CHEMICAL ENGINEERING SENIOR LABORATORY
CHEG 4139

3D-Printed Continuous Reactor Prototypes

Objective:
Additive manufacturing is a way to quickly print and test devices on the small-scale. A chemical engineer can design a small-scale prototype reactor, characterize it using minimal reagents, and then scale that design up as appropriate. In this experiment, you will design a small continuous flow tubular reactor, evaluate it as a plug-flow reactor (PFR), model the reactor in COMSOL, and test the device using actual reagents. After you have designed one reactor, your goal will be to design a second reactor that will yield better conversion and repeat the process.

Major Topics Covered: Chemical reaction kinetics, reactor design, computer modeling

Theory:
The reaction taking place is an alkali bleaching reactions of a Triphenylmethane, Malachite Green (MG). This reaction has the following rate equation:

$$r = k\,[MG]^{\alpha}\,[NaOH]^{\beta}$$

Note that you are being asked to determine the conversion of reagents for a small tubular reactor. At the scales these tests will be performed, the flow rate of reagents is limited to the laminar regime. What assumptions must be made to assume that the reactor is a PFR? If the reactor is not a PFR nor a CSTR, what is it? What variables will have the greatest impact on your overall conversion, assuming that your inlet concentrations of reagent are equal?

As you are limited to the laminar regime, mixing of the two reagents is limited by diffusion of reagents across the channel. You should review the mass transfer Peclet number, particularly how Peclet number relates to how long a channel has to be before it is fully mixed by diffusion. Refer to the references for more information.

You will also want to take into account the relationship between diffusion time and residence time in the reactor. Chapter 4 of Kirby's "Micro- and Nanoscale Fluid Mechanics Transport in Microfluidic Devices" is a good resource and can be found on the ChegLabs website.

You will be using an Arduino spectrophotometer for data collection. The code will be provided to you and will be pre-loaded onto the board. An Arduino board is a basic input-output board. For this experiment, the board uses a photo cell and an LED to create a spectrophotometer. The LED transmits light through the fluid in the reactor, and the photo cell resistivity increases or decreases based on the amount of light received. The photo cell becomes more conductive when more light is absorbed. A blue solution, like those containing MG, transmits blue light easily; we want to be as sensitive to a change in MG concentration as possible. Orange, on the other end of the spectrum, would probably be best for a blue solution, but only red, blue or green LEDs are available.

Safety Precautions:

1. In this lab, you will use Malachite Green and Sodium Hydroxide. Use caution when handling these reagents. Review the SDS for each chemical. Wear appropriate personal protective equipment at all times (lab coats and safety glasses).
2. If the reagents used in this experiment come in contact with skin, immediately rinse with water and alert an instructor.
3. Be careful when sampling your reactor. It may leak or drip.
4. Mix reagents in well-ventilated areas.
5. When working with the 3D printer, wear gloves at all times. 3D printer resin should not be handled with bare hands. If some gets on you, apply some isopropyl alcohol to the affected area, then wash with soap and water.
6. Be careful when removing your reactor from the 3D printer stage. The spatula is sharp. If you apply too much force, it can slip and cut your hand. If you are having difficulty removing your part, call an instructor. There are cut-resistant gloves available for protection.
7. Do not operate the 3D printer without instructor permission.

Available Variables: Reactor design (channel length, channel width, channel spacing, static mixers), reagent flow rates

Procedure:
The proposed schedule for this experiment is as follows:

Lab Period 1: SolidWorks tutorial & design Device 1. Predict performance using COMSOL. Print Device 1.
Lab Period 2: Create calibration curve; test Device 1 with reagents.
Lab Period 3: Design Device 2 & predict performance using COMSOL. Print Device 2.
Lab Period 4: Test Device 2 with reagents.
Lab Period 5: Test Devices 1 & 2 for more variables/data points.

You are free to work on SolidWorks and COMSOL outside of the laboratory period. If your group has more than two reactor designs to test, and if time permits, you will be allowed to print and test them.

For SolidWorks design and COMSOL tutorials, refer to the appendices. An instructor will give 3D printer operation and post-print part finishing instructions during your lab period.

Experimental Procedure:
Calibration: Using the provided calibration single-channel device, create a calibration curve of known MG concentrations against the PC output.

- In the past, groups have found it beneficial to calibrate at the start of each lab period.
- Start at the lower concentrations and increase the concentration as you create the curve. Do not exceed a concentration of 1e-4 M MG when calibrating.
- Make sure the sensors are as close to the outlet channel as possible.

Device Testing:

1. Prepare solutions of NaOH and MG. Use a glass container for the MG solution.
2. Secure your device to a ring stand with a clamp.
3. Fill one 60-mL syringe with Malachite Green. Fill a second 60-mL syringe with Sodium Hydroxide.
4. Attach the provided tubing to the syringes and load them into the syringe pump.
5. Attach the tubing to the appropriate ports on your device, Insert the spectrophotometer box to the outlet port of the reactor, then attach a short piece of tubing to the outlet of your device.
6. **Carefully** remove trapped air from the syringes and the tubing using the syringe pump.
7. Insert the LED and the Photo Cell (PC) into the appropriate ports on the spectrophotometer box. Make sure the sensors are as close to the outlet channel as possible. Use the black putty to secure these sensors; this also acts as a block for ambient light.
8. Ensure the device is level.
9. Place a glass waste beaker under the outlet tube of your device. Turn on the syringe pump and set the flow rate. When you are ready, start the pump and wait for the entire device to fill. You may need to **gently** tap the side of your reactor to expel all the air bubbles. Once all air bubbles are out of your device, set the pump to the appropriate flow rate. Make sure the device is level!
10. Make sure the sensors are as close to the outlet channel as possible. Wait for the photo cell (PC) reading to become stable, then record the value.
11. When data collection is complete, use the wash bottle or the syringe to rinse the reactor with 0.05M Sodium Hydroxide. If you plan on testing this reactor again, rinse the reactor with DI water.

Analysis:

Your analysis **must** include:

1. A calculated analysis of each device your group designs as if it were a PFR. Report conversions at various flow rates.
2. A simulation of each device your group designs using COMSOL. Report conversions at various flow rates.
3. The results of your actual device tests. Report conversions at various flow rates.
4. A discussion of how your devices differ and why you expected one to have better conversion than the other(s).
5. A discussion of how your prediction methods compared to the results of your device tests. How accurate were the predictions? How accurate was your experimental technique?

Report:

Describe the design of your experiments and the results obtained, including an error analysis. Provide thoughtful and quantitative discussion of results, explain trends using physical principles, and relate your experimental observations to predicted results. Express any discrepancies between observed and predicted results in terms of quantified experimental uncertainties or limitations of the correlations or computational software used.

Pro Tips:

1. Use COMSOL to optimize your experiments. When modeling in COMSOL, see what flow rates allow you to reach noticeable differences in conversion of NaOH. Also consider the limitations of the syringe pump.
2. Check the ambient temperature during each test. Reactor temperature isn't regulated, so this information is important to develop accurate models.
3. Use this online simulation to look at the reaction as it progresses over time: http://vstem.org/app/SpecKinetics

References:

1. Fogler, H.D., *Elements of Chemical Reaction Engineering*, Prentice-Hall, Inc., Englewood Cliffs, NJ, 2nd Ed., 1992.
2. Bramford, C.H. and C.F.H. Tipper, eds. *Comprehensive Chemical Kinetics*, vol. 10
3. "Ester Formation and Hydrolysis," Elsevier, New York, NY, 1973. International Critical Tables, 7, 129 (1930).
4. Schmidt, L.D., *The Engineering of Chemical Reactions*, Oxford University Press, New York, NY, 2nd Ed., 2005.
5. Levinspiel, O. *Chemical Reaction Engineering*, Wiley, Hoboken, NJ, 3rd Ed. 1998.

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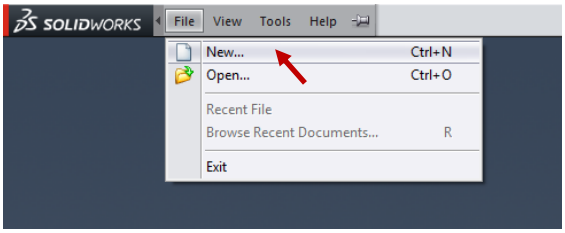
SolidWorks Reactor Design Tutorial

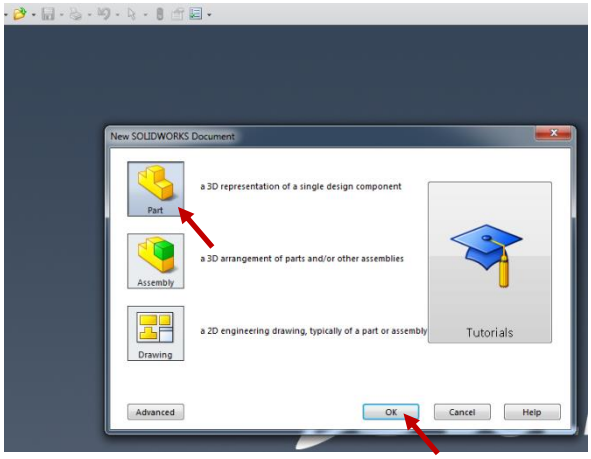
This tutorial will teach you how to design a 3D-printable reactor prototype. The tutorial assumes you already know how some of the basics of SolidWorks (such as opening a new file, defining your scales, sketching, using Smart Dimensions, viewing from different angles, extruding a boss, and extruding a cut). If you need more information about these methods, it is recommended that you try out the SolidWorks tutorial provided in the software itself before proceeding.

Note: Make sure SolidWorks is using the correct unit system for your design. To change the units, go to Options → Document Properties → Units.

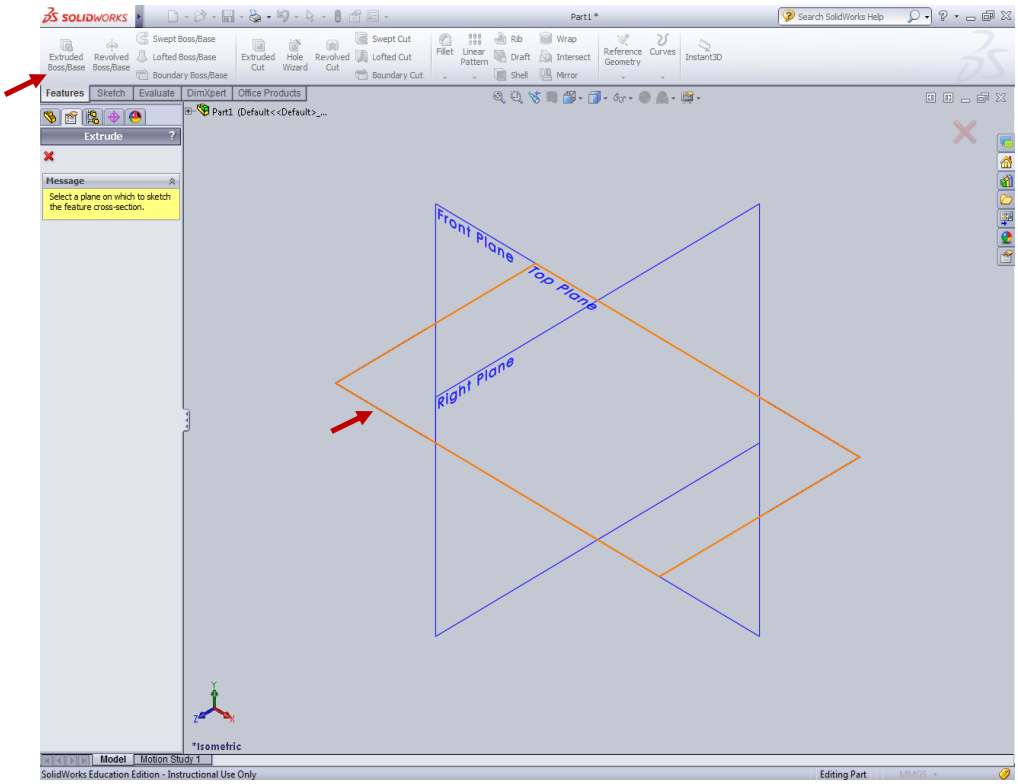
Part 1: Creating the Base

1) Click "New File" and create a new "Part file".

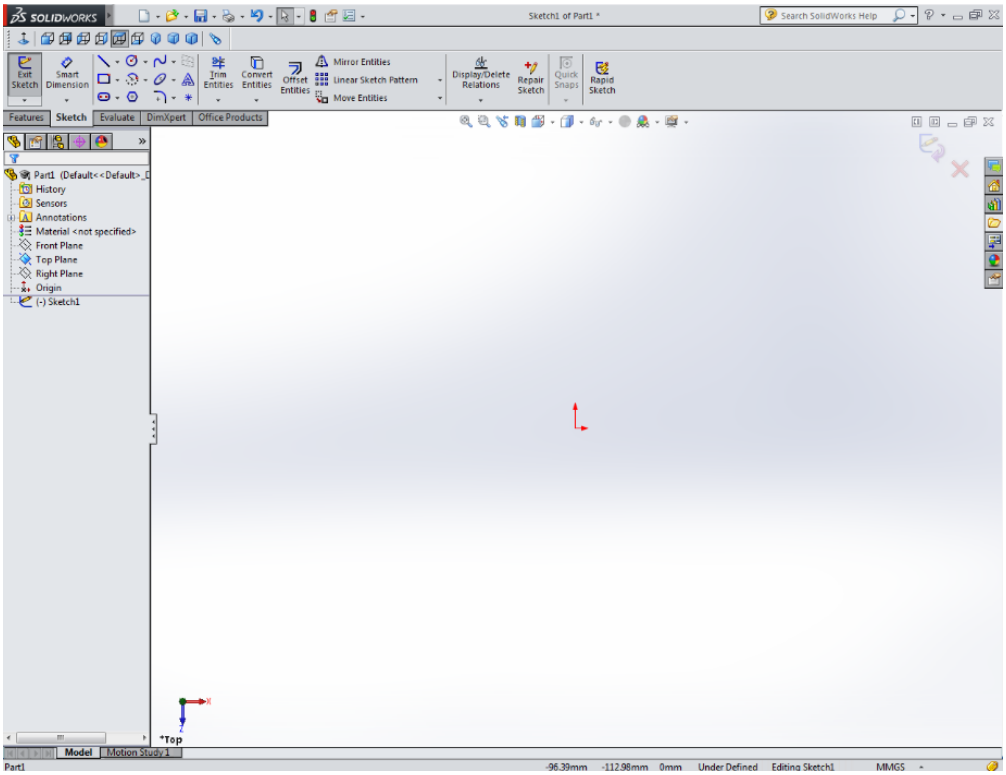




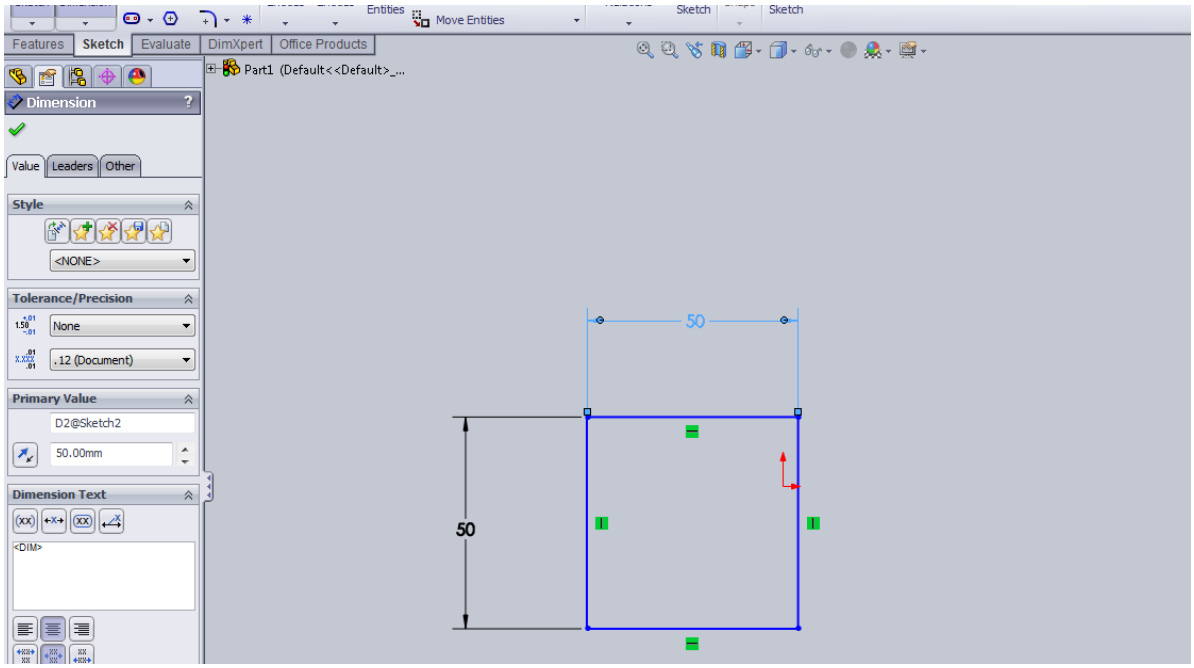
2) Click “Extruded Boss/Base” and select the Top Plane.



