High field model SECCM with pH

Report date

Jul 16, 2024, 3:14:54 PM

Contents

1 Global Definitions

Date	Jul 11, 2024, 5:27:24 PM

GLOBAL SETTINGS

Name	High field model SECCM with pH Hu.mph
Path	C:\Users\Admin\OneDrive - McGill University\Doctorat_Danny Chhin\Desktop\Hu\High field model SECCM with pH_Hu.mph
Version	COMSOL Multiphysics 6.2 (Build: 290)

USED PRODUCTS

Electrodeposition Module
COMSOL Multiphysics

COMPUTER INFORMATION

CPU	AMD64 Family 25 Model 33 Stepping 2, 12 cores, 127.88 GB RAM
Operating system	Windows 11

1.1 PARAMETERS

1.1.1 Geometry

GEOMETRY

Name	Expression	Value	Description
r_tip	1[um]	1E−6 m	radius of pipette
Hdrop	1[um]	1E−6 m	Height of drop
rdrop	0.62[um]	6.2E−7 m	Radius of drop
d_QCRE	1.5[cm]	0.015 m	Distance from QCRE to tip
L_tip	5[mm]	0.005 m	
L_taper	L_tip*1.15	0.00575 m	
r_taper	L_tip*0.15	7.5E−4 m	

1.1.2 CV parameters

CV PARAMETERS

Name	Expression	Value	Description
E0	-1[V]	−1 V	CV: lower vertex potential
Ef	1[V]	1 V	CV: upper vertex potential
scan_rate	100[mV/s]	0.1 V/s	CV: scan rate
tsim	(Ef - E0)/scan_rate	20 s	CV: time for single cycle
C_dl	16[uF/cm^2]	0.16 F/m^2	

Name	Expression	Value	Description
T	298[K]	298 K	

1.1.3 High field parameter

HIGH FIELD PARAMETER

Name	Expression	Value	Description
A	6.5e-12[A/m^2]	6.5E−12 A/m^2	
B	3.2e-6[cm/V]	3.2E−8 C/N	
M_Al2O3	102[g/mol]	0.102 kg/mol	
rho_Al2O3	3[g/cm^3]	3000 kg/m^3	
Fdiss	M_Al2O3/rho_Al2O3	3.4E−5 m^3/mol	
Epass	-1.75[V]	−1.75 V	Redox potential for passivation
d0	2.73[nm]	2.73E−9 m	Initial oxide layer thickness
Rdiss	1e-12[mol/cm^2/s]	1E−8 mol/(m^2·s)	Chemical dissolution rate
nH	1	1	Number of proton released
min_eff	0.6	0.6	

1.1.4 pH parameter

PH PARAMETER

Name	Expression	Value	Description
c0_H3O	1e-7[M]	1E−4 mol/m^3	Initial concentration of acid
c0_HA	0[M]	0 mol/m^3	Initial concentration of weak acid
c0_A	0[M]	0 mol/m^3	Initial concentration of conjugate base
c0_OH	0	0	Initial concentration of base

1.1.5 Cathodic reaction parameter

CATHODIC REACTION PARAMETER

Name	Expression	Value	Description
i0cat	8.3[uA/cm^2]	0.083 A/m^2	Tafel: corrosion current density
Ecat	-0.4[V]	−0.4 V	
tslope_cat	-750[mV]	−0.75 V	

2 Component 1

2.1 DEFINITIONS

2.1.1 Variables

Passivation efficiency

SELECTION

Geometric entity level	Entire model

Name	Expression	Unit	Description
pass_eff	1/(1 + 1.7e6*cH3O[m^3/mol]/1000)		
Fpass	pass_eff*M_Al2O3/(6*rho_Al2O3*F_const)	$m^3/(s \cdot A)$	
d_avg	comp1.aveop1(d)	m	

