Simulating microfluidics in COMSOL

Department of Biomedical Engineering

LTH, Lund University

Introduction

In this lab, you will get acquainted with COMSOL Multiphysics, a program package that uses the Finite Element Method (FEM) to numerically solve partial differential equations and thus physics problems. The COMSOL software is partitioned into so-called *modules* that make it simple to stepwise increase the complexity of the models.

In this first lab, you will study a microfluidic chip using numerical simulations. You will compute the velocity fields and visualize the laminar flow inside a microfluidic chip. Then we will look at diffusion and convection processes inside the chip.

First, we will solve a stationary problem and then we will calculate time-dependent solutions and animate the flow fields. Due to the limited time available for the lab exercise, we will only use 2D-simulations. Although, the workflow for setting up 3D simulations is very similar to the 2D case, they require much more computational power.

The typical workflow in COMSOL is as follows:

1. Chose the appropriate physics module
2. Set up the model geometry
3. Enter material parameters
4. Define boundary conditions
5. Mesh the geometry
6. Compute the solution
7. Visualise the solution

Simulation software packages are powerful tools that can give you clues on the best way to design a system. However, a simulation always contains simplifications and is a more or less accurate representation of reality.

The COMSOL program is available for all LTH-students through the computer management group (DDG) at http://program.ddg.lth.se. Follow the instructions for students and download version 6.2. The required modules are (1) CFD, (2) Chemical Reaction Engineering, and (3) Particle Tracing. Note that if you run a newer or older version than Comsol 6.2, the instructions may differ slightly. Comsol requires that your computer is either located on Campus or connected via (how to set up VPN). The option using *Forticlient* seems to be the more stable way to go if there are problems.

Examination

The examination takes place on Zoom and you explain what you did and the results individually to a supervisor. Make sure you have documented the results for instance by taking screen dumps of the different plots. Make sure you have answered all the questions marked **Q#**.

Model wizard

1. Start COMSOL version 6.2. Save new versions of your file every ~30 minutes. This way you can always go back to a previous version in case you run into problems.
2. Click on *File > New > Model Wizard***,** and COMSOL will guide you through the mandatory steps in building your model.
3. In the Model Wizard, click on *Space Dimension 2D*.
4. Expand *fluid flow > single phase flow,* click on *laminar flow* and press the 'add'-button. We have now specified that we want to investigate fluid flow in the laminar, i.e. non-turbulent, regime. Here, we are only interested in single phase flows. A two-phase flow such as oil and water together in a channel would be modelled using the multiphase flow option.
5. Press the *Study* button.
6. Select *stationary* as the study type. This way the time derivatives are dropped from the equation and the results show the steady state. We include the time dependency at a later stage, for now press the *Done* button.

You may need to change the graphics settings

If you experience any of the following issues it may be necessary to change the default graphics settings in COMSOL. (1) The graphics window is black, (2) It is not possible to mouse-select objects in the graphics window, (3) The COMSOL application crashes unexpectedly, for example directly after mesh generation or after a simulation has completed. (4) COMSOL starts and then disappears without error messages. (5) The graphics window is scrambled, shows unwanted artifacts, or there are other graphics issues. In the menu bar, go to *File>Preferences>Graphics* and Plot Windows. Change Rendering from *OpenGL* to *Software* instead. Click Ok. Save the simulation file with a suitable filename, then restart COMSOL. Open the saved file.)

Setting up the simple geometry

We will start by setting up a simple channel geometry. The channel is 6 cm long (L), 800 μm high (H) and, in this example, infinitely wide.

7. Expand *Global Definitions* and select *Parameters*. Then add a parameter with *Name*: L and *Expression*: 6 [cm]. Add a second parameter H = 800 [μm] (note: in COMSOL you can use [um] to denote μm). It is good practice to define parameters that are kept constant throughout the study in this Parameter list.
8. Under *Component 1*, right-click on *Geometry 1* and select *Rectangle*. Now a rectangle named *Rectangle 1* appears under *Geometry 1*.
9. Go to the *Settings* menu of the *Rectangle 1* and set the width to L and height to H. Edit the corner position of the rectangle to be at (0, -H/2) so that the channel is centred around the x-axis. Press *Build Selected*.

Figure 1 The geometry inside the Graphics panel after step 9.