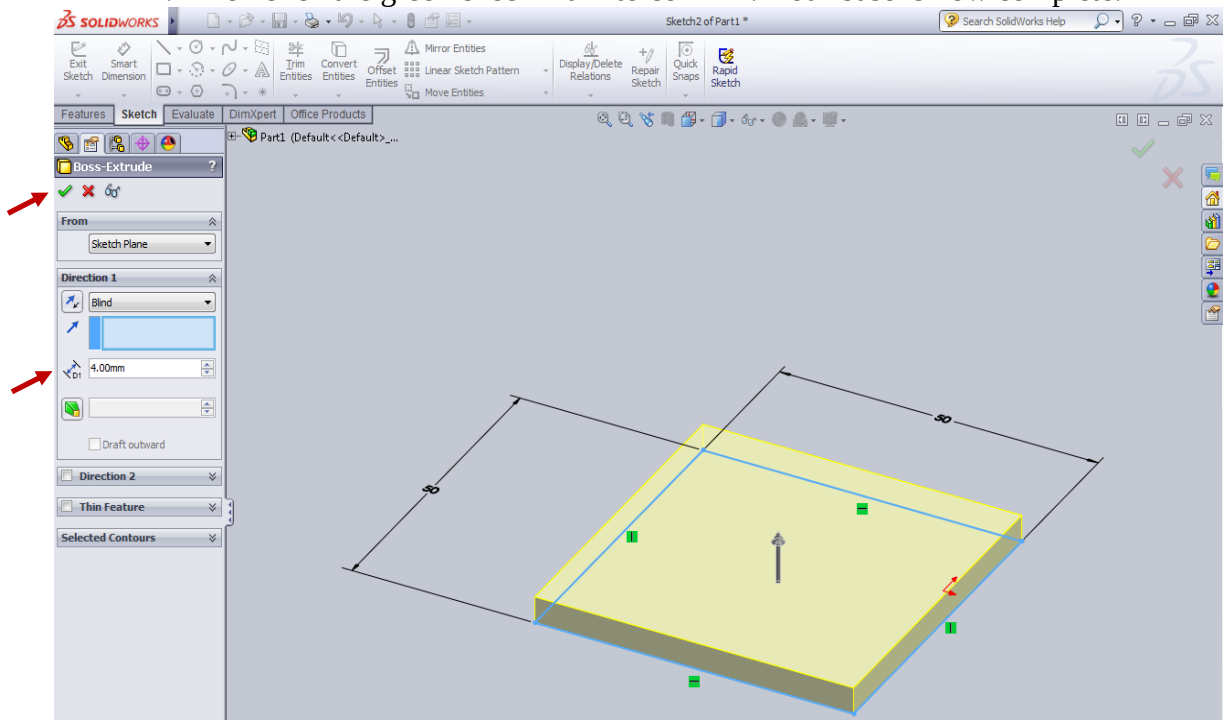
The following window will pop up:



3) You should now be in “Sketch” mode. Draw a rectangle. Use “Smart Dimension” tool to make it a square with sides **50 mm** in length.

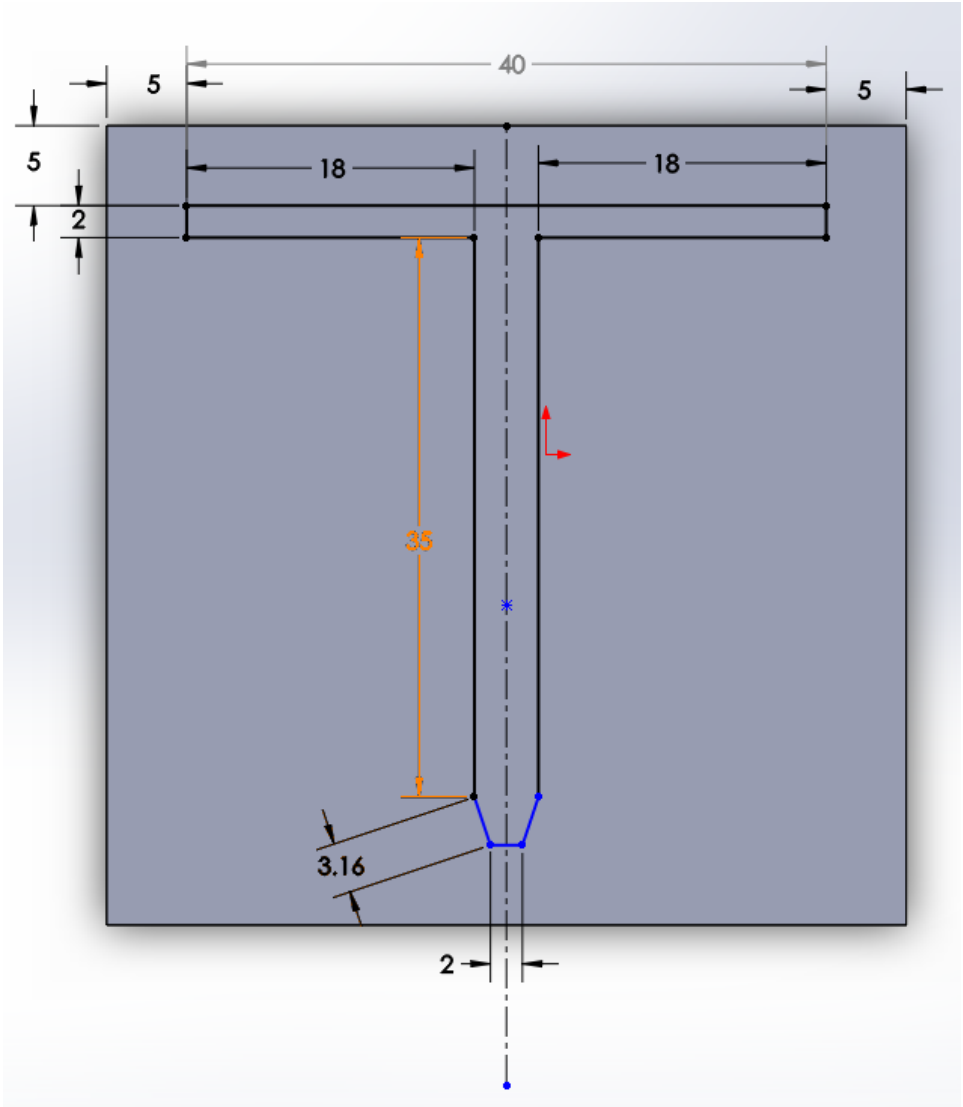


4) Exit “Sketch” using the button in the top left. Set the thickness of your extruded base to **4 mm**. Then click the green check mark to confirm. Your base is now complete.



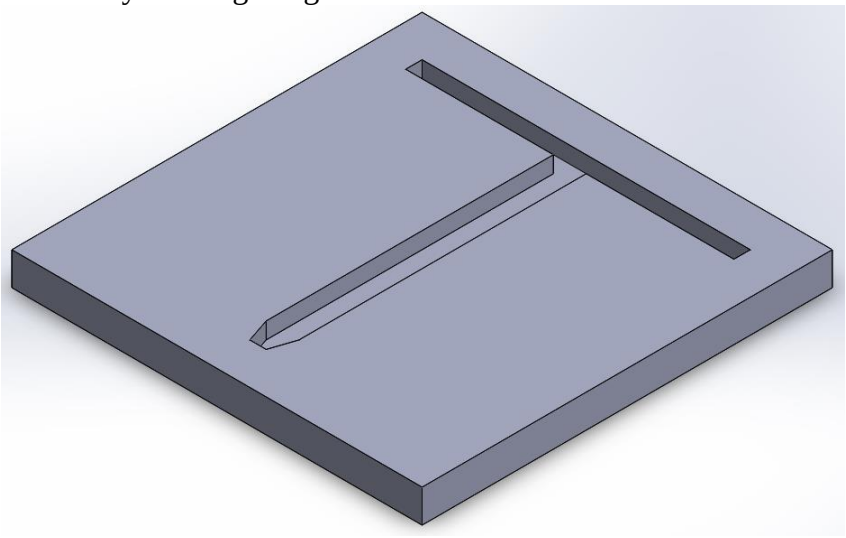
Part 2: Drawing & Extruding Your Channel

1) Click "**Sketch**" and select the top surface of your extruded base.
2) Draw the shape of the main body of your reactor.
   Note: *Keep the following points in mind:*
   a. *Your reactor will need three ports. One for the malachite green, one for sodium hydroxide, and one for the products.*
   b. *Avoid overlapping sketch lines whenever possible.*
   c. *Do not sketch closer than* ***5 mm*** *from the edge of your base. The ports for tubing will be added in later.*
   d. ***REMEMBER*** *to use Smart Dimension to make sure all your feature sizing is precise0*
   e. *Feel free to change aspects of this device; just make sure the outlet port in your design is centered in the device!*



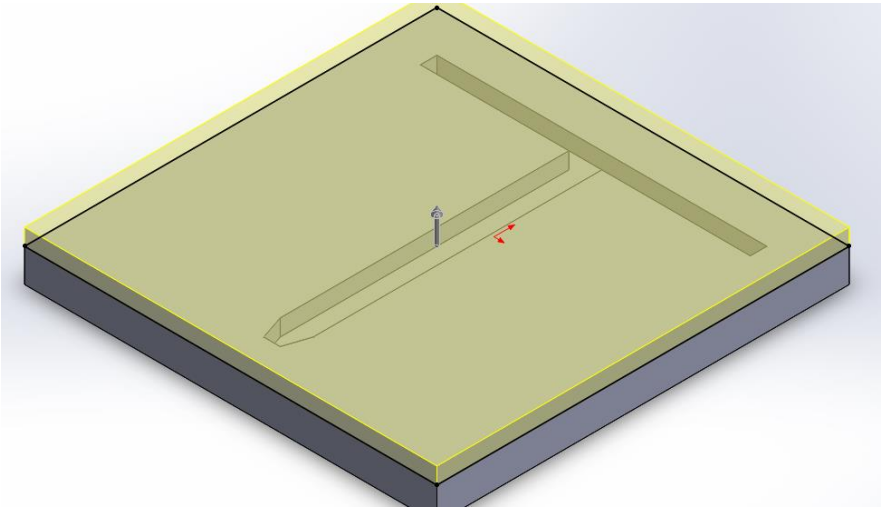
Note: This design is intentionally basic for the purpose of this tutorial. Feel free to experiment with design in ways that you think will yield better conversion!

3) Return to the Features tab. Click "Extruded Cut" and extrude the channel down **2 mm**. Confirm the cut by clicking the green check mark.



Part 3: Finishing the Reactor

1) Click "Extruded Boss/Base" and then click the **top surface** of your device (Do not click inside the channel you just extruded).
2) Draw a rectangle over the entire surface. If you drag the cursor from corner-to-corner over your device, you should not need to Smart Dimension.
3) Click "Exit Sketch" and select **2 mm** as the thickness for this extruded layer. Click the green check mark to confirm. If done correctly, your hollow channel should be inside the solid block.

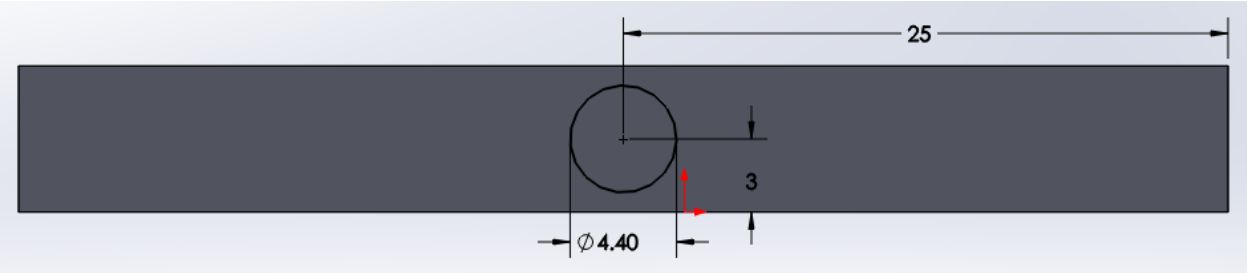


Part 4: Adding the Outlet Port

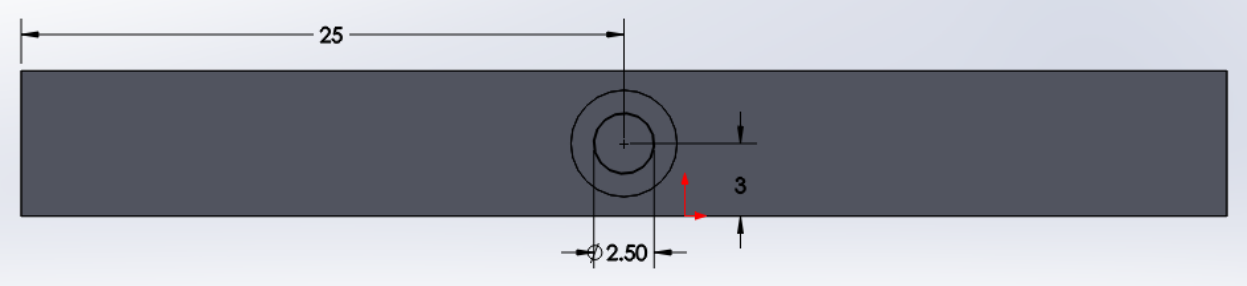
Note: If creating barbed ports, skip this step and go to that tutorial now.

1) View the front of your device (where the outlet stream will go).

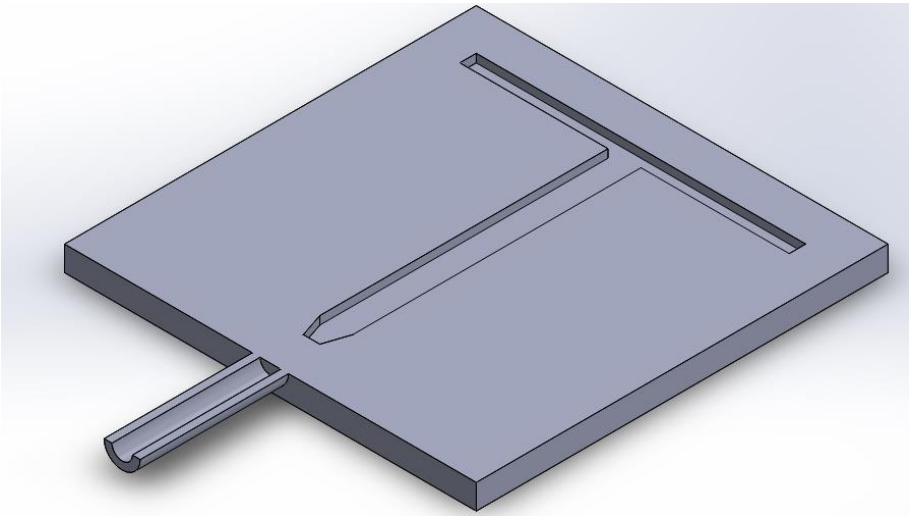
2) On this plane, select “Sketch”, select the plane and draw one circle. **It should have a diameter of 4.4 mm**. If your channel extends to exactly 5 mm from the sides of your device, the center of the circle should be 3 mm from the top. This circle should be centered on the device.
3) Return to the “Features tab”. If not selected already, select the circle you just drew and click “Extrude Boss/Base”. Extrude the circle out **18 mm**. Select the green checkmark to confirm.



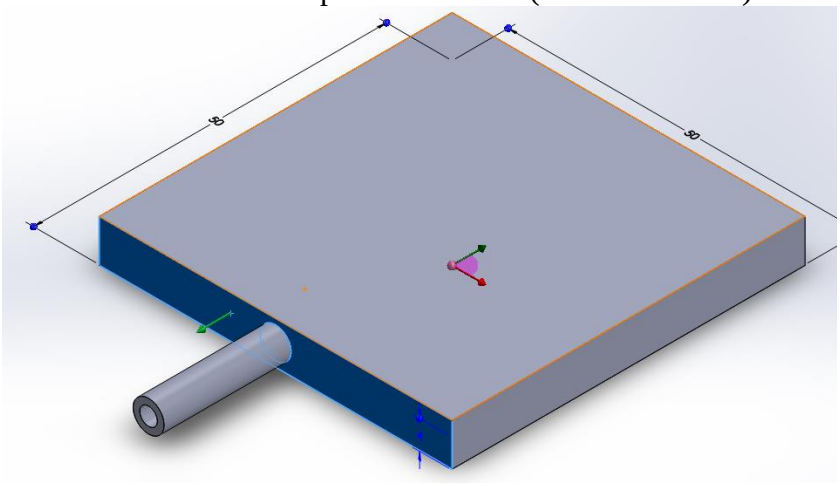
4) Return to “Sketch” and draw a circle with a **diameter of 2.5 mm** in the center of the larger circle. Use Smart Dimension to make sure it is centered.



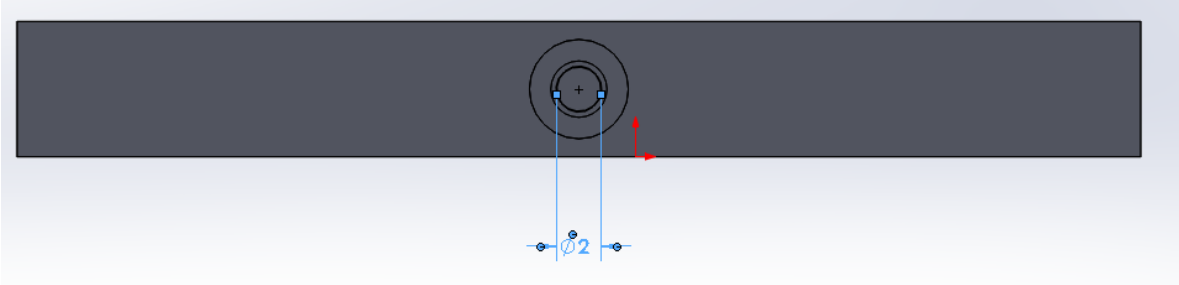
5) Return to the Features tab. If not selected already, select the smaller circle. Use “Extruded Cut” to extrude it down 18 mm. Click the green check mark to confirm. Check that this was done correctly in Section View. The device should look like the part below.



