Finite Element Modules for Enhancing Undergraduate Transport Courses: Application to Fuel Cell Fundamentals

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Example 1: Newtonian and Non-Newtonian Fluid Flow in a Capillary Rheometer

Note: This example problem will be used in the required course "Transport / Unit Operations 1" which is taken by junior-level chemical engineering students.

Problem Statement: A capillary viscometer consists of a very small diameter, cylindrical capillary tube. A liquid is forced through the capillary by imposing a pressure drop. The very small diameter of the tube and the very large length to diameter ratio minimizes entrance and exit effects and ensures a fully developed velocity profile.

For all fluids, the shear stress at the pipe wall (τ_{wall} in units of Pa) is given as

$$\tau_{\mathrm{wall}} = (\Delta P\, R)/(2L) = (\Delta P\, D)/(4L) \qquad (1)$$

Where: ΔP= pressure drop across the capillary tube, Pa
D = inside capillary tube diameter, m
R = inside capillary tube radius, m
L = capillary tube length, m

For a laminar, incompressible, Newtonian fluid, the shear rate at the circular pipe wall, $\dot{\gamma}_{wall}$ can be calculated from the microscopic balances[4]. The result is shown below.

$$\dot{\gamma}_{wall} = (4Q)/(\pi R^3) = (32Q)/(\pi D^3)\ 8V/D = 4V/R \qquad (2)$$

Where: Q= volumetric flow rate, m^3/s
V= average fluid velocity, m/s

The Hagan-Poiseuille equation can also be calculated from the microscopic solution for this problem[4], and may be used to calculate the viscosity of a laminar, Newtonian, incompressible fluid

$$V = \frac{\Delta P R^2}{8\mu L} \qquad (3)$$

The equations for Reynolds number and entrance length[2], L_e, are shown below.

$$\mathrm{Re} = \frac{DV\rho}{\mu} \qquad (4)$$

$L_e = 0.035 D \,\mathrm{Re}$

If you plot τ_w as a function of $\dot{\gamma}_{wall}$ for a Newtonian fluid, the slope is the viscosity of the fluid.

$$\tau_{wall} = \mu \, \dot{\gamma}_{wall} \tag{5}$$

Where: μ = viscosity of fluid (Pa-s)

For a power law fluid, you still use equation 1 to determine $\tau_{wall.}$ However, the following equation is used to relate wall shear stress and shear rate at the wall[4]:

$$\tau_{wall} = m(\dot{\gamma}_{wall})^n \tag{6}$$

Where: m = flow consistency index, Pa-s^n, noting that m = μ = viscosity of fluid if the fluid is a Newtonian fluid (The fluid is Newtonian when n = 1)
n = flow behavior index, dimensionless

When n > 1 the fluid is shear-thickening (also called dilatant) meaning that as the shear rate is increased the fluid becomes more viscous, and when n < 1 it is shear-thinning (also called pseudoplastic) meaning that as the shear rate is increased the fluid becomes less viscous.

In this module we are going to model the flow of water through a capillary rheometer with a radius of 0.5 mm and a length of 20mm. The fluid enters the tube at an average velocity of 0.0125 m/s downward and exits at a pressure of 0 Pa. From the module you will be able to determine the pressure drop over the length of the tube and you will view the velocity profile at the exit of the tube. You can then rerun the model for a non-newtonian fluid: Vectra A950RX Liquid Crystal Polymer, which has potential use as a matrix material for recyclable fuel cell bipolar plates.

Part 1: Start the program

1.Start Comsol Multiphysics
2.Within the "New" tab of the "Model Navigator" window there should be a pull-down menu labeled "Space Dimension." Within this pull-down menu select "Axial Symmetry (2D)."
3. Expand the folder "Chemical Engineering Module" by clicking the "+" sign to the left of the folder followed by the same for Momentum Balance, Non-Newtonian Flow, and then select Steady-State Analysis. Click "OK." The program should then open to the main screen of the program with a red, vertical axis on it.