Applied potential: Linear Scan Voltammetry

SELECTION

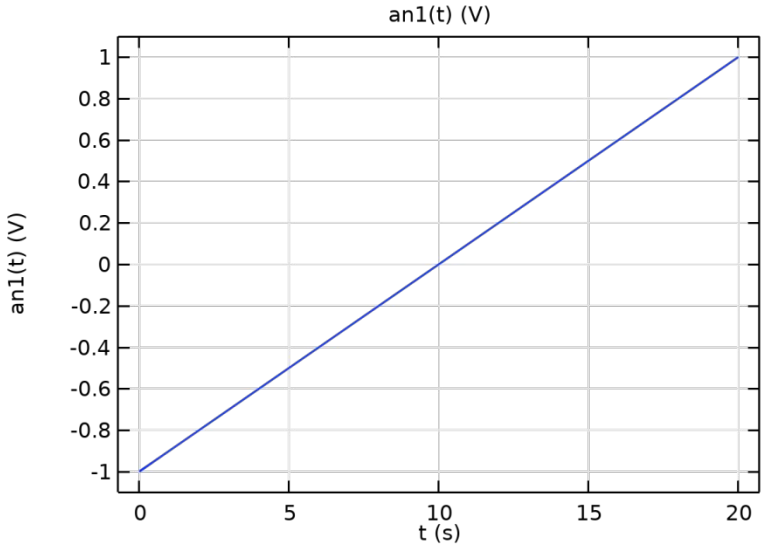
Geometric entity level	Entire model

Name	Expression	Unit	Description
Eapp	an1(t)	V	

2.1.2 Functions

Linear potential scan

Function name	an1
Function type	Analytic



Linear potential scan

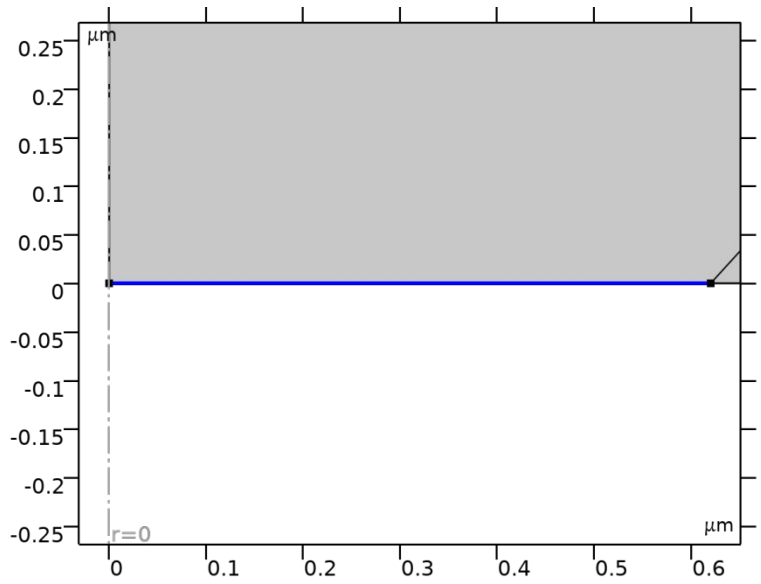
2.1.3 Nonlocal Couplings

Integration 1

Coupling type	Integration
Operator name	intop1

SELECTION

Geometric entity level	Boundary
Selection	Geometry geom1: Dimension 1: Boundary 2



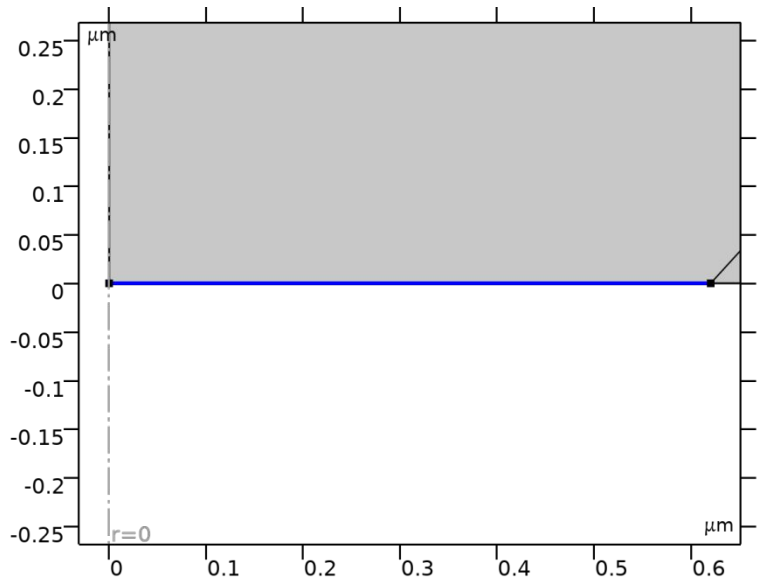
Selection

Average 1

Coupling type	Average
Operator name	aveop1

SELECTION

Geometric entity level	Boundary
Selection	Geometry geom1: Dimension 1: Boundary 2