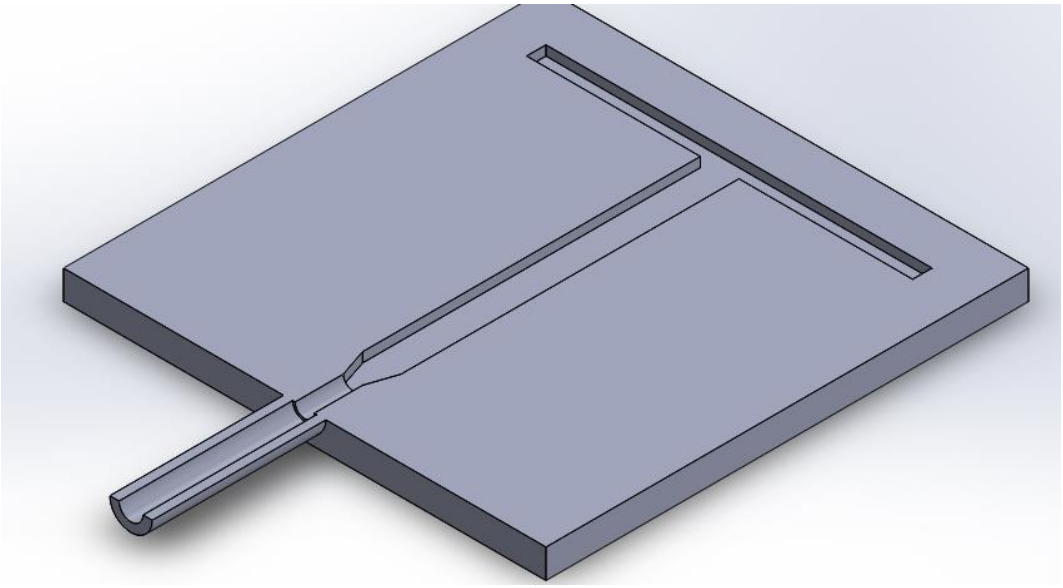
6) Exit Section View and return to Isometric View, if not there already. Select the face of the reactor from which the outlet port is extruded (blue face below):



7) On this plane, select “Sketch” and draw one circle. It should have a diameter of **2 mm**. The circle should be concentric with the other circles.

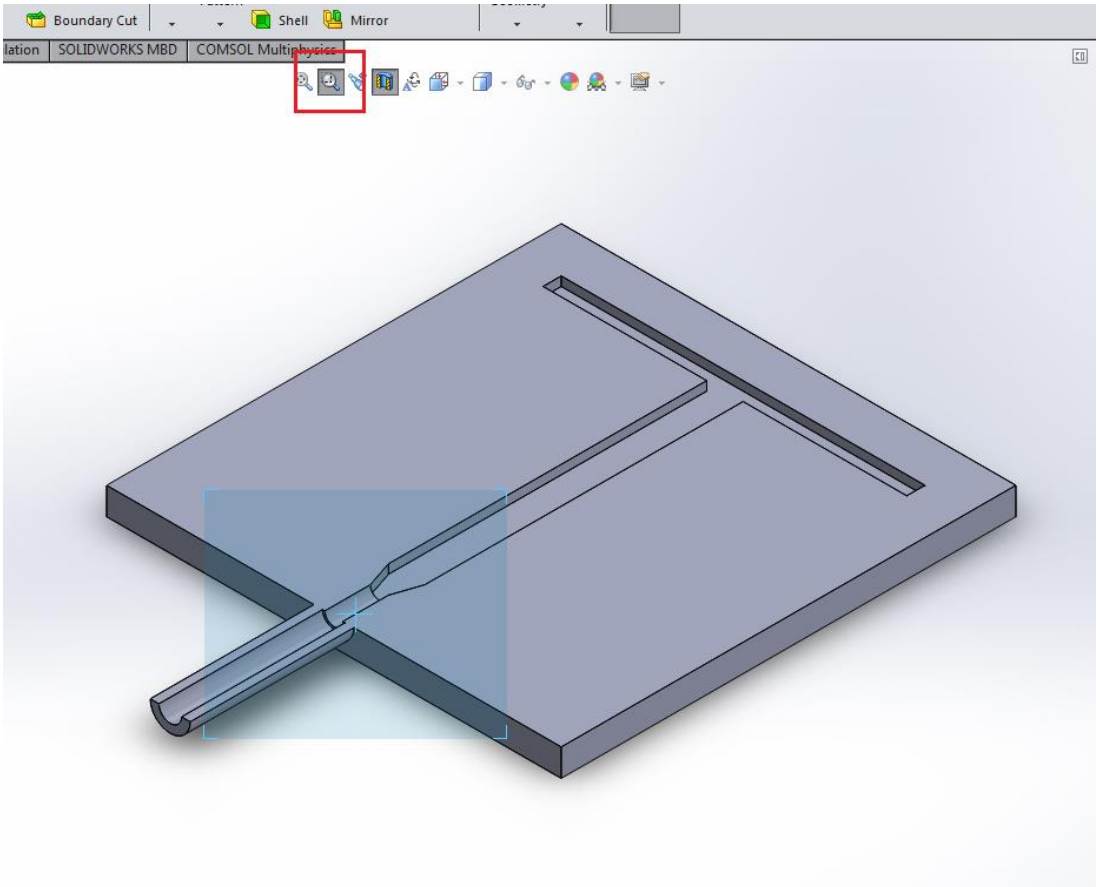


8) In the Features tab, select “Extruded Cut” and extrude this circle down 5mm. In Section View, your device should now look like this:

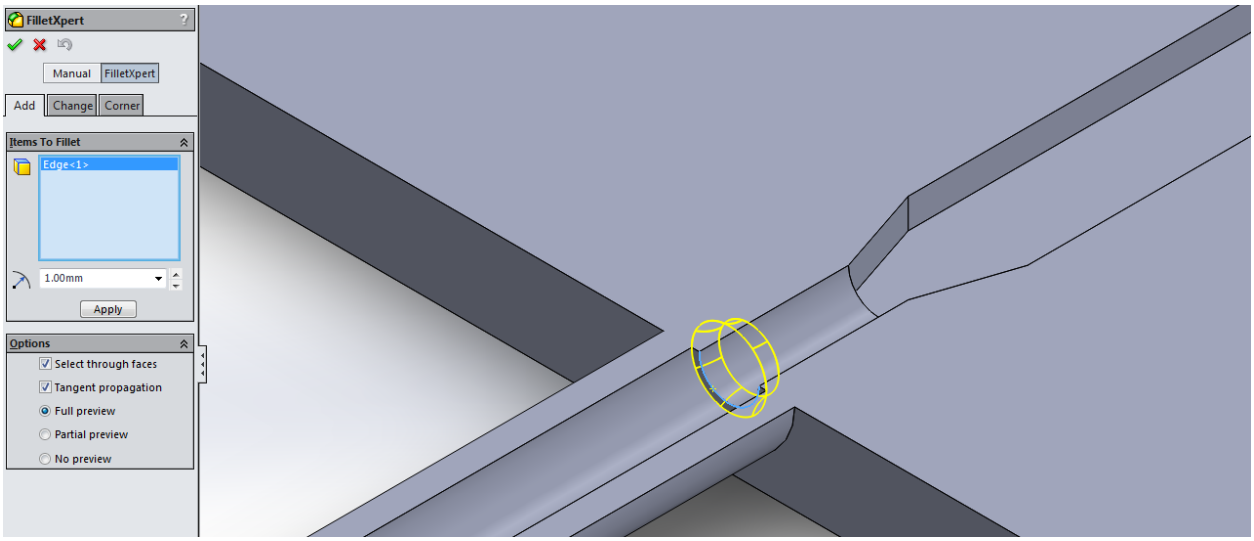


Note: Fillet steps #9)-#12) are optional

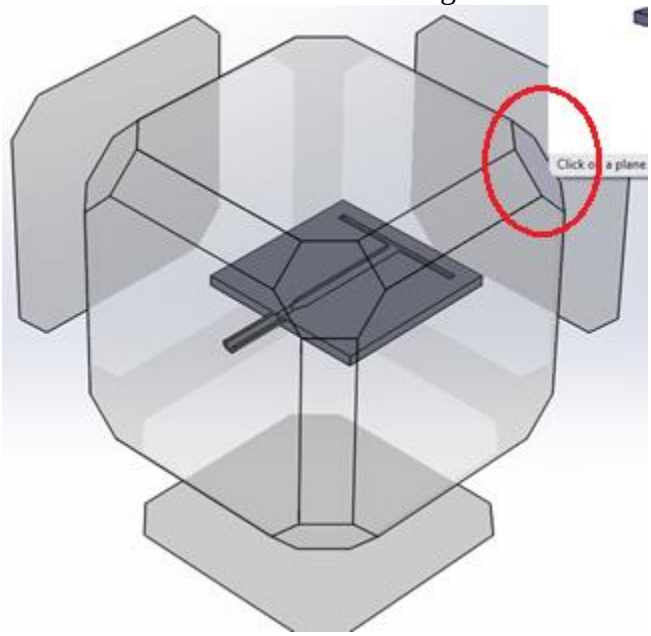
9) Use the “Zoom to Area” button to zoom in on the channel.



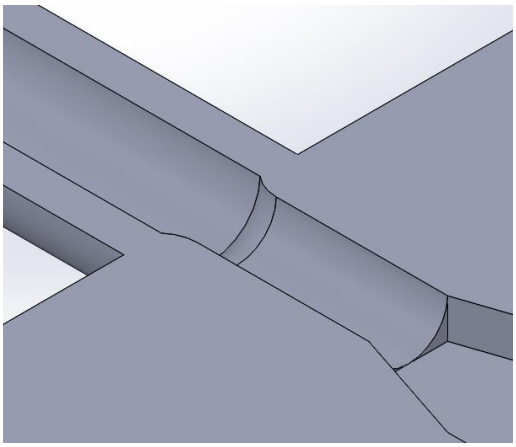
10) Under the Features tab, select “Fillet” and select the edge between the two channels (blue line below). Set the angle to 1.00mm, then select “Apply”. Select the green checkmark to confirm.



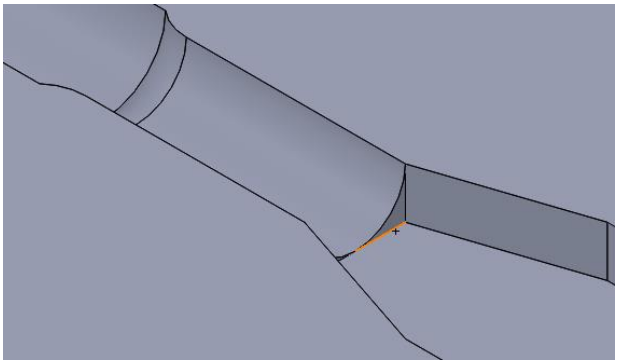
11) Change your view orientation to view the other edge of the channel:

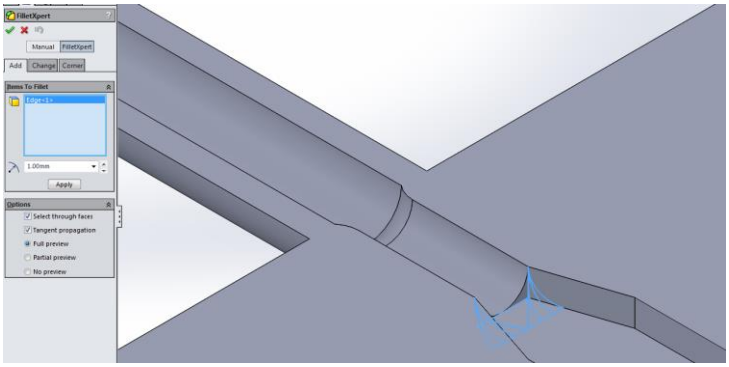


Use the Zoom to Area tool to zoom in to the channel edge.

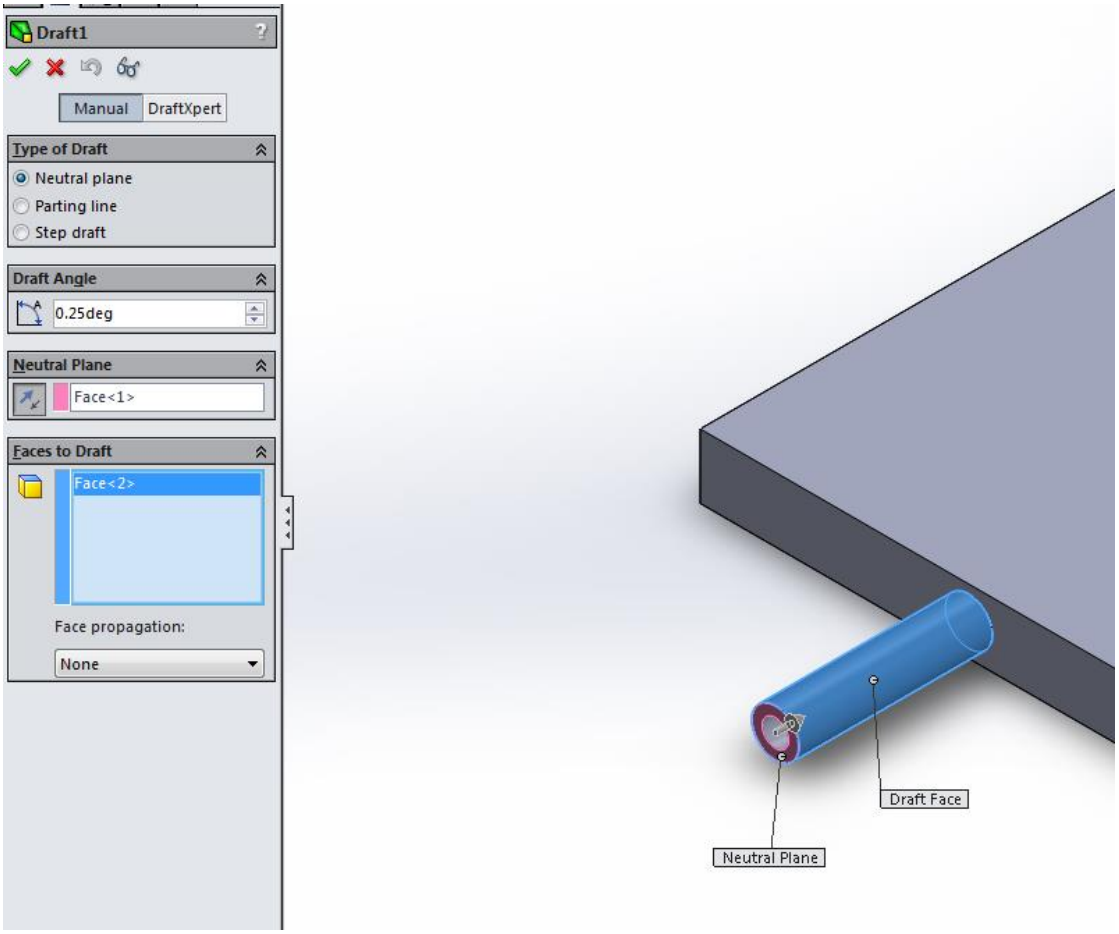


12) Under the Features tab, select “Fillet” and select the edge between the two channels (orange line below). Set the angle to 1.00mm, then select “Apply”. Select the green checkmark to confirm.

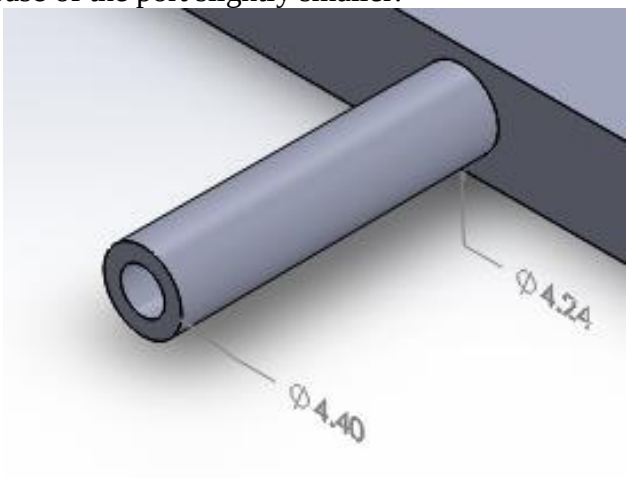




13) Return to Isometric View; under the Features tab select “Draft.” The Draft angle should be 0.25 degrees; the neutral plane is the outer plane of the port, and the draft plane is the cylindrical body of the port. If necessary, change the direction of the draft to be towards the device by changing the direction of the neutral plane; the grey arrow should be pointing towards the device. Select the green checkmark to confirm.

