

# Design of Integrated Microrobotic Fish

## Presentation 3 - Physical Model (Improving) & COMSOL Simulation (Debugging)

Yihua Liu

UM-SJTU Joint Institute

March 9, 2021

# Contents

- 1 Antecedent
- 2 Improved Model
- 3 COMSOL Simulation

# Antecedent

Total Impedance  $Z$

$$\text{In}[1]:= R = \frac{\text{Pi} * x * (\sqrt{k} + \frac{1}{\sqrt{k}})}{2\sigma * \delta x};$$

$$C_{DL} = \frac{\epsilon * \delta x * \sqrt{k}}{\lambda_D};$$

$$C_{DS} = \frac{\epsilon * \delta x}{\sqrt{k} * \lambda_D};$$

$$Z_x = R + \frac{1}{I * \omega * C_{DL}} + \frac{1}{I * \omega * C_{DS}}$$

$$\text{Out}[4]= \frac{(\frac{1}{\sqrt{k}} + \sqrt{k}) \pi x}{2\delta x \sigma} - \frac{i \lambda_D}{\sqrt{k} \delta x \epsilon \omega} - \frac{i \sqrt{k} \lambda_D}{\delta x \epsilon \omega}$$

$$\text{In}[10]:= \text{Simplify}[Z_x]$$

$$\text{Out}[10]= \frac{(1+k) (\pi x \epsilon \omega - 2 i \sigma \lambda_D)}{2 \sqrt{k} \delta x \epsilon \sigma \omega}$$

# Total Impedance $Z$

Remind the formula given in the article

$$Z = \frac{\pi \left( \sqrt{k} + \frac{1}{\sqrt{k}} \right)}{2l\sigma} \frac{\ln A - i\theta}{(\ln A)^2 + \theta^2}$$

where

$$A = \frac{\sqrt{\left[ (2\lambda_D\sigma)^2 + (\omega\varepsilon\pi)^2 + x_{min}x_{max} \right]^2 + [2\lambda_D\sigma\omega\varepsilon\pi (x_{max} - x_{min})]^2}}{(2\lambda_D\sigma)^2 + (\omega\varepsilon\pi x_{min})^2}$$

and

$$\theta = \arctan \frac{2\lambda_D\sigma\omega\varepsilon\pi (x_{max} - x_{min})}{(2\lambda_D\sigma)^2 + (\omega\varepsilon\pi)^2 x_{min}x_{max}}$$

The author probably made a mistake of  $A$ . The correct formula is

# Total Impedance $Z$

$$\ln[\cdot] = \left( \star A = \frac{\sqrt{\left((2\lambda_0 \star \sigma)^2 + (\omega \star \epsilon \star P i)^2 + X_{\min} \star X_{\max}\right)^2 + (2\lambda_0 \star \sigma \star \omega \star \epsilon \star P i (X_{\max} - X_{\min}))^2}}{(2\lambda_0 \star \sigma)^2 + (\omega \star \epsilon \star P i \star X_{\min})^2} \right); \star$$

$$A = \frac{(2\lambda_0 \star \sigma)^2 + (\omega \star \epsilon \star P i \star X_{\max})^2}{(2\lambda_0 \star \sigma)^2 + (\omega \star \epsilon \star P i \star X_{\min})^2};$$

$$\theta = \text{ArcTan} \left[ \frac{2\lambda_0 \star \sigma \star \omega \star \epsilon \star P i (X_{\max} - X_{\min})}{(2\lambda_0 \star \sigma)^2 + (\omega \star \epsilon \star P i)^2 X_{\min} \star X_{\max}} \right];$$

[反正切]

$$Z_0 = \frac{P i \left( \sqrt{k} + \frac{1}{\sqrt{k}} \right)}{1 \star \sigma \star (\text{Log}[A] + 2 I \star \theta)}$$

$$\text{Out}[\cdot] = \frac{\left( \frac{1}{\sqrt{k}} + \sqrt{k} \right) \pi}{1 \star \sigma \left( 2 i \text{ArcTan} \left[ \frac{2 \pi \epsilon \sigma \omega |X_{\max} - X_{\min}| \lambda_0}{\pi^2 \epsilon^2 \omega^2 X_{\max} X_{\min} + 4 \sigma^2 \lambda_0^2} \right] + \text{Log} \left[ \frac{\pi^2 \epsilon^2 \omega^2 X_{\max}^2 + 4 \sigma^2 \lambda_0^2}{\pi^2 \epsilon^2 \omega^2 X_{\min}^2 + 4 \sigma^2 \lambda_0^2} \right] \right)}$$

