# Solutions to the diffusion equation with Comsol

Comsol is a finite element software. You can use it to obtain numerical solutions to the diffusion equation (and many other equations). In some of the cases below (where the geometry is simple) these solutions exist in analytical form. We will use the software to gain intuition about the behavior of solutions. We will demonstrate Comsol use in class and use it throughout the course. Comsol can be pretty easy to learn and can solve a number of problems quite readily. It can be sometimes be hard to force it to do what you want. Don't get too frustrated and please seek help if you get stuck. The purpose of using finite element software in this course is to gain some insight into solutions, not to master the software.

Don't get too worried if you can't force the graphics and plots to do exactly what you want. If your graphs are a little clunky, you can print and annotate things by hand. If on any given problem, you find there is something more interesting to look at than what I selected here, go for it. The questions and things for you to explore are only suggestions. It is always best to do some simple estimates first - i.e. for a transient problem estimate how long it might take and object to equilibrate before solving so you know how long in time to solve for. The default for comsol is to solve a transient problem for 1 second - this will not be appropriate for most problems. For this set of problems we will select at the beginning of creating a new model, "Chemical species transport", "Transport of diluted species".

Finally, you don't have to do all the problems here. Give yourself a budget for time, work that much and then put it away. If you get stuck on the software, ask google for help. If you can't figure it out in a reasonable amount of time ask someone else before randomly clicking for two hours. Ask a friend or one of your friendly instructors. Generate a few plots for whatever problems you work and just show us that you spent time doing this. Also, the questions here are written intetionally in a somewhat vague form. The goal is to learn the software, explore diffusion, and see you can use the simulation to help guide some intuition.

## I. DIFFUSIVE MASS TRANSFER

1. Solve the following problem numerically with Comsol.

$$\frac{\partial c}{\partial t} = \mathcal{D}\frac{\partial^2 c}{\partial x^2}$$

$$c(t=0,x)=0; \quad c(t,x=0)=1; \quad c(t,x=5cm)=0;$$

   Solve the problem on the domain $0 < x < 5$ cm. Set the properties to that of salt in water, $\mathcal{D} \sim 10^{-9}$ m$^2/s$. Adjust the time of the solution to capture the most interesting transients. Based on what we have done already, check that your answers are sound. Explore the evolution of the concentration field to gain some intuition. Try adjusting the initial and boundary conditions. Try changing the diffusivity to see if the diffusion time scale estimate $\tau \sim L^2/\mathcal{D}$ is reasonable.

   How would you make this problem dimensionless? How do you change the Comsol simulation to dimensionless form? What is the final equilibrium state, without Comsol?

2. Solve the 2D steady state diffusion equation on a dimensionless square, 1x1. The dimensionless diffusivity is 1. Set three of the boundaries to have a concentration of 0 and the other one to have a concentration of 1. Plot contours of constant concentration as well as the mass flux vectors. Look at the concentration field as a mesh plot to explore what a zero curvature surface looks like (remember, at steady state the field has no curvature).

3. Consider the 1D diffusion equation on a domain that extends sufficiently far for the length scales of interest (could assume infinite). The equation is

$$\frac{\partial c}{\partial t} = \mathcal{D}\frac{\partial^2 c}{\partial x^2}$$

   on the domain $0 < x < \infty$. Initially the concentration of the whole domain is 0. The boundary condition at $x = 0$ is

$$c(x=0,t>0)=1$$

   In the simulation, make the domain sufficiently large such that the solution could be considered the same as you would have on an infinite domain. Plot the concentration as a function of time at various instances in time.

Make the equation dimensionless and solve it in comsol. If the diffusivity were $\mathcal{D} = 10^{-9}\ m^2/s$, how far would the diffusion layer penetrate after 1 day, 1 week, and 1 year?

This situation has a known analytical solution

$$c(x,t) = 1 - \text{erf}\left(\frac{x}{\sqrt{4\mathcal{D}t}}\right)$$

where erf is the error function. You can look up the definition of the error function and MATLAB or Wolfram Alpha will know how to plot it. Compare Comsol to the analytical solution.