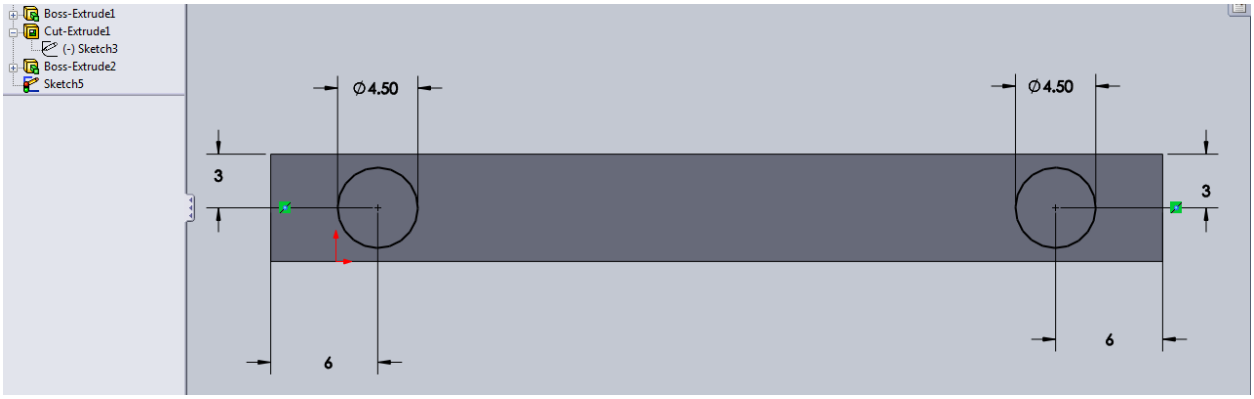


The draft made the base of the port slightly smaller:



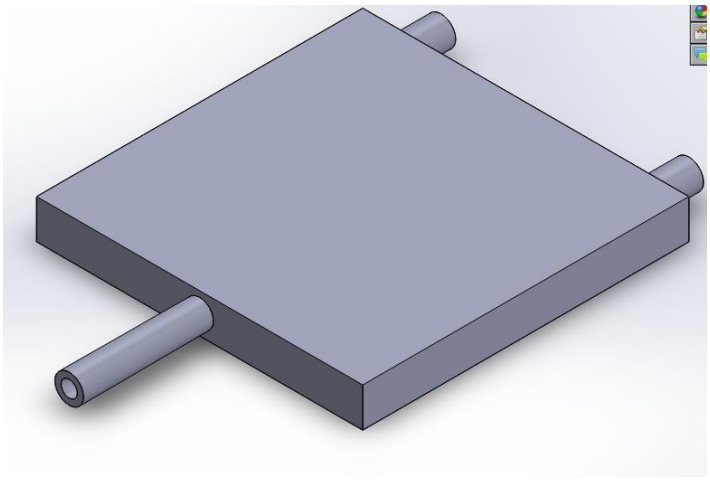
Part 5: Adding Inlet Ports

1) Change the view orientation to the Back Face. Select "Sketch", select the back face and draw two circles. **They should have a diameter of 4.5 mm**. If your channel extends to exactly 5 mm from the sides of your device, the centers of the circles should be 3 mm from the top. The circles should be centered on the device.
2) Return to the "Features tab". If not selected already, select both circles you just drew and click "Extrude Boss/Base". Extrude the circles out **6 mm**. Click the green check mark to confirm.



3) Return to the "Features tab". If not selected already, select both circles you just drew and click "Extrude Boss/Base". Extrude the two circles out **6 mm**. Click the green check mark to confirm.
4) Select "Sketch" again. In the center of each of the two circles you just extruded, draw a circle with a diameter of **2 mm**. Use Smart Dimension to make sure they are centered.

5) Return to the Features tab. If not selected already, select both of the smaller circles and extrude them down **11 mm** (enough to cut through the ports and into the channels themselves). Click the green check mark to confirm.
6) When your device is complete, it should look something like the part shown below:

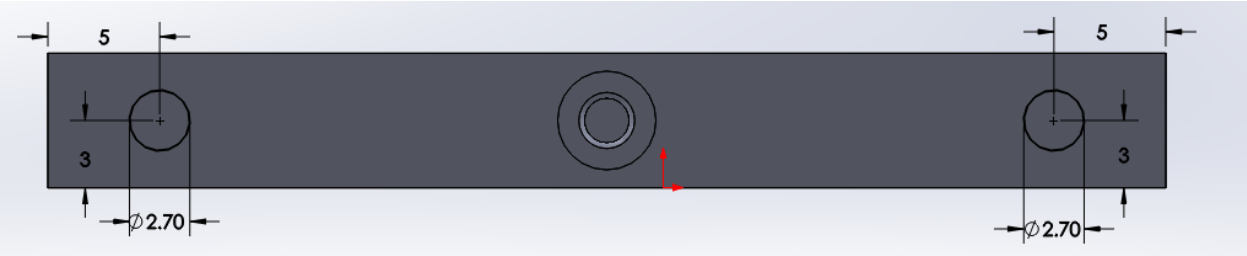


Isometric View

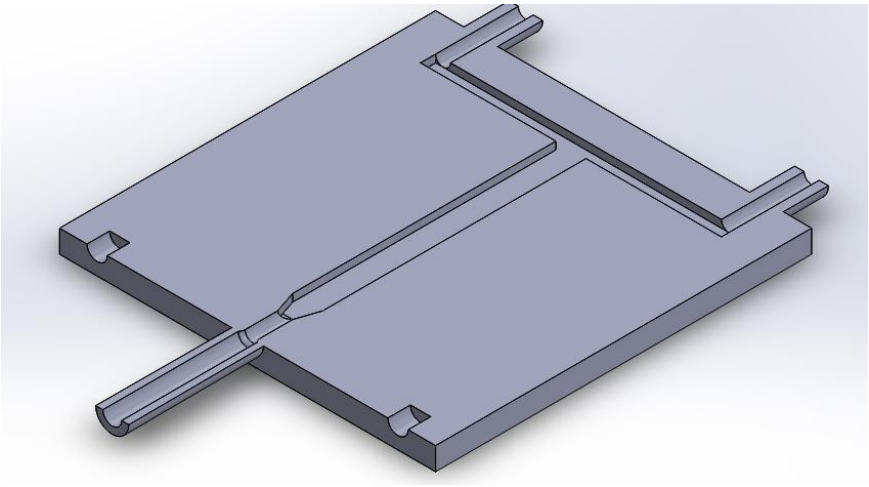
Part 6: Adding Stability Tabs

1) Change the view orientation to view the front of the device.

2) On this face, select “Sketch”, select the face and draw two circles. **They should have a diameter of 2.7 mm**. The centers of the circles should be 3 mm from the top.



3) Return to the “Features tab”. If not selected already, select the circles you just drew and click “Extruded Cut”. Extrude the circles down 3mm. Select the green checkmark to confirm.



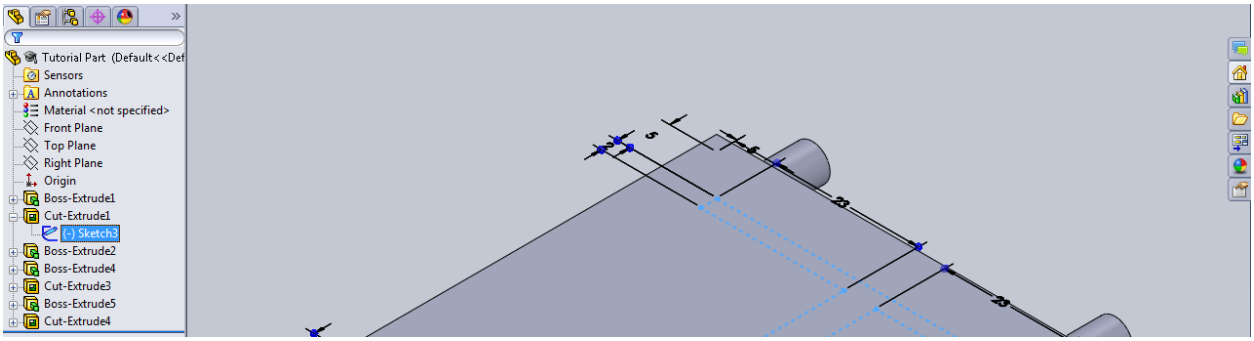
Section View

Part 7: Getting Your Part Ready to Print

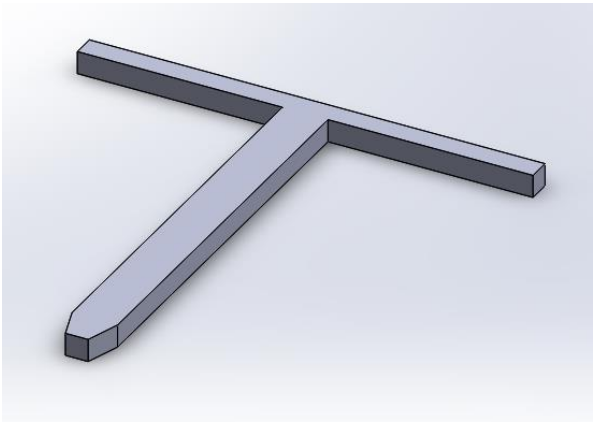
1) You should save your part as both a .SLDPRT file and a .STL file.
    a. The .SLDPRT file is the SolidWorks file extension. You may continue to edit this file.
    b. The .STL file is a stereolithography file. This is the only type of file the 3D Printer software can read, but you cannot edit something that has been saved as a .STL file
2) If completing this device outside of lab, send both the .SLDPRT and .STL files to Leslie and Emily. If there are any issues with the file, they will notify you and suggest improvements.

Part 8: Preparing Your Design for COMSOL

1) On the left-hand side bar, locate the sketch you used to design your channel.
2) Select that sketch and copy it (Ctrl+C works).



3) **Open a New SolidWorks Part file.** Do not skip this step!
4) Click "Extruded Boss/Base" and select the Top Plane.
5) Paste your channel into this space (Ctrl + V) and click "Exit Sketch".
6) Extrude the sketch up **2 mm** (or whatever the height of your channel is, if you have changed the geometry). Click the green check mark to confirm.



7) Save this file as a .STL file. You may import the .STL file into COMSOL to begin your simulation.

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Modeling Flow, Diffusion, and Chemical Reaction in a 3D-Printed Microreactor: A COMSOL Demonstration

Part I. Introduction

COMSOL is a computer modeling software package that will allow you to model heat transfer, pressure-driven flow, diffusion, chemical reactions, and other physical phenomena occurring in various chemical engineering applications. COMSOL has a graphic user interface where you can define the governing physics and/or chemistry for a user-defined 2- or 3-dimensional geometry, define initial and boundary conditions, and perform a fine element model without writing any code. Take some time and look through the COMSOL web site, including the model gallery, animations, and tutorials for relevant models: http://www.comsol.com.

For an example of a 2D microfluidic channel coupling laminar flow and diffusion physics, see the following video tutorial:

http://www.comsol.com/products/tutorials/Microfluidics_Simulation_of_an_H-Cell/.

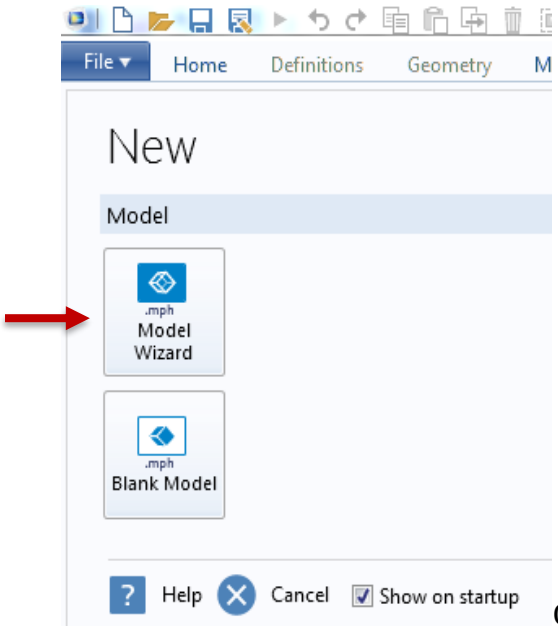
** Please note that they use a shallow channel approximation in this simulation because the channel is a true microfluidic channel and very small. However, our channel is much larger and we cannot make this assumption.*

In this lab, we will be performing a simple exercise together to help you become more familiar with how to use COMSOL in a 3D microchannel application. The software is available to you free in the SoE computer labs and on your own computer with UConn SKYBOX through the SoE: http://skybox.uconn.edu/. However, the SKYBOX can be prone to crashing, so we recommend doing as much of this modeling in the SoE computer lab as possible – **and save frequently!**

In this demonstration, we will be modeling fluid flow, diffusion, and a chemical reaction in a 3D-printed microreactor. In this example, we will be using simple materials, but the material library (which contains all pertinent parameters e.g. heat transfer coefficients, density, viscosity etc.) for COMSOL is extensive.

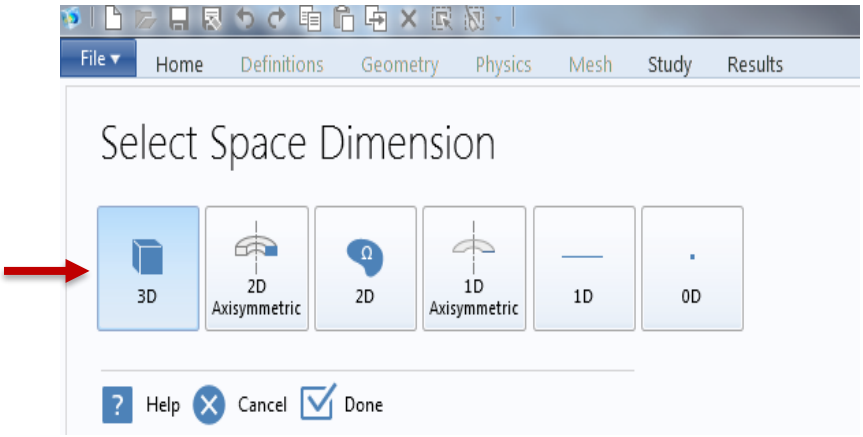
Part II. Step-by-Step Modeling Instructions

First, you have to create the type of model you want to solve.

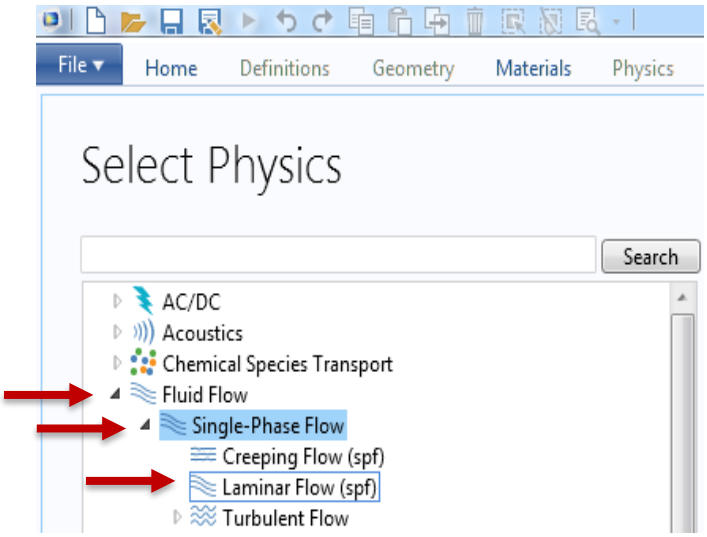
1. 

On the first window for creating a new model, select "**Model Wizard**".

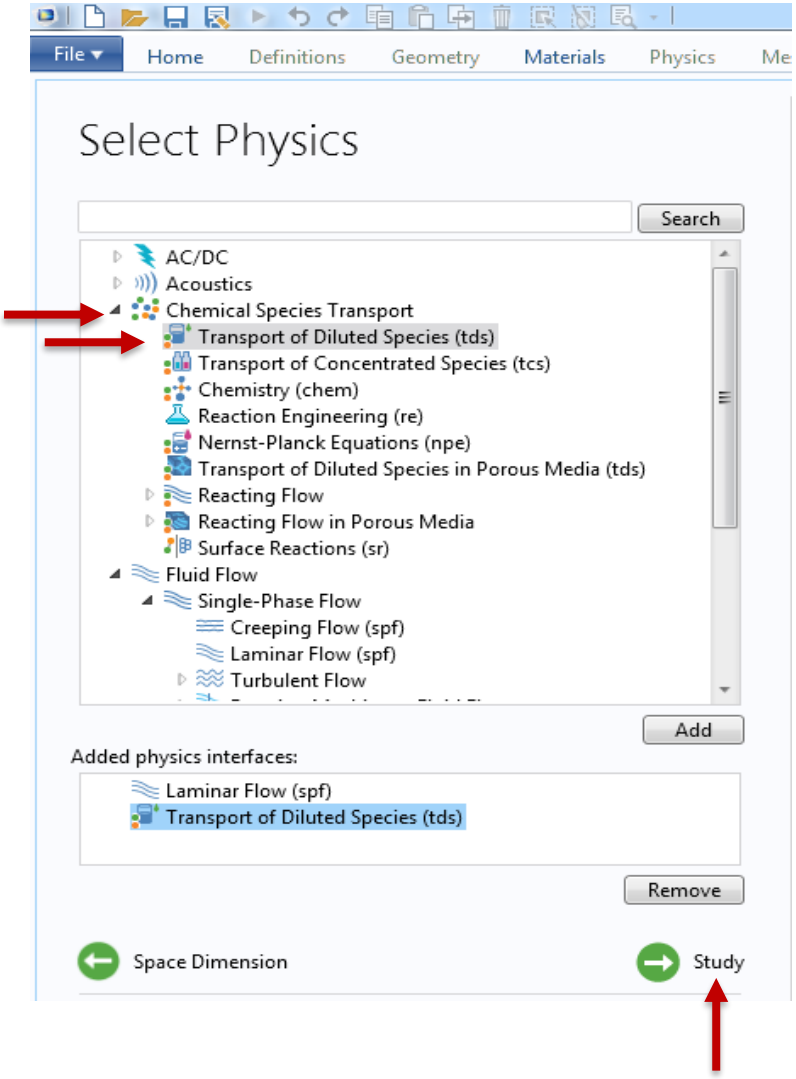
2. In the window of "Select Space Dimension", select "**3D**" for a three dimensional model.



