Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Modelling Ohmic Drop in Cyclic Voltammetry

Report date	Jan 4, 2021 4:54:10 PM

Contents

1 Global Definitions

Date	Nov 6, 2020 6:26:53 PM

GLOBAL SETTINGS

Name	2020-11-06-Modelling Ohmic Drop in Cyclic Voltammetry. mph
Path	F: \Paper SI\2020-11-06-Modelling Ohmic Drop in Cyclic Voltammetry.mph
Version	COMSOL Multiphysics 5.5 (Build: 359)

USED PRODUCTS

COMSOL Multiphysics
Chemical Reaction Engineering Module

1.1 PARAMETERS

1.1.1 Parameters (General)

PARAMETERS (GENERAL)

Name	Expression	Value	Description
L	10 [mm]	0.01 m	Domain length
Point1	0.5 [mm]	5E−4 m	Electrode radius - r coordinate for point 1 of the electrode
T	298.15[K]	298.15 K	Temperature (25°C)
v	0.1 [V/s]	0.1 V/s	Scan rate
f	(n*F_const)/(R_const*T)	38.922 1/V	nF/RT
R_U	5000 [V/A]	5000 Ω	Uncompensated Resistance
Area	pi*(Point1^2)	7.854E−7 m^2	Electrode area

1.1.2 Paramaters (CV Waveform)

PARAMATERS (CV WAVEFORM)

Name	Expression	Value	Description
V_i	E0 + 0.5	0.34 V	Initial E
V_sw	E0 - 0.5	−0.66 V	Switching E
SegmentDuration	ScanRange/v	10 s	
ScanRange	abs(V_i - V_sw)	1 V	Potential window scanned

1.1.3 Parameters (Redox Couple)

PARAMETERS (REDOX COUPLE)

Name	Expression	Value	Description

Name	Expression	Value	Description
DcOx	8.8*10^ - 6[cm^2/s]	8.8E−10 m^2/s	Diffusion coefficient oxidised species ([Ru(NH3)6]+3)
DcRed	DcOx	8.8E−10 m^2/s	Diffusion coefficient reduced species ([Ru(NH3)6]+2)
cOx0	1 [mM]	1 mol/m^3	Initial concentration of oxidised species ([Ru(NH3)6]+3)
k0	1 [cm/s]	0.01 m/s	Rate constant (fast)
alpha	0.5	0.5	Transfer coefficient
n	1	1	number of electrons transferred
E0	-0.160 [V]	−0.16 V	Standard redox potential for [Ru(NH3)6]+3/+2 vs SCE

2 Component 1

SETTINGS

Description	Value
Unit system	Same as global system
Avoid inverted elements by curving interior domain elements	Off

2.1 DEFINITIONS

2.1.1 Variables

Butler Volmer HET Equations

SELECTION

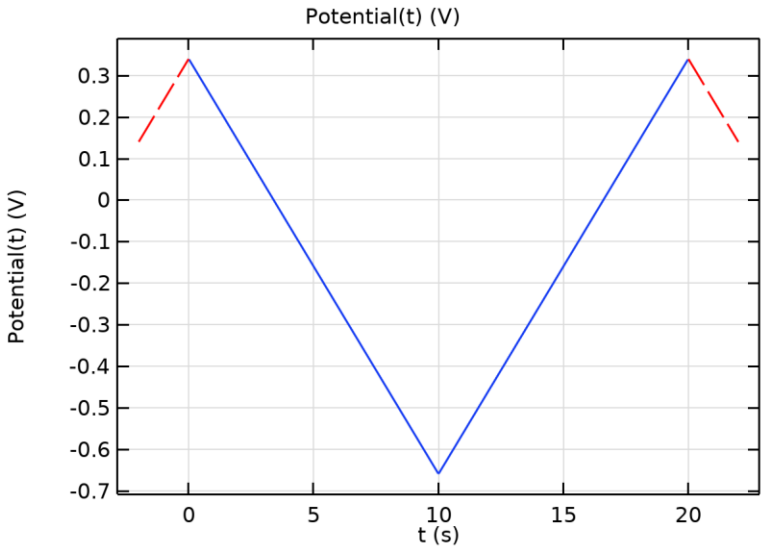
Geometric entity level	Boundary
Selection	Geometry geom1: Dimension 1: Boundary 2

Name	Expression	Unit	Description
kf	k0*exp((-alpha*f*(Potential(t) - E0 - bnd1*R_U)))	m/s	Forward rate constant with Ohmic drop included
kb	k0*exp(((1 - alpha)*f*(Potential(t) - E0 - bnd1*R_U)))	m/s	Reverse rate constant with Ohmic drop included

2.1.2 Functions

Piecewise 1

Function name	Potential
Function type	Piecewise



Piecewise 1

DEFINITION

Description	Value
Argument	t
Extrapolation	Periodic
Smoothing	No smoothing

DEFINITION

Start	End	Function
0	SegmentDuration	V_i-v*t
SegmentDuration	2*SegmentDuration	V_sw+v*(t-SegmentDuration)

UNITS

Description	Value
Arguments	s
Function	V

2.1.3 Selections

Electrode

Selection type
Box[cuboid]