Selection

2.1.4 Coordinate Systems

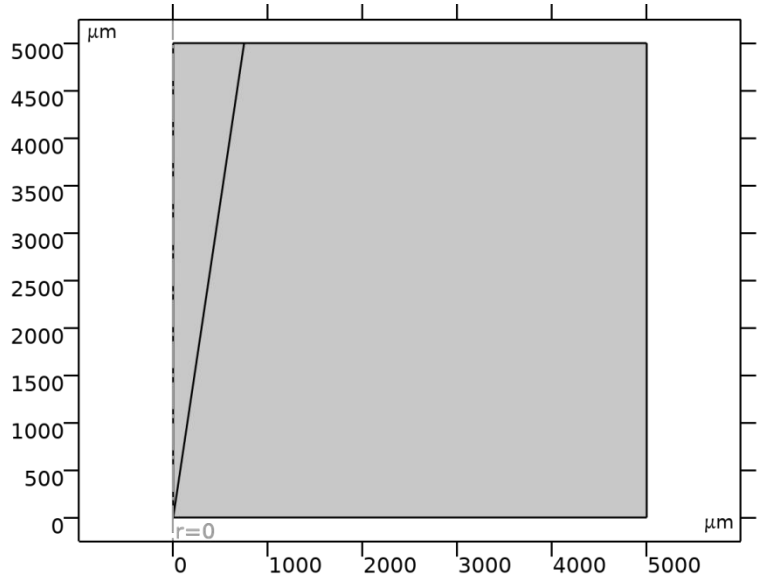
Boundary System 1

Coordinate system type	Boundary system
Tag	sys1

COORDINATE NAMES

First	Second	Third
t1	to	n

2.2 GEOMETRY 1



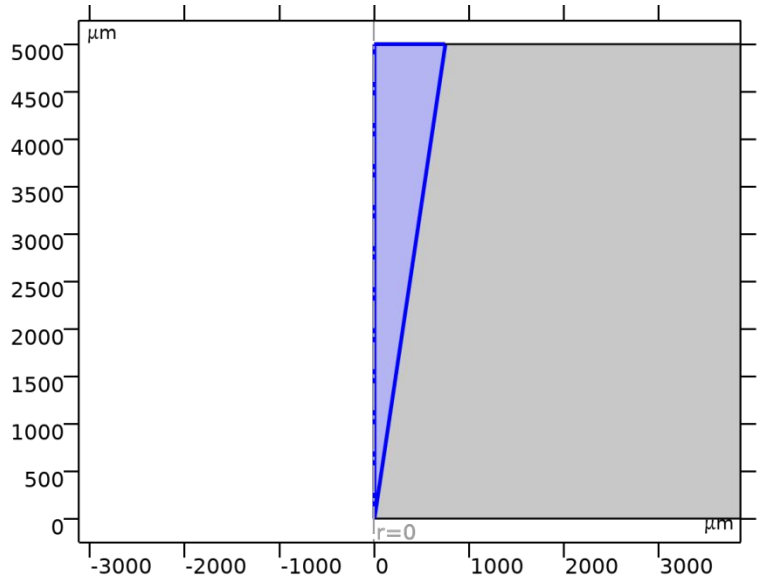
Geometry 1

UNITS

Length unit	µm
Angular unit	deg

2.3 MATERIALS

2.3.1 Water

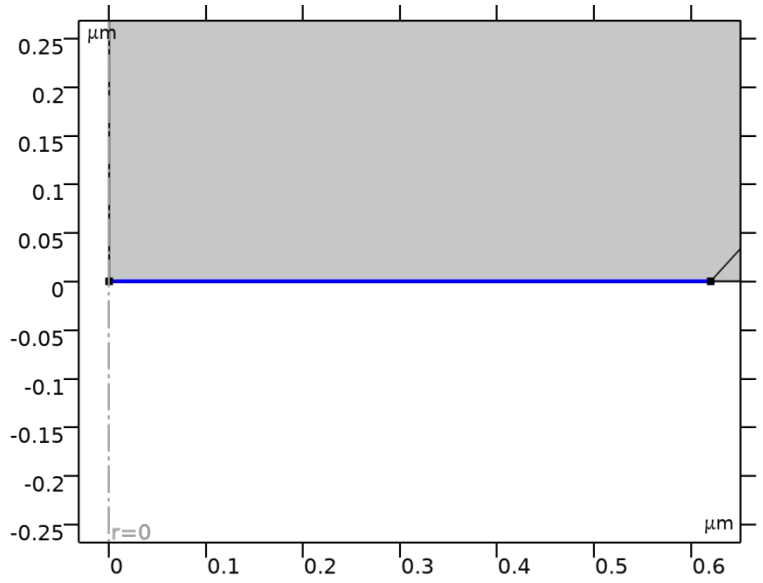


Water

SELECTION

Geometric entity level	Domain
Selection	Geometry geom1: Dimension 2: Domain 2

2.4 BOUNDARY ODES AND DAES



Boundary ODEs and DAEs

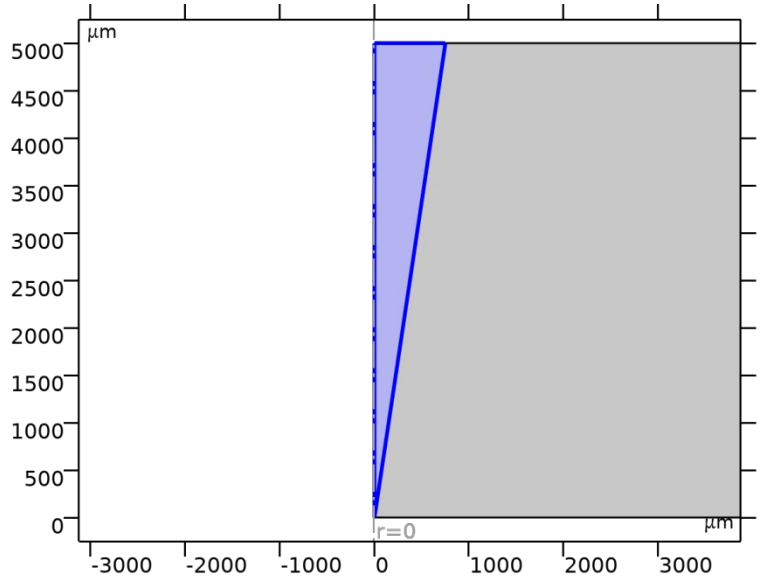