$$\ln[\cdot] = Z = \frac{1}{\int_{X_{\min}}^{X_{\max}} \frac{2 \sqrt{k} \epsilon \sigma \omega}{(1+k) (\pi X \epsilon \omega - 2 i \sigma \lambda_0)} dx}$$

$$\text{Out}[\cdot] = \frac{(1+k) \pi}{\left( \sqrt{k} \sigma \left( 2 i \text{ArcTan} \left[ \frac{\pi \epsilon \omega X_{\max}}{2 \sigma \lambda_0} \right] - 2 i \text{ArcTan} \left[ \frac{\pi \epsilon \omega X_{\min}}{2 \sigma \lambda_0} \right] + \text{Log} \left[ \frac{\pi^2 \epsilon^2 \omega^2 X_{\max}^2 + 4 \sigma^2 \lambda_0^2}{\pi^2 \epsilon^2 \omega^2 X_{\min}^2 + 4 \sigma^2 \lambda_0^2} \right] \right) \right) \text{ if } \text{condition} \star$$

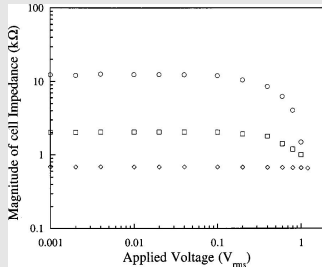
# Total Impedance $Z$

```

In[ ]:=  $\lambda_D = 4.56 * 10^{-9};$ 
 $\sigma = 0.018;$ 
 $k = 6.12;$ 
 $v_{Le} = 2.82 * 10^{-9};$ 
 $x_{min} = 1.6 * 10^{-6};$ 
 $x_{max} = 12 * 10^{-6};$ 
 $\Psi_0 = 0.1;$ 
 $\omega = 2 \text{ Pi} * 1000;$ 
| 圆周率
 $l = 0.235;$ 
 $c_0 = 299792458;$ 
 $\mu_0 = 4 * \text{Pi} * 10^{-7};$ 
| 圆周率
 $\epsilon_0 = \frac{1}{\mu_0 * c_0^2};$ 
 $\epsilon = 80 \epsilon_0;$ 
 $\frac{Z}{1}$ 
Zo
Out[ ]:= 667.159 - 1265.49 i
Out[ ]:= 667.159 - 1265.49 i

```

# Total Impedance $Z$



Here we restore the resistance to three-dimensional by dividing by the total length of the electrodes in the cell  $l = 23.5$  cm.

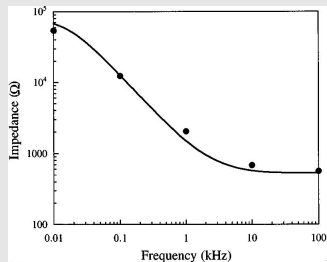
We again made a mistake here last time. What the paper gives in its FIG. 7. is the magnitude of cell impedance, i.e.,

$$\text{Abs}[Z] = 1430.58 \Omega$$

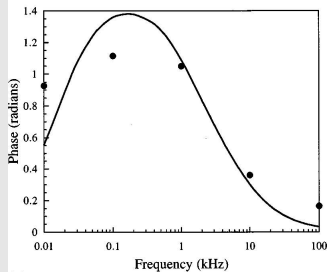
which is closed to the corresponding value in FIG. 7. We can directly found that the frequency is not correlated with the applied voltage.

Next, the left side is FIG. 8. in the paper and the right side is our result.

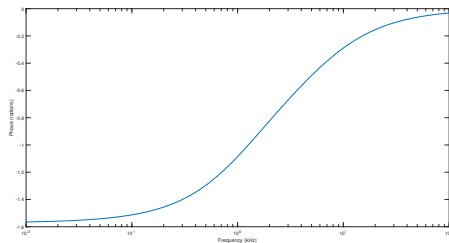
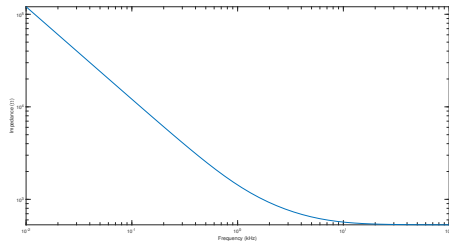
# Total Impedance $Z$