Selection
Boundaries 1–2, 4

GEOMETRIC ENTITY LEVEL

Description	Value
Level	Boundary

OUTPUT ENTITIES

Description	Value
Include entity if	Entity intersects box

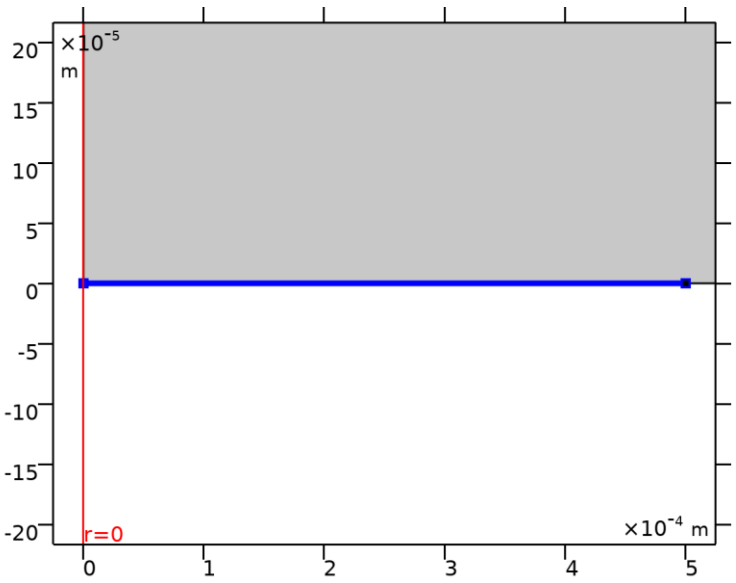
2.1.4 Probes

Boundary Probe - Calculate Current

Probe type	Boundary probe

SELECTION

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



Selection

PROBE TYPE

Description	Value
Type	Integral

EXPRESSION

Description	Value
Expression	-(tds.ntflux_cOx)*F_const*n
Table and plot unit	A

Description	Value
Description	-(tds.ntflux_cOx)*F_const*n

INTEGRATION SETTINGS

Description	Value
Integration order	2
Frame	Mesh

TABLE AND WINDOW SETTINGS

Description	Value
Output table	Probe Table 12
Plot window	Probe Plot 2

2.1.5 Coordinate Systems

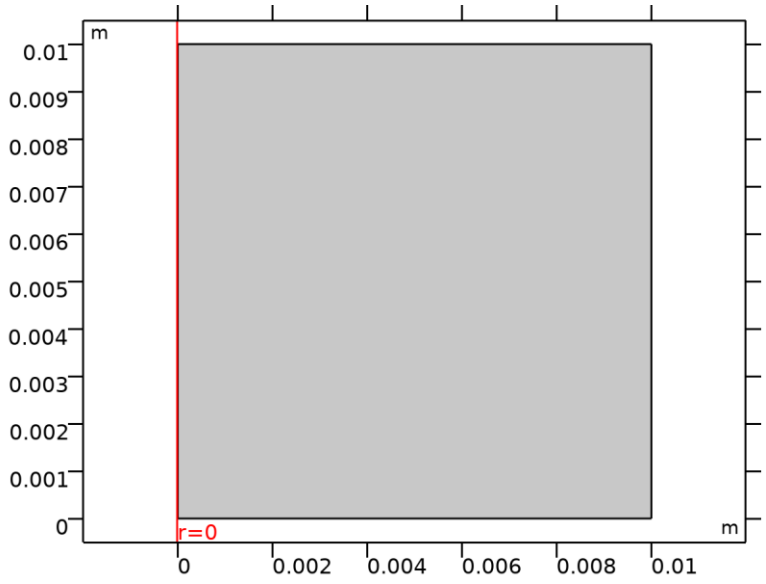
Boundary System 1

Coordinate system type	Boundary system
Tag	sys1

COORDINATE NAMES

First	Second	Third
t1	to	n

2.2 GEOMETRY 1



Geometry 1

UNITS

Length unit	m
Angular unit	deg

GEOMETRY STATISTICS

Description	Value
Space dimension	2
Number of domains	1
Number of boundaries	5
Number of vertices	5

2.2.1 Domain (sq1)

POSITION

Description	Value
Position	{0, 0}

SIZE

Description	Value
Side length	L

2.2.2 Point 1 - Electrode (pt1)

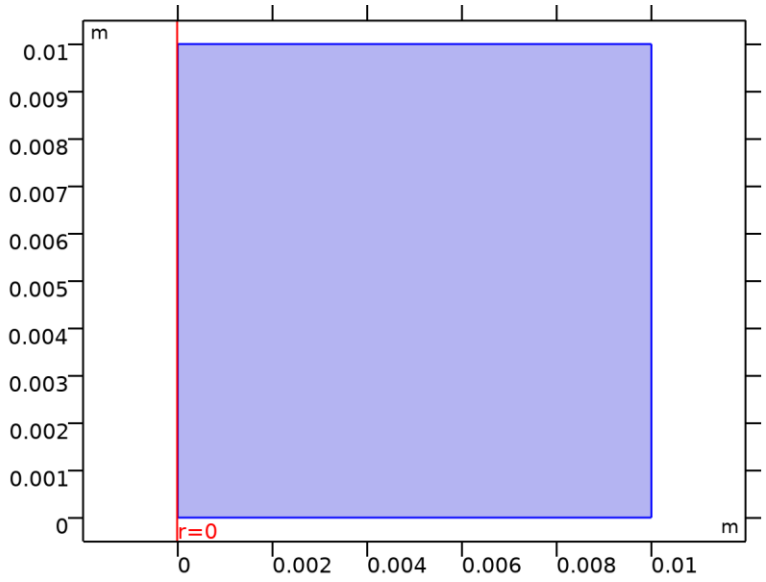
POINT

Description	Value
Point coordinate	{5.0E-4, 0}

2.3 TRANSPORT OF DILUTED SPECIES

USED PRODUCTS

COMSOL Multiphysics
Chemical Reaction Engineering Module



Transport of Diluted Species

SELECTION

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

EQUATIONS

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

2.3.1 Interface settings

Discretization

SETTINGS

Description	Value
Concentration	Linear
Compute boundary fluxes	On
Apply smoothing to boundary fluxes	On
Value type when using splitting of complex variables	Real