Part 2: Create the domain

In this module, a fluid will be modeled flowing through a capillary tube. The domain will be half of the vertical cross section of this tube, which when rotated completely around the z-axis creates the entire tube.

1.To draw a tube, select “Draw” from the tool bar and then “Specify Object” and select rectangle.
2. A box to specify the rectangle should appear on the screen as in the figure to the left below. For this problem we will enter length in meters, time in seconds, and mass in kilograms. Enter 5e-4 for “Width” (corresponding to the tube radius) and 2e-2 for “Height” (corresponding to the tube length) in the window that appears. Click “OK.” The rectangle that appears represents a tube with a length-to-diameter of 20.

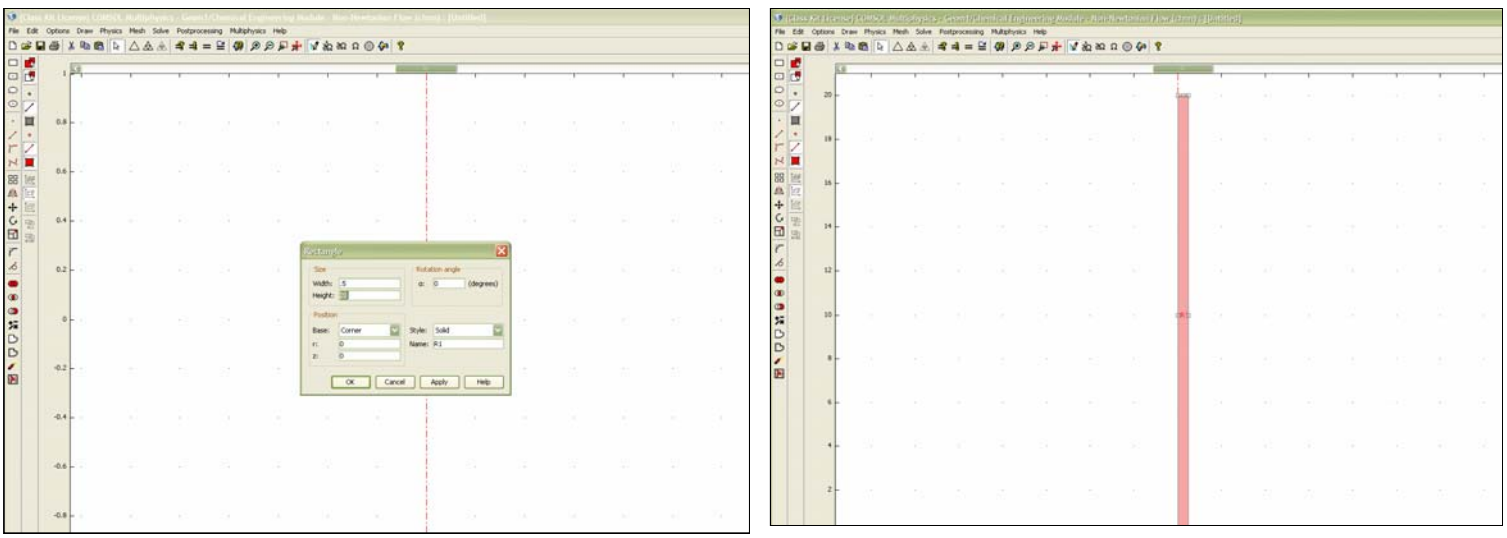

Figure 1.1. Setting up the model geometry.

3. Click the “Zoom Extents” button on the main toolbar. It looks like a red cross with a magnifying glass. This allows the user to view the entire geometry, as seen in the figure on the right above.

Part 3: Apply physical properties
1. From the top menu, select Physics, then Subdomain Settings
2. On the left hand side of the pop-up window, there will be a box labeled “Subdomain Selection.” In this box select the subdomain (1).
3. On the right hand side of the pop-up window (under the “General” tab there is a box labeled “Fluid properties and sources/sinks.” The third item from the top is Viscosity Model; make sure that the pull-down menu is set to “Power Law.”
4. Switch from the “General” tab to the “Power Law” tab, then enter m=1e-3 corresponding to the viscosity of water in kg/m-s and 1 as the n value to specify the Newtonian flow
5. Click “OK”, or repeat steps if there are multiple subdomains.

