Modeling an Electrochemical Printer (EcP)

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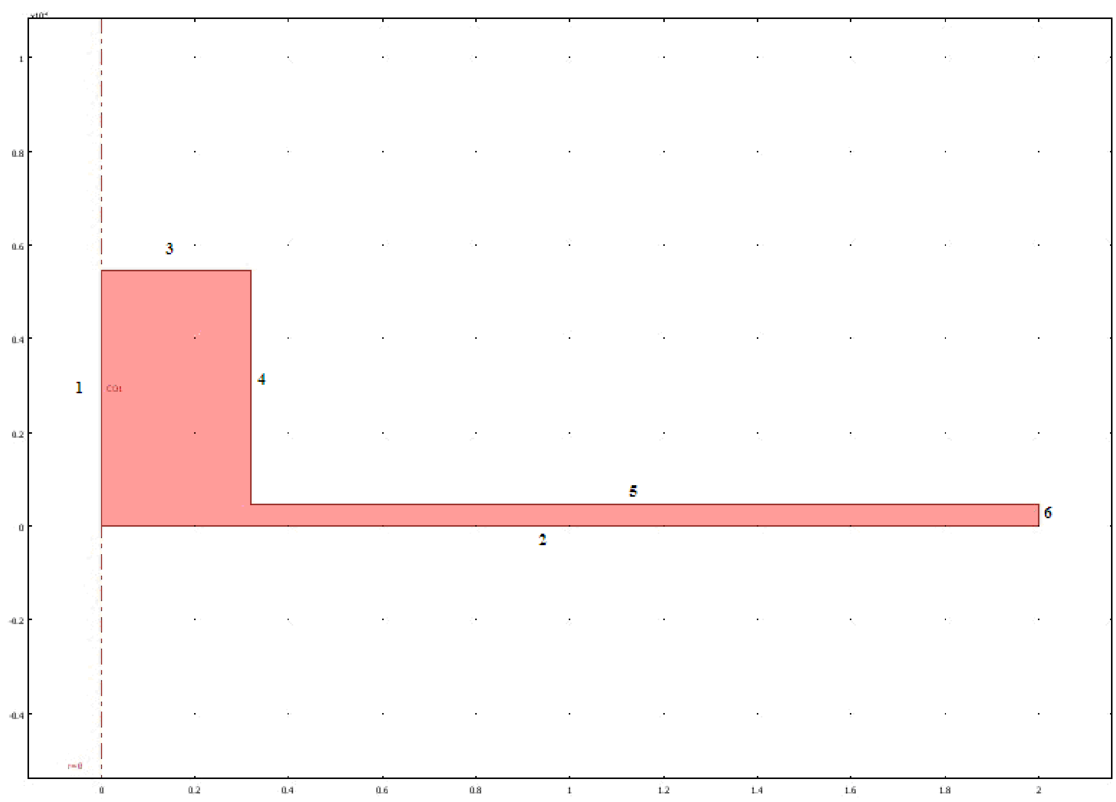
Introduction

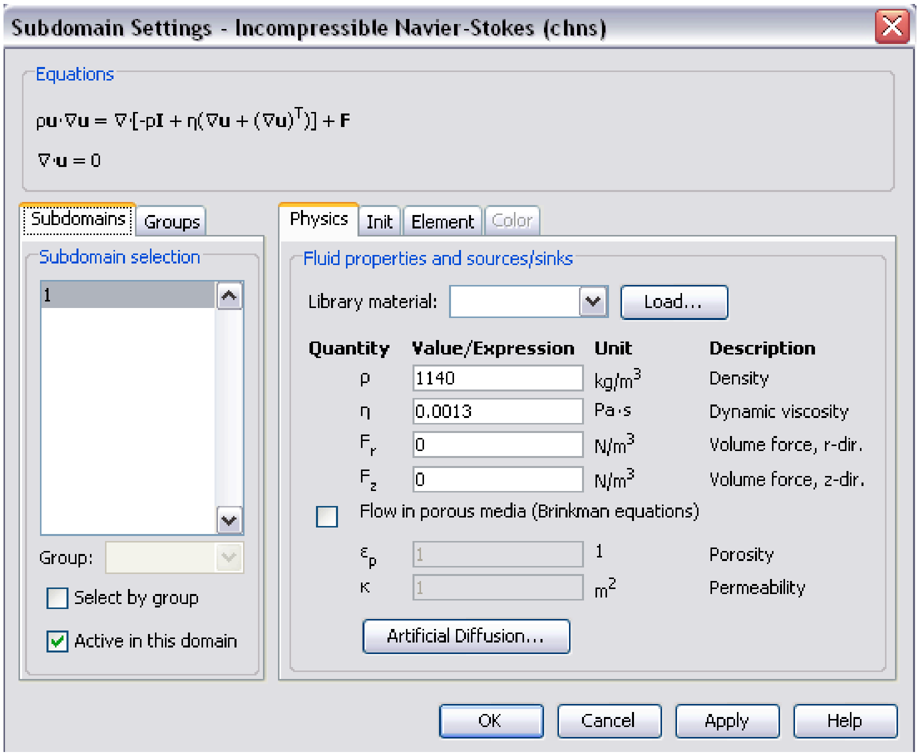
Electrochemical printing is a micro scale printing process that deposits metal ions onto conductive material with the oppositely charged jet nozzle. Experiments have been done previously to find out the general working conditions and components' dimensions. The object of this project is to extend the model developed previously by including the chemistries occurring on the print. Our goal is to get the model to converge at the most practical condition.