EQUATIONS

$$e_a\frac{\partial^2 d}{\partial t^2}+d_a\frac{\partial d}{\partial t}=f$$

FEATURES

Name	Level
Distributed ODE 1	Boundary
Initial Values 1	Boundary

2.5 TERTIARY CURRENT DISTRIBUTION, NERNST-PLANCK 2



Tertiary Current Distribution, Nernst-Planck 2

EQUATIONS

$$\frac{\partial c_i}{\partial t} + \nabla \cdot \mathbf{J}_i + \mathbf{u} \cdot \nabla c_i = R_i$$

$$\nabla \cdot \mathbf{i}_s = Q_s$$

$$\mathbf{J}_i = -D_i \nabla c_i$$

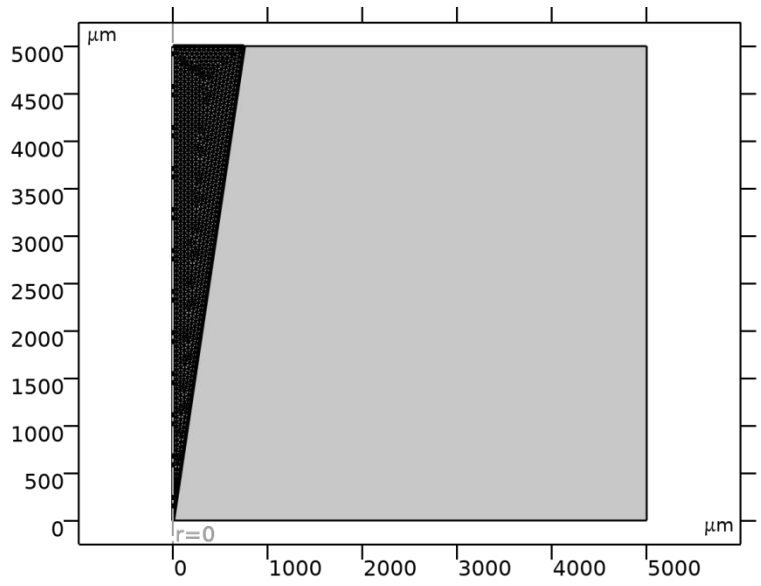
$$\mathbf{i}_s = -\sigma_s \nabla \phi_s$$

