

## Boundary Value Problem Solved in Comsol 4.1.

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See also *Introduction to Chemical Engineering Computing*, Wiley (2006).

### INTRODUCTION TO COMSOL MULTIPHYSICS

In this chapter step-by-step instructions are provided for these one-dimensional problems. Many features of Comsol Multiphysics are not used or needed until you solve two- and three-dimensional problems, and these features are explained in Chapters 10-11 and Appendix D. For the boundary value problems treated here, we generally follow these steps:

1. Open Comsol Multiphysics and choose the dimensions of the problem (here 1) and the Physics modules we wish to solve.
2. Establish our preferences.
3. Create the geometry.
4. Insert the variables that define the problem and set the boundary conditions.
5. Create a mesh.
6. Solve the problem.
7. Examine the solution; here we limit ourselves to plots and integrals of the solution.

The icons shown in Figure 9.2 are ones that are used frequently in these examples. They are worth remembering.








Setup: Next: ; Finish: ; Show: ; Create geometry/mesh: Build: ;  
Plot: Expression button: ; Plot: ; Range of parameters: 

Figure 9.2. Icons used for Setup, Creation of geometry and mesh, and Plotting

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This example considers flow in a pipe for a Newtonian fluid, Eq. (9.6). You'll solve this problem using Comsol Multiphysics with  $\Delta p = 2.8 \times 10^5$  Pa,  $\mu = 0.492$  Pa s,  $L = 4.88$ ,  $R = 0.0025$  m. You must expand the differential equation because the one-dimensional option does not contain cylindrical geometry. (This limitation is removed in 2D and 3D problems, but here a one-dimensional solution suffices.) So, rewrite Eq. (9.6) as

$$\frac{d^2 v}{dr^2} = - \frac{1}{\mu} \frac{\Delta p}{L} - \frac{1}{r} \frac{dv}{dr} \tag{9.30}$$
$$\frac{dv}{dr}(0) = 0, \quad v(R) = 0$$

**Step 1: choose the problem.** To solve Eq. (9.30), we must select the equation. In Comsol, the 1D option will be appropriate for planar geometry; the 1D, axisymmetric option is appropriate for cylindrical geometry, which is what we want. Select from the first menu: 1D, axisymmetric, next. The next screen indicates that there is no 1D option for Fluid Flow. Thus, we will use the Transport of Diluted Species option and change the variable names in it. Choose Transport of Diluted Species, next; and Stationary, finish.

**Step 2: set the variables.** Then working down the Model Builder, we right click on Definitions and choose variables. Define dpL as  $2.8e5/(0.492*4.88)$  [this avoids having to get out your calculator; alternatively you could insert the pressure drop, length, and viscosity here and define dpL as  $dp/(\mu*L)$ ].

**Step 3: define the geometry.** Then right click on Geometry and choose Intervals. The default interval is (0,1), so change it to (0,0.0025); click Build All.

**Step 4: define the problem.** Click on Transport of Diluted Species. Select the domain if it isn't highlighted in the Selection box. You can also take convection out of the problem by unselecting the Convection box, or keep the velocity as zero, since there is no velocity in this problem. To see the equation being solved, choose Equation. Near the bottom of the settings panel is the panel for Dependent Variables. Click it, and note that the concentration is called c; change it to v. Under Transport, select Diffusion and change the diffusivity to 1 in the Settings panel (the problem is dimensionless). Make sure the domain is selected and appears in Domains. Go back and right click Transport and choose Reactions; select the domain and + to add it to the Domain box. Set RsubC to dpL. (Why no minus sign? Check the equation in Transport and compare it with Eq. (9.30).)

**Step 5: set the boundary conditions.** To set the boundary conditions, right click on Transport and choose Concentration. Then click on point 2 (the right-most point), click + to add it to the box, click Species c, and keep the value of 0. Select the No Flux button and notice that the boundary 1 not applicable, since the program satisfies it without intervention by us due to the

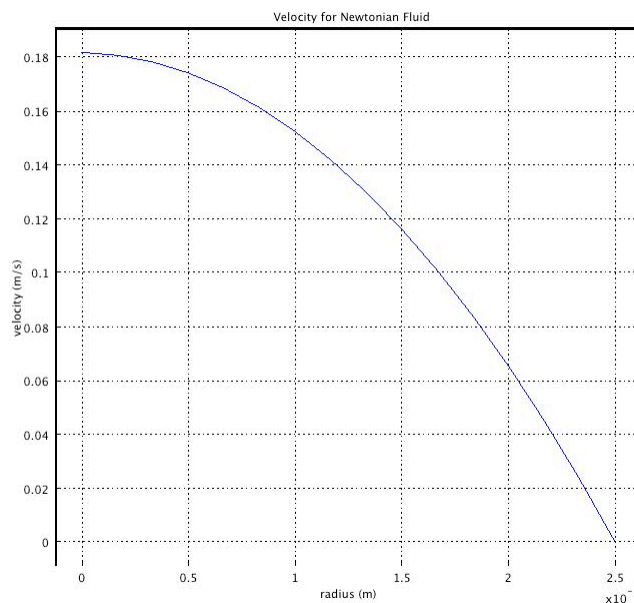
axisymmetric geometry. Thus, the boundary conditions are correct.

**Step 6: set the mesh.** In the Model Builder, right click on Mesh and choose Build All to create the mesh. Alternatively, select Mesh and then in the Settings window choose Build All. The default mesh uses 16 points and the points are added to the plot of the geometry.

**Step 7: solve the problem.** Right click Study and choose = to solve the problem. If an error occurs, click on the Error node in the Model Builder to see what the problem is and trace it down.

**Step 8: examine the solution.** The plot appears automatically. To change the axis labels and title, select the 1D Plot Group Node and click the x-axis and y-axis labels and change them to radius (m) and velocity (m/s). Click on the Title to change it to Velocity for Newtonian Fluid and click the plot icon to redo the plot. To save the plot, choose the camera and follow the instructions.

**Step 9: calculate the average velocity.** To compute the average velocity, you need to be careful to get the integrals in Eq. (9.8). Right click on the sub-node Derived Values under Results and choose Line Integration. Then in the settings window, open the panel Integration settings. A box there is clicked to have the integration be appropriate for cylindrical geometry. First, insert the value 1.0 for the expression; click =. Look in the results for the tabular value,  $1.9635e-5$ . This is appropriate for integrating  $2\pi r dr$  from 0 to 0.0025. Next insert  $v$  for the expression. The integral this time is  $1.779e-6$ . The ratio of these is the average velocity, 0.0906 m/s. Note that this is exactly half of the peak velocity, which is expected since that is true of the exact solution. It is also possible to look at the velocity gradient (a straight line from zero at the center to a maximum at the wall). The shear stress is the viscosity multiplied by the velocity gradient, and that is linear with distance, too, for a Newtonian fluid.



**Figure 9-10. Velocity profile for fully-developed Newtonian flow in a pipe**