Transport mechanisms

SETTINGS

Description	Value
Convection	Off
Migration in electric field	Off

Description	Value
Mass transfer in porous media	Off

Advanced settings

SETTINGS

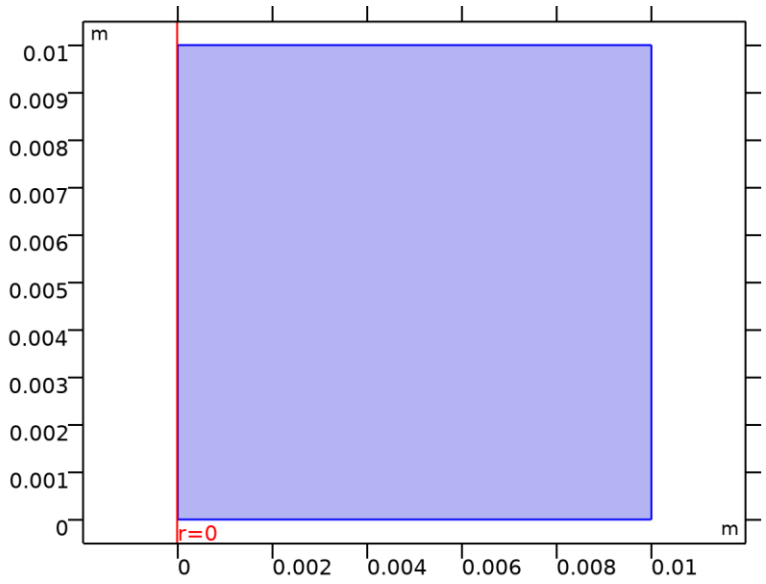
Description	Value
Convective term	Nonconservative form

2.3.2 Variables

Name	Expression	Unit	Description	Selection	Details
tds.R_cOx	0	mol/(m³·s)	Total rate expression	Domain 1	+ operation
tds.cP_cOx	0	mol/kg	Concentration species absorbed to the solid	Domain 1	+ operation
tds.cP_cOx	0	mol/kg	Concentration species absorbed to the solid	Boundaries 1–5	+ operation
tds.KP_cOx	0	m³/kg	Adsorption isotherm, first concentration derivative	Domain 1	+ operation
tds.KP_cOx	0	m³/kg	Adsorption isotherm, first concentration derivative	Boundaries 1–5	+ operation
tds.R_cRed	0	mol/(m³·s)	Total rate expression	Domain 1	+ operation
tds.cP_cRed	0	mol/kg	Concentration species absorbed to the solid	Domain 1	+ operation
tds.cP_cRed	0	mol/kg	Concentration species absorbed to the solid	Boundaries 1–5	+ operation
tds.KP_cRed	0	m³/kg	Adsorption isotherm, first concentration derivative	Domain 1	+ operation
tds.KP_cRed	0	m³/kg	Adsorption isotherm, first concentration derivative	Boundaries 1–5	+ operation

Name	Expression	Unit	Description	Selection	Details
tds.epsilon_p	1	1	Porosity	Domain 1	
tds.theta	tds.epsilon_p	1	Liquid volume fraction	Domain 1	
tds.av	0	1	Gas volume fraction	Domain 1	
tds.nr	dnr	1	Normal vector, r component	Boundaries 1–5	
tds.nphi	0	1	Normal vector, phi component	Boundaries 1–5	
tds.nz	dnz	1	Normal vector, z component	Boundaries 1–5	
tds.nrmesh	dnrmesh	1	Normal vector (mesh), r component	Boundaries 1–5	
tds.nphimesh	0	1	Normal vector (mesh), phi component	Boundaries 1–5	
tds.nzmesh	dnzmesh	1	Normal vector (mesh), z component	Boundaries 1–5	
tds.nrc	root.nrc/tds.ncLen	1	Normal vector, r component	Boundaries 1–5	
tds.nphic	0	1	Normal vector, phi component	Boundaries 1–5	
tds.nzc	root.nzc/tds.ncLen	1	Normal vector, z component	Boundaries 1–5	
tds.ncLen	sqrt(root.nrc^2+root.nzc^2+eps)	1	Help variable	Boundaries 1–5	

2.3.3 Transport Properties 1



Transport Properties 1

SELECTION

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

EQUATIONS

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

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

Diffusion

SETTINGS

Description	Value
Material	None
Diffusion coefficient	User defined
Diffusion coefficient	{{DcOx, 0, 0}, {0, DcOx, 0}, {0, 0, DcOx}}
Diffusion coefficient	User defined
Diffusion coefficient	{{DcRed, 0, 0}, {0, DcRed, 0}, {0, 0, DcRed}}

