Cr \ll 1$
• He who knows and knows not he knows is asleep, awaken him, $Cr \gg 1$
• He who knows and knows he knows is wise, follow him $Cr \sim 1$
Dimensionless Proverb

• Child ~ Wise person
Dimensional Analysis NoteBook

Buckingham Pi method (dimensional analysis)

This notebook has been written in Mathematica by

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More recent versions of this notebook should be available at the web site:
http://www.nd.edu/~mjm/dimensional_analysis.nb
Mathematica Note Books

Many of these (and other useful materials) are also available from MathSource, at the Wolfram Research website. This and other courses that use Mathematica materials can be found at the Mathematica Courseware web site.

A simple Mathematica primer,
Mathematica_primer_1.nb, (Notebook)
Mathematica Primer (html)

A basic introduction to dimensional analysis including physical motivation and how to solve pipe flow.
dimensional_analysis.nb, (Notebook)
dimensional_analysis.html (html)

A simple primer on why we use log-log plots and what they mean,
Primer on log-log and semilog plots, (Notebook)
Primer on log-log and semilog plots (html)

An exhaustive solution of the lubricated flow example ("core-annular flow") from Middleman 3.2.3, pp79-82). It demonstrates a number of Mathematica features and several important basic ideas from this course,
lubricatedflow.nb (notebook format)
lubricatedflow.html (html, this is not as good as the Mathematica version, but you don't need MathReader.)

This one shows how to use the chain rule to nondimensionalize differential equations. It also makes a point that the Resulting dimensionless terms are of order 1.
Making a differential equation dimensionless (Notebook format)
Making a differential equation dimensionless (html)
Finite Difference and Finite Element solution to flow in a Rectangular Duct

The numerical code for this problem is adapted from a Fortran program and discussion given by C. A. J. Fletcher (1991) Computational Techniques for Fluid Dynamics, Springer vol. 1 p 112.

Homework problem

1. Plot the solution for different values of the the aspect ratio, ba. Explain what is happening.
2. What do you have to do to get accurate answers as ba is changed ??
3. If you use the finite element method with nx=6 and ba>=6, there will be two cells of flow. How do you know that this is incorrect? One of the important issues that you may face when using numerical codes is that they may not be correct !!!!
4. It is rather significant that the solution depends only on the geometric parameter, ba. There is no qualitative change in the flow field with flow rate. The group, (-eta/b^2/DPDZ) scales the velocity to make this possible, discuss this physical meaning of this group.
Objectives for “CFD”

• BS engineers, whether we like it or not, will increasingly be using computational packages and analytical instruments that are “turn key” (they don’t understand how they work). We need to instill in them both a healthy skepticism that they need to verify the answers, and enough fundamental understanding of the different subject so that they can.
As the aspect ratio is varied from one, the solution become increasingly inaccurate. The finite different method works better.
Comparison of solutions

Analytical

Finite diff.

Finite element
Boundary-Layer flows

Boundary-layer flow over a flat plate and wedge

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http://www.nd.edu/~mjm/boundarylayer.nb

Version: 6/19/00
Boundary-Layer Flow (cont)

Summary

This notebook examines the boundary-layer flow over a flat plate and a wedge. The solution is given using numerical scheme and several important physical aspects of boundary layers are elucidated.

Reference

Sample Homework problem for this note book

1. How does the boundary layer thickness change with Reynolds number??
2. How does the wall shear stress change with Reynolds number??
3. What are two physical characteristics of boundary layers??
4. Run the code to find is the approximate location of the outer edge of the boundary layer.
5. Run the code to find the value of the stress at the wall.
6. Run the code to show how the boundary-layer thickness and shear stress change when the imposed pressure gradient changes (i.e. the wedge problem)
Boundary Layer Flow

*Flow past a flat plate*

- Governing equations and problem set up
- Numerical Solution
- Plots of the results
Problem set-up

Governing equations and problem set up

Boundary layers are regions where two competing transport effects are about the same order of magnitude. It is expected that the gradients are also "large" in this region. This Mathematica program gives numerical code for the boundary velocity field for flow over a flat plate and below, the Falkner-Skan problem for flow over a wedge.

The boundary layer equations are

$$\frac{\partial v_x}{\partial x} + \frac{\partial v_y}{\partial y} = 0$$

$$\rho \left( v_x \frac{\partial v_x}{\partial x} + v_y \frac{\partial v_x}{\partial y} \right) = - \frac{\partial p}{\partial x} + \eta \frac{\partial^2 v_x}{\partial y^2}$$

If the plate is flat, there is no change in pressure because of a change in the fluid local velocity, say for example if the flow were converging or diverging. You might have a slight pressure drop in a closed system, but this can usually be neglected.