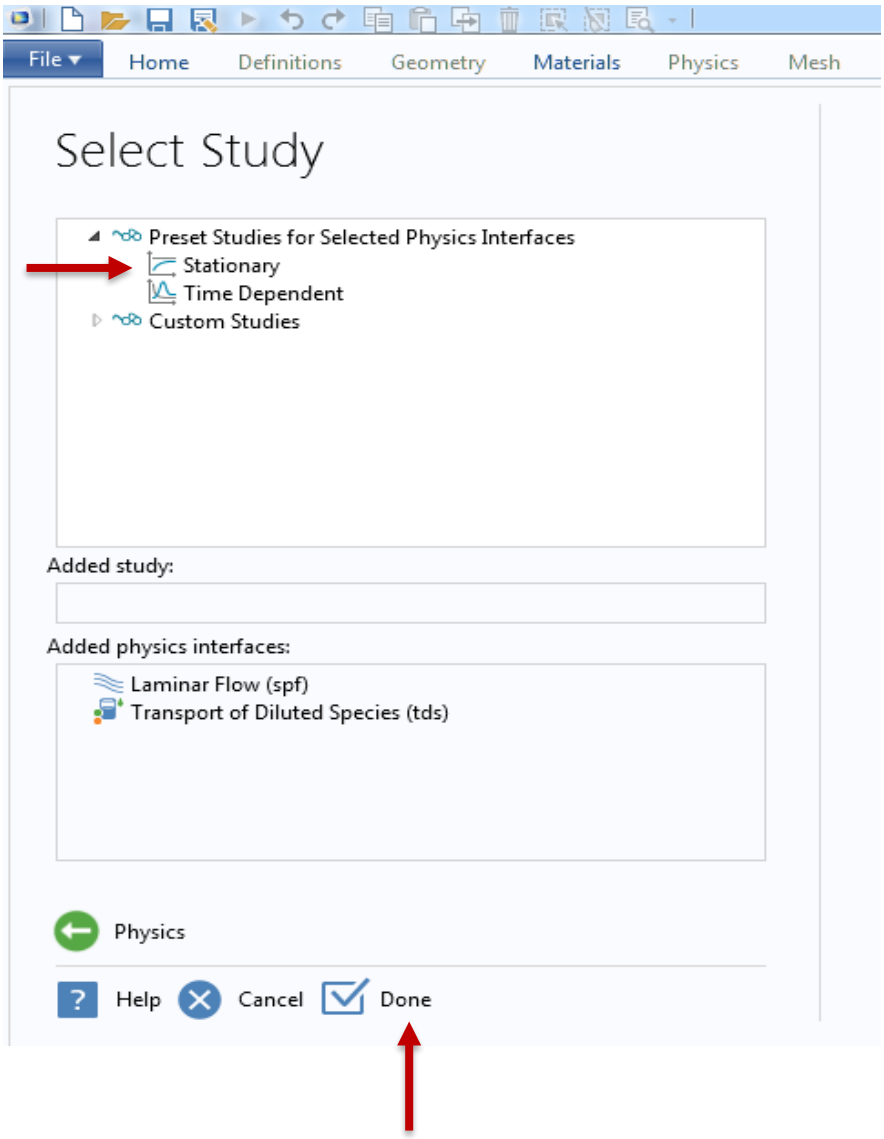
3. **Add Physics**:
   a. Double click on "**Fluid Flow**". In the drop down list, double click "**Single-Phase Flow**" and then double click on "**Laminar Flow (spf)**."



b. Next, double click on "**Chemical Species Transport**" and double click "**Transport of Diluted Species (tds)**" (aka Fickian diffusion). Click the "**Study**" arrow.

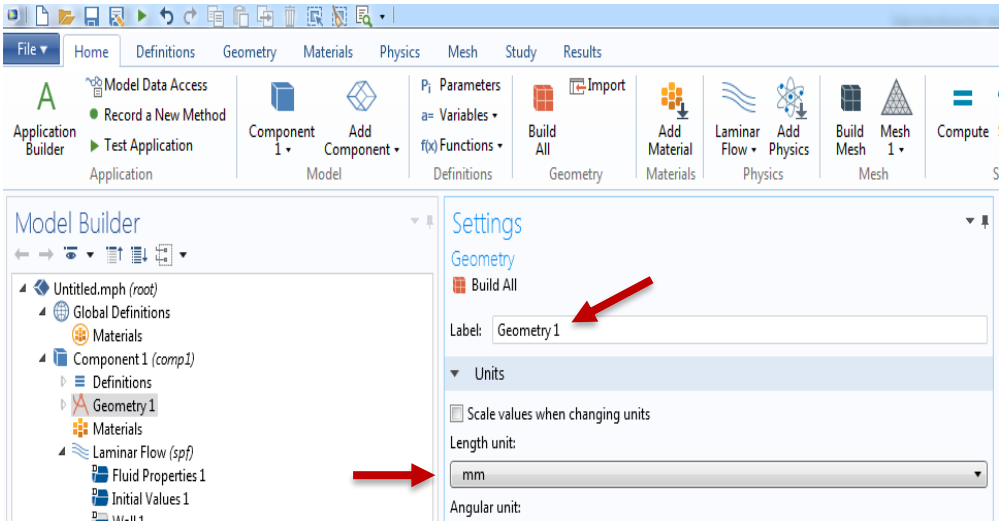


c. Select Study Type—"Stationary" for steady state (you can try "Time Dependent" another time if you're interested in the unsteady state solution). Click the "Done" checkbox.

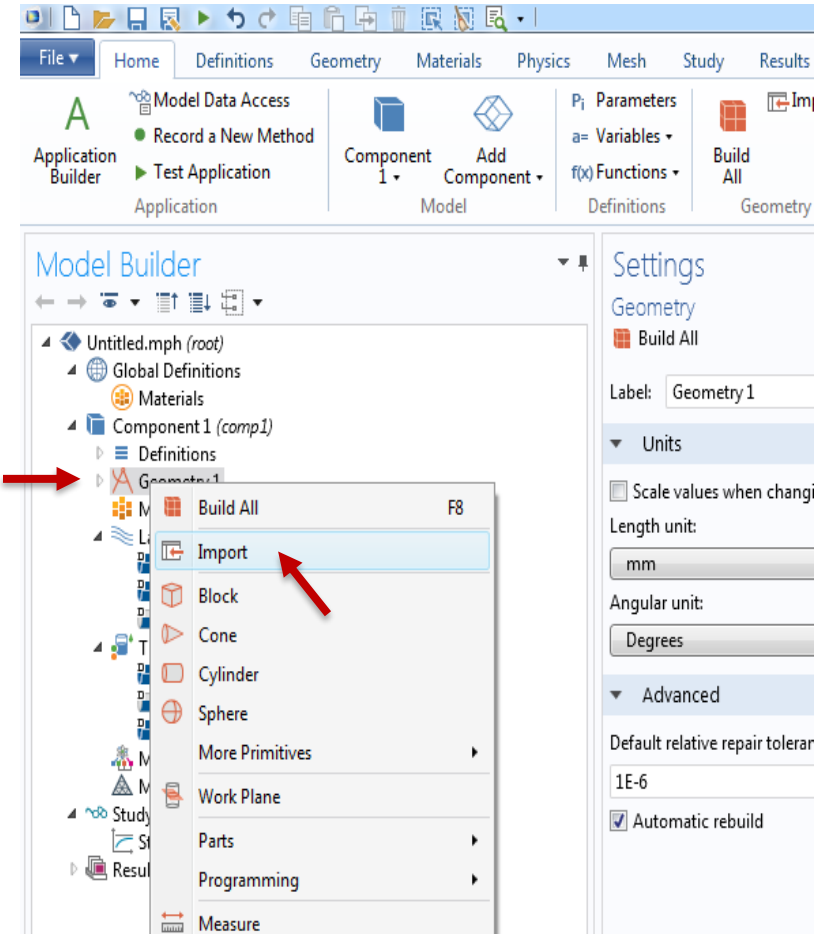


Second, you have to import the geometry of your system.

1. A Settings tab labeled "**Geometry**" should automatically pop up; select **mm** for the length unit.

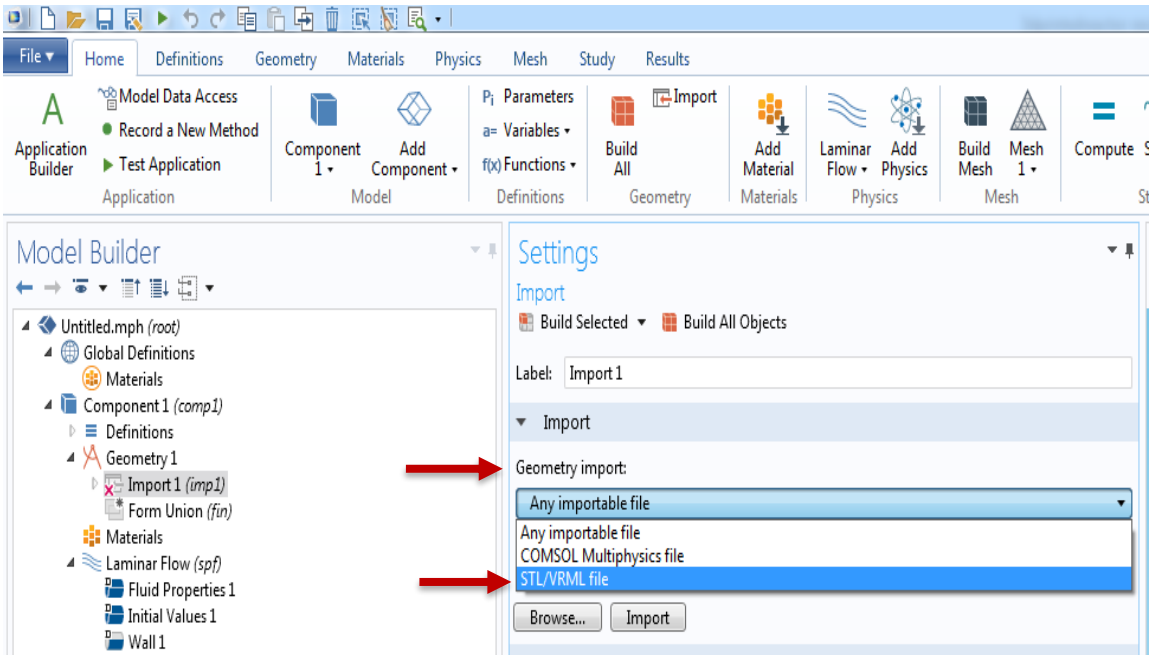


2. In the Model Builder tab, right click on "**Geometry 1**" and click on "**Import**".

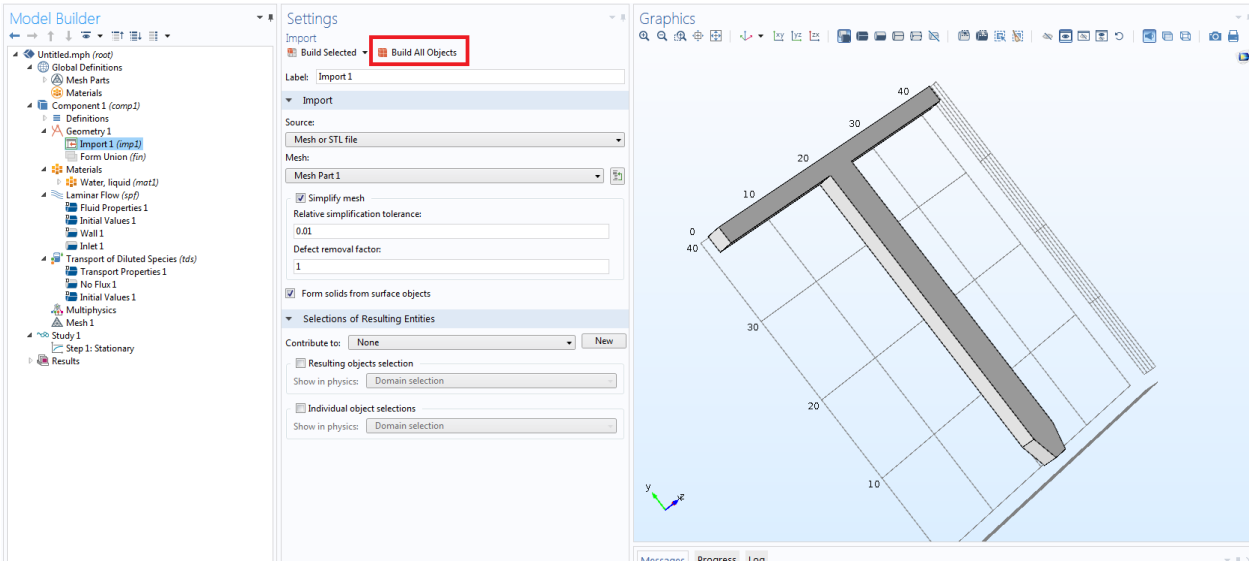


3. Under "**Geometry Import**", select "**STL/VRML file**".

Note: You will have to import a .stl file of your design where the channels are solid shapes in order for COMSOL to model it properly.

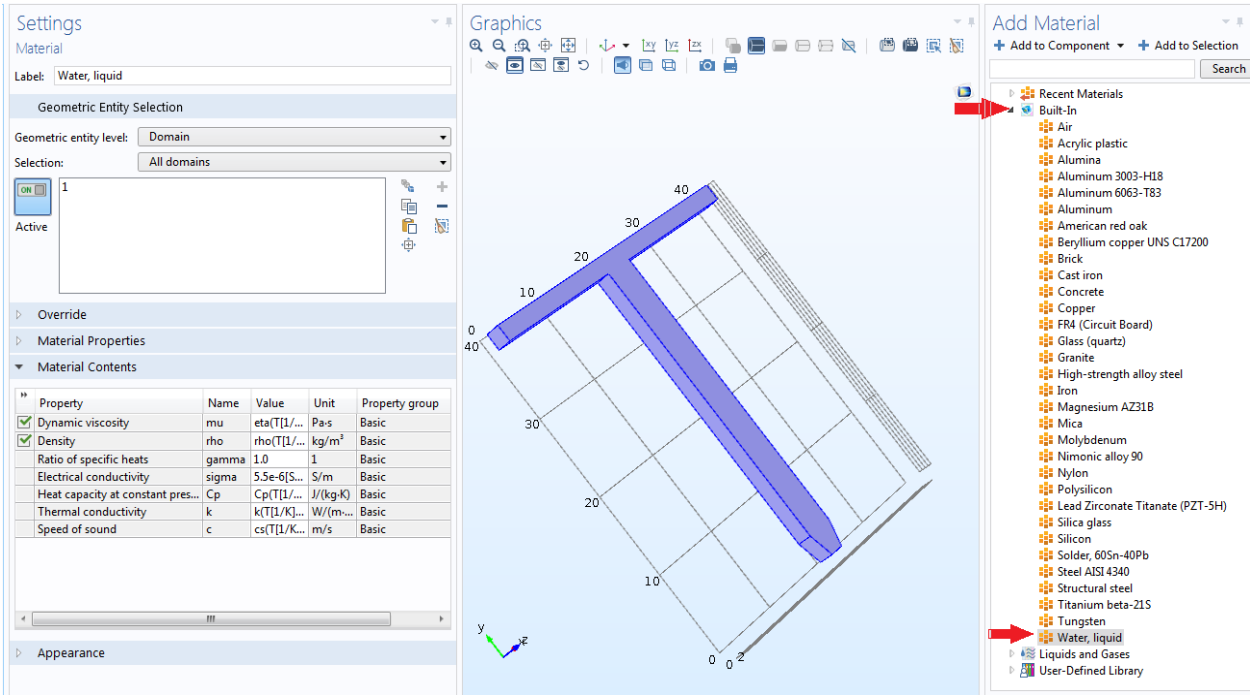


4. Click the "**Browse**" button and find the desired .stl file of your design.
5. Click "**Import**" and then "**Build All Objects**" at the top of the Import tab. Make sure the units are in "mm."



Third, you have to define material types for domains of your object.

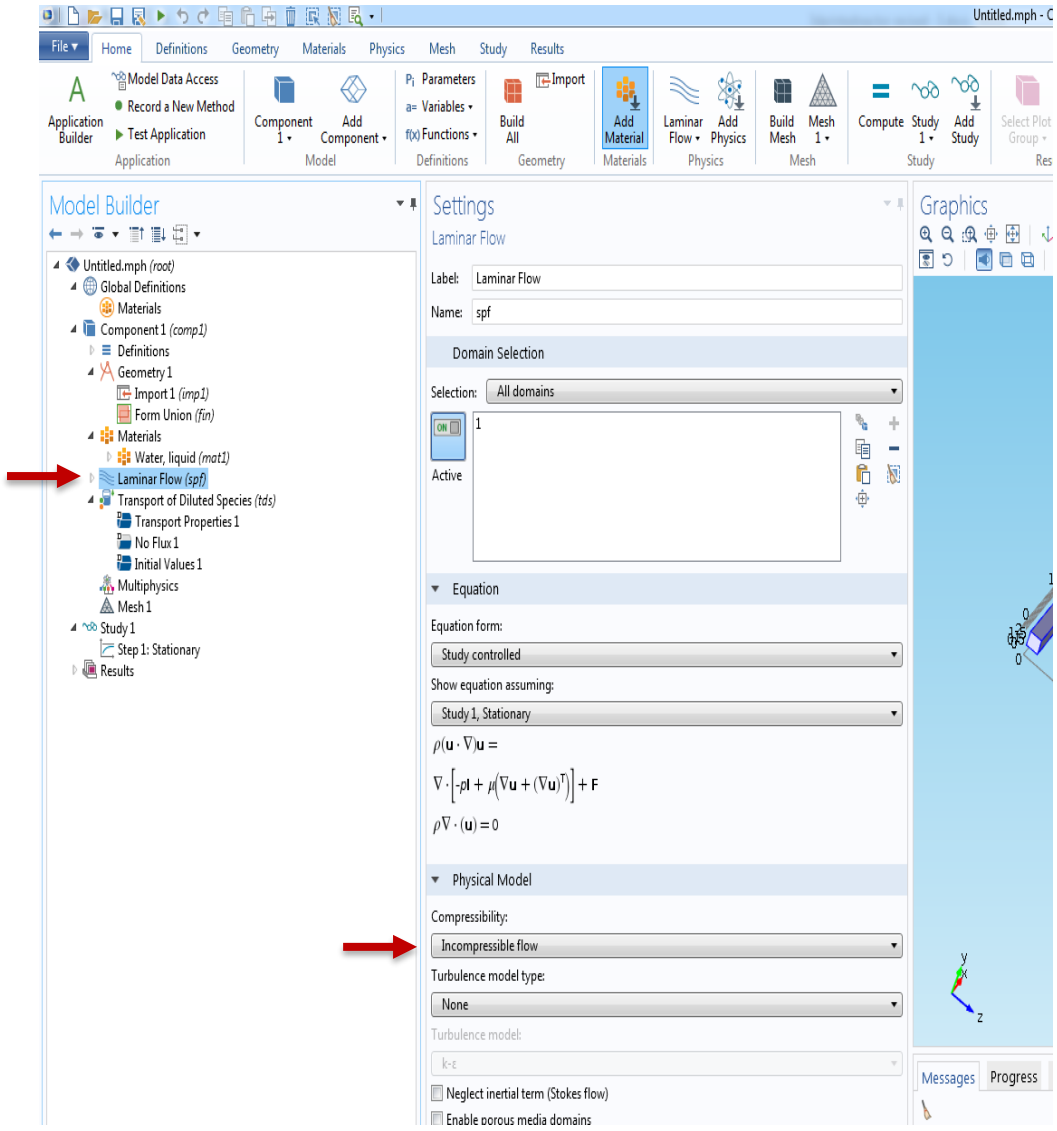
1. Under the Model tab, click on "**Add Materials**", "Add Material" will pop-up at the right side of screen (You could also right click on the "**Material**" under "Model Builder" and then click on "**Add Material**"). Double click "**Built-In**", then right-click on "**Water, liquid**" and then click on "**Add to Component 1**".