Coordinate system selection

SETTINGS

Description	Value
Coordinate system	Global coordinate system

Model input

SETTINGS

Description	Value
Temperature	User defined
Temperature	T

Variables

Name	Expression	Unit	Description	Selection	Details
domflux.cOxr	2*tds.dflux_cOxr*pi*r	mol/(m·s)	Domain flux, r component	Domain 1	
domflux.cOxz	2*tds.dflux_cOxz*pi*r	mol/(m·s)	Domain flux, z component	Domain 1	
domflux.cRedr	2*tds.dflux_cRedr*pi*r	mol/(m·s)	Domain flux, r component	Domain 1	
domflux.cRedz	2*tds.dflux_cRedz*pi*r	mol/(m·s)	Domain flux, z component	Domain 1	
tds.ndflux_cOx	tds.bndFlux_cOx	mol/(m²·s)	Normal diffusive flux	Boundaries 2–5	
tds.ntflux_cOx	tds.bndFlux_cOx	mol/(m²·s)	Normal total flux	Boundaries 2–5	
tds.ndflux_cRed	tds.bndFlux_cRed	mol/(m²·s)	Normal diffusive flux	Boundaries 2–5	
tds.ntflux_cRed	tds.bndFlux_cRed	mol/(m²·s)	Normal total flux	Boundaries 2–5	
tds.bndFlux_cOx	if(r>0.001/sqrt(sqrt(mean(emetric2))),-0.5*dflux_spatial(cOx)/(pi*r),NaN)	mol/(m²·s)	Boundary flux	Boundaries 1–5	
tds.bndFlux_cRed	if(r>0.001/sqrt(sqrt(mean(emetric2))),-0.5*dflux_spatial(cRed)/(pi*r),NaN)	mol/(m²·s)	Boundary flux	Boundaries 1–5	
tds.D_cOxrr	DcOx	m²/s	Diffusion coefficient, rr component	Domain 1	+ operation
tds.D_cOxphir	0	m²/s	Diffusion coefficient, phir component	Domain 1	+ operation
tds.D_cOxzr	0	m²/s	Diffusion coefficient, zr component	Domain 1	+ operation
tds.D_cOxrphi	0	m²/s	Diffusion	Domain 1	+ operation

Name	Expression	Unit	Description	Selection	Details
			coefficient, rphi component		
tds.D_cOxphiphi	DcOx	m^2/s	Diffusion coefficient, phiphi component	Domain 1	+ operation
tds.D_cOxzphi	0	m^2/s	Diffusion coefficient, zphi component	Domain 1	+ operation
tds.D_cOxrz	0	m^2/s	Diffusion coefficient, rz component	Domain 1	+ operation
tds.D_cOxphiz	0	m^2/s	Diffusion coefficient, phiz component	Domain 1	+ operation
tds.D_cOxzz	DcOx	m^2/s	Diffusion coefficient, zz component	Domain 1	+ operation
tds.D_cRedrr	DcRed	m^2/s	Diffusion coefficient, rr component	Domain 1	+ operation
tds.D_cRedphir	0	m^2/s	Diffusion coefficient, phir component	Domain 1	+ operation
tds.D_cRedzr	0	m^2/s	Diffusion coefficient, zr component	Domain 1	+ operation
tds.D_cRedrphi	0	m^2/s	Diffusion coefficient, rphi component	Domain 1	+ operation
tds.D_cRedphiphi	DcRed	m^2/s	Diffusion coefficient, phiphi component	Domain 1	+ operation
tds.D_cRedzphi	0	m^2/s	Diffusion coefficient, zphi component	Domain 1	+ operation
tds.D_cRedrz	0	m^2/s	Diffusion coefficient, rz component	Domain 1	+ operation
tds.D_cRedphiz	0	m^2/s	Diffusion coefficient, phiz component	Domain 1	+ operation

Name	Expression	Unit	Description	Selection	Details
tds.D_cRedzz	DcRed	m^2/s	Diffusion coefficient, zz component	Domain 1	+ operation
tds.Dav_cOx	0.5*(tds.D_cOxrr+tds.D_cOxzz)	m^2/s	Average diffusion coefficient	Domain 1	
tds.Dav_cRed	0.5*(tds.D_cRedrr+tds.D_cRedzz)	m^2/s	Average diffusion coefficient	Domain 1	
tds.tflux_cOxr	tds.dflux_cOxr	$mol/(m^2·s)$	Total flux, r component	Domain 1	+ operation
tds.tflux_cOxphi	tds.dflux_cOxphi	$mol/(m^2·s)$	Total flux, phi component	Domain 1	+ operation
tds.tflux_cOxz	tds.dflux_cOxz	$mol/(m^2·s)$	Total flux, z component	Domain 1	+ operation
tds.dfluxMag_cOx	sqrt(tds.dflux_cOxr^2+tds.dflux_cOxphi^2+tds.dflux_cOxz^2)	$mol/(m^2·s)$	Diffusive flux magnitude	Domain 1	
tds.tfluxMag_cOx	sqrt(tds.tflux_cOxr^2+tds.tflux_cOxphi^2+tds.tflux_cOxz^2)	$mol/(m^2·s)$	Total flux magnitude	Domain 1	
tds.tflux_cRedr	tds.dflux_cRedr	$mol/(m^2·s)$	Total flux, r component	Domain 1	+ operation
tds.tflux_cRedphi	tds.dflux_cRedphi	$mol/(m^2·s)$	Total flux, phi component	Domain 1	+ operation
tds.tflux_cRedz	tds.dflux_cRedz	$mol/(m^2·s)$	Total flux, z component	Domain 1	+ operation
tds.dfluxMag_cRed	sqrt(tds.dflux_cRedr^2+tds.dflux_cRedphi^2+tds.dflux_cRedz^2)	$mol/(m^2·s)$	Diffusive flux magnitude	Domain 1	
tds.tfluxMag_cRed	sqrt(tds.tflux_cRedr^2+tds.tflux_cRedphi^2+tds.tflux_cRedz^2)	$mol/(m^2·s)$	Total flux magnitude	Domain 1	
tds.dflux_cOxr	-tds.D_cOxrr*cOxr-tds.D_cOxrz*cOxz	$mol/(m^2·s)$	Diffusive flux, r component	Domain 1	
tds.dflux_cOxphi	-tds.D_cOxphir*cOxr-tds.D_cOxphiz*cOxz	$mol/(m^2·s)$	Diffusive flux, phi component	Domain 1	
tds.dflux_cOxz	-tds.D_cOxzr*cOxr-tds.D_cOxzz*cOxz	$mol/(m^2·s)$	Diffusive flux, z component	Domain 1	
tds.grad_cOxr	cOxr	mol/m^4	Concentration	Domain 1	