Method and procedure

A simulation was setup using an axial symmetric model with the upper boundary equals to 32E-6 and bottom boundary equals to 200E-6. Using the fly-height and radius ratio given from the previous experiment, the fly-height was set to be 4.48E-6, and the total height of the model was chosen to be 54.48E-6.



The fluid properties were input into the sub-domain settings with the properties of water.



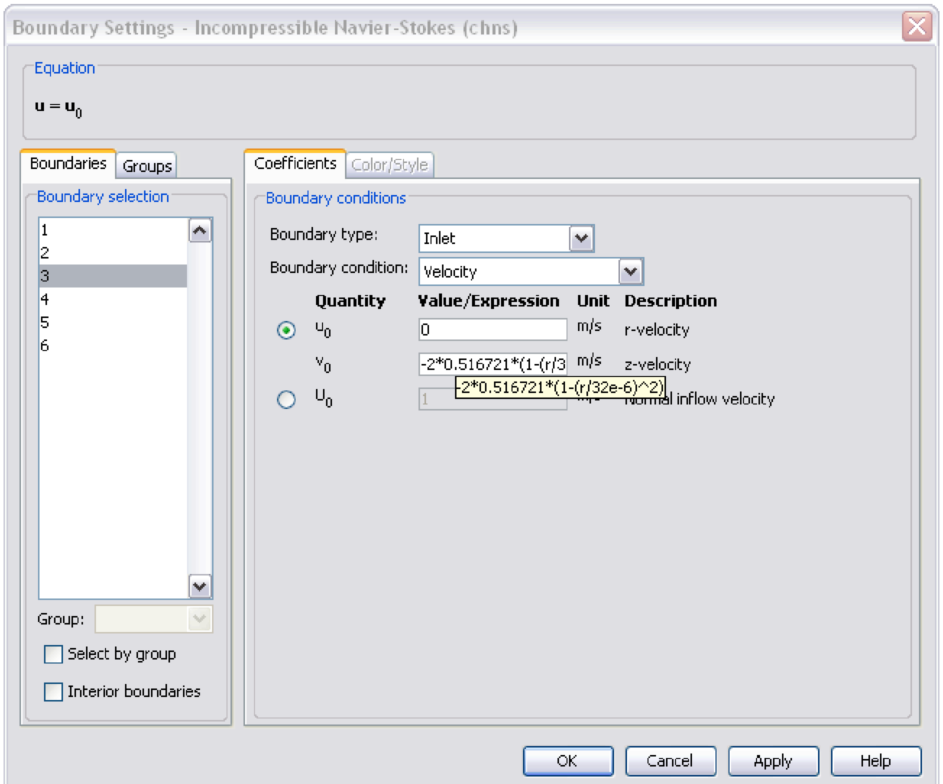
At the boundary settings, axial symmetry was set for boundary 1. Bounary 2,4, and 5 was set to be no slip. At the entrance of the fluid, which is boundary 3, a parabolic velocity distribution was set according to

$$v_0 = -2 < v > \left(1 - \left(\frac{r}{r_0}\right)^2\right)$$

, where <v> is the average z-velocity, r is the radius at any point, and r_0 is the radius at the opening. The average z-velocity was calculated from the Reynold's number,

$$Re = \frac{\rho < v > d}{\eta}$$

where ρ is the density, d is the diameter of the opening, and η is the viscosity. The Reynold's number that we chose is 29 so that the number we put into <v> is 0.516721.