10. To specify the liquid in the channel right-click *Component 1/Materials > Add Material from Library*. In the rightmost panel on the screen, under the *Add Material* menu, select *Liquids and Gases>Liquids> Water*. After selecting water as a liquid for the model, click on *Add to Component.*

Boundary conditions

Boundary conditions define the variables on the boundary of the model and are needed to achieve a unique solution to the partial differential equation. Choosing boundary conditions is an important modelling task that requires a very good understanding of the underlying physics.

11. Under *Component 1* expand the *Laminar Flow (spf)* tab. Left click on *Laminar Flow (spf)* and expand the *Equation* tab to have a look at the equation that COMSOL solves.
12. Underneath *Equation* expand the *Physical Model* and set *Compressibility* to *Incompressible flow*.
13. Open the *Fluid properties 1* tab, chose *User defined* in the *Temperature* tab and set the value to 293.15 [K]. Check that the values for the density and viscosity are taken from the material (water).
14. Under the *Laminar Flow (spf)* tab, click on *Wall 1*. By default, the *No slip* boundary condition is applied to all 4 boundaries of our microfluidic channel.
15. Add an inlet to our channel by right clicking on *Laminar Flow (spf)* and selecting *Inlet*. Select the left boundary as inlet by left clicking on the corresponding boundary in the graphics window and then set the *Boundary Condition* to *Fully Developed Flow* with an *Average velocity* of 1 [mm/s].

Figure 2 Selecting the left boundary.

16. Add an outlet to our channel by right-clicking *Laminar flow (spf)* and selecting *Outlet*. Specify the right boundary and set the *Pressure* to 0.

Mesh

To solve our partial differential equation (PDE) with the finite element method the geometry is discretized using a mesh.

17. We start our analysis using a very simple mesh. Under *Component 1*, click on *Mesh 1* and set the *Element size* to *Finer*. Press the *Build all* button.
18. Zoom in on the channel and have a look at the mesh structure.

Solving the model

We are now ready to compute the solution.

19. Since we already selected a *stationary study* in the *Model Wizard*, all we need to do is right-click *on Study 1* under *Component 1*, and select *Compute (or simply press F8).* Just relax while COMSOL does the computations for you. If you have a slow computer, the meshing and solving can take some time. If it takes more than a minute, you can consider increasing the mesh size. Then your results will be less accurate.

Visualization and plotting

20. When the simulation is finished, a surface graph of the velocity field inside your chip will be shown on the screen.
21. Under *Component 1*, go to *Results* > *Velocity* > *Surface*. The default plot is the velocity magnitude (*spf.U*). You can select and change the plotted field by pressing the little *Replace Expression* button (red-green arrow logo) next to the *Expression* tab. Take some time and play around with different settings.
22. It is often helpful to add velocity vectors to the flow field. Right-click *Velocity (spf)* and choose *Arrow Surface*. Change the arrow *Color* to *Black* at the bottom of the *Settings* tab. Update by pressing *Plot* at the top of the tab. Adjust the number of arrows by changing the *Number of points* in the *Arrow Positioning* tab.
23. To measure a quantity, you can either look at the colour legend at the right side of the screen, or you can click somewhere in the graph and get a point-value presented in a table at the bottom of the screen.

A cross-section plot of the channel will give a clear picture of the velocity profile in the channel.

24. Right-click on *Data Sets* under the *Results* menu and select *Cut Line 2D*. Enter the values as shown in Figure 3 and then click *Plot*.

Figure 3 The input data for step 24.

25. Add a line plot by right clicking on *Results* and add a *1D Plot Group*. Under *Data*, select *Dataset: Study1/Solution 1(sol1)*.
26. Right-click on the new *1D Plot Group* and select *Line Graph*. This will add a new tab, *Line Graph 1*, under the *1D Plot Group* tab.
27. Click on *Line Graph 1*, and select *Data set>Cut Line 2D*.
28. Under *y-Axis Data*, in *Expression*: enter the x-component of the velocity field *u*.
29. Under *x-Axis Data* in *Parameter*: choose *Expression* and type in *y*.
30. Click *Plot*, then examine the velocity profile.

Q1. What shape does the velocity profile have?

Q2. Does the velocity profile change along the channel length? (tip add more cut lines)

31. Make a horizontal cut line **along** the channel and examine the pressure drop along the flow in the channel.

Q3. How does the pressure change along the channel length?

Q4. How does the pressure depend on the distance from the walls?