Part 4: Apply boundary conditions

1. From the top menu, select Physics, then Boundary Settings. To specify boundaries highlight a number in the left portion of the box that appears (as shown below).
2. For the right edge of the geometry (edge that is not on the center line), select boundary condition "No Slip."

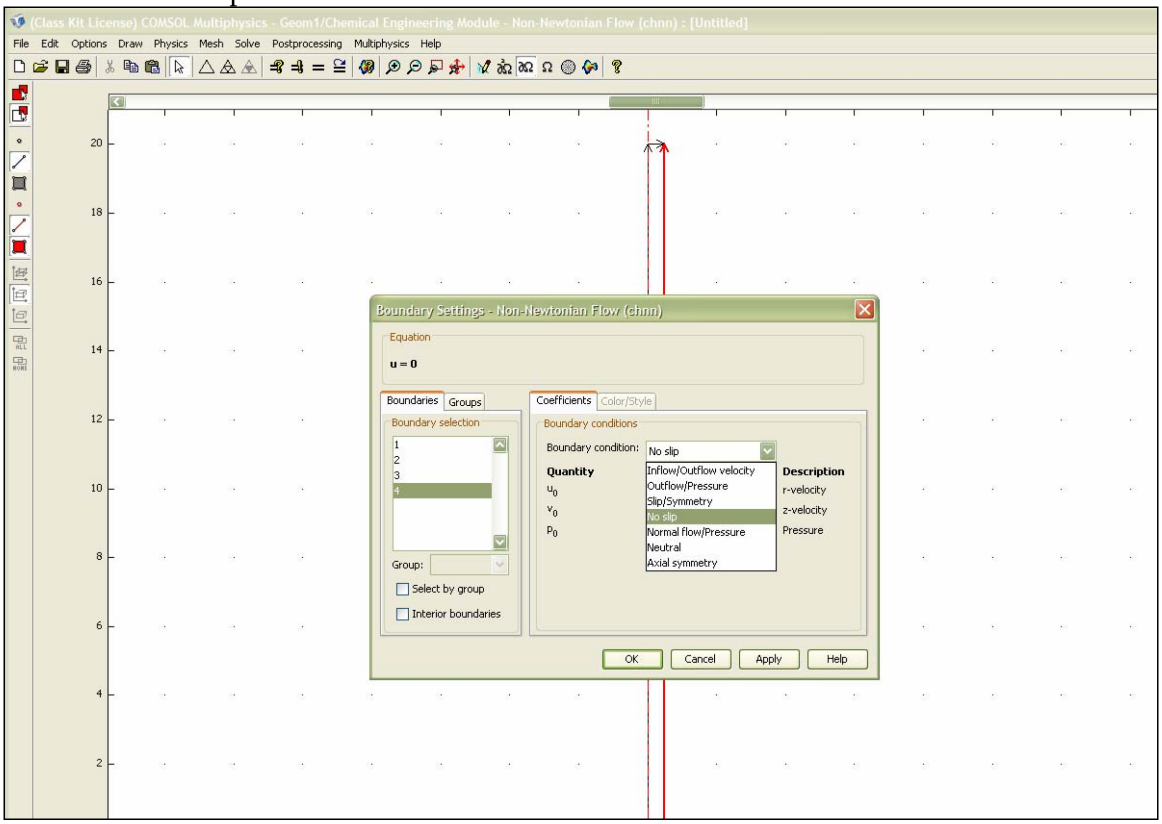

Figure 1.2. Setting boundary conditions.

