Examples for calculations with Comsol

A. Friction of a sphere. Check with a Comsol simulation that the friction of a Sphere in laminar flow is 6*Pi*eta*r*v with radius r, velocity v, viscosity eta. Choose a good symmetry to make the calculation fast (3D is not the way to go). You will see that the boundaries has to be chosen rather far away to minimize the error. Make a parameter variation simulation that varies the simulation box and plots the error from above analytical expression with respect to the size of the simulation box.

B. Design a microfluidic mixer. Two laminar flows (10µm/s flow speed) should be mixed within a minimal time and volume. What are good geometries of mixing? First start with a T-mixer and change the geometries to your taste.

C. Convective PCR. Make a laminar convection cell between 95°C and 60°C and implement into this cell a convective PCR reaction. Use diffusion coefficients for 10mer, 100mer and 1000mer of DNA and assume a replication speed of 50 bases per second. Think of the kinetic rate equations for the replication. To model the DNA, assume a constant, near-diffusion limited kon-rate (the experimental value is 0.1..1.5 1/(µM*s) according to e.g. doi:10.1093/nar/gkl422 or doi:10.1093/nar/gkt687) and an exponentially varying koff with the rough formula koff in 1/s given by 10^([Temp[°C]-20°C]/10°C + 3 - #Bases/2). While this formula is OK for short DNA, you might need to research a better formula for longer strands. Check that it shows a reasonable melting transition first by plotting the probability of double stranded DNA with respect to the total concentration of DNA– it should be between the warm and cold temperatures of your convective PCR. If above formula does not work in your hand, use a temperature dependent koff that gives you a melting transition that match published data. Alternatively, you can add thermophoretic accumulation – or even combine both.

D. Insulation around a window. Insulation of houses is very important to fight against climate change. Typically, 30-40cm of insulation is added to the outside (Do you know why insulation from the inside will rot your house if you do not make it absolutely air tight? Perhaps you can speculate why this is the case). Now since the windows are typically exchanged against insulating 3-fold glasses, the question is where to put these windows: at the same location as before (say right in the center of the wall), or do you find less thermal heat flow if you move them say more to the inside or more to the outside? Make a parameter variation to plot the heat flow versus the location of the window. Do you understand the resulting curve?

E. Airplane wind tunnel. Make a wind tunnel of an arbitrary shaped airplane profile. Of course for simplicity you do this in 2D - neglecting the rotational flow at the end tip of the wing. The central parameter for constructing a good profile for an airplane is its behavior with respect to its angle of attack, i.e. the angle between the line through the center of the airfoil and the wind flow. You would want to calculate both the friction of the profile and its lift – the ratio between lift versus friction is a central design parameter to make an efficient wing. Make a variation of the angle of attack and plot both of above parameters. Of course you can calculate this only here for laminar flow, so choose an arbitrarily slow plane speed (compare it for example to a para-glider, one of the slowest airplanes).

F. Embryo gradients. In Drosophila embryos, a gradient of a protein is produced. It is both the result of the degradation of the RNA that makes the protein and the initial point-like concentration of RNA at one side of the Embryo. Think of a minimal model and assume a cylinder-symmetrical shape of the embryo. Some embryos can create a surface flow through the embryo by flow generated at its surface. Implement one of these flows and see how the gradient can be steepened by the flow. Use parameters from literature for your model (see e.g. Bicoid as model example).