Therefore, $\frac{\partial p}{\partial x} = 0$. 
Problem set-up continued

Using the variable changes given in Denn, pp292-293, the boundary layer equations become simply

\[ f''' + f \frac{f''}{2} = 0. \]

The primes (') denote derivatives with respect to the similarity variable. This nonlinear ode does not have a known analytical solution. However, it can be easily solved numerically.

Numerical solutions for ode's are often done by creating a system of first order odes. This is done by defining

\[
\begin{align*}
y_1 &= f, \\
y_2 &= f' \\
y_3 &= f''
\end{align*}
\]

These have to be related.

Thus we have

\[
\begin{align*}
y_1' &= y_2 \text{ (by definition)} \\
y_2' &= y_3 \text{ (by definition)} \\
y_3' &= -\frac{1}{2}y_1^*y_3 \text{ (which is from the original ode.)}
\end{align*}
\]

In the first part I solve the flat plate problem separately using a crude numerical scheme that usually converges, although not real fast. It is a shooting method. I have picked \( y = 15 \) as the end of the integrate. The NDSolve routine uses a Runge-Kutta method with built in step size adjustment.
Flow over a flat plate solution

```plaintext
Numerical Solution

fppinit = 1;
eps = 1;

While[Abs[eps] > .000001,
    zz = NDSolve[{{y1'[x] == y2[x], y2'[x] == y3[x],
                    y3'[x] == -1/2 y1[x] y3[x], y1[0] == 0, y2[0] == 0,
                    y3[0] == fppinit}, {y1[x], y2[x], y3[x]}, {x, 0, 15}];
    xx = (zz /. x -> 15)[[1, 2, 2]]; eps = 1 - xx; fppinit = fppinit/(1 - eps);
    Print["U = ", xx, " error= ", eps, " f''[0]= ", fppinit];
]
U = 2.08541 error= -1.08541 f''[0]= 0.479523
U = 1.27761 error= -0.277607 f''[0]= 0.375329
U = 1.08509 error= -0.085088 f''[0]= 0.345897
U = 1.02759 error= -0.0275943 f''[0]= 0.336608
U = 1.00911 error= -0.00911473 f''[0]= 0.333568
U = 1.00303 error= -0.00302905 f''[0]= 0.32561
U = 1.00101 error= -0.00100866 f''[0]= 0.32225
U = 1.00034 error= -0.000336106 f''[0]= 0.332114
U = 1.00011 error= -0.000112022 f''[0]= 0.332077
U = 1.00004 error= -0.0000373392 f''[0]= 0.332064
U = 1.00001 error= -0.0000124462 f''[0]= 0.33206
U = 1. error= -4.1487\times10^{-6} f''[0]= 0.332059
U = 1. error= -1.38289\times10^{-6} f''[0]= 0.332058
U = 1. error= -4.60962\times10^{-7} f''[0]= 0.332058
```

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Flow past a wedge

We again need to make a system of first order ODE's. These are

\[
\begin{align*}
y_1' &= y_2 \\
y_2' &= y_3 \\
y_3' &= -(m+1)/2 \ y_1 \ y_3 + m^*(1-y_2^2)
\end{align*}
\]

This time I use a real shooting method, with a pseudo Newton-Raphson iteration. It works for most cases. If the angle is too negative, the stress will go through 0, this means that there is no layer and thus it is not surprising that the answer blows up. Of course if we look at the physical situation, we might be surprised that we can get any solution for negative \( \beta \). The trend is correct and it is interesting to examine the case of a diverging flow.

- Numerical solution
- Plots of the results at different angles
Flow past a wedge

Governing equations and problem set up

From Denn the flow past a wedge (figure 15-1) is given by

\[ U(x) = A x^m, \text{ } m = \beta/(2 \pi - \beta) \]

Recall that the pressure gradient, \( \frac{\partial p}{\partial x} \), will change as \(-V(x) V'(x)\). This gives

\[ \rho \left( v_x \frac{\partial v_x}{\partial x} + v_y \frac{\partial v_x}{\partial y} \right) = V(x) V'(x) + \eta \frac{\partial^2 v_x}{\partial y^2} \]

******* Thus, the flow past a wedge is a model problem for telling how the boundary layer will change as the pressure gradient changes. *******

Denn tells us that the equation can be reduced to a nonlinear ode again taking advantage of similarity of solution profiles. This gives

\[ f''' + (m+1)/2 f f''/2 + m (1-f'^2) = 0. \]