Parametric Sweep

32. We would like to study the influence of the fluid viscosity to the flow profile in our chip using a so-called Parametric Sweep. First, introduce a new parameter eta = 1 [mPa*s] in your parameter list (*Global Definitions>Parameters*).
33. Under *Component 1>Laminar Flow>Fluid Properties*, set the *Dynamic viscosity* to *User defined* and type in the parameter *eta*.
34. Right-click *Study 1* and select *Parametric Sweep*. Add the parameter *eta* by clicking the plus sign under *Study Settings*. Type 1, 2, 3 in the *Parameter value list* and enter mPa*s as *Parameter unit* and compute the solution.

Q5. How does the pressure drop along the channel scale with viscosity?

Reminder: Log your results and save versions of your file every 30 minutes

Convection and Diffusion

In COMSOL it is relatively simple to add multiple physical phenomena to a single model. The first model consisted of a single *module* to simulate the laminar fluid flow in a channel. We now add another *module* to study diffusion as well.

35. For this part we use a more detailed channel structure. Download from Canvas and open the file *SIM_lab_trifurcation_channel_comsol61.mph* in the Simulationlab-folder on your desktop (use a version that is lower than your installed Comsol version).
36. Under *Results*, investigate velocity field near the trifurcation inlet.

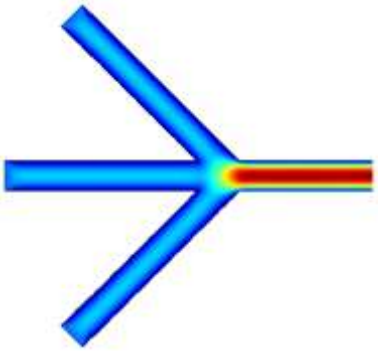

Figure 4 Snapshot of the velocity field at the trifurcation inlet. Red and blue indicate a high or low velocity amplitude, respectively.

37. Right-click on *Component 1* and choose *Add Physics*.
38. In the panel to the right of the screen, choose *Chemical Species Transport>Transport of Diluted Species*, then click on the *Add to Component 1* button. A new entry appears in the *Model builder* menu, we now have a new entry under *Component 1* called *Transport of Diluted Species (tds)*.
39. Right-click on the *yourfilename.mph* at the top of *Model Builder*, and then click on *Add Study*.
40. Select *Stationary* under the *Add Study* tab in the panel to the right of the screen and click *Add Study*.

First, we set the diffusion coefficient and couple the diffusion module to the laminar flow module that we have previously solved.

41. Go to *Global Definitions > Parameters* and add the diffusion coefficient Dc = 1*10^(-9) [m^2/s] to the list.
42. Add our diffusion constant to *Transport of Diluted Species > Transport Properties 1 > Diffusion*.
43. Under *Convection* select *Velocity Field (spf)* as our velocity field. This way, molecules will be transported along the channel by the previously simulated velocity field while they undergo diffusion.
44. Select *Water (mat1)* to be our *Material.*
45. For now, we assume isotropic diffusion.
46. To set the diffusion in- and outlets, right-click on *Transport of Diluted Species* and select *Inflow*.
47. Add the two side inlets, Boundary 4 and 6, to the list and set the concentration to 1 mol/m^3.
48. Right click on *Transport of Diluted Species* again, choose *Outflow* and select all outlets. The central inlet can also be selected as an outlet although no molecules will escape that way due to the inflow of water.

We only solve the diffusion problem since the velocity profile has already been computed.

49. Expand *Study 1* and select *Step1: Stationary*. Under *Physics and Variables Selection*, disable Transport of diluted species and make sure that laminar flow is enabled. Now go to *Study 2* and *Step1: Stationary* and disable Laminar flow and leave *Transport of diluted species (tds)* enabled. Near the bottom of this tab, you will find something called *Values of Dependent Variables*. Under *Values of variables not solved for>Settings*, choose *User controlled*. Then

Method: Solution, *Study: Study1* and *Selection: Automatic*. These settings allow Study 2 to use the results from Study 1 for the consecutive computations.

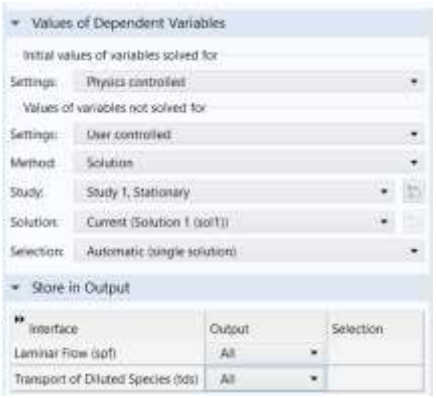

Figure 5: Values of Dependent variables.