2. Click on your component to add the material to model. You should see the number 1 show up in the "Selection" box in the "Geometric Entity Selection" tab and the component should become a light blue color (see screen shot on next page). To view properties of the material, you can look under the "Material Contents" or "Material Properties" tabs for more detail.

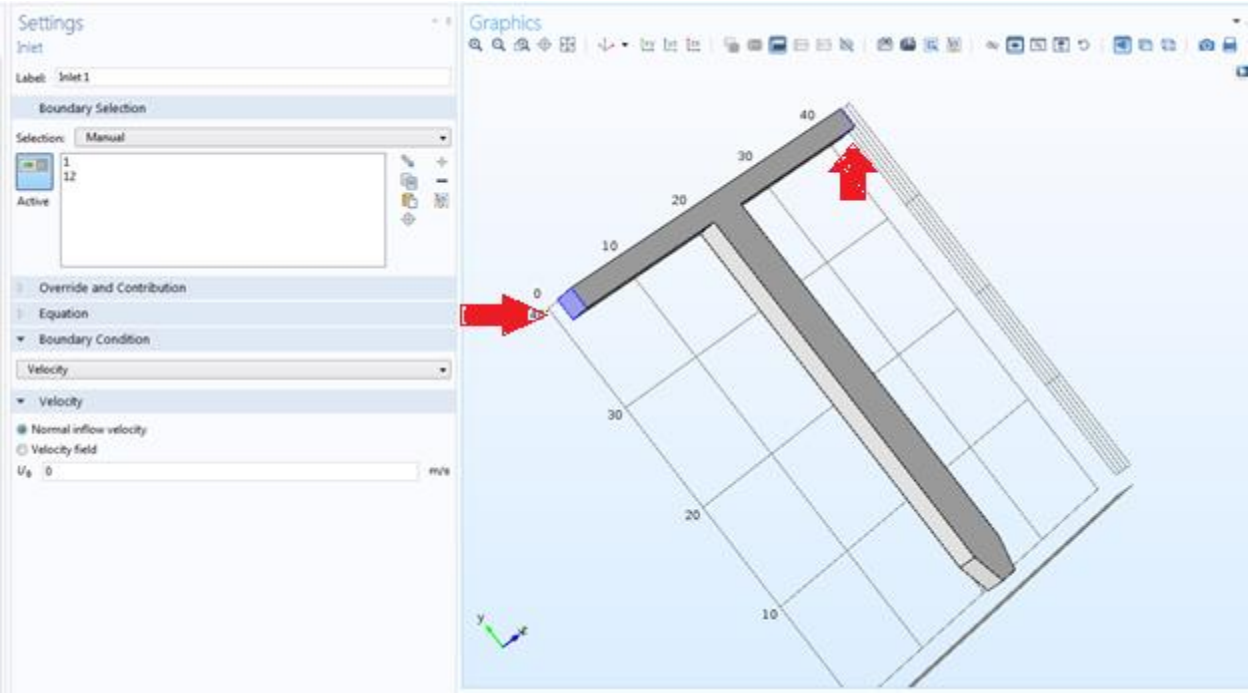
Fourth, you have to define modeling conditions.

1. Laminar Flow: Define initial and boundary conditions.
   a. Click "**Laminar Flow**" and first of all select "**Incompressible Flow**" from the drop down menu under "Compressibility" (to make it a less complicated problem for the model for now).

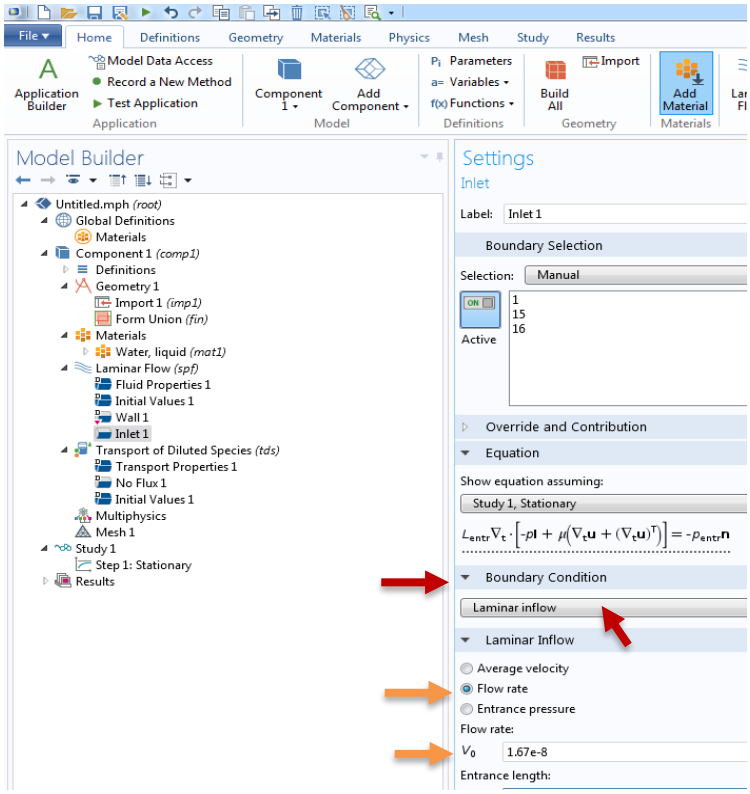


   b. COMSOL automatically assumes a no-slip condition along the walls and an initial fluid flow of zero. You can look at these assumptions in "Fluid Properties", "Wall", and "Initial Values", which can all be found under the "Laminar Flow" heading in the Model Builder tab.

c. Now we need to set the inlet flows coming into the microreactor. Right click "**Laminar Flow**" and select "**Inlet**". Left click the two inlet faces so that they appear on the list for the "Boundary Selection" – they should be faces 1 and 12, and should appear blue after they are selected (see screen shot on next page).

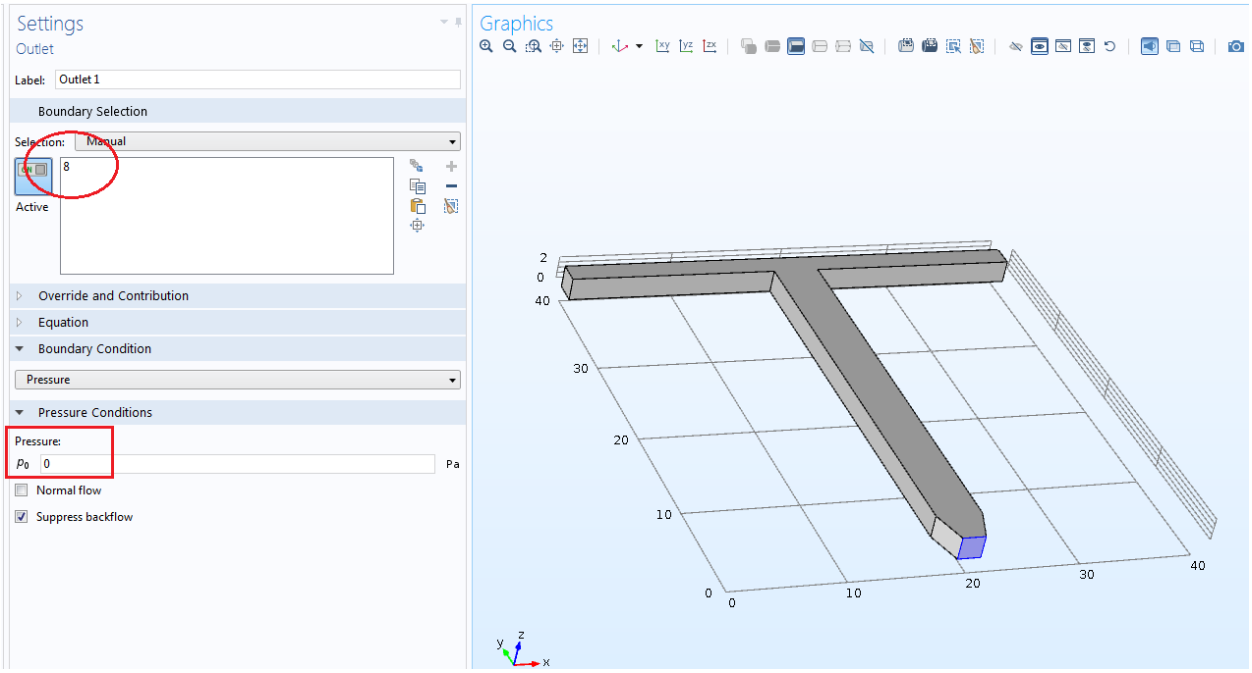


d. Under the "**Boundary condition**" drop down menu, select "**Laminar inflow**" and then select the "**Flow Rate**" (this is the volumetric flow rate). Enter your volumetric flow rate in the space below. We can start with 1.67e-8 m^3/s (1 mL/min).



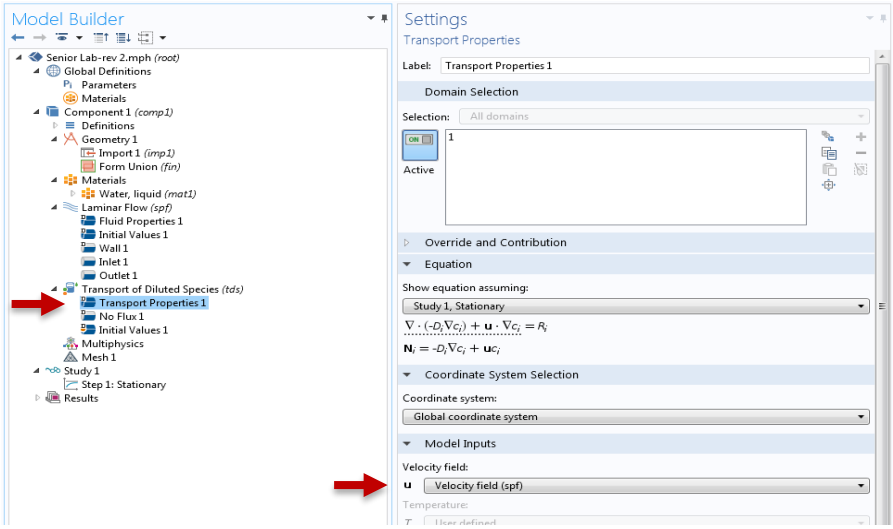
** You can enter in an actual number, or you can assign a name to this parameter so that you can do a parameter sweep of the flow rate later on. Expand "Global Definitions" in the Model Builder tab and right click on "Parameters." Here you can define your parameters and any initial values.*

e. Next, we will select the outlet conditions. Right click "**Laminar Flow**" and select "**Outlet**". Select the outlet face at the end of the microreactor (8) and leave the boundary condition at "Pressure" and $p_0 = 0$ Pa.



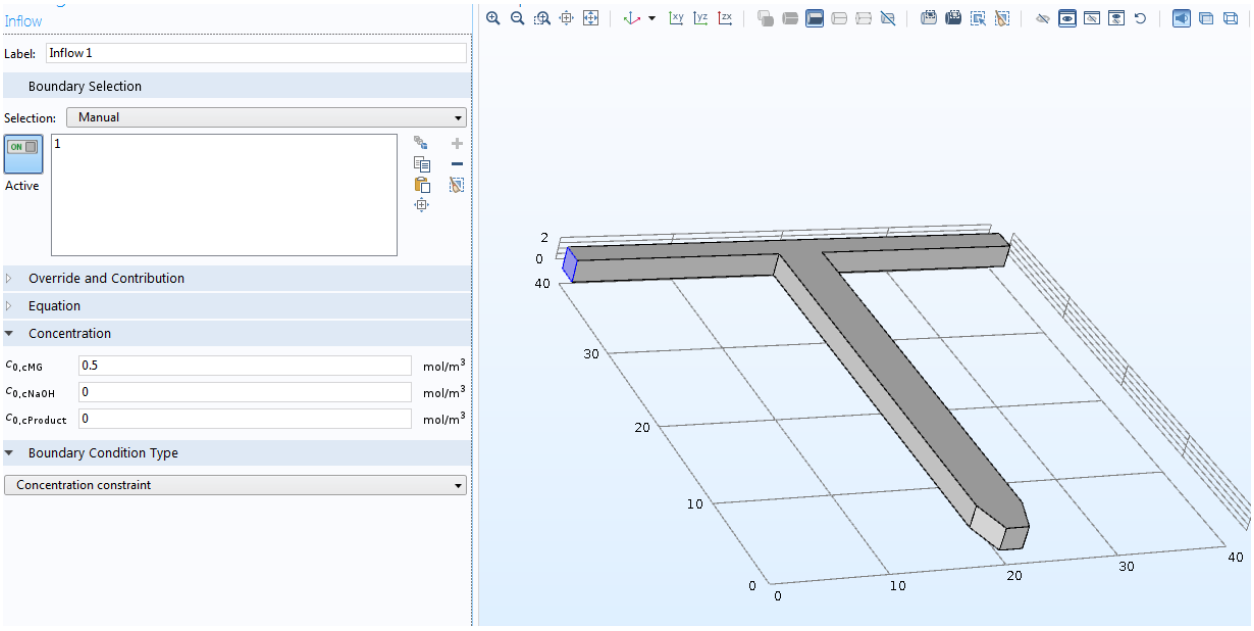
2. Transport of Diluted Species: Define initial and boundary conditions.
   a. Click on "**Transport of Diluted Species**" and make sure that the "**Convection**" box is checked.
   b. We will also need to make sure we have the proper number of variables for the species concentrations. Still in the "**Transport of Diluted Species**" menu, expand the "**Dependent Variables**" section. Change the number of species to **3** and enter the following concentration variables: "**cMG**" (Malachite Green), "**cNaOH**" (Sodium Hydroxide), and "**cProduct**"
   c. Next, click on "**Transport Properties 1**" under "**Transport of Diluted Species**." For model inputs, make sure you select "**Velocity field**", NOT "User defined".

      Note: Your model will not be able to calculate both physics together if this box is not checked and the velocity field connected to the flow regime from your other physics.



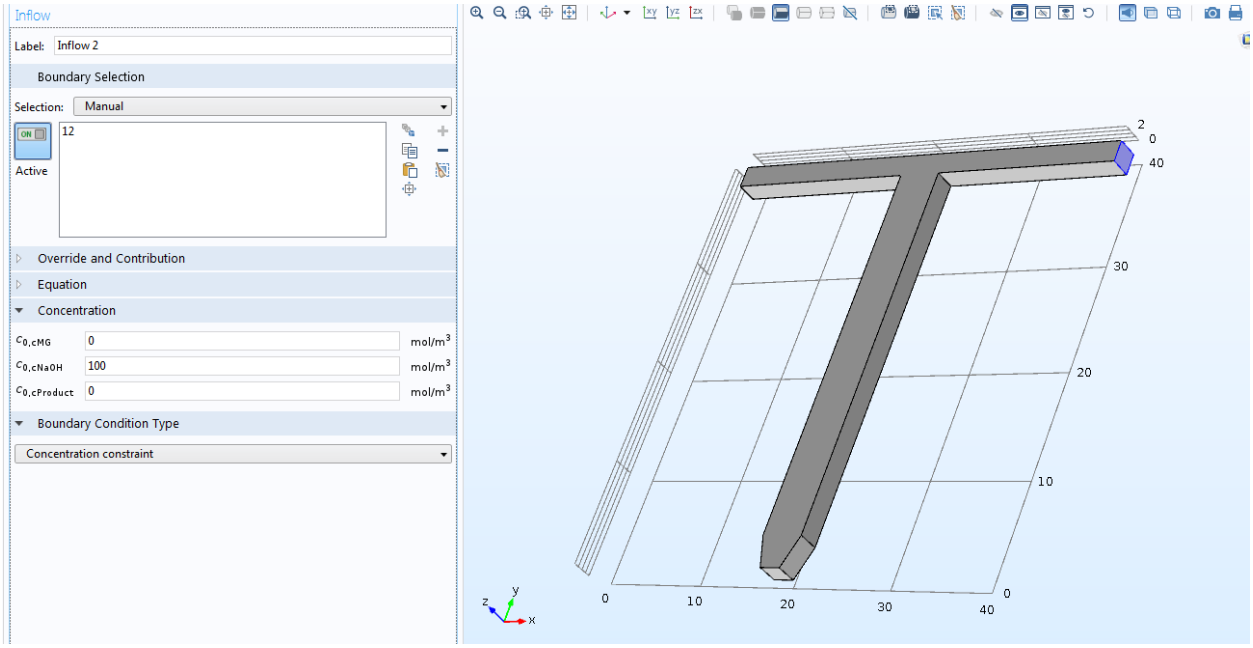
d. Note that COMSOL automatically assumes a diffusion coefficient of 1e-9 m^2/s for all species. This is fairly close to actual values for the species we're using, but this may be something you can adjust (by looking up actual values) to improve your model.

e. Now, we will be setting the inflow concentrations of your species. Right click "**Transport of Diluted Species**" and select "**Inflow**". Select the inlet face of your upper-left inlet channel (face 1) and select an **MG** concentration of 0.05 mol/m^3 (5e-5M). Leave everything else at 0.