If \( m = 0 \), the equation is the same as for the flat plate.
Solution code

Numerical solution

Note that you will want to run this several times changing the value of $\beta$ over the possible range. If $\beta=0$, the result is the same as a flat plate.

```plaintext
fppinit = 1;
eps = 1;
beta = 0 * \frac{\pi}{2} ;
\eta = \frac{\beta}{2 \pi - \beta} ;
\rhoouter = 10 ;

angleindegrees = \eta \left[ \frac{\beta \times 180}{\pi} \right] ;
```

0.
need to run one time to get a value for the outer f'[infinity]

```
z = NDSolve[
{y'[x] == y2[x], y2'[x] == y3[x],
  y3'[x] == -1/2 (m + 1) y1[x] y3[x] - m (1 - y2[x]^2),
  y1[0] == 0, y2[0] == 0, y3[0] == fppinit},
{y1[x], y2[x], y3[x]}, {x, 0, youter}];
z = (z /. x -> youter)[[1, 2, 2]]; eps = 1 - z;
Print["U = ", z, " error= ", eps, " f'[0]= ", fppinit];
U = 2.08541 error = -1.08541 f'[0] = 1

fppinitold = fppinit;
fppinit = fppinit + .01;
xzold = z;

While[Abs[eps] > .000001,
z = NDSolve[
{y'[x] == y2[x], y2'[x] == y3[x],
  y3'[x] == -1/2 (m + 1) y1[x] y3[x] - m (1 - y2[x]^2),
  y1[0] == 0, y2[0] == 0, y3[0] == fppinit},
{y1[x], y2[x], y3[x]}, {x, 0, youter}];
z = (z /. x -> youter)[[1, 2, 2]]; eps = 1 - z;
xCorrect = (1 - z) (fppinit - fppinitold) /
(z - xzold)

fppinitold = fppinit; xzold = z;
fppinit = fppinitold + xcorrect;
Print["U = ", z, " xzold= ", xzold, 
  " error= ", eps, " f'[0]= ", fppinit, " xc= ", xcorrect]; xzold = z;]
```

U = 2.09929 xzold = 2.09929 error =
-1.09929 f'[0] = 0.217988 xc = -0.792012

U = 0.755344 xzold = 0.755344 error =
0.244656 f'[0] = 0.362168 xc = 0.144181

U = 1.95957 xzold = 1.95957 error =
Plots at different angles
Solution of natural convection boundary-layer flow near a heated flat plate

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Version: 5/25/00
More recent versions of this notebook may be available at the web site:
http://www.nd.edu/~mjm/thermal_boundarylayer.nb
Problem overview

Derivation of the ODE's from the original PDE's.

Correlation of the experimental data

Numerical solution of the coupled ODE's that result after a similarity variable is introduced to the natural convection boundary-layer equations for flow near a flat plate.

Conclusions
## Problem overview

- Physical situation of interest
- High Grashof number heat transfer
- Boundary-layer physics
- The basic mass, momentum and energy equations for a free convection boundary-layer
Numerical solution uses a shooting method and a Runge-Kutta Integration.
Reference: Numerical Recipes in Fortran, See also the notes from ChEg 258, (D. T. Leighton).
http://www.nd.edu/~dtl/cheg258/cheg258-1999/notes/137/overheads.html

Return to conclusions

The key equations for the shooting method are:

\[ \alpha \cdot \delta \mathbf{V} = -\mathbf{F} \]
\[ \mathbf{V}_{\text{new}} = \mathbf{V}_{\text{old}} + \delta \mathbf{V} \]

where \( \alpha \) is the Jacobian Matrix obtained by varying the initial guesses for the unknown initial conditions, \( \mathbf{F} \) is the error in the solution produced from the current initial guesses, \( \mathbf{V}_{\text{old}} \), and \( \delta \mathbf{V} \) is the correction to the initial guesses for the next step.

This turns out to be a touchy calculation. Here are a set of initial conditions that give a solution with some trouble. You will find that higher \( Pr \) is harder and that if \( y_{\text{outer}} \) is too large, the calculation does not work.

\[ \text{finit} = \{.8\},\{-0.25\}; \]
\[ \text{pr} = 10; (* \text{Prandtl number}*), \]
\[ \text{youter} = 5.5; (* \text{outer value of } \eta \text{ } *) \]
\[ \delta \mathbf{v} = .0006; (* \text{increment on the initial guesses used to generate the Jacobian} * ) \]
Here is the numerical solution

- Initialize some variables.

- We need to run through the integration once to get a first values for the error.