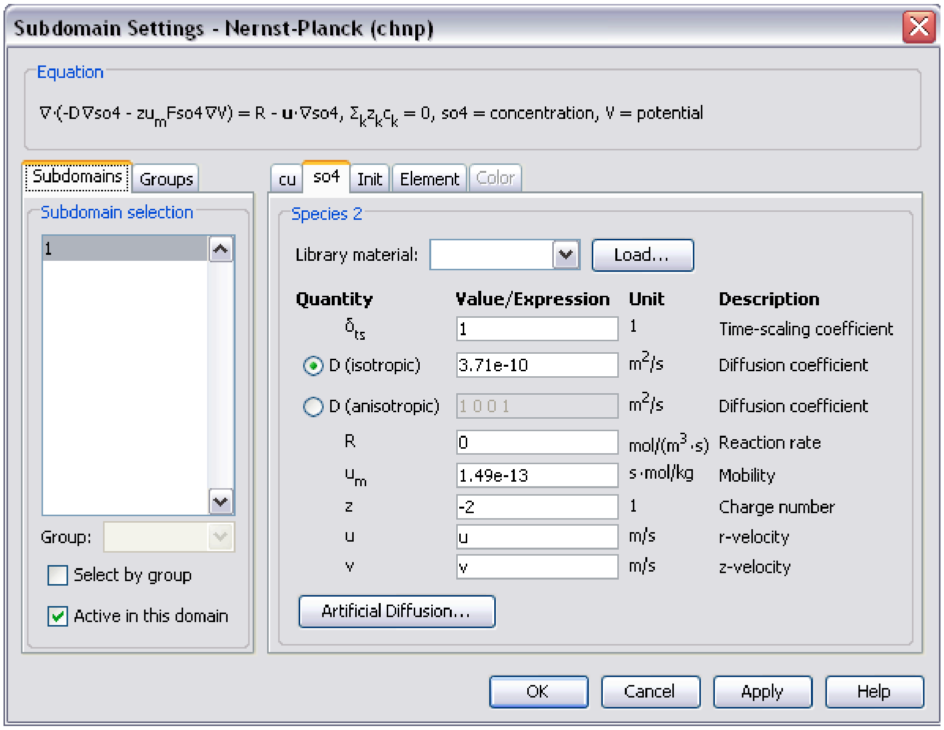


For the exit, boundary 6, atmospheric pressure was specified.

After the simulation was run till convergence, the current and concentration distribution was then setup using the Nernst-Planck simulation model with copper and sulphate as the only components. In the sub-domain settings, the diffusion coefficient and mobility of each species were entered according to the following table.

	Cu^{2+}	SO_4^{2-}
D_i (m^2s^{-1})	2.07E-10	3.71E-10
$u_{m,I}$ (mol $m^2J^{-1}s^{-1}$)	8.35E-14	1.49E-13
z	2	-2

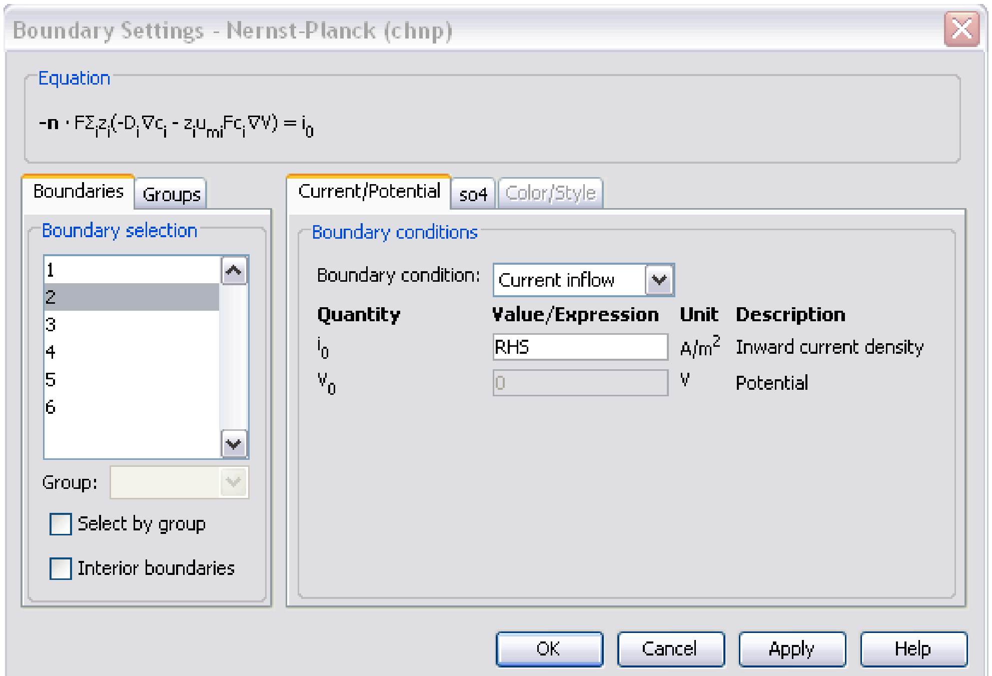
However, in order to get the model converge, the magnitude of the parameters were scaled up by 1000, and then scaled down by 10 till they went back to the actual values.