Name	Expression	Unit	Description	Selection	Details
			gradient, r component		
tds.grad_cOxphi	0	mol/m^4	Concentration gradient, phi component	Domain 1	
tds.grad_cOxz	cOxz	mol/m^4	Concentration gradient, z component	Domain 1	
tds.dflux_cRedr	-tds.D_cRedrr*cRedr-tds.D_cRedrz*cRedz	mol/(m^2·s)	Diffusive flux, r component	Domain 1	
tds.dflux_cRedphi	-tds.D_cRedphir*cRedr-tds.D_cRedphiz*cRedz	mol/(m^2·s)	Diffusive flux, phi component	Domain 1	
tds.dflux_cRedz	-tds.D_cRedzr*cRedr-tds.D_cRedzz*cRedz	mol/(m^2·s)	Diffusive flux, z component	Domain 1	
tds.grad_cRedr	cRedr	mol/m^4	Concentration gradient, r component	Domain 1	
tds.grad_cRedphi	0	mol/m^4	Concentration gradient, phi component	Domain 1	
tds.grad_cRedz	cRedz	mol/m^4	Concentration gradient, z component	Domain 1	
tds.Res_cOx	d(cOx,t)-tds.R_cOx	mol/(m^3·s)	Equation residual	Domain 1	
tds.Res_cRed	d(cRed,t)-tds.R_cRed	mol/(m^3·s)	Equation residual	Domain 1	

Shape functions

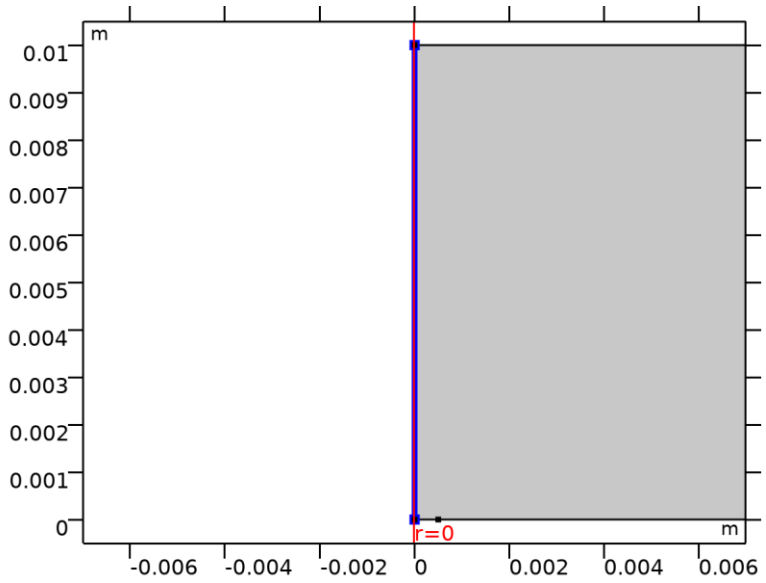
Name	Shape function	Unit	Description	Shape frame	Selection
cOx	Lagrange (Linear)	mol/m^3	Concentration	Spatial	Domain 1
cRed	Lagrange (Linear)	mol/m^3	Concentration	Spatial	Domain 1

Weak expressions

Weak expression	Integration order	Integration frame	Selection
2*(-cOxt*test(cOx)+tds.dflux_cOxr*test(cOxr)+tds.dflux_cOxz*test(cOxz))*pi*r	2	Spatial	Domain 1

Weak expression	Integration order	Integration frame	Selection
2*(-cRedt*test(cRed)+tds.dflux_cRedr*test(cRedr)+tds.dflux_cRedz*test(cRedz))*pi*r	2	Spatial	Domain 1
2*tds.streamline*(isScalingSystemDomain==0)*pi*r	2	Spatial	Domain 1
2*tds.crosswind*(isScalingSystemDomain==0)*pi*r	4	Spatial	Domain 1

2.3.4 Axial Symmetry 1

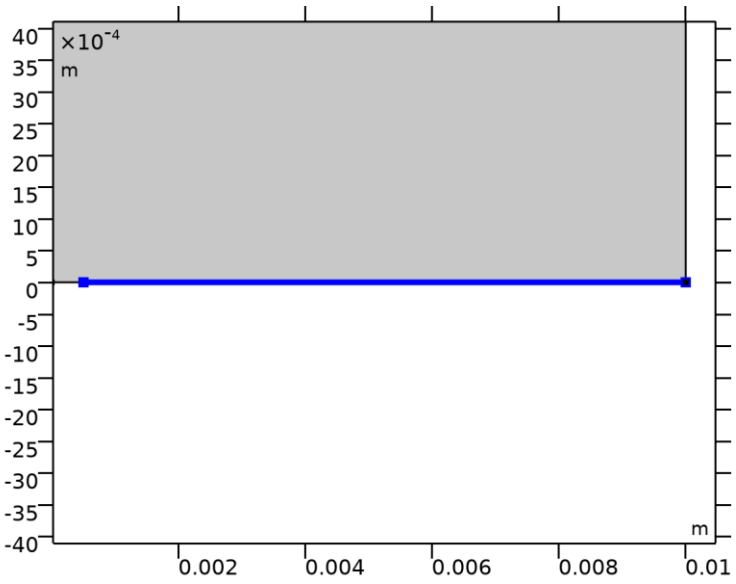


Axial Symmetry 1

SELECTION

Geometric entity level	Boundary
Selection	Geometry geom1: Dimension 1: All boundaries