$$\phi_l = 0, \quad \phi_s = \text{phis3}$$

FEATURES

Electrolyte 1	Domain
Axial Symmetry 1	Boundary
No Flux 1	Boundary
Insulation 1	Boundary
Initial Values 1	Domain
Electrode Surface 1	Boundary
Reactions 1	Domain
Concentration 1	Boundary

2.6 MESH 1



Mesh 1

3 Study 1

COMPUTATION INFORMATION

Computation time	37 s

3.1 PARAMETRIC SWEEP 2

Parameter name	Parameter value list	Parameter unit
scan_rate	0.025, 0.05, 0.1, 0.2	V/s

STUDY SETTINGS

Description	Value
Sweep type	Specified combinations
Parameter name	scan_rate
Unit	V/s

PARAMETERS

Parameter name	Parameter value list	Parameter unit
scan_rate (CV: scan rate)	0.025, 0.05, 0.1, 0.2	V/s

3.2 TIME DEPENDENT

Times	Unit
range(0,tsim/100,tsim)	s

STUDY SETTINGS

Description	Value
Include geometric nonlinearity	Off

STUDY SETTINGS

Description	Value
Output times	{0, 38.922, 77.844, 116.77, 155.69, 194.61, 233.53, 272.46, 311.38, 350.3, 389.22, 428.14, 467.07, 505.99, 544.91, 583.83, 622.75, 661.68, 700.6, 739.52, 778.44, 817.37, 856.29, 895.21, 934.13, 973.05, 1012, 1050.9, 1089.8, 1128.7, 1167.7, 1206.6, 1245.5, 1284.4, 1323.4, 1362.3, 1401.2, 1440.1, 1479, 1518, 1556.9, 1595.8, 1634.7, 1673.7, 1712.6, 1751.5, 1790.4, 1829.3, 1868.3, 1907.2, 1946.1, 1985, 2024, 2062.9, 2101.8, 2140.7, 2179.6, 2218.6, 2257.5, 2296.4, 2335.3, 2374.3, 2413.2, 2452.1, 2491, 2529.9, 2568.9, 2607.8, 2646.7, 2685.6, 2724.6, 2763.5, 2802.4, 2841.3, 2880.2, 2919.2, 2958.1, 2997, 3035.9, 3074.9, 3113.8, 3152.7, 3191.6, 3230.5, 3269.5, 3308.4, 3347.3, 3386.2, 3425.1, 3464.1, 3503, 3541.9, 3580.8, 3619.8, 3658.7, 3697.6, 3736.5, 3775.4, 3814.4, 3853.3, 3892.2}
Tolerance	User controlled
Relative tolerance	1E-4

PHYSICS AND VARIABLES SELECTION

Physics interface	Solve for	Equation form
Boundary ODEs and DAEs (bode)	On	Automatic (Time domain)
Tertiary Current Distribution, Nernst-Planck 2 (tcd2)	On	Automatic (Time dependent)

STORE IN OUTPUT

Interface	Output	Selection
Boundary ODEs and DAEs (bode)	Physics controlled	
Tertiary Current Distribution, Nernst-Planck 2 (tcd2)	Physics controlled	

MESH SELECTION

Component	Mesh
Component 1	Mesh 1

4 Results

4.1 DATASETS

4.1.1 No Solution (1)

SOLUTION

Description	Value
Component	Component 1 (comp1)

4.1.2 No Solution (2)

SOLUTION

Description	Value
Component	Component 1 (comp1)