- Here is the main iteration loop.

- Here are some plots of the results
Conclusions

1. For natural convection flows where the Grashof number is larger, a boundary layer can be expected close to a solid surface.

2. For situations where a natural convection boundary-layer is occurring, heat transfer will be governed by coupled energy and momentum equations.

3. For transport processes that occur on a semi-infinite domain, where there is no geometric length scale, it is often possible to define a (dimensionless) similarity variable that contains the natural length scale.

4. It is often possible to reduce PDE's to ODE's through simplifications made possible by use of the similarity variable.

5. From the scaling identified by the similarity variable, it is often possible to predict the macroscopic behavior without solving the differential equations. In this case \( \text{Nu} \sim Gr^{1/4} \).

6. This prediction agrees with the recommended correlation for high Gr heat transfer.

7. The coupled, nonlinear ODE's can be readily solved with a shooting method.

8. Note the shape of the temperature profile and the location of the maximum velocity.

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Show[Upr10, Upr01, Upr100, Upr1];

\[ \frac{u_k}{2} \gamma Gr^{-\frac{1}{2}} \]

return to conclusions

Show[Tpr10, Tpr01, Tpr100, Tpr1];
The basic mass, momentum and energy equations for a free convection boundary-layer

Continuity

$$\frac{\partial u(x, y)}{\partial x} + \frac{\partial v(x, y)}{\partial y} = 0$$

Momentum

$$u(x, y) \frac{\partial u(x, y)}{\partial x} + v(x, y) \frac{\partial u(x, y)}{\partial y} = g (T(x, y) - T0) \beta + \nu \frac{\partial^2 u(x, y)}{\partial y^2}$$

Energy

$$u(x, y) \frac{\partial T(x, y)}{\partial x} + v(x, y) \frac{\partial T(x, y)}{\partial y} = \alpha \frac{\partial^2 T(x, y)}{\partial y^2}$$

These equations are coupled, meaning you cannot solve any of them without simultaneously solving the other two. Further, the momentum equation is nonlinear.
Demonstration of the effect of flow regime on pressure drop in multifluid flows

Summary

This notebook is intended to give a first introduction to multifluid flows through the use of “model” flow regimes calculated from exact solutions for laminar flow in different configurations. By comparing pressure drop over a range of flow rates for these different configurations, that show differences of factors of up to 30, the importance of knowing the flow regime is demonstrated. Insight into the physical reasons for the variation in pressure drop with flow rates and physical properties is given.

Preview of Major points

Flow rate pressure drop relations for the three regimes.

Pressure drop comparisons

Recap of Major points

Suggestions for future study
Recap of Major points

(same as the preview above)

[BACK to Preview]

We have shown, using simple models for flow regimes, stratified, slug and dispersed, that

1. The qualitative as well as the quantitative behavior of multiphase flows will change as the ratios of flow rates and physical properties change.

2. The pressure drop predictions differ substantially with flow configuration. The pressure drop for dispersed flow was predicted to be a factor of 35 higher than for slug flow in one case and a factor of 20 greater than stratified flow for another case. This key result is true for process flows and makes correct prediction of the flow regime crucial to successful design of multifluid systems. Most engineering designs cannot stand an uncertainty of a factor of 2 in the main design variable, let alone 30.

3. Stratified flow is the most efficient configuration, of the three tested here (compare stratified/slug, dispersed/stratified), for fluid transport when the more viscous fluid has a higher flow rate. This is due to the lubricating effect of the less viscous fluid that reduces shear in the more viscous fluid. This is the basis of lubricated pipeline transport of heavy oil (See D. D. Joseph and Y. Y. Renardy, Fundamentals of Two-Fluid Dynamics, Springer-Verlag, 1993, Vol. 2.) If the more viscous fluid is present in less amounts the advantage is lost because it is subjected to high shear and acts to reduce the available flow area for the less viscous fluid.

4. The loss of lubricating effect of a less viscous fluid in stratified flow can cause a region where decreasing the flowrate of the less viscous fluid, increases the pressure drop (click for specifics about retrograde pressure drop) -- contrary to physical intuition gained from most other flow situations.