4. Imagine a spherical micro-organism that is unable to move in an stationary liquid environment. The organism consumes dissolved oxygen. The diffusivity of oxygen in water is $\mathcal{D} = 2 \times 10^{-9}\ m^2/s$. Take the concentration of dissolved oxygen in the bulk liquid to be 1. Assume the organism consumes oxygen fast enough that it maintains the concentration of zero at it's surface. The organism is 2 microns in radius, $a$. Therefore you will want to solve

$$\frac{\partial c}{\partial t} = \nabla^2 c$$

where $c(\mathbf{r}, t = 0) = 1$, $c(r = a, t > 0) = 0$, and $c(r \to \infty) = 1$. Solve the transient problem (you can use 2D axisymmetric). How long does it take for the result to reach a steady state?

Look up the $\nabla^2$ operator in spherical coordinates. Assuming spherically symmetric and steady state, by hand, compute the radial concentration distribution and compare to comsol. Note that the two solutions should be the same, however you may notice some departure depending on the finite size of the computational domain. Using your analytical solution, can you come up with a formula for the rate of uptake of oxygen by the organism?

Using comsol, try changing to some ellipsoidal shapes and observe whether or not the shape has much influence.

## II. CONVECTIVE MASS TRANSFER

Mass transfer is significantly modified by fluid motion. Using Comsol we can introduce fluid motion quite easily, again using the "Transport of diluted species" model.

We will do all these problems in dimensionless form. Set up a 2D rectangle to be 2 units high (in the y-direction) by 20 units long (in x-direction). The vertical dimension of the domain should go from -1 to 1. You can just leave comsol in units of m and we will control the important dimensionless parameter via changing the diffusivity by hand (rather than using a built in material property). Once you have the geometry specified, under "transport of diuted species" on the left, select "transport properties". Set the velocity field to be a parabola, $u(y) = 1 - y^2, \quad v = 0$, where $u$ and $v$ are the $x$-$y$ components of velocity respectively. We will soon learn why the parabolic velocity profile holds when we have flow between two plates. For now, just trust us. Set the diffusivity to be 0.01 initially, but you will change this parameter. Solve the following problems.

1. Solve a transeint problem. Set the $y = 1$ and $y = -1$ boundaries to be no flux (the default). Set the $x = 20$ boundary to be outflow. Set the $x = 0$ boundary to be $c = 1$. Change the integration time to be 50. Run the simulation and watch the animation. After running with $\mathcal{D} = 0.01$, change $\mathcal{D} = 0.001$, then 0.00001. Observe the behavior. This simulation is dye being introduce to a channel flow.

2. Solve a transeint problem. Set the $y = 1$ and $y = -1$ boundaries to be no flux (the default). Set the $x = 20$ boundary to be outflow. Set the $x = 0$ boundary between $0 < y < 1$ to be $c = 1$. Set the $x = 0$ boundary between $-1 < y < 0$ to be $c = 0$. Change the integration time to be 50. Run the simulation and watch the animation. After running with $\mathcal{D} = 0.01$, change $\mathcal{D} = 0.001$, then 0.00001. Observe the behavior. This problem is dye introduced to a channel flow, only the top half and bottom half of the channel has different concentrations.

3. Solve a steady state problem. Set the $y = 1$ boundary to be no flux (the default). Set the $x = 20$ boundary to be outflow. Set the $x = 0$ to be $c = 0$. Set the $y = -1$ to be $c = 1$. After running with $\mathcal{D} = 0.01$, change $\mathcal{D} = 0.001$, then 0.00001. Observe the behavior. This problem is setting the concentration of the lower wall to introduce the dye, while the inlet is a fluid with no dye.

4. Solve a transient problem. For this one, it will help to make the channel a little longer, say 50 units of length. Set the $y = \pm 1$ boundaries to be no flux (the default). Set the $x = L$ boundary to be outflow. Set the $x = 0$ to be $c = 0$. For this one, the initial condition will be zero everywhere, except for a small region between

$4 < x < 6$. After running with $\mathcal{D} = 0.01$, change $\mathcal{D} = 0.1$, then 1 and observe the behavior. In the transient solver, change the time scale such that the plug reaches the end of the channel. This is a classic problem called Taylor dispersion (yes, the same Taylor) and we can discuss the relevance in class.