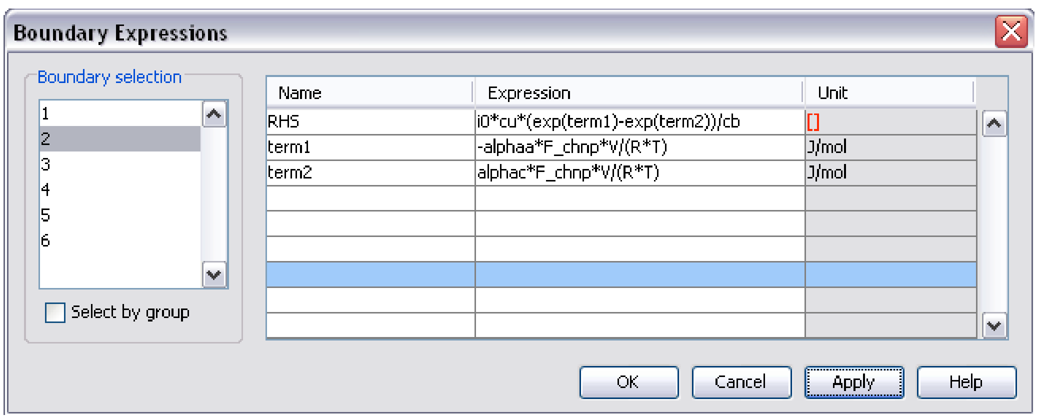


The neutrality equation, $\sum z_i c_i = 0$, is already implemented into the Comsel model; therefore, the boundary condition of the first component, which was copper for this experiment, will not be needed to be specified. The boundaries conditions for Current/ Potential are Electric insulation for boundaries 4, 5, and 6, and axial symmetry for boundary 1. On boundary 2, the inflow current density is specified as follow,

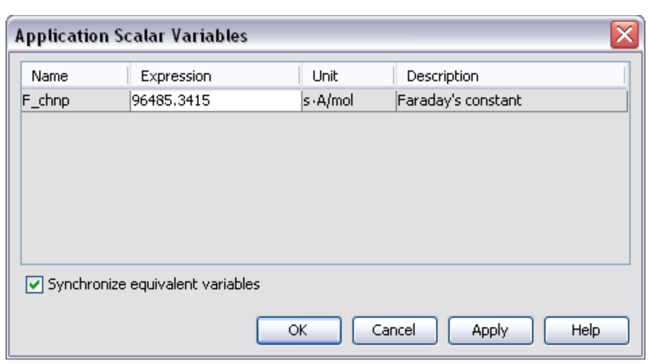
$$\mathbf{n} \bullet \sum_i z_i (z_i u_i F c_i \nabla V) = \frac{i_0}{nF} \left(\frac{c^s}{c^b}\right) \left[\exp\left(\frac{-\alpha_a F V}{RT}\right) - \exp\left(\frac{\alpha_c F V}{RT}\right) \right]$$

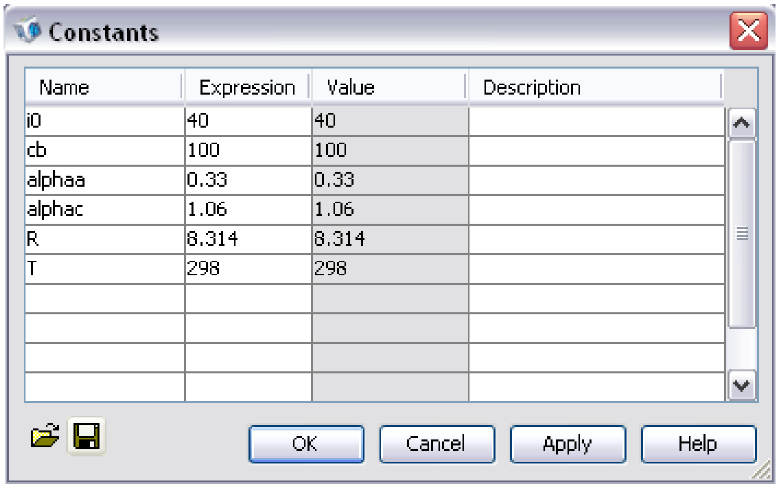
where i_0 is the exchange current density (A m-2), c^s is the cupric ion surface concentration, c^b is the cupric ion buld concentration, F is the Faraday's constant, n is the number of change per ion, V is the potential, R is the gas constant, T is the temperature, α_a_ is the anodic transfer coefficient, and α_c is the cathodic transfer coefficient.





However, in order to balance our equation with the unit given, we took out the nF, which turns the unit of the equation from mass flux to charge flux. The values of the parameters are as follow,