3. For the axial side of the tube (edge that is on the center line), select the boundary condition "Axial Symmetry."
4. For the top boundary select "Inflow/Outflow Velocity" and enter $v_0 =$ -0.0125 (Description: average z-velocity in m/s) for a uniform downward flow at the inlet. This inflow velocity corresponds to a shear rate of 100s^{-1}.
5. For the bottom boundary (the outlet of the tube) select "Outflow/Pressure" and enter $p_0 = 0$ in Pa. We are interested in the pressure drop over the length of the capillary tube, so 0 is used as a reference pressure, rather than the atmospheric pressure that would actually appear at the outlet of the tube. Click "OK."

Part 5: Create the mesh

1. From the top menu, click on the hollow triangle to initialize the mesh. In the bottom left of the screen it should say there are 120 elements in the mesh
2. The button next to "Initialize Mesh" is called "Refine Mesh" (which appears as a triangle within a triangle). This button takes the current mesh and simply makes it more detailed. Click the button once to make the mesh more refined. There should be 480

elements. Please note that problems may occur depending on graphics capabilities of your computer. If this occurs start over but do not refine the mesh.

Part 6: Solve

1.Click "Solve" from the pull-down menu and select "Solver Parameters"
2. On the left hand side of the pop-up window there will be a box labeled "Solver:."
Make sure that "Stationary nonlinear" is selected. Click "OK."
3. From the top menu, click the "=" sign to solve. A window will appear showing how much progress has been made in solving the problem. After the problem is solved and the window disappears, you should see the geometry with a color spectrum indicating a velocity-concentration profile, as seen in the figure below. If you don't see anything, click on "Zoom Extents." This plot is called a Surface Plot. Notice the velocity is zero at the boundary and maximum at the center.