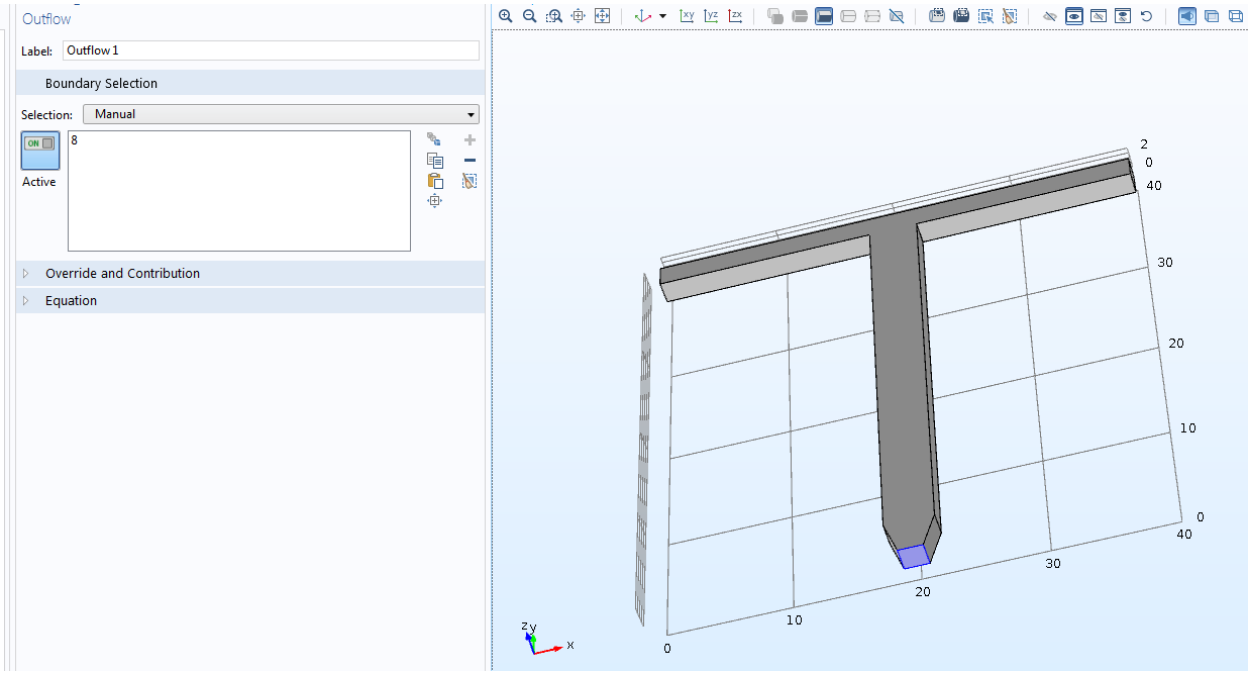


f. Repeat the previous step for the inlet face of the upper-right inlet channel (face 12) and select an **NaOH** concentration of 100 mol/m^3 (0.1M). Leave everything else at 0.

* You should now have “Inflow 1” and “Inflow 2” under “Transport of Diluted Species”.



g. To set up the outflow, right click “**Transport of Diluted Species**” and select “**Outflow**”. Select the outlet face at the end of the microreactor (face 8).

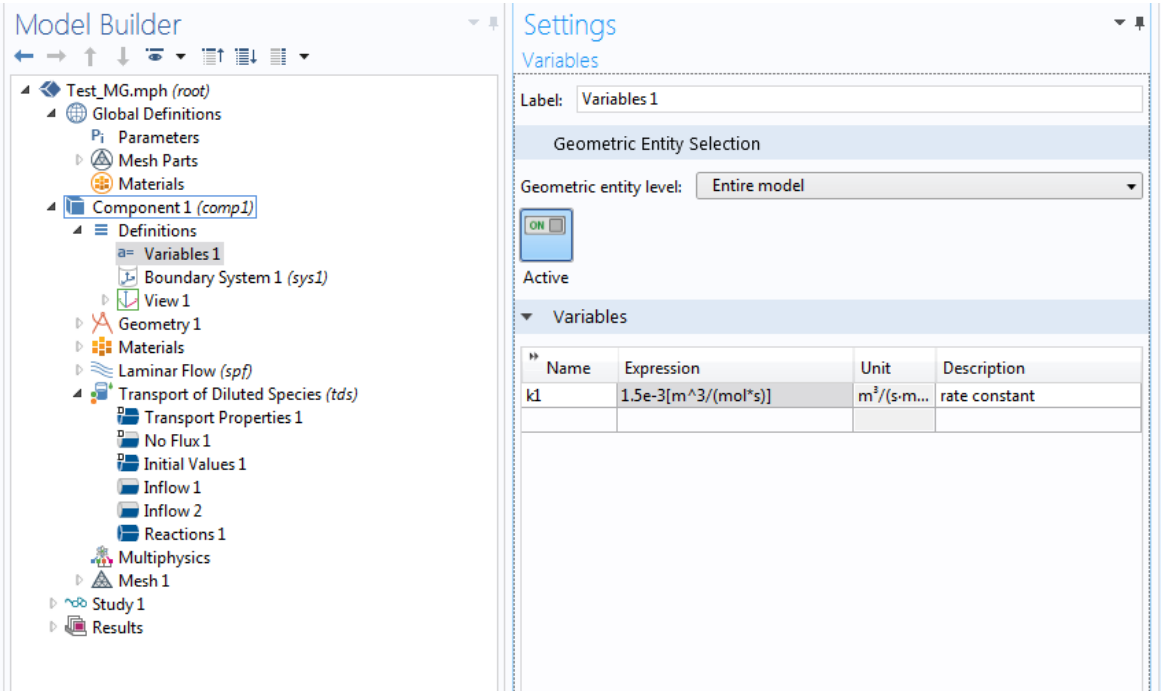


3. Transport of Diluted Species: Define Chemical Reaction

Now we will define the following chemical reaction in COMSOL:

NaOH + MG → Product

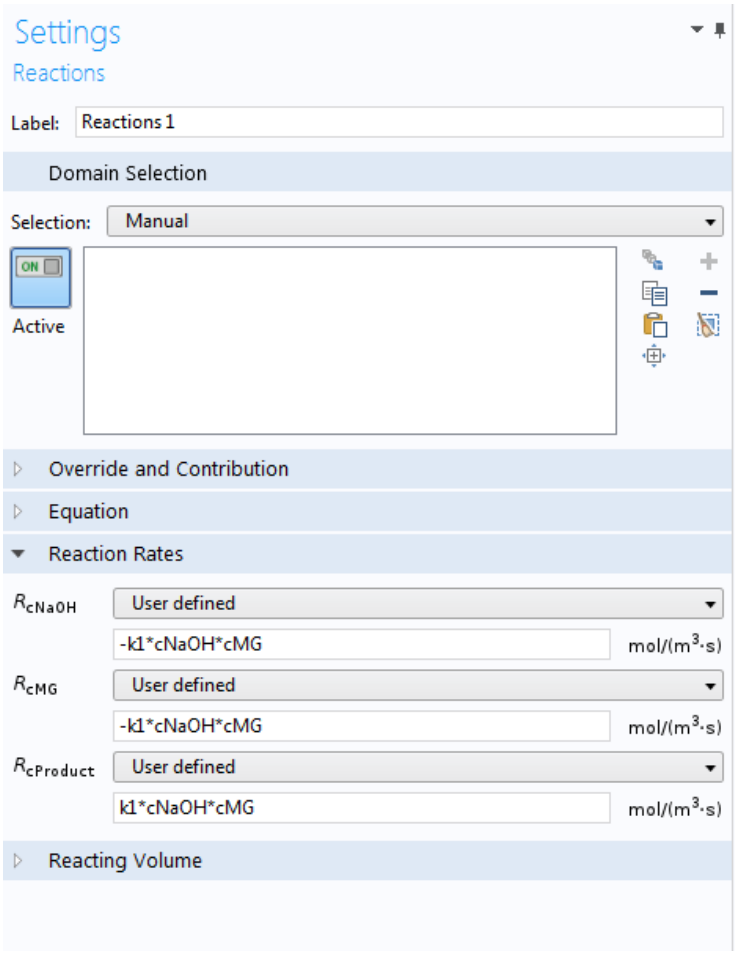
a. First, we will define the rate constant, k. Under "**Component1**" in the Model Builder, right-click on "**Definitions**" then select "**Variables**." Define rate constant, "**k1**", as 1.5e-3 m^3/(mol*s).



b. Second, right click on "**Transport of Diluted Species**" and select "**Reactions**." Make sure **the entire domain** is selected (it should be light blue and the number 1 should appear in the "**Domain Selection**" window). Expand the "**Reaction rates**" section and specify the reaction rates for each of the species as shown below:

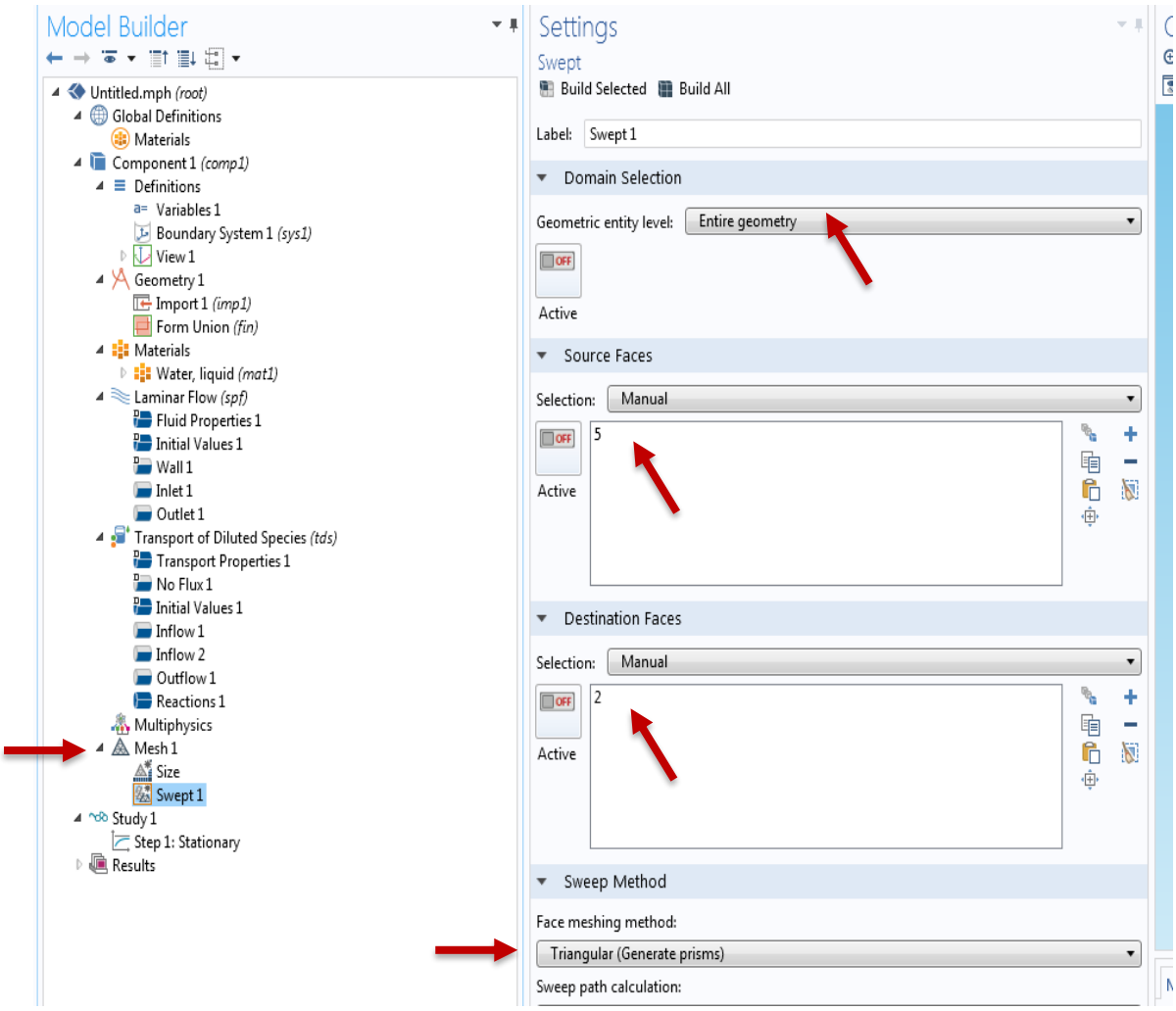
R_{cMG}	**-k1*cMG*cNaOH**	**mol/(m^3/s)**
R_{cNaOH}	**-k1*cMG*cNaOH**	**mol/(m^3/s)**
$R_{cProduct}$	**k1*cMG*cNaOH**	**mol/(m^3/s)**

Note: the reaction rate is negative for the reactants because they are being consumed, but positive for the products because they are being produced.

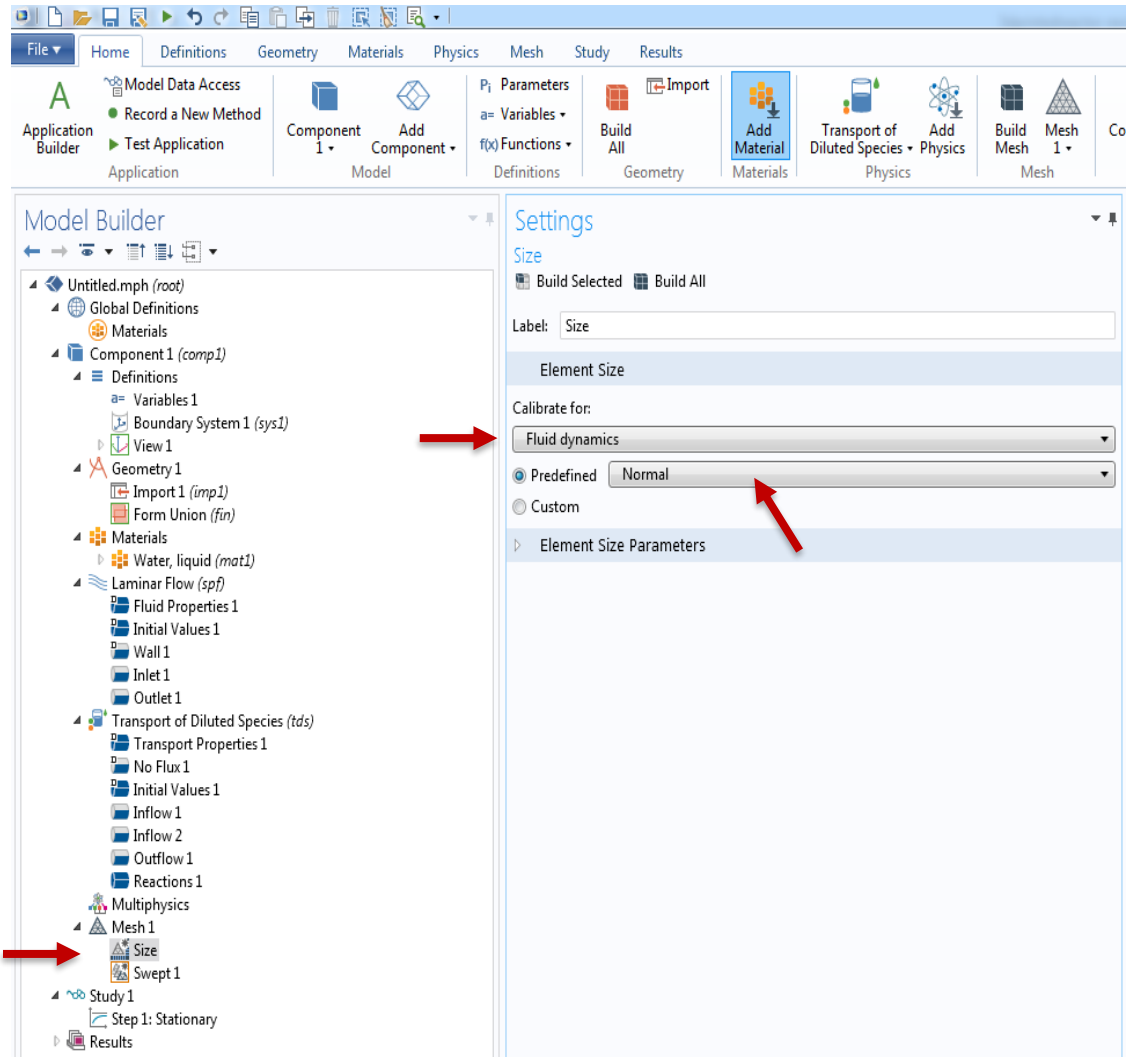


After completing model setup, you have to create mesh over the objects (domains) that you are interested in.

1. Right click on "**Mesh 1**" and select "**Swept**".
2. Make sure you have "**Entire geometry**" selected for the "Domain Selection".
3. Select the top face of your microreactor as the "source face".
4. Select the bottom face of your microreactor as the "destination face".
5. Under "Sweep Method", select "**Triangular**" for your "Face meshing method".



6. Under "Mesh 1", click on "**Size**". Under the element size heading, make sure it is calibrating for "**Fluid dynamics**" and select "**Normal**" under the "Predefined" drop down menu.



7. Click "**Build All**" at the top of the tab to build the mesh.

Then you're ready to compute the model.