50. Right click on *Study 2* and choose *Compute*.
51. Under *Results* section a new tab named *Concentration* will appear. Click on it to visualize the diffusion process along the channel. Some distortions, caused by a too coarse mesh, can sometimes be seen in the channel or at the inlets. Then try to make a smaller mesh by selecting *Extra fine*.

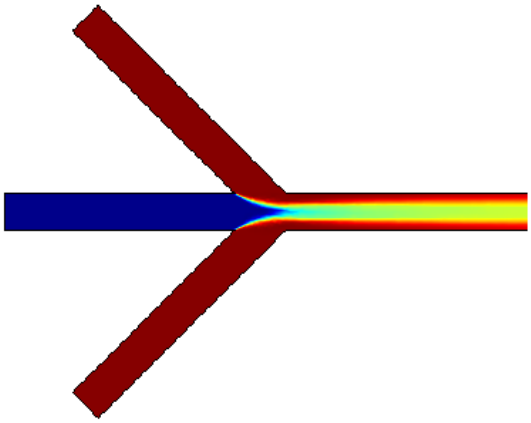

Figure 6 Ilustration of the diffusion process along the channel. Red and blue indicate high and low concentrations, respectively.

52. Investigate the influence of the diffusion coefficient on the concentration field by configuring a parametric sweep [e.g. Dc = 1*10^(-9), 1*10^(-8)]. If you get this Error: Failed to find a solution for the initial parameter. Then try making the mesh finer and re-compute both solutions.
53. Use the previously defined *Vertical Cut Line 2D* to add a cross-section plot. Reconfigure the settings of *Results>Data Sets>Vertical Cut Line 2D*. Under *Data*, select *Data set: Study2/Solution 2 (sol2)*. Do the same change for the horizontal cut line.
54. Click on *Results>Vertical Cut Line 2D>Line Graph 1*. Under y-Axis Data, click on the *Replace Expression* arrows and select *Transport of Diluted Species>Species c > c-Concentration*. Or just type in *Expression: c*.
55. Click Plot, then examine the concentration profile at different distances from the inlets. The graph is automatically scaled and sometimes does not cover more than a few decimals.

Q6. How does increasing the diffusion constant by a factor of 10 affect the concentration profile?

56. Examine the pressure along a horizontal cut-line from the central inlet to the outlet.

Q7. Why is the pressure gradient steeper in the main channel as compared to the central inlet?

Even if the mesh is set to *Finer*, there are only a few nodes across the channel height. Proper meshing is very important in FEM simulations and typically the mesh needs to be refined in regions where the computed variables have strong gradients.

Time-dependent simulations

Time-dependent simulations are more computationally demanding than their time-independent counterparts. However, in certain setups, we must explicitly consider the time-dependency. We will now study the time-dependent dispersion of a plug of molecules in the channel. You will be able to select both the time interval and the number of time-steps. To save some time during the lab we will cut our geometry in half and only study the inlet.

57. Go to *Geometry 1* and add a new *Rectangle*. Set the rectangle to have a width of L/2 and a height of H*20. Set the corner to be at (L/2, -H*10). Press *Build Selected*.
58. Now right click on *Geometry 1* and select *Booleans and Partitions>Difference*.
59. By left clicking on the geometry in the graphics window: 1. add our original structure, *uni1*, to *Objects to add* and 2. add the new rectangle, *r3*, to *Objects to subtract*. When you click *Build Selected*, everything inside the new rectangle is deleted from our structure.