(a)



(b)





# Total Impedance Z

## MATLAB Code

```

lambda_D = 4.56*10^(-9);
sigma = 0.018;
k = 6.12;
v_L0 = 2.82*10^(-9);
x_min = 1.6*10^(-6);
x_max = 12*10^(-6); % Psi_0 = 0.1;
l = 0.235;
c_0 = 299792458;
mu_0 = 4*pi*10^(-7);
epsilon_0 = 1/(mu_0*c_0^2);
epsilon = 80 * epsilon_0;
f = logspace(1,5);
omega = 2*pi*f;
A = ((2*lambda_D*sigma)^2+(omega*epsilon*pi*x_max).^2)/((2*lambda_D*sigma)^2+(omega*epsilon*pi*x_min |
↪ ).^2);
% A = sqrt(((2*lambda_D*sigma)^2+(omega*epsilon*pi).^2*x_min*x_max).^2+(2*lambda_D*sigma*omega*epsilon*pi |
↪ pi*(x_max-x_min)).^2)/((2*lambda_D*sigma)^2+(omega*epsilon*pi*x_min).^2);
theta = atan((2*lambda_D*sigma*omega*epsilon*pi*(x_max-x_min))/((2*lambda_D*sigma)^2+(omega*epsilon*pi |
↪ pi).^2*x_min*x_max));
Z = pi*(sqrt(k)+1/sqrt(k))./(1*sigma*(log(A)+2i*theta));
figure(1);
loglog(f/1000,abs(Z)); % ylim([100,10^5]);
xlabel('Frequency (kHz)'); ylabel('Impedance (\Omega)');
figure(2);
semilogx(f/1000,angle(Z));
xlabel('Frequency (kHz)'); ylabel('Phase (radians)');

```



# Time-Averaged Velocity

Given  $v_{DL} = \frac{\lambda_D \rho_{DL} E_{HL}}{\eta}$ , how to derive its time-averaged value?

Note that both  $\rho_{DL} = \frac{\Psi_{DL} \varepsilon}{\lambda_D}$  and  $E_{HL} = -\frac{\Psi}{\sqrt{k(1+k)}} \frac{\frac{i\omega\varepsilon\pi}{2\lambda_D\sigma}}{(1+\frac{i\omega\varepsilon\pi x}{2\lambda_D\sigma})^2}$  have the part

$\Psi = \Psi_0 \exp i\omega t$ . Remind the method we use in calculating the time-averaged power:

$$\langle P \rangle = \frac{1}{T} \int_0^T V_0 I_0 \cos(\omega t + \phi_1) \cos(\omega t + \phi_2) dt$$

Using the formula

$$\cos(A + B) = \cos A \cos B - \sin A \sin B$$

we have

$$\langle P \rangle = \frac{1}{T} \int_0^T V_0 I_0 (\cos \omega t \cos \phi_1 - \sin \omega t \sin \phi_1) (\cos \omega t \cos \phi_2 - \sin \omega t \sin \phi_2) dt$$

# Time-Averaged Velocity

$$\begin{aligned} \langle P \rangle = & \frac{1}{T} \int_0^T (\cos^2 \omega t \cos \phi_1 \cos \phi_2 + \sin^2 \omega t \sin \phi_1 \sin \phi_2 \\ & - \cos \omega t \sin \omega t (\cos \phi_1 \sin \phi_2 + \cos \phi_2 \sin \phi_1)) dt \end{aligned}$$

Since  $\int_0^T \sin^2 \omega t = \frac{T}{2}$ ,  $\int_0^T \cos^2 \omega t = \frac{T}{2}$ , and  $\int_0^T \sin \omega t \cos \omega t = 0$ ,

$$\langle P \rangle = \frac{1}{2} V_0 l_0 (\cos \phi_1 \cos \phi_2 + \sin \phi_1 \sin \phi_2) = \frac{1}{2} V_0 l_0 \cos(\phi_1 - \phi_2)$$

Thus,

$$\langle P \rangle = \frac{1}{2} \text{Re} \left( l_0 V_0 e^{i\phi_1} e^{-i\phi_2} \right) = \frac{1}{2} \text{Re} \left( \tilde{l}_0 \tilde{V}_0^* \right)$$