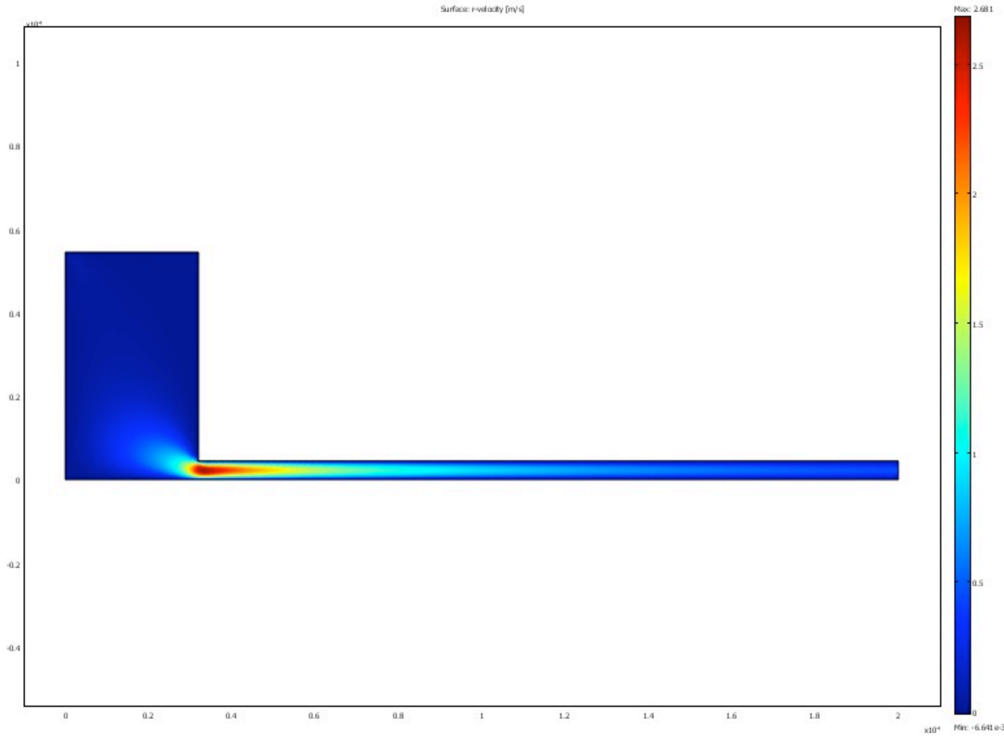
Constants

Name	Expression	Value	Description
i0	40	40	
cb	100	100	
alphaa	0.33	0.33	
alphac	1.06	1.06	
R	8.314	8.314	
T	298	298	

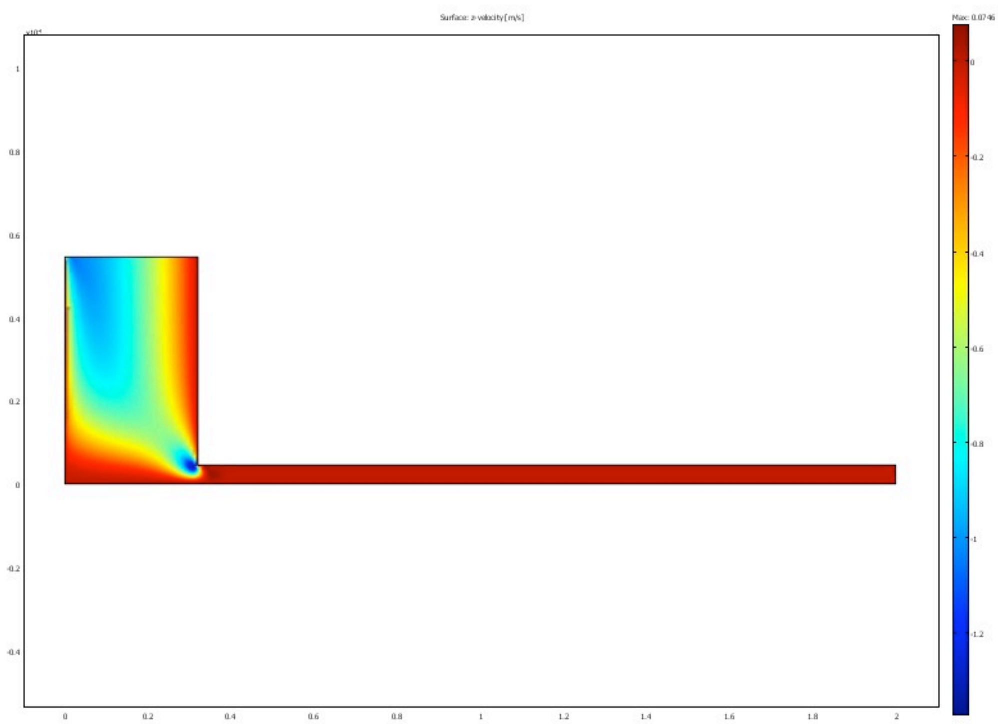
In order to approach the real scenario happening in the printing process, an apply inlet current density was chosen to be 1000A. For the convention/diffusion boundary settings, the flux on boundary 3 was specified as 0 since none of the ions is going in or out on the boundary. For boundary 6, convective flux was set, and for the rest of the boundaries, Insulation/Symmetry was set.

Results and discussion

The surface plot of the r-velocity profile is very smooth due to the number of mesh in the model. And we can see there is a dramatic increase of velocity at the constriction site at the entrance of the jet nozzle tip, where we would expect to see a big different on the deposit of ions before and after it. However, there is not much to see from the z-velocity profile because the velocity is very close to zero after the constricted site.