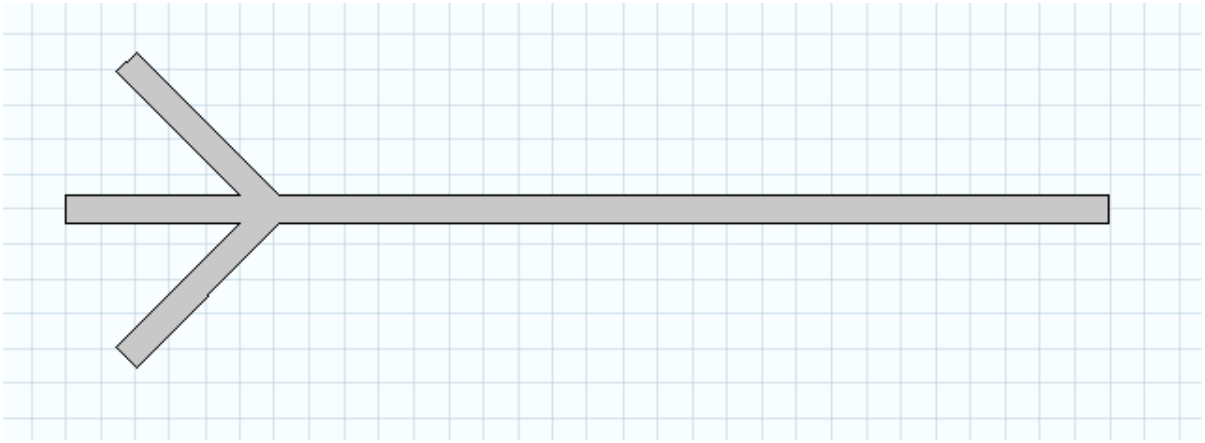

Figure 7 The geometry after the difference is applied.

60. Since we deleted our outlets, we need to go back to the *Laminar flow(spf)* tab and reassign the outlet boundary.
61. Go to *Transport of Diluted Species (tds)* and reassign the outflow for the molecules.
62. Since we cut our channel in half, we will have to solve the laminar flow problem again. Start by right clicking *Study 1* and choose *Compute*.

Since the velocity field is time independent, we will perform the time-dependent study only for the diffusion problem.

63. Right-click on the file name at the top of the *Model Builder, select add study*. In the panel to the right select *time dependent* and click *Add Study*.
64. *Step 1: Time dependent* from the new *Study 3*. Set the range to 0:1:10 seconds. If you want a larger time span, or a finer time resolution, you can go back and change this value later.
65. To use the previously calculated velocity field, disable the *Laminar Flow* in the *Physics interface* and set *the Values of variables not solved for* to *User controlled*, *Solution, Study1: Stationary, Automatic (single solution)*.
66. Now right-click on *Study 3* and choose *Compute*. It will take a little longer to compute as COMSOL computes 10 solutions, one for each time step.

67. As soon as the simulation is finished, the solution at the very last time step is shown by default. Look at *Concentration (tds) 1*. In the *Time* drop-down menu, you can select the solutions from 0-10 s, and then click *Plot*. Or you can click the arrows next to *Plot* to step through time.

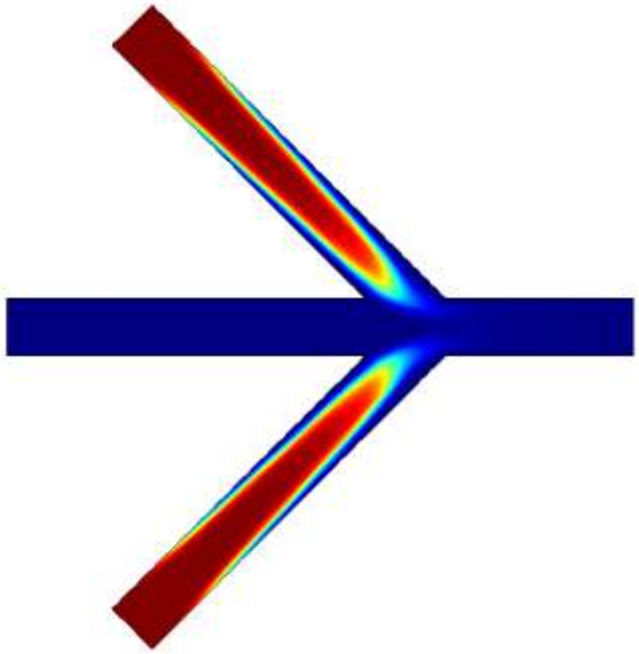

Figure 8 The concentration profile in the channel at t=4s. Red and blue indicate areas of high and low concentration, respectively.

Animation

The animation feature can be used to visualize time-dependent processes.

68. On the *Results tab*, right-click *Export* and choose *Animation>Player*.
69. In the new menu that appears, choose *Subject: Concentration (tds) 1*. COMSOL automatically chooses the time instants that your time dependent simulation ran over. If you wish to animate only a time interval, you change the settings under *Animation Editing*.
70. To start the animation, click on the *Play* button in the *Graphics* window.
71. If you wish to export the animation as a movie, you can right-click *Export* and choose *Animation>File* instead of the *Player*.