Similarly, we can write

$$\langle v_{DL} \rangle = \frac{1}{2} \text{Re} \left\{ \frac{\lambda_D \rho_{DL} E_{HL}^*}{\eta} \right\}$$

# Improved Model

## Electrical Problem

Let's start from Poisson's equation:

$$\nabla^2 \phi = \frac{\rho}{\varepsilon} = \frac{e(n_- - n_+)}{\varepsilon}$$

and the continuity equation (charge conservation equation):

$$\nabla \cdot \mathbf{J} = -\frac{\partial \rho}{\partial t}$$

Remind in VE320 Chapter 5: Carrier Transport Phenomena 5.2 Carrier Diffusion 5.2.2 Total Current Density Eq. (5.36) is the sum of electric drift and diffusion density:

$$\mathbf{J} = en\mu_n \mathbf{E} + ep\mu_p \mathbf{E} + eD_n \nabla n - eD_p \nabla p$$

Adding drift due to the fluid motion:

$$\mathbf{J}_{\pm} = \mp en_{\pm} \mu \nabla \phi - eD \nabla n + en_{\pm} \mathbf{u}$$

where  $\mathbf{u}$  is the liquid velocity,  $\rho$  is the (volume) charge density.

# Electrical Problem

## Scales and parameters

Here to simplify our calculation, we use a dimensional analysis technique called "nondimensionalization" or "scaling" in order to suggest that certain quantities are better measured relative to some appropriate unit that is especially useful for systems that can be described by differential equations.

Next, we plan to use this method (or not) to calculate the electric field.

# Electrical Problem

The electrical potential in the bulk electrolyte satisfies Laplace's Equation

$$\nabla^2 \Phi = 0$$

$\Phi$  is the potential just outside the double layer.

Low voltage assumption: the voltage drop across the double layer is linear to the surface charge  $\frac{\partial q_s}{\partial t} = -\sigma E_y$ . The surface charge conservation equation:

$$\sigma \frac{\partial \Phi}{\partial y} = i\omega C_{DL}(\Phi - V_j)$$

Note that different from previous definition, here  $C_{DL}$  is the capacitance per unit of **area** of the total double layer.

Boundary condition at the interface between the electrolyte and the glass:

$$(\sigma + i\varepsilon\omega) \frac{\partial \Phi}{\partial y} = (\sigma_g + i\varepsilon_g\omega) \frac{\partial \Phi_g}{\partial y}$$

# Electrical Problem

Remind the Ampère's circuital law with Maxwell's addition (differential equations SI convention):

$$\nabla \times \mathbf{H} = \mathbf{J}_f + \frac{\partial \mathbf{D}}{\partial t}$$

Since the electric potential is alternating as  $\Phi = \Phi_0 \exp(i\omega t)$ ,

$$\mathbf{j} + \frac{\partial \mathbf{D}}{\partial t} = \mathbf{j} + i\epsilon\omega \frac{\partial \Phi}{\partial y} = (\sigma + i\epsilon\omega) \frac{\partial \Phi}{\partial y}$$

not to be confused with the electromagnetic wave  $E = E_0 \exp(i(\mathbf{k} \cdot \mathbf{r}) - \omega t)$ , which leads to  $\sigma - i\epsilon\omega$ .

# Electrical Prolem

Material	Conductivity $\sigma$ at 20 °C (S/m)
Glass	$10^{-15}$ to $10^{-11}$
Sea water	4.8
Drinking water	$5 \times 10^{-4}$ to $5 \times 10^{-2}$
Deionized water	$4.2 \times 10^{-5}$

Since  $\varepsilon_g \ll \varepsilon$  and  $\omega \ll \frac{\sigma}{\varepsilon}$ , we can simplify the equation to

$$\frac{\partial \Phi}{\partial y} = 0$$

Besides,

$$\int_{-\frac{l}{2}}^{-\frac{l}{2}} \frac{\partial \Phi}{\partial y} dx = 0$$



# Fluid Dynamic

Debye-Hückel theory: surface capacitance

$$C_{DL} = \frac{\varepsilon}{\lambda_D}$$

Helmholtz-Smoluchowski formula: electro-osmotic slip velocity

$$u = \frac{\varepsilon \Delta \Phi}{\eta} E_x = -\frac{\varepsilon \Delta \Phi}{\eta} \frac{\partial \Phi}{\partial x}$$