2.3.5 No Flux - Glass



No Flux - Glass

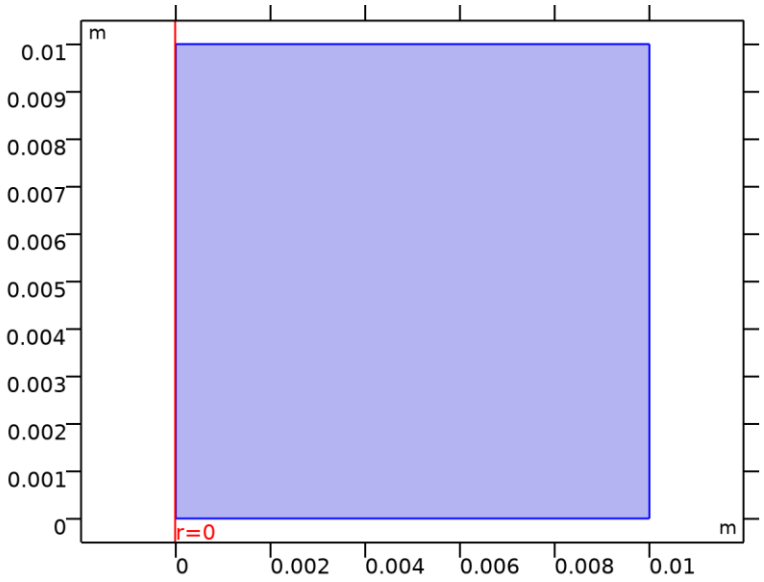
SELECTION

Geometric entity level	Boundary
Selection	Geometry geom1: Dimension 1: All boundaries

EQUATIONS

$$-\mathbf{n} \cdot \mathbf{J}_i = 0$$

2.3.6 Concentration Initial Values



Concentration Initial Values

SELECTION

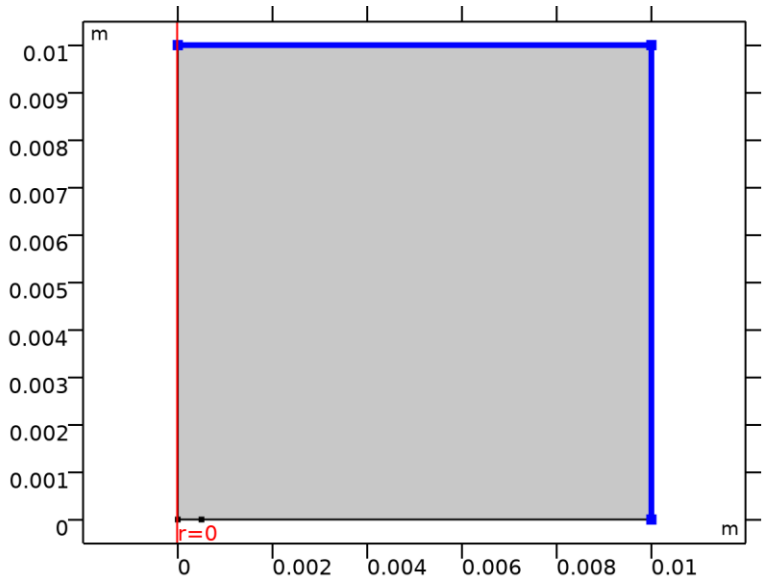
Geometric entity level	Domain
Selection	Geometry geom1: Dimension 2: All domains

Initial values

SETTINGS

Description	Value
Concentration	{cOx0, 0}

2.3.7 Concentration Outer Boundary



Concentration Outer Boundary

SELECTION

Geometric entity level	Boundary
Selection	Geometry geom1: Dimension 1: Boundaries 3, 5

EQUATIONS

$c_i = c_{0,i}$

Concentration

SETTINGS

Description	Value
Species cOx	On
Species cRed	On
Concentration	{cOx0, 0}

Constraint settings

SETTINGS

Description	Value
Apply reaction terms on	All physics (symmetric)
Use weak constraints	Off
Constraint method	Elemental

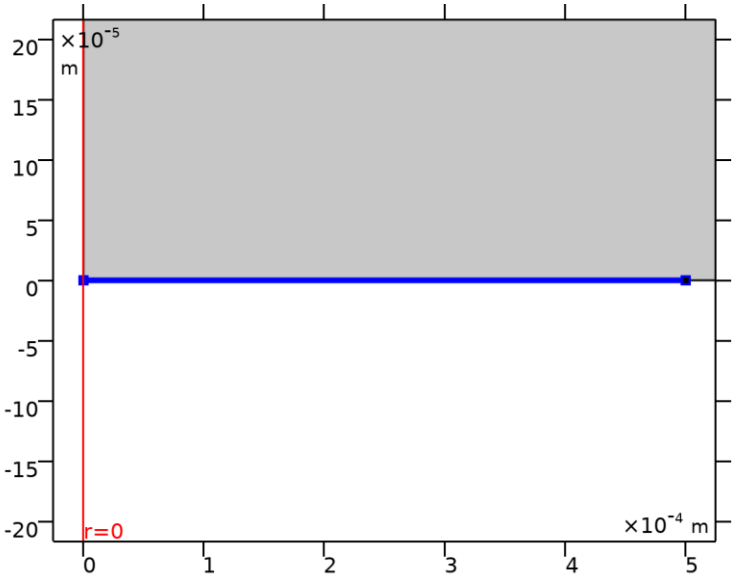
Variables

Name	Expression	Unit	Description	Selection
tds.c0_cOx	cOx0	mol/m³	Concentration	Boundaries 3, 5
tds.c0_cRed	0	mol/m³	Concentration	Boundaries 3, 5