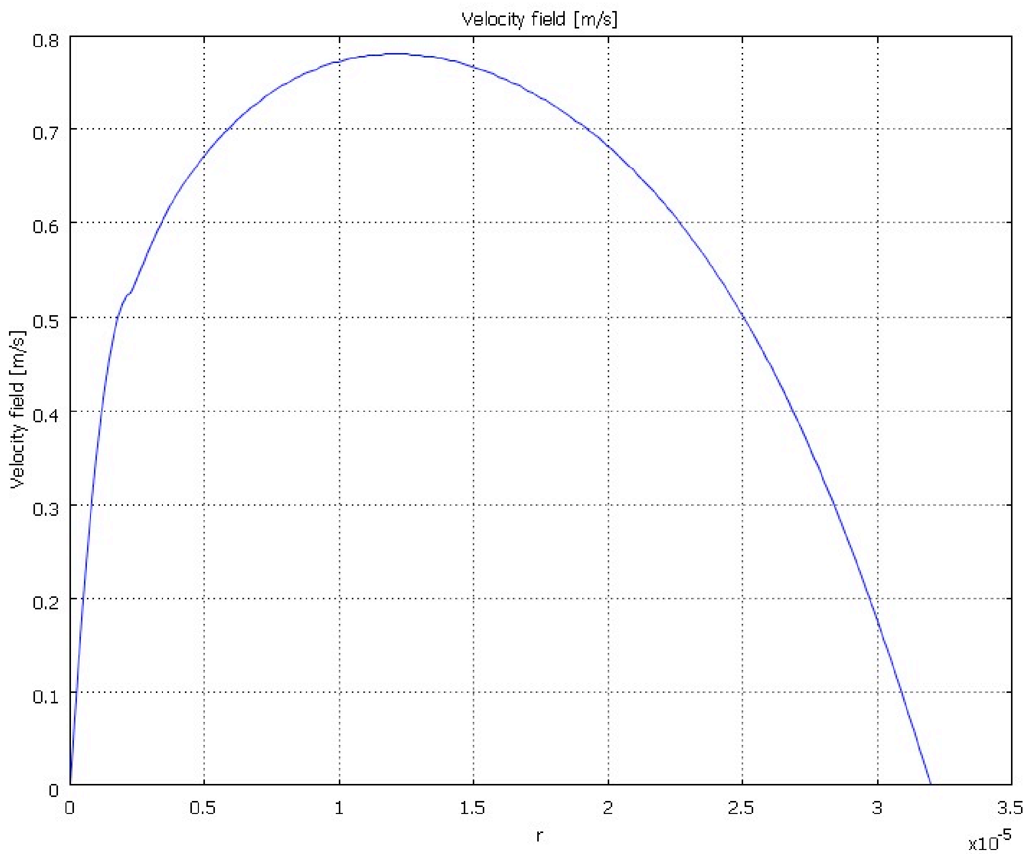


r-velocity surface plot

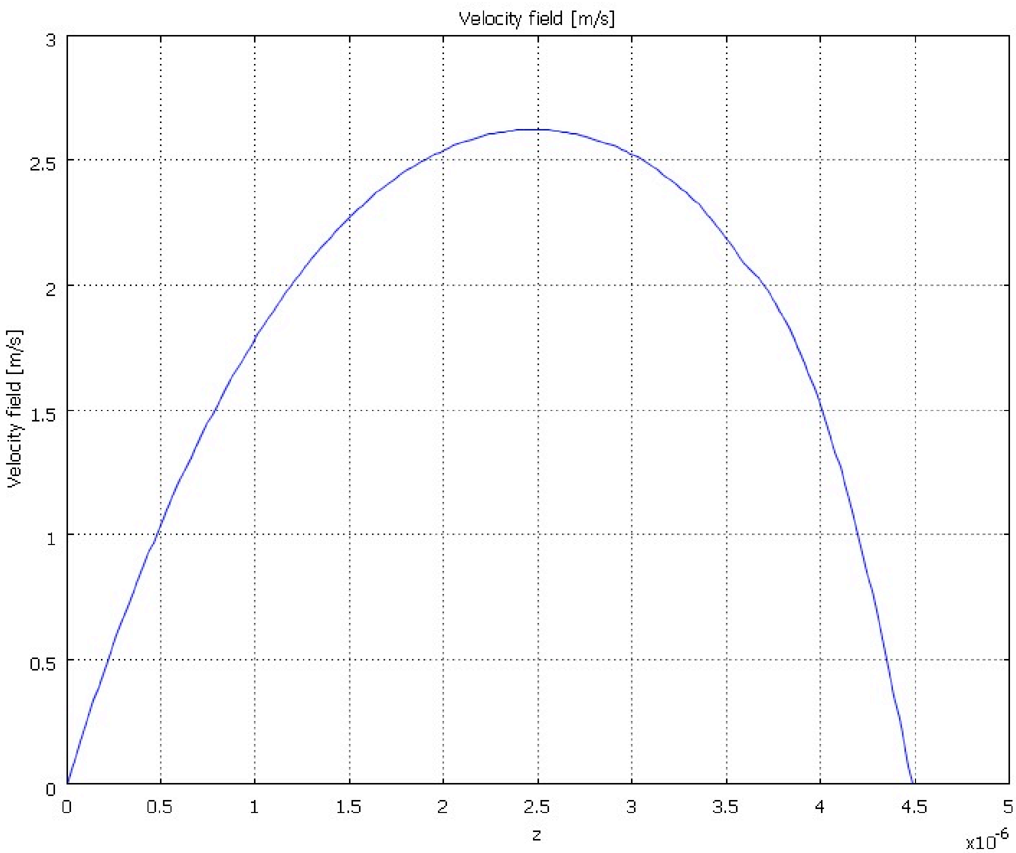


z-velocity surface plot

To confirm the flow was fully developed on everywhere in the model, we had plotted two cross-sectional graphs, one within the nozzle and one within the fly-height outside the nozzle. Both of them demonstrate a fully developed flow pattern.