4.1.3 Revolution 2D 1

DATA

Description	Value
Dataset	No Solution (2)

AXIS DATA

Description	Value
Axis entry method	Two points
Points	{{0, 0}, {0, 1}}

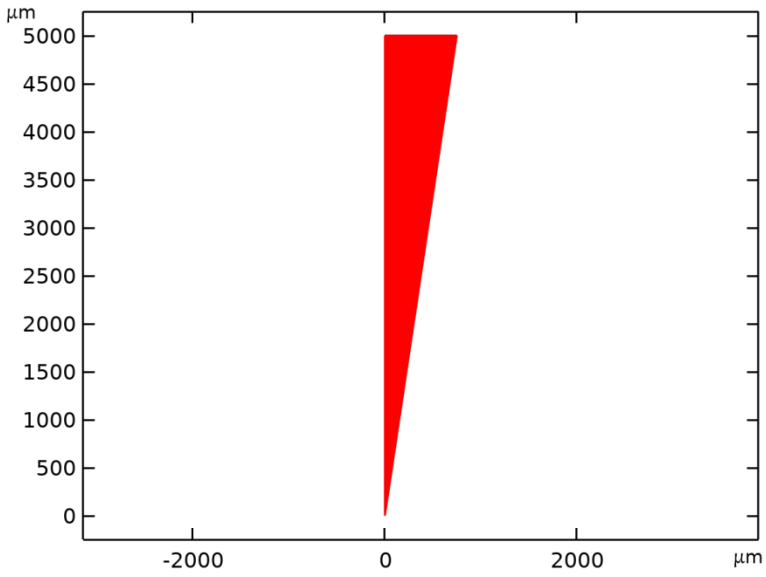
REVOLUTION LAYERS

Description	Value
Start angle	-90
Revolution angle	225

4.1.4 Study 1/Solution 1

SOLUTION

Description	Value
Solution	Solution 1 (sol1)
Component	Component 1 (comp1)

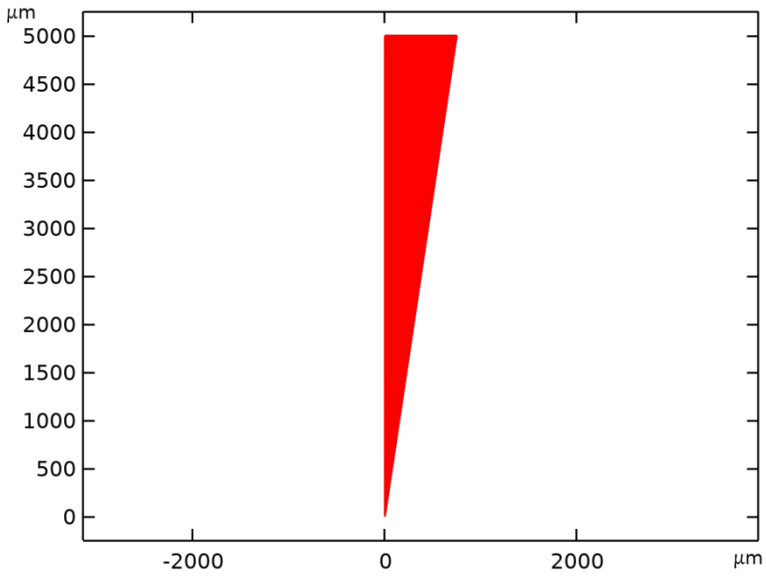


Dataset: Study 1/Solution 1

4.1.5 Study 1/Parametric Solutions 1

SOLUTION

Description	Value
Solution	Parametric Solutions 1 (sol2)
Component	Component 1 (comp1)