5. The specific conclusions for dispred/slug, disperes/d/stratified and stratified/slug can be accessed directly.

6. The reason for the differences in the pressure drop with configuration for the examples in this notebook is that the dissipation is altered. Differences in dissipation arise primarily when fluids of different viscosities are located in regions of different stress. We also find that changing the effective flow area (i.e., by having a stratified region of more viscous fluid) for the fast moving fluid changes the dissipation significantly. These general observations should hold for either laminar flow (as shown here) or turbulent flow. However, if the primary contributions to pressure drop are from fluid acceleration, or gravity, then the pressure drop differences caused by the flow regime could be less than shown here. Examples are unsteady or transient flows, developing flows or vertical flows.
Slug (Alternating)

View the slug flow movie, Slug Flow

Stratified flow

Two-layer, horizontal two-fluid flow
Surprising result

Pressure drop comparison for dispersed vs. slug flow

Plot[Evaluate[dispslungratio /. {ReL -> 100, μL -> .01, μG -> .00018, ρL -> 1, ρG -> 1/899, H -> 1}]], {ReG, 1, 10000}, AxesLabel -> {"ReG", "dispersed/slur ratio"}];

dispersed/slur ratio

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Creeping flow past a stationary sphere

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Version: 8/8/00
More recent versions of this notebook should be available at the web site:
http://www.nd.edu/~mjm/creepingsphere.nb
This notebook shows how to solve creeping (inertialess) flow past a stationary sphere (Stokes's Problem)

Flow past a sphere problem

Problem of interest

Learning Objectives

Mathematical Formulation

Solution of the equations with the boundary conditions

Examination of the solution

Conclusions

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Learning Objectives

- Physical Issues

1. We are restricting the problem to the case where inertia forces are much weaker than viscous forces. Thus we expect that the inertia terms of the Navier-Stokes equation should be much smaller than the viscous and pressure terms and that thus they can be neglected. For this case the Reynolds number is very small. If we make the equations dimensionless all terms are no larger in magnitude than about unity. Thus the parameters that appear in these equations, and which can have values much different from one, determine which terms are needed for the solution. In the nondimensional equations, the Reynolds number multiplies the inertia terms and these will consequently be neglected in the solution.

2. Since the Reynolds number is small, the fluid goes only where specifically pushed and it will stop if the forcing is stopped. Thus the geometry of the flow field is determined by the boundaries.

3. Because viscous forces dominate the flow field, the fluid can never accelerate above the free stream value even if an obstacle causes the fluid to be squeezed. Thus the velocity in the region of the sphere just slows down and then returns to the free stream value.

4. Both normal stresses and tangential stresses contribute to the drag on the sphere. These can be termed form drag and skin drag.

5. Consistent with the fluid not accelerating, the pressure never increases above the free stream value. The fluid has no inertia that would cause a pressure increase as the fluid slows down.

6. The velocity decays slowly (as \( \frac{1}{r} \)) and thus the disturbance is felt very far away from the sphere. This makes it difficult to do a real experiment, in a reasonable size container, that allows that sphere to fall at a speed specified by the drag that is predicted from the analysis here. The very high Reynolds number case decays much faster.
Conclusions

1. Creep flow is a term used for a flow that have effectively no inertia. In this case the inertia terms are neglected and the solution is obtained from the resulting linear equations. The Reynolds number is very much smaller than unity.

2. The solution technique involves using a solution form that is deduced from boundaries of the flow field, far away from the sphere.

3. Because viscous forces dominate the flow field, the fluid can never accelerate above the free stream value even if an obstacle causes the fluid to be squeezed. Thus the velocity in the region of the sphere just slows down and then return to the free stream value.

4. Both normal stresses and tangential stresses contribute to the drag on the sphere. These can be termed form drag and skin drag. Note that both of these are linear in the velocity (consistent with the linear governing equations) and fluid viscosity. The density, and thus the Reynolds number, does not appear.

5. Consistent with the fluid not accelerating, the pressure never increases above the free stream value. The fluid has no inertia that would cause a pressure increase as the fluid slows down.

6. The velocity decays slowly (as \( \frac{1}{r} \)) and thus the disturbance is felt very far away from the sphere. This makes it difficult to do a real experiment, in a reasonable size container, that allows that sphere to fall at a speed specified by the drag that is predicted from the analysis here. The very high Reynolds number case decays much faster.
Velocity field magnitude
Conclusions

• Some elements of mixing are incorporated into the fluid dynamics course
  – Laboratory experiment
  – Dimensional analysis

• The main idea we attempt to convey about computational fluid dynamics is that it is wonderful if it works, but make sure your solution is correct.
  – Strategy is like using different excess Gibbs Free Energy models to design distillation columns with a process simulator
Conclusions (cont.)

• *Mathematica* notebooks can be used to show students
  – Computations
  – To do algebra that is too tedious for them to do
  – To allow them to explore the solution
  – To incorporate other media

• Questions remain as to if our approach gives a significant or incremental benefit to the students.