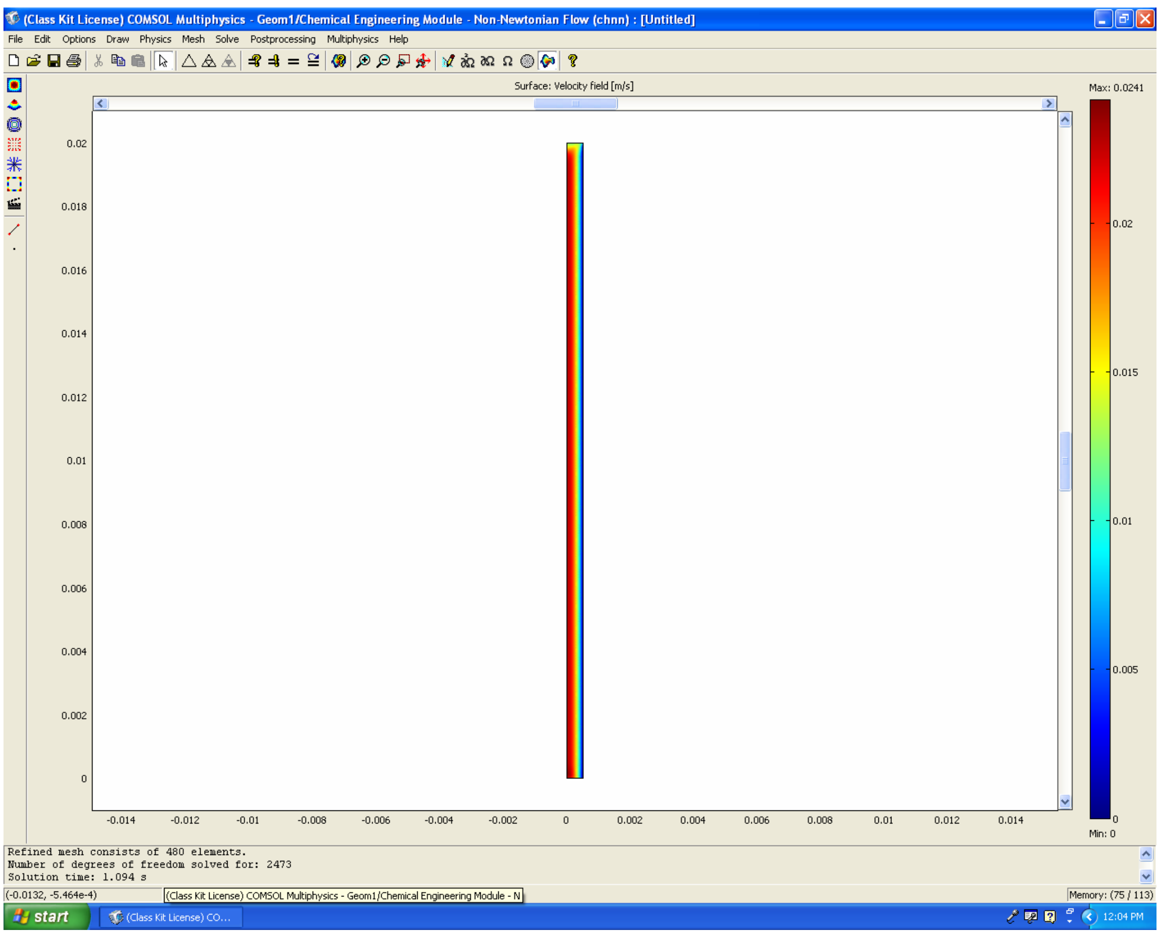

Figure 1.3 Velocity surface plot for water.

Part 7: Post-Processing

In this part you will produce a plot with the pressures at the inlet and outlet of the tube, and therefore be able to estimate the pressure drop across the length of the tube. You can compare this value to the change in pressure as calculated with the Hagen-Poiseuille law. You will also produce a plot of the velocity profile at the outlet of the tube.

1. From the top menu, select “Postprocessing” then “Cross-sectional plot parameters…”
2. Under the “Line/Extrusion” tab, in the “y-axis data” section, from the “Predefined Quantities” pull down menu, select Pressure as the desired field.
3. In the “Cross-section Line Data section” select the coordinates between which you would like the measurements to be made. You want to do this once for the pressure at the top of the tube and once at the bottom, at a constant z value to see the profile across the tube radially—that is at a height of 0.0 and 0.02. First, for the outlet, use r0=0, r1=5e-4, z0=1e-6, and z1=1e-6. These values are sufficiently close to zero, but still within the domain of interest. Under the “General” tab, select “keep current plot.” Hit “OK” to complete a calculation of the pressure across the exit of the tube. Then, for the inlet repeat the calculation, starting again with selecting “Postprocessing” in step 1, using z0=0.019995 and z1=0.0199995. You should now have a plot of the pressures at the inlet and outlet, radially across the tube.
4. From the top menu of the plot, select “ASCII” and save in desired location. From there you can import data to a program such as Matlab or Excel and plot it in comparison to theoretical values. Close the Comsol Plot, but leave the main screen open.
5. To find the velocity profile at the exit of the tube repeat steps 1-4, selecting “Velocity Field” as the desired field and using 1e-6 as the z-values. This will produce a plot of the velocity profile at just the one location. By selecting the “keep current plot” option under the “General” tab however, the velocity profiles in other locations can be added.

Part 8: Practice

1. Calculate ΔP using the Hagen-Pouseuille law and compare to the value found using the model.
2. Find the Reynolds number to determine whether the flow is laminar or turbulent.
3. Find the velocity profile at the entrance of the tube in order to observe the entrance effect.
4. Rerun the module from the start and do practice problems 1-3 using Vectra A950RX Liquid Crystal Polymer (n=0.54, m=690).

Example 2: Flow in a Fuel Cell Bipolar Plate

Note: This example problem will be used in the required course "Transport / Unit Operations 1" which is taken by junior-level chemical engineering students.

Problem Statement: A fuel cell bipolar plate has channels etched in it to allow for the flow of reactant gases. The flow path is rather complicated to allow for equal gas distribution so that there is a uniform fuel concentration at the catalyst. This design will result in better efficiency for the fuel cell. Refer to figure 2.1 below for the simplified geometry that we will be studying here.