Dataset: Study 1/Parametric Solutions 1

4.1.6 Revolution 2D 2

DATA

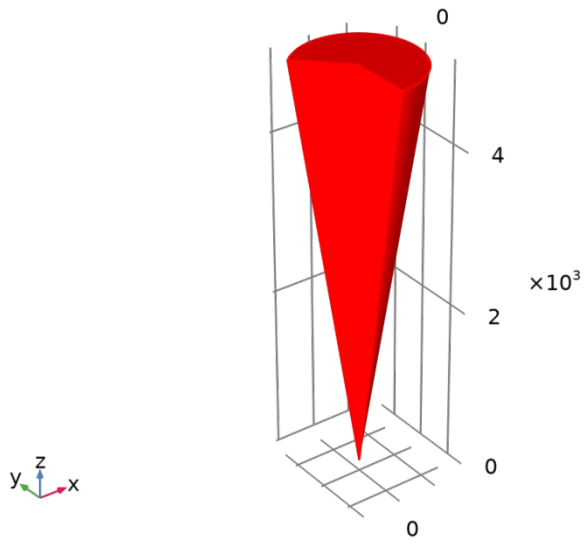
Description	Value
Dataset	Study 1/Parametric Solutions 1 (sol2)

AXIS DATA

Description	Value
Axis entry method	Two points
Points	{{0, 0}, {0, 1}}

REVOLUTION LAYERS

Description	Value
Start angle	-90
Revolution angle	225



Dataset: Revolution 2D 2

4.2 TABLES

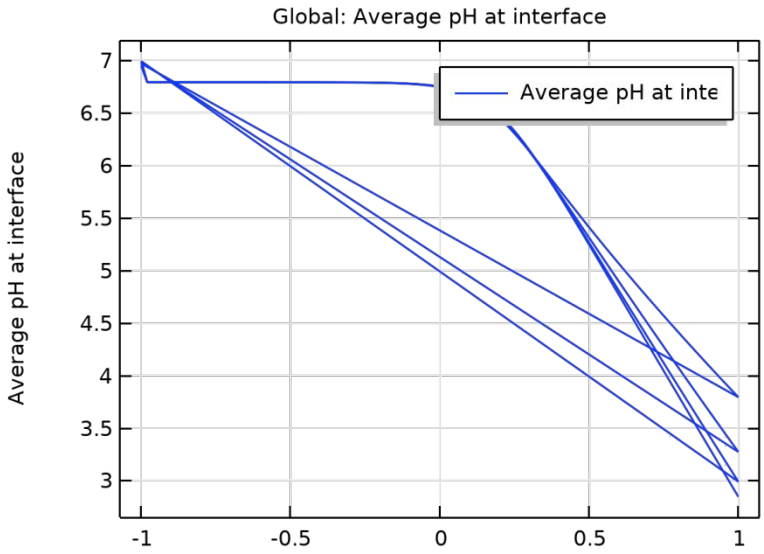
4.2.1 Evaluation 2D

Interactive 2D values

x	y	Value