Using the same strategy introduced before, the time-averaged horizontal fluid velocity at the interface between the double layer and the bulk is

$$\langle u \rangle = -\frac{\varepsilon}{2\eta} \text{Re} \left[ \Delta \Phi \frac{\partial \Phi^*}{\partial x} \right] = -\frac{\varepsilon}{2\eta} \Lambda \text{Re} \left[ \Delta \Phi_{DL} \frac{\partial \Phi^*}{\partial x} \right] = -\frac{\varepsilon}{2\eta} \Lambda \frac{\partial}{\partial x} |\Phi - V_j|^2$$

$\Phi$  is the potential just outside the double layer;  $V_j$  is the potential applied to electrode  $j$ ;  $\Phi_{DL}$  is the total double layer potential drop.

# Fluid Dynamic

## The solution in the diffuse layer

The slip electro-osmotic velocity

$$\langle u \rangle = -\frac{\varepsilon}{2\eta} \Lambda \frac{\partial}{\partial x} [(\Phi - V_j)(\Phi - V_j)^*]$$

where  $\Lambda$  is the ratio of the diffuse double layer impedance to the total double layer impedance given by

$$\Lambda = \frac{(i\omega C_d)^{-1}}{(i\omega C_{DL})^{-1}} = \frac{C_s}{C_s + C_d}$$

where  $C_d$  and  $C_s$  are the capacitances of the diffuse layer and the Stern or compact layer respectively. Boundary condition:

$$\sigma \frac{\partial \Phi}{\partial y} = i\omega C_{DL}(\Phi - \Phi_g) = i\varepsilon_g \omega \frac{\partial \Phi_g}{\partial y}$$

# Fluid Dynamic

The solution in the bulk

Incompressible Navier-Stokes equations (convective form)

$$\overbrace{\rho \left( \underbrace{\frac{\partial \mathbf{v}}{\partial t}}_{\text{Unsteady acceleration}} + \underbrace{(\mathbf{v} \cdot \nabla) \mathbf{v}}_{\text{Convective acceleration}} \right)}^{\text{Inertia}} = \underbrace{-\nabla p}_{\text{Pressure gradient}} + \underbrace{\mu \nabla^2 \mathbf{v}}_{\text{Viscosity}} + \underbrace{\mathbf{f}}_{\text{Other forces}}$$

For microsystems, the Reynolds number  $\text{Re} = \frac{\rho V D}{\eta} = \frac{V D}{\nu}$  is very small ( $D \sim 2 \times 10^{-5} \text{m}$ ,  $V \sim 5 \times 10^{-4} \text{m/s}$ ,  $\nu = \mu/\rho \sim 10^{-6} \text{m}^2/\text{s}$ ,  $\text{Re} \sim 10^{-2}$ ), so inertial terms (and the externally applied body forces) can be neglected:

$$\eta \nabla^2 \mathbf{u} - \nabla p = 0$$

$$\nabla \cdot \mathbf{u} = 0$$

Next, we plan to solve the differential equations.

# COMSOL Simulation

## Parameters

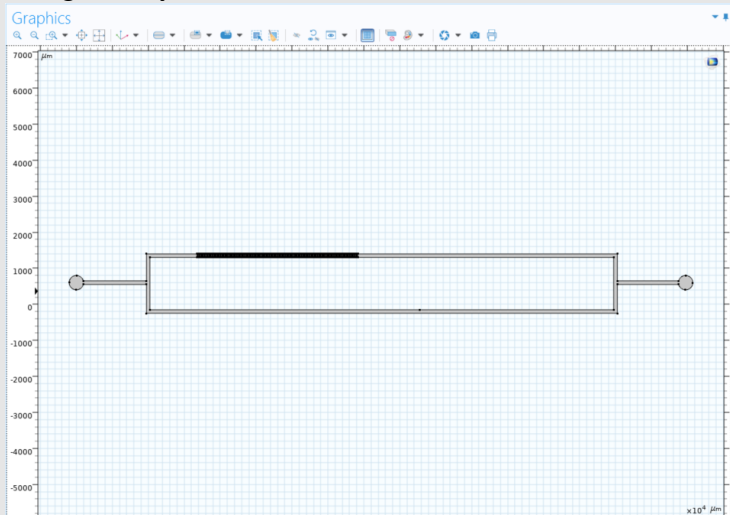
To simulate our model, we mainly referred to a COMSOL sample "Electroosmotic Micromixer". Our parameters are:

Name	Expression	Value	Description
sigma	0.00123[S/m]	0.00123 S/m	Conductivity of the ionic solution
epsilon_r	80.2	80.2	Relative permittivity of the fluid
V0	0.1*sqrt(2)[V]	0.14142 V	Maximum value of the AC poten...
omega	2*pi[rad]*1000[Hz]	6283.2 Hz	Angular frequency of the AC po...
zeta	-0.120596[V]	-0.1206 V	Zeta potential
U0	0[mm/s]	0 m/s	Mean inflow velocity

# COMSOL Simulation

## Geometry

Our geometry is:



# COMSOL Simulation

## Material

Settings

Material

Label:

**Geometric Entity Selection**

Geometric entity level:

Selection:

1

**Override**

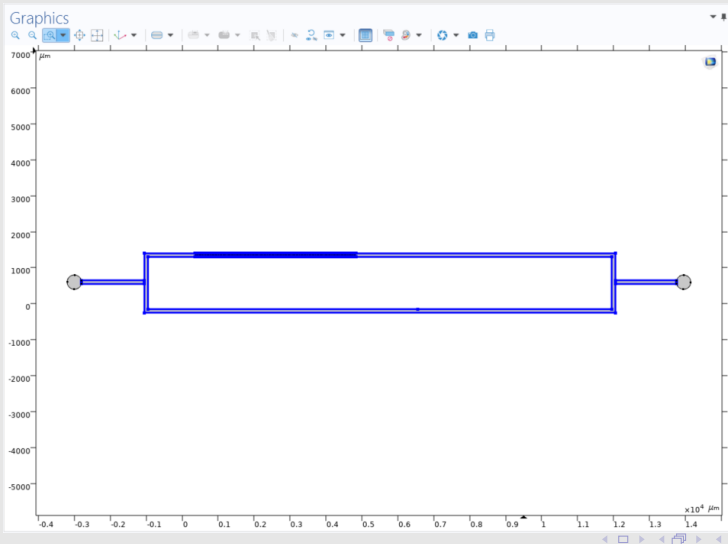
**Material Properties**

**Material Contents**

	Property	Variable	Value	Unit	Property group
<input checked="" type="checkbox"/>	Electrical conductivity	sigma_is...	sigma	S/m	Basic
<input checked="" type="checkbox"/>	Dynamic viscosity	mu	epsilon_r/(...	Pa-s	Basic
<input checked="" type="checkbox"/>	Relative permittivity	epsilon_r...	epsilon_r	1	Basic
<input checked="" type="checkbox"/>	Density	rho	1e3[kg/m^3]	kg/m³	Basic

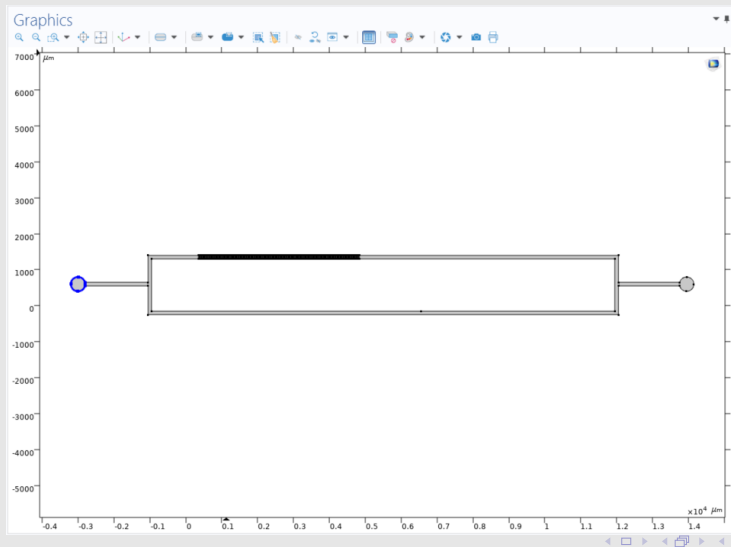
# Creeping Flow

Wall ( $U_{av} = U_0$ )