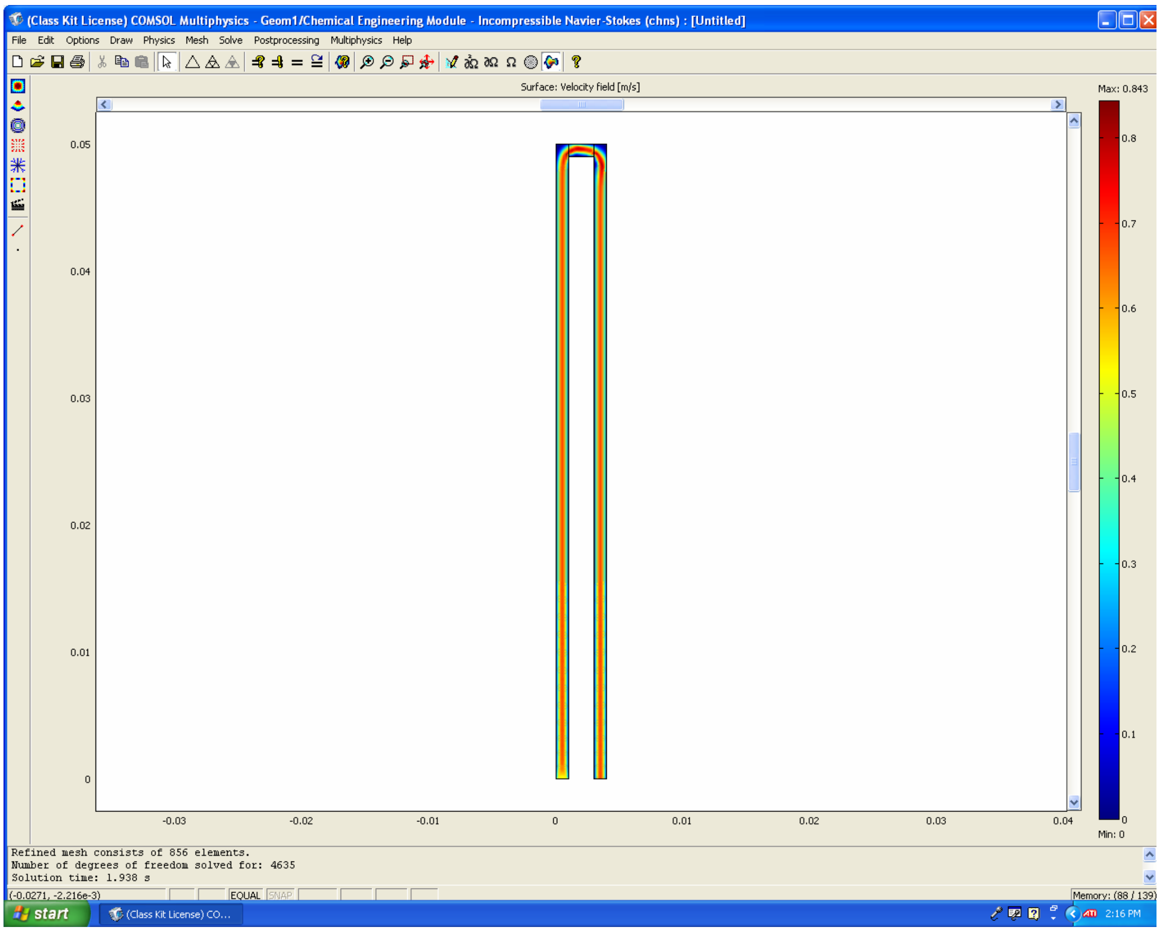

Figure 2.1. Velocity surface plot.

Part 1: Start the program

1.Start Comsol Multiphysics

2.Within the "New" tab of the "Model Navigator" window there should be a pull-down menu labeled "Space Dimension." Within this pull-down menu select "2D".