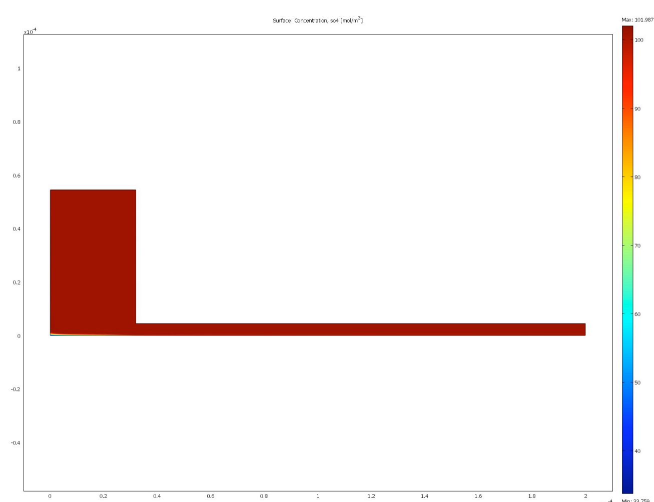


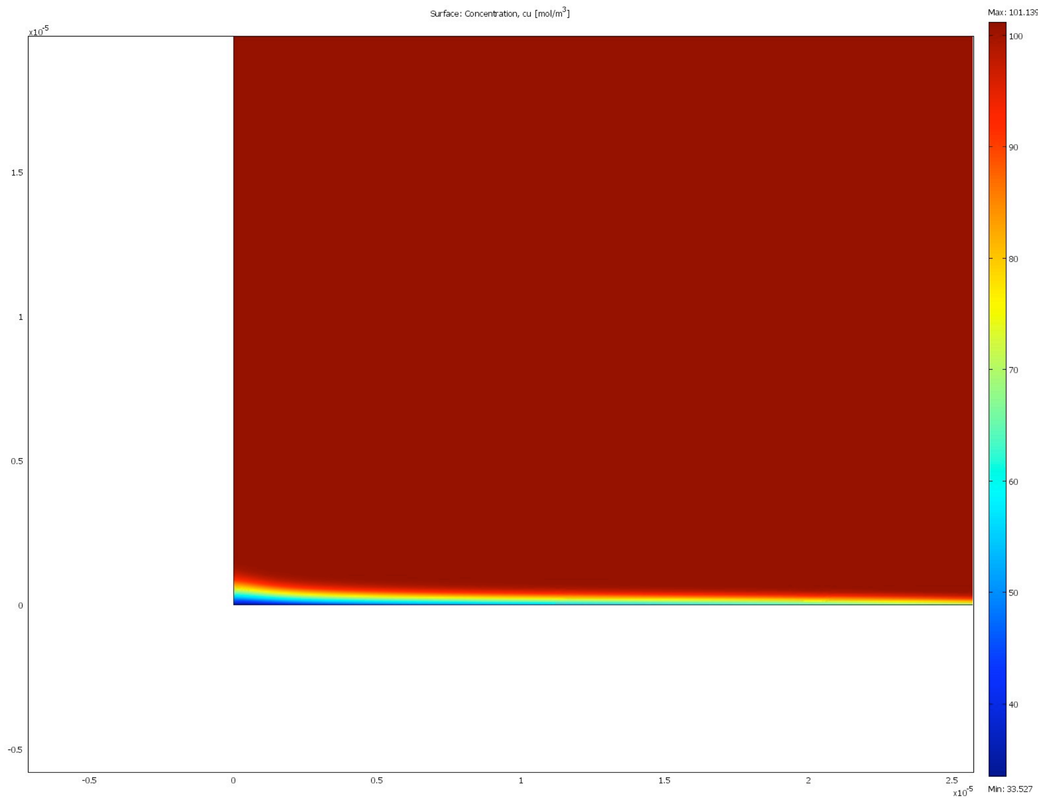
Cross-sectional plot for r-velocity with respect to radius inside the printer's nozzle



Cross-sectional plot for r-velocity with respect to height outside the printer's nozzle