# Creeping Flow

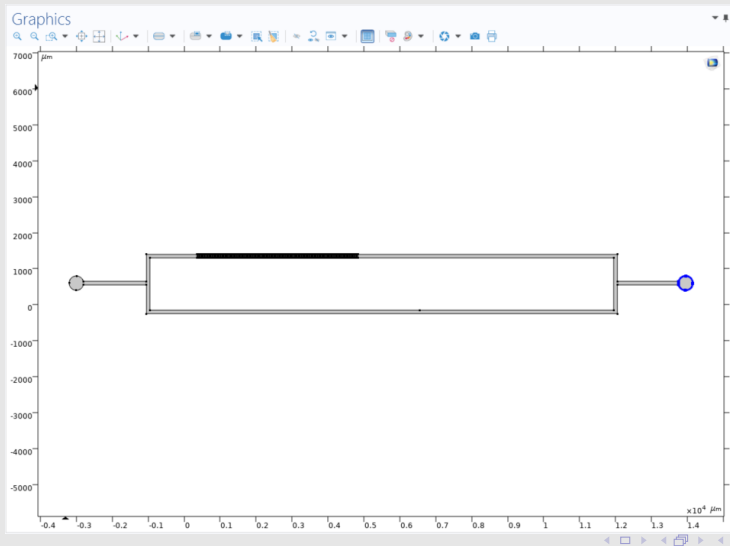
Inlet





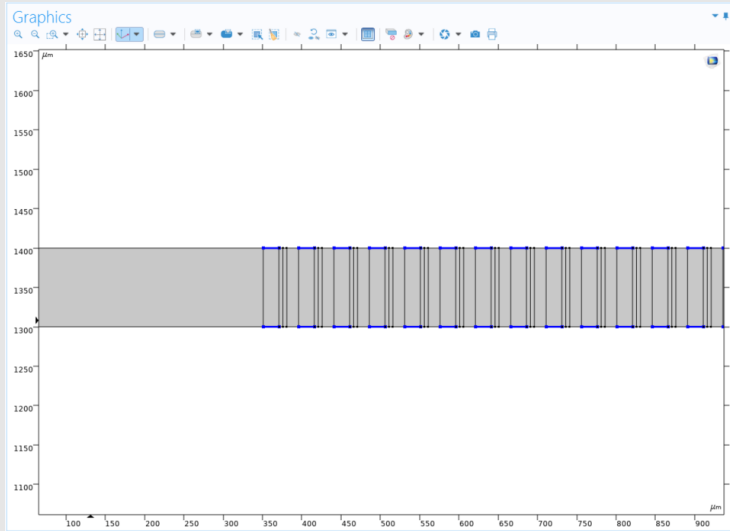
# Creeping Flow

## Outlet



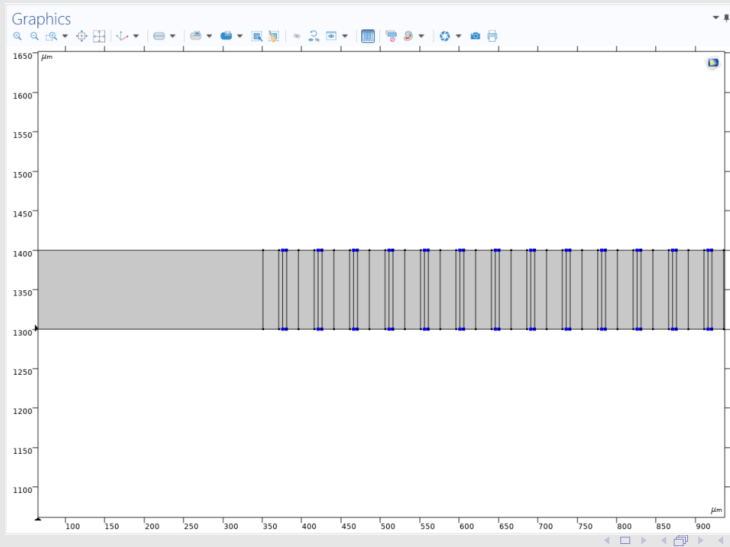
# Electric Currents

Electric Potential 1 ( $V_0 = V_0$ )



# Electric Currents

Electric Potential 2 ( $V_0 = -V_0$ )



# COMSOL Simulation

## Material

Then, we set up a study using time-dependent solver to solve the fluid flow. After computing, we can derive the results including:

- Velocity, streamlines
- Electric potential

Next, we plan to modify the original layout in GDS file in AutoCAD to fit the COMSOL geometry requirements.

Thanks!