3. Expand the folder "Chemical Engineering Module" by clicking the "+" sign to the left of the folder followed by the same for Momentum Balance, Incompressible Navier-Stokes, and then select Steady-State Analysis. Click "OK." The program should then open to the main screen.

Part 2: Create the domain
In this module, a fluid will be modeled flowing through a U shaped tube.

1.Select "Draw" from the tool bar and then "Specify Object" and select rectangle.
2. A box to specify the rectangle should appear on the screen. For this problem we will enter length in meters, time in seconds, and mass in kilograms. Enter 1e-3 for "Width" and 5e-2 for "Height" in the window that appears. Make sure the base is x = 0 and y = 0. Click "OK."
3. Click the "Zoom Extents" button on the main toolbar. It looks like a red cross with a magnifying glass. This allows the user to view the entire geometry, as seen in the figure on the right above.
4.Once again, select "Draw" from the tool bar and then "Specify Object" and select rectangle. Enter 2e-3 for "Width" and 1e-3 for "Height" in the window that appears. Change the base to x = 1e-3 and y = 4.9e-2. Click "OK." You now have a bend in your geometry.
5.Once again, select "Draw" from the tool bar and then "Specify Object" and select rectangle. Enter 1e-3 for "Width" and 5e-2 for "Height" in the window that appears. Change the base to x = 3e-3 and y = 0. Click "OK." You now have a bend in your geometry. Click "OK." You have now finished your bend!
6. While holding down the shift key, click on each rectangle. Then click on the overlapping two red circles on the icons on the left side of the page. This function is called "Union" and joins the rectangles together.

Part 3: Apply physical properties
1. From the top menu, select Physics, then Subdomain Settings
2. On the left hand side of the pop-up window, there will be a box labeled "Subdomain Selection." In this box select the subdomains 1-3 by holding down the shift key.
3. Enter the dynamic viscosity of 9.6e-6 Pa-s and click "OK." Note that this is a steady-state problem and density is not needed.

Part 4: Apply boundary conditions
1. From the top menu, select Physics, then Boundary Settings. To specify boundaries highlight a number in the left portion of the box that appears (as shown below).
2. For the bottom of the first rectangle (boundary 2), select a y-velocity of 0.5 m/s.
3. For the bottom of the second rectangle (boundary 9), select outflow/pressure = 0 Pa.
4. Make sure all other boundaries are "no slip."

Part 5: Create the mesh
1. From the top menu, click on the hollow triangle to initialize the mesh. In the bottom left of the screen it should say there are 214 elements in the mesh
2. The button next to "Initialize Mesh" is called "Refine Mesh" (which appears as a triangle within a triangle). This button takes the current mesh and simply makes it more detailed. Click the button once to make the mesh more refined. There should be 856 elements. Please note that problems may occur depending on graphics capabilities of your computer. If this occurs start over but do not refine the mesh.

Part 6: Solve

1.Click “Solve” from the pull-down menu and select “Solver Parameters”
2. On the left hand side of the pop-up window there will be a box labeled “Solver:.” Make sure that “Stationary nonlinear” is selected. Click “OK.”
3. From the top menu, click the “=” sign to solve. A window will appear showing how much progress has been made in solving the problem. After the problem is solved and the window disappears, you should see the geometry with a color spectrum indicating a velocity-concentration profile, as seen in the figure below. If you don’t see anything, click on “Zoom Extents.” This plot is called a Surface Plot. Notice the velocity is zero at the boundary and maximum at the center.

Part 7: Post-Processing

In this part you will produce a surface plot of the pressure at the inlet and outlet of the channel.

1. From the top menu, select “Postprocessing” then “Plot parameters…”
2. Make sure the “surface” tap is selected, and choose the predefined quantity “Pressure.” Select “OK.”
3. Verify the maximum pressure of 5.6 Pa.