Particle tracing

In a next step, we add particles to the flow field. Using COMSOL, we can choose between particles with and without mass. The particle tracing can be done either in stationary or time-dependent mode. If you choose a stationary solution, you will only see the streamlines that the particles would follow. In a time-dependent solution, you can see and follow the particles as they move along the channel.

72. To add a particle tracing to our time dependent diffusion solution, right click on the *Concentration (tds) 1* under *Results* and click *More point plots > Particle tracing*.
73. COMSOL automatically applies the fluid velocity field as the driving mechanism for the particle trajectories. Under *Particle Positioning* you can choose where to "inject" the particles into the system. This can either be done at a boundary or selected coordinates.
74. To inject the particles into the central inlet, choose *Start point controlled* as *positioning setting* and put *L*/20 as x-value. For the y-axis, put 10 values between *–H*/2 and *H*/2 (range(-H/2, H/9, H/2)). When entering the values, click on the menu on the right-hand side, choose the start value, end value and the number of values in between. Make sure that *Number of values* is chosen as input method.
75. The release time can be controlled under the *Release* menu. For the moment, we leave it as it is.
76. Under *Coloring and Style* we can add a *Point style: Point,* so we can see the particle easier. Choose point under type, set the radius to H/20 and specify a scaling factor of 1. Chose a line color.
77. When you click on *Plot*, the particle positions for the chosen time will be displayed together with their corresponding trajectories.

Dispersion

Another example of a time-dependent solution is the dispersion of a ”concentration plug” that enters our channel.
We simply introduce a time dependency for a given parameter by using the COMSOL-variable *t*. For instance, by multiplying a parameter with the expression ($\underline{t} < 1$), it will only have this value for times between 0 and 1. You can use the syntax stated here but this will often lead to problems with discontinuities at the end values.
In COMSOL you have the possibility to use smoothed Heaviside functions to achieve a smoother transition between the Boolean states.

78. Go to *Transport of Diluted Species > Inflow*. Change the concentration value from 1 to 1*(flc2hs(t [1/s]-0.5,0.5)-flc2hs(t [1/s]-1,0.5)). This way we will create a ”pulse” of amplitude 1 between times 0.5 and 1. The second value (0.5) is a smoothing parameter.
79. Under *Study 3*, refine the time step to 0:0.1:10 s and *Compute*.
80. You can now either study the dispersion by looking at the surface plots or you can animate the process.

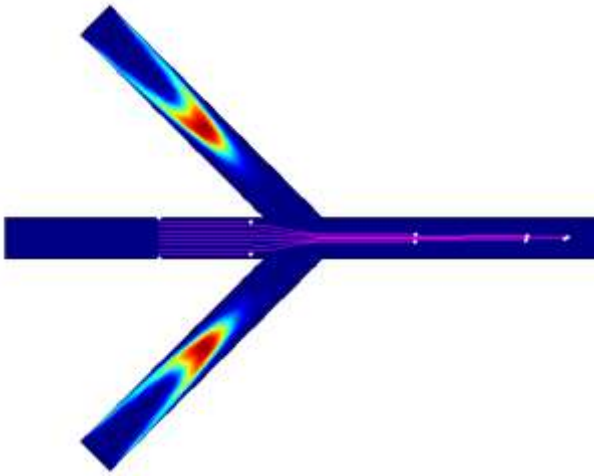

Figure 9 Convection diffusion of a concentrated plug.

Application Libraries

In COMSOL, there is a rather large library of solved problems. You can find the library under *File > Application Libraries*. Look through the different examples and see how the professionals have solved their problems.

Summary

You have now tried different modelling and simulation techniques in COMSOL. No matter the problem you are trying to solve, the approach is almost always the same: draw your model, set the boundary conditions, set the subdomain settings, add a mesh, compute the solution and visualize the field that you are interested in.

Getting a solution in COMSOL does not necessarily mean that it is a true representation of a real system. Do not trust the simulations blindly. You can have missed a step, made a wrong assumption or the solution might not have converged. Correctly used, however, a simulation can be a powerful tool to visualize concepts that are otherwise hard to grasp and it can strengthen the link between theory and experiments.