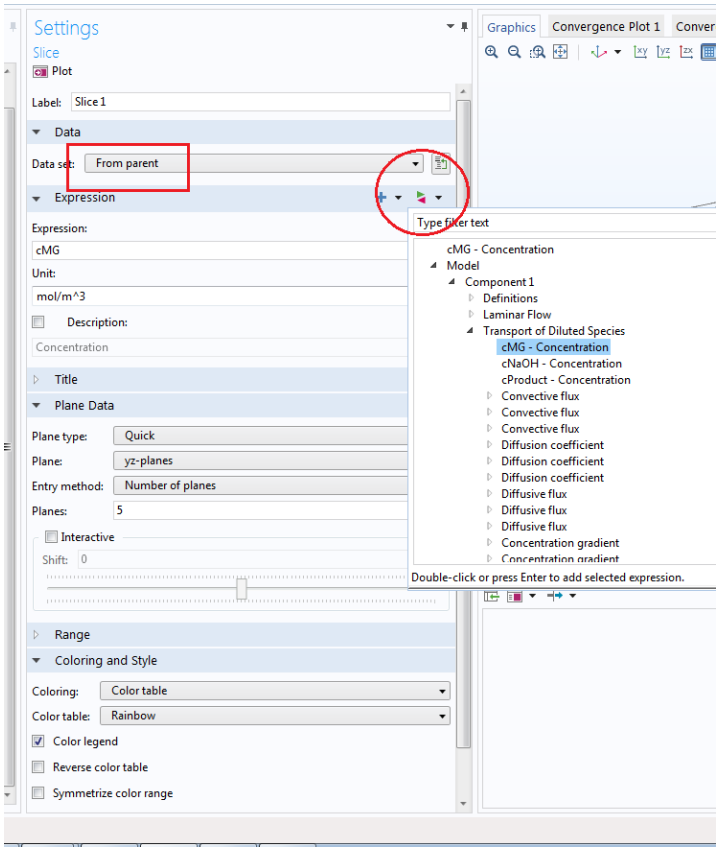
1. Right click on "**Study 1**", select "**Compute**". This may take several minutes depending mostly on the number of nodes in mesh and number of time steps of computing.

Having issues computing? Try these changes:

- Use a coarser mesh
- Check your boundaries and boundary conditions
- Try running a Time Dependent Study
    - Add Study → Time Dependent
    - Change the time range: (0, step size, end time)
        - Ex: (0, 1.0, 240) evaluates every second for 240 seconds

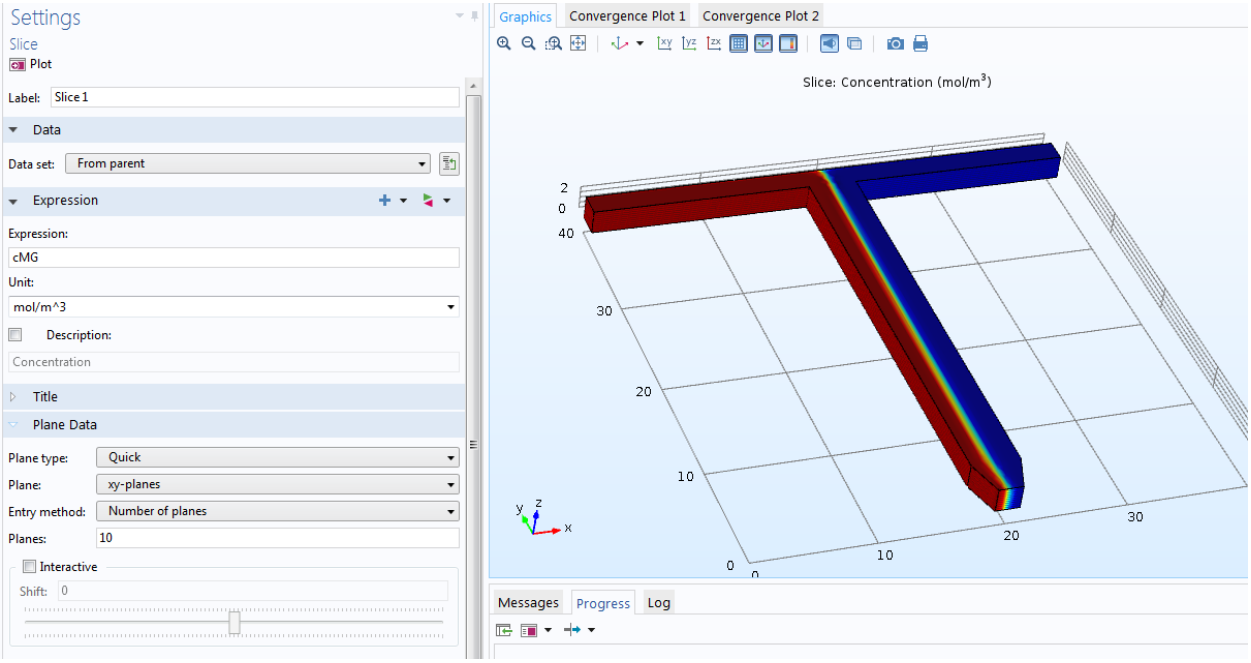
Finally, you can analyze computed data and create plots of species concentrations.

1. COMSOL will automatically plot a few parameters, such as the concentration, velocity, and pressure, but you will most likely want to customize these to learn more about the system.
2. First, we'll look at the species diffusion results.
    a. COMSOL's automatic plot will most likely be a surface plot, but this only tells you what is happening at the channel surfaces, not what's going on inside the channel.
    b. Right click on the "**Concentration (tds) 1**" plot and select "**Duplicate**". Rename this new plot whatever you'd like – we want to look at the concentration profiles for each of the species separately, e.g. "**MG Concentration**".
    c. Right click "**Surface**" on the drop-down menu under the name of your new plot and select "**Delete**".
    d. Right click the name of your new plot and select "**Slice**". Click on "Slice" and under the "Slice" tab, make sure the Data set says "**from parent**" and make sure the expression is the correct variable you want to look at (i.e., cMG). You can change this expression by clicking on the red and green arrows at the top of the "Expression" top down.



e. In the z-x plane, we look at 1 plane in the middle of the structure.

f. You can also add slices in the x-y plane to show you the concentration profile in the direction perpendicular to flow along the length of the channel:

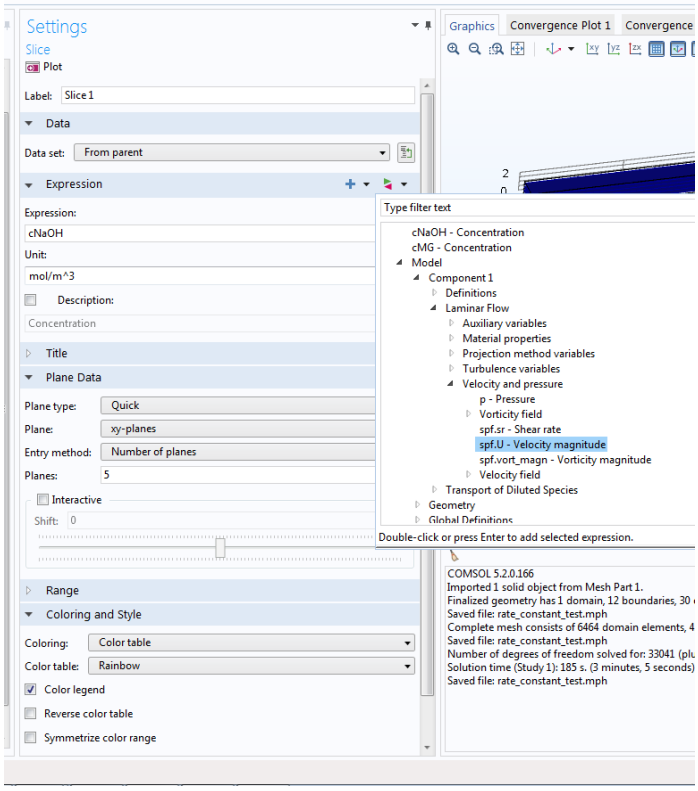


g. You can repeat these steps with the other species.

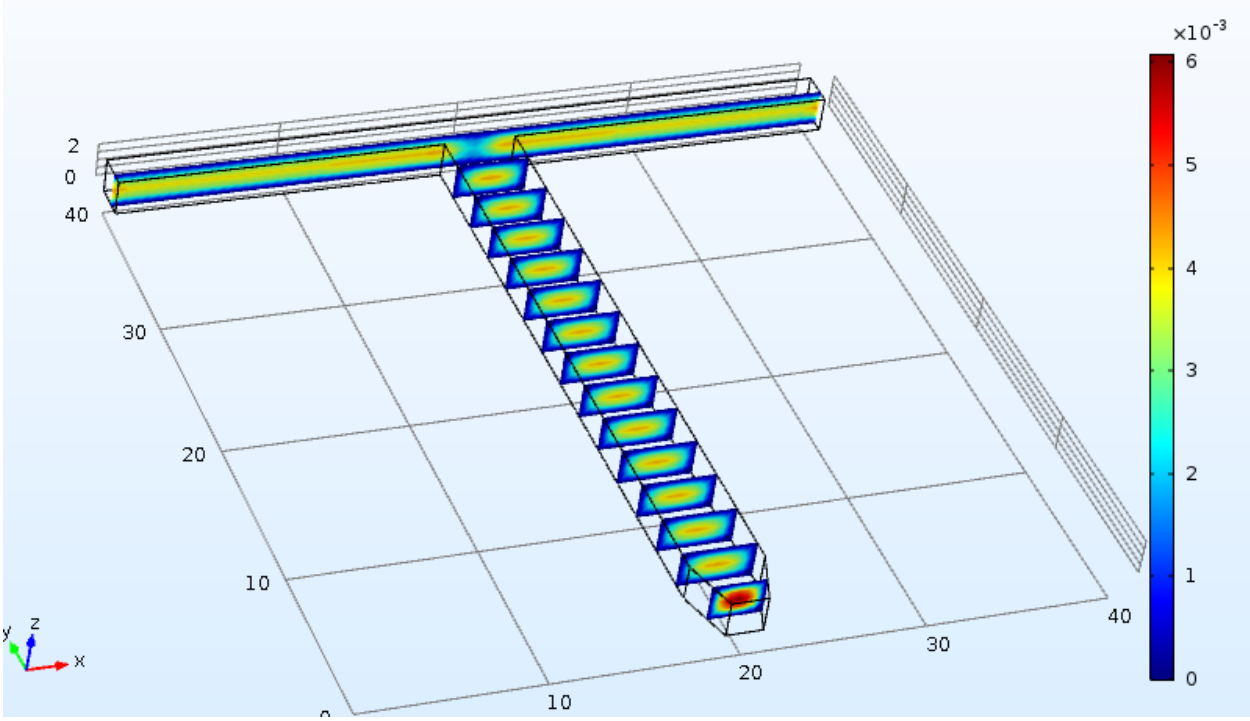
3. Next, we'll look at the velocity profile.

a. To make life easier, we'll just duplicate one of the concentration plots you just made. Rename this plot "**Velocity**".

b. For each of the slices, replace the expression with the expression for "**Velocity Magnitude**". To change, highlight the current expression and click on the red/green arrow "Change Expression" button. Then expand "Laminar Flow" and select "Velocity Magnitude." (see screen shot on next page)



c. In the plot, you should see low flow rates at the edges of the walls, but higher flow rates in the middle of the channel:

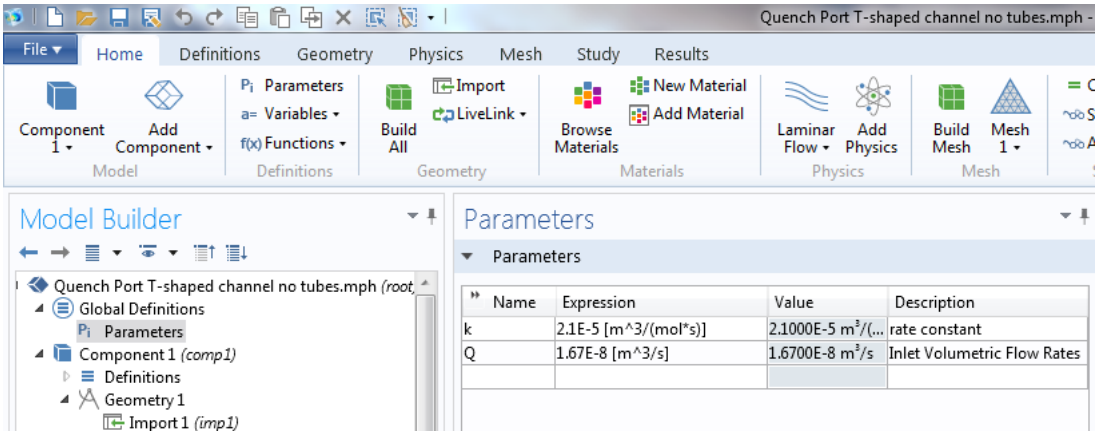


4. Last, we want to look at the outlet concentrations so we can have a better understanding of the reaction conversion and better optimize our operating parameters.
   a. First, we'll look at the average outlet concentrations. We'll look at the outlet concentration of the product.
   b. COMSOL will calculate the average outlet concentrations. Right click on "**Derived Values**" under the "**Results**" node and select "**Average**" and then "**Surface Average**". Rename this however you like, e.g. "Product Surface Average".
   c. Select the microreactor outlet face (face 8) so that it appears in the "Selection" space. Make sure you have the correct variable in the "**Expression**" space (cProduct). Click the orange equal sign "**Evaluate**" button to calculate the surface average. It should appear in the table under your graphics window.
   d. Right click and duplicate this surface average and repeat these steps for NaOH (rename and use cNaOH for your expression).
   e. You can also use these derived values to calculate the outlet molar flow rate (concentration average x total outlet volumetric flow). For the NaOH, you can compare this to the inlet molar flow rate (inlet concentration x inlet flow rate) to determine the reaction conversion.

5. Additional data for plots:
   a. To view any calculated variable at defined coordinates, right click on "**Data Sets**". Select "**Cut Point 3D**". Enter the desired coordinate. Right click on "**Derived Values**". Select "**Point Evaluation**". Select the point you want to evaluate in "**Data set**". Choose either the variable you would like as "Expression". Hit the orange "Evaluate" (equal sign) button at upper left.
   b. You may also find Cut Lines, Cut Planes, or Surfaces to be useful for generating plots – just choose those instead of Cut Point and specify your desired coordinates.
   c. To make a plot from scratch, right click on "**Results**" and select the plot type you might want. We have been using 3D plots for the previous selections, but you can use 1D plots to make line plots of different variables along Cut Lines.

You can do a parameter sweep – for this example we'll look at how changes in the flow rate affect the reaction.

1. In the "Parameters" node under "Global Definitions," define your flow rate variable name (e.g.: Q for volumetric flow), an initial number to use (with units), and a description.



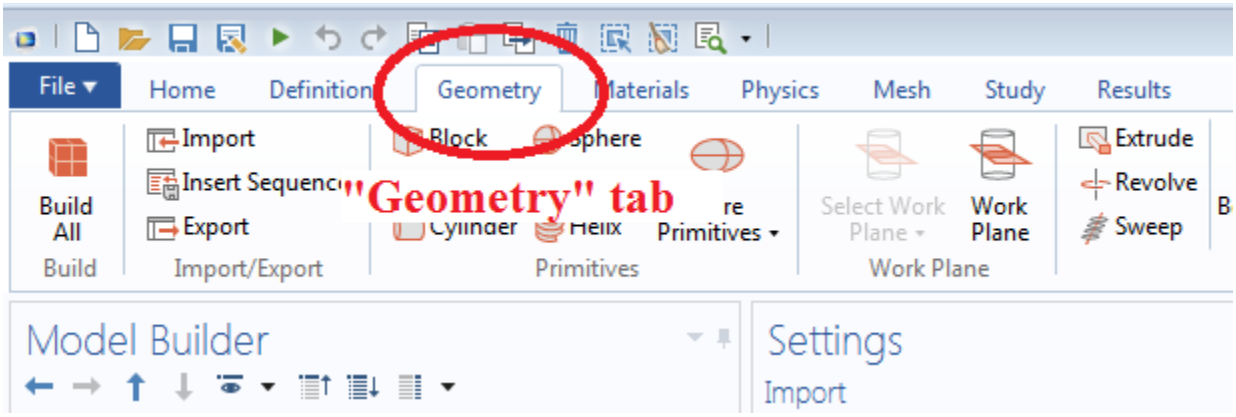
2. Make sure you use this new parameter name for your laminar flow inlets and anywhere else you may have put in a number for your volumetric flow rate.
3. Right click "**Study 1**" and select "**Parametric Sweep**".
4. In the "**Parametric Sweep**" tab, click the plus sign and select the parameter name you assigned from the list (i.e., Q). In the "**Parameter Value List**" you can write out each of

the values you wish to test, or if you select the button that looks like a miniature graph, you can type in a start, stop, and step that you wish to test.

5. Hit the "**= compute**" button when you're ready, but be aware that this may drastically increase the computation time.
6. For your plots, data sets, and derived values, make sure you have the correct solution selected in the "Data Set" drop down at the top of the tab – often when you do a parameter sweep, this will make a whole new solution. You can tell you did everything right if there is another drop-down menu beneath the "**Data Set**" one called "Parameter Selection" and you can pick which parameter value you want to look at.
7. It might be particularly interesting to look at changes in your conversion rates and outlet molar flow rates of your products and reactants – use this to think about how you might want to optimize your operating conditions!

To find dimensions and volume of reactor in COMSOL:

1. In the Graphics View of your reactor, there are selection tools in the toolbar. Use these to select edges, faces, or domains.



2. Under the "Geometry" tab, select the tool called "Measure." Based on your selections from step 1, it will tell you the length of the line, area of the face, or surface area and volume of the domain.