Constraints

Constraint	Constraint force	Shape function	Selection	Details
-cOx+tds.c0_cOx	test(-cOx+tds.c0_cOx)	Lagrange (Linear)	Boundaries 3, 5	Elemental
-cRed+tds.c0_cRed	test(-cRed+tds.c0_cRed)	Lagrange (Linear)	Boundaries 3, 5	Elemental

2.3.8 Butler Volmer HET on the Electrode



Butler Volmer HET on the Electrode

SELECTION

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

EQUATIONS

$$-\mathbf{n}\cdot\mathbf{J}_i = J_{0,i}$$

Inward flux

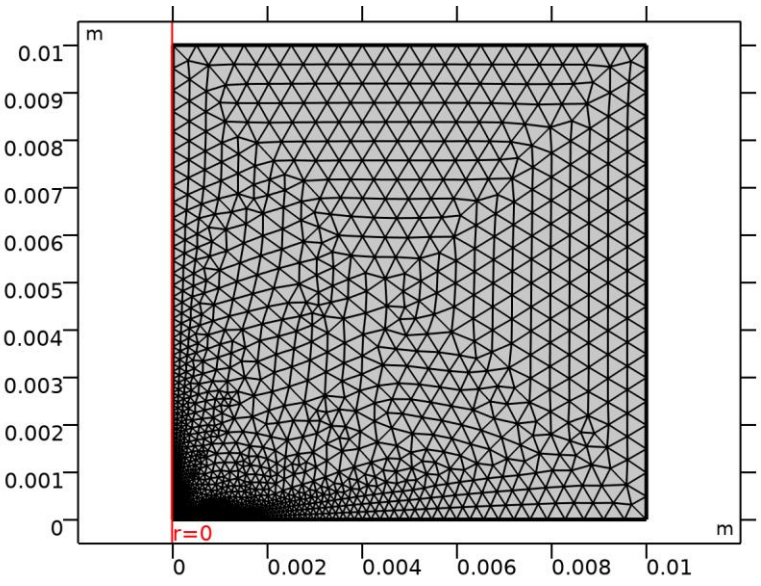
SETTINGS

Description	Value
Flux type	General inward flux
Species cOx	On
Species cRed	On
	{-kf*cOx + kb*cRed, -(-kf*cOx + kb*cRed)}

Weak expressions

Weak expression	Integration order	Integration frame	Selection
2*(-kf*cOx+kb*cRed)*test(cOx)*pi*r	2	Spatial	Boundary 2
-2*(-kf*cOx+kb*cRed)*test(cRed)*pi*r	2	Spatial	Boundary 2

2.4 MESH 1



Mesh 1

2.4.1 Size (size)

SETTINGS

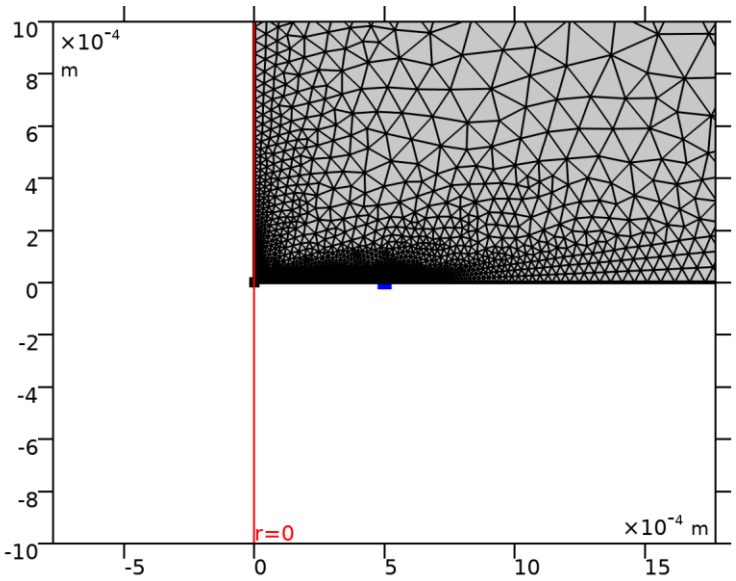
Description	Value
Maximum element size	5E-4
Minimum element size	1E-8
Curvature factor	0.3

Description	Value
Maximum element growth rate	1.2
Custom element size	Custom

2.4.2 Size 1 (size1)

SELECTION

Geometric entity level	Point
Selection	Geometry geom1: Dimension 0: Point 3



Size 1

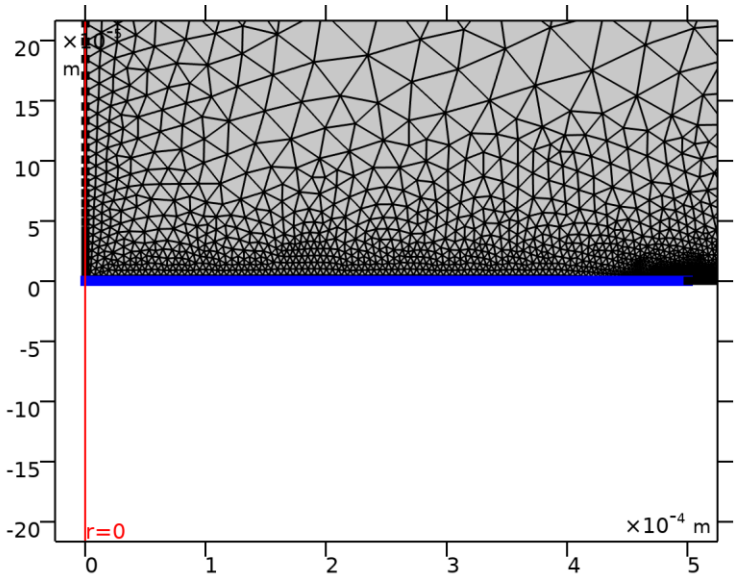
SETTINGS

Description	Value
Maximum element size	1E-7
Minimum element size	1E-8
Curvature factor	0.3
Curvature factor	Off
Resolution of narrow regions	Off
Maximum element growth rate	1.05
Custom element size	Custom