35.539	1356.9	8.8861

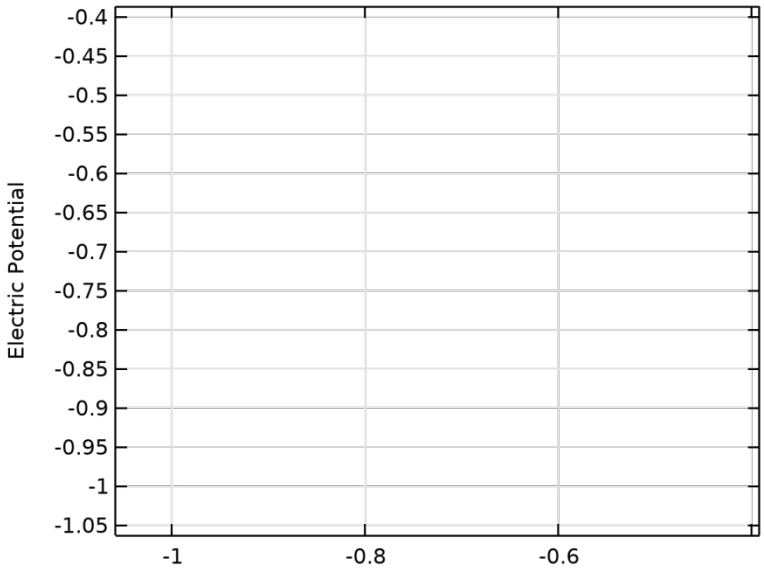
4.3 PLOT GROUPS

4.3.1 pH change at interface vs time



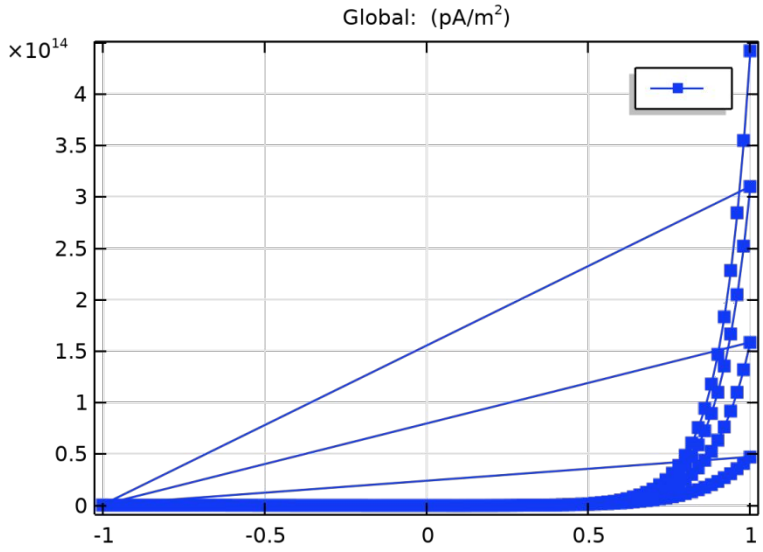
Global: Average pH at interface

4.3.2 Electrode Potential (tcd)



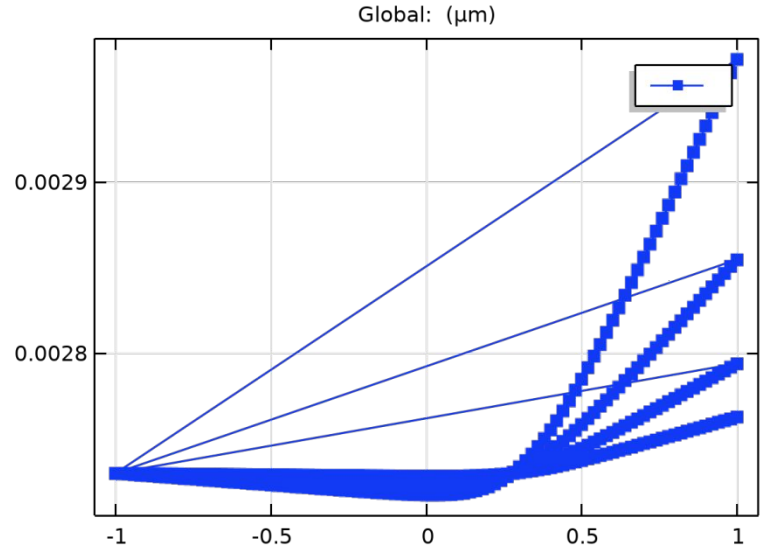
Global: Electric Potential

4.3.3 Current



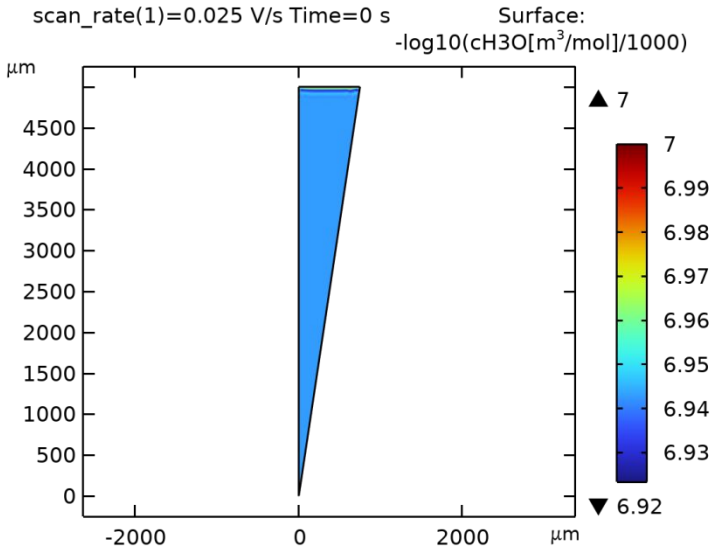
Global: (pA/m²)

4.3.4 d thickness oxide



Global: (µm)

4.3.5 pH



Surface: -log10(cH3O[m³/mol]/1000)