Part 8: Practice

1. Calculate a surface plot of velocity and pressure for the geometry shown below which is a first step in a complex bipolar plate geometry. Note there are two separate channels. The “outer” channel is of the same length as in the above module (50 mm), but the channels are separated by a wider margin. The “inner” channel is 2 mm shorter than the “outer” channel (thus 48 mm). The gap between channels is 1 mm. How would you adjust this system to provide equal velocity in each channel? What would happen if there were a manifold connecting the two inner channels?

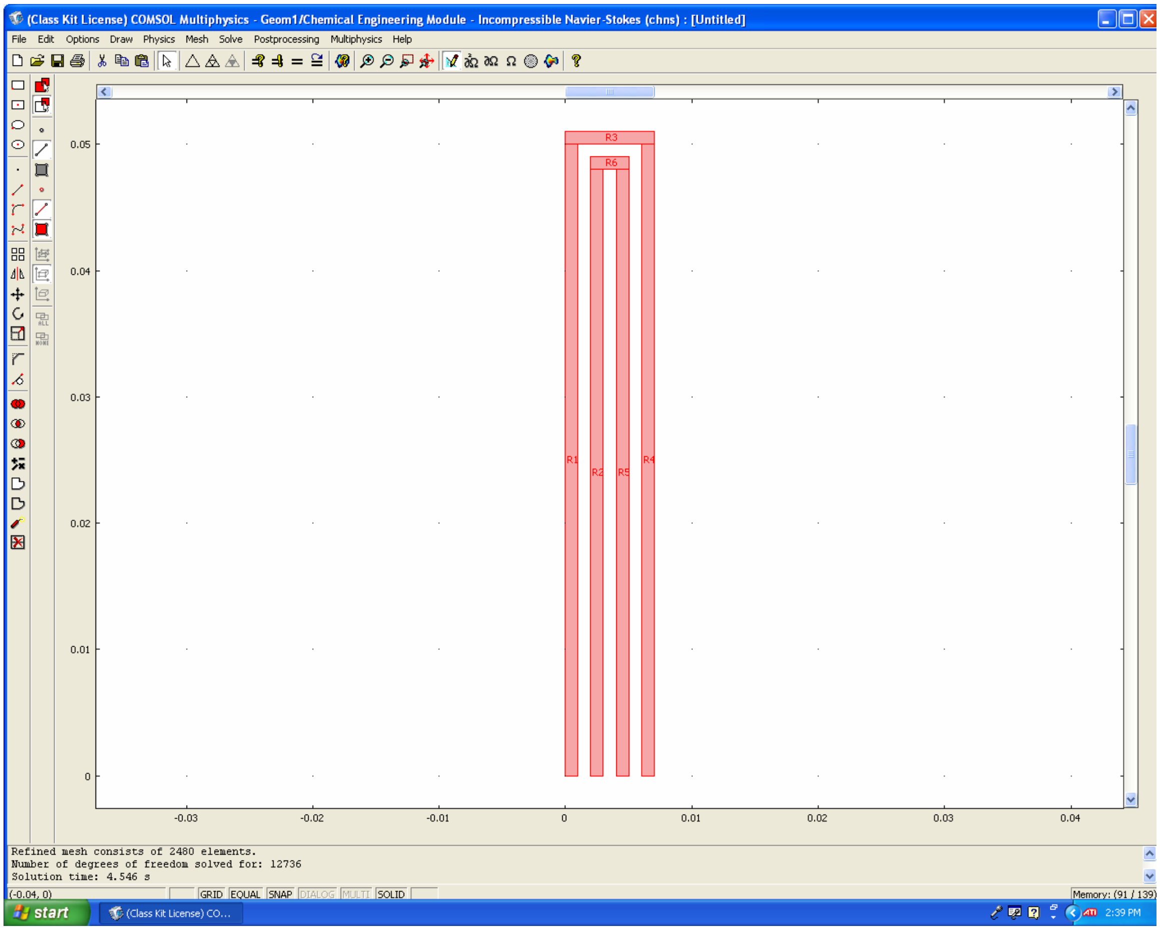

Figure 2.2. Geometry for practice problem.