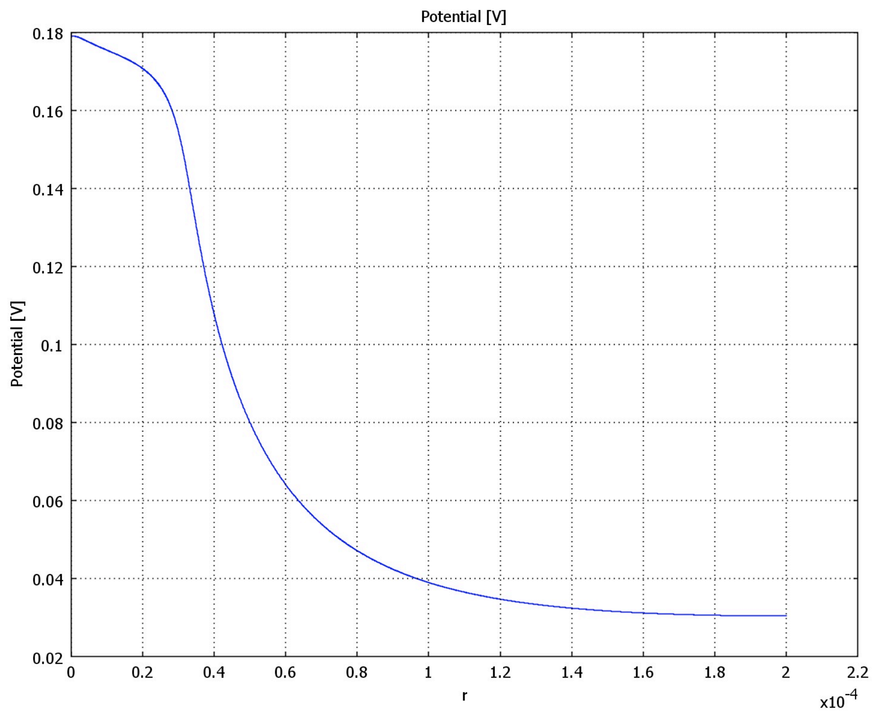
After confirming the flow pattern, we looked into the concentration profile of the model and plotted a surface plot for the concentration of copper with zoom up at the bottom right under the nozzle head.


Surface plot of the concentration of copper

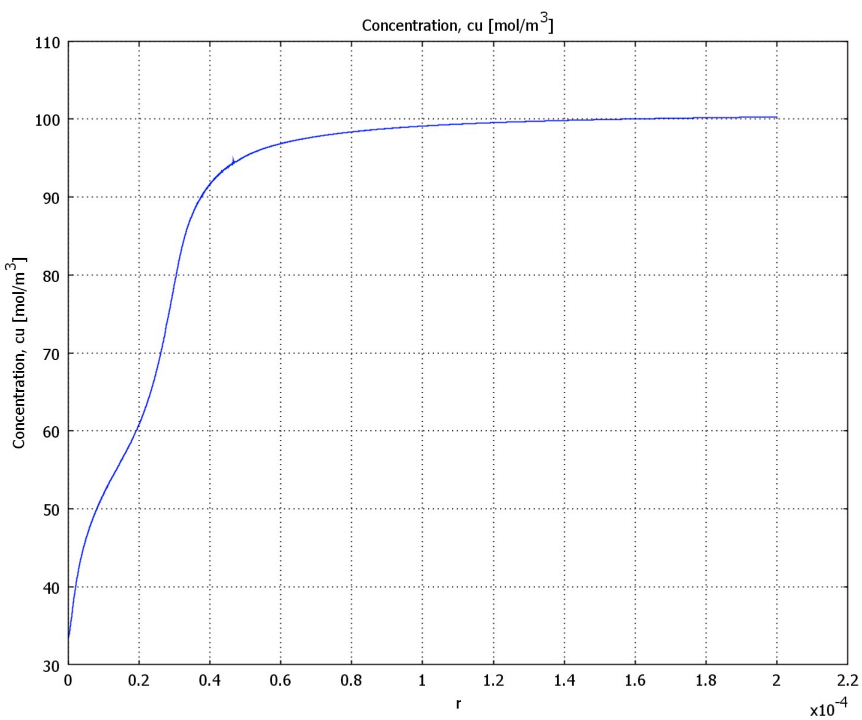


Close-up surface plot of concentration of copper at the bottom under the nozzle

We can tell that the reaction takes place at a very fast time in a very thin layer compare to the dimension of whole model. This could be resulted from the high current density and ultra-low diffusivity of the species, and so it is mass transfer limited. Next, domain plots were used to demonstrate the velocity profile and the copper deposition profile.



Domain plot of potential with respect to radius



Domain plot of concentration of copper with respect to radius

As we can see, the concentration of copper drastically increases back to the bulk concentration after the constriction site, which corresponds to the great drop in the velocity profile at the same area. And this proves that our expectation from the velocity profile was reasonable.

Conclusion

By comparing our result with the previous experiment, we concluded that our simulation was valid and the implementation of the Nernst-Planck was a success. However, future work can be done with different Re and fly-height to radius ratio to see how they changes the pattern of the deposit in order to manipulate different output patterns in the printing process.

References

[1] Jeffrey B Nelson, Zudtky Wisecarver and Daniel T Schwartz, Electrochemical printing: mass transfer effects. 2007.