2.4.3 Size 2 (size2)

SELECTION

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



Size 2

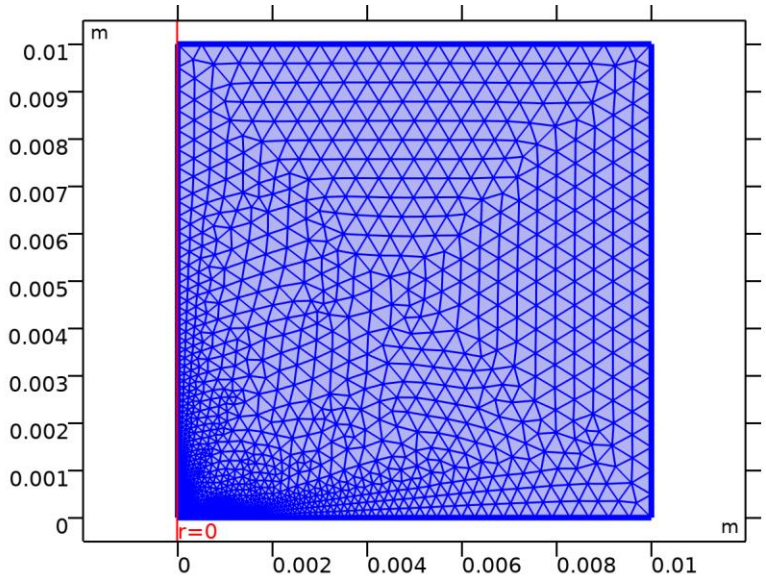
SETTINGS

Description	Value
Maximum element size	Point1/100
Minimum element size	0.5[mm]/100
Minimum element size	Off
Curvature factor	0.3
Curvature factor	Off
Resolution of narrow regions	Off
Maximum element growth rate	1.05
Custom element size	Custom

2.4.4 Size 3 (size3)

SELECTION

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



Size 3

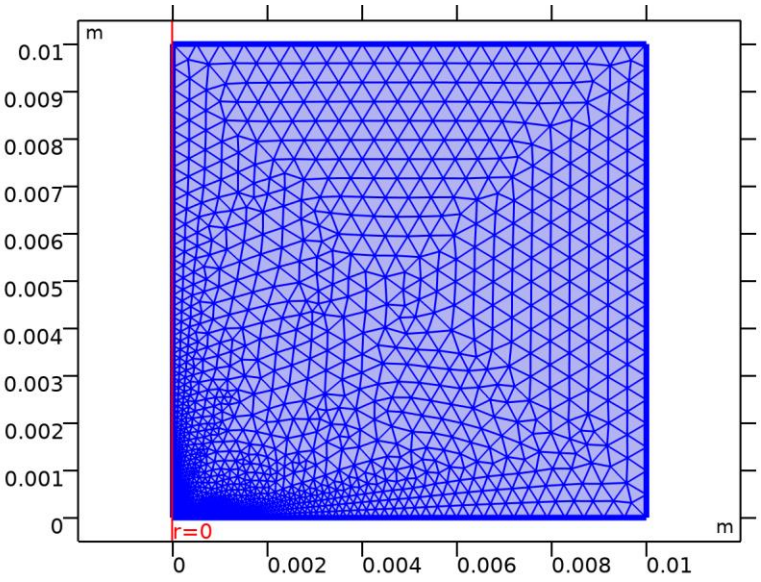
SETTINGS

Description	Value
Maximum element size	5E-4
Minimum element size	1E-8
Curvature factor	0.3
Curvature factor	Off
Resolution of narrow regions	Off
Maximum element growth rate	1.3
Maximum element growth rate	Off
Custom element size	Custom

2.4.5 Free Triangular 2 (ftri2)

SELECTION

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



Free Triangular 2

3 Study

COMPUTATION INFORMATION

Computation time	46 min 42 s
CPU	Intel64 Family 6 Model 158 Stepping 9, 4 cores
Operating system	Windows 10

3.1 PARAMETRIC SWEEP

Parameter name	Parameter value list	Parameter unit
R_U	0, 5000, 50000	Ω

STUDY SETTINGS

Description	Value
Sweep type	Specified combinations
Parameter name	R_U
Unit	Ω

PARAMETERS

Parameter name	Parameter value list	Parameter unit
R_U (Uncompensated Resistance)	0, 5000, 50000	Ω

3.2 TIME DEPENDENT

Times	Unit
range(0,(2*SegmentDuration-0)/4000,2*SegmentDuration)	s

STUDY SETTINGS

Description	Value
Include geometric nonlinearity	Off

PHYSICS AND VARIABLES SELECTION

Physics interface	Discretization
Transport of Diluted Species (tds)	physics

MESH SELECTION

Geometry	Mesh
Geometry 1 (geom1)	mesh1

3.3 SOLVER CONFIGURATIONS

3.3.1 Solution 7

Compile Equations: Time Dependent (st1)

STUDY AND STEP

Description	Value
Use study	Study
Use study step	Time Dependent

Dependent Variables 1 (v1)

GENERAL

Description	Value
Defined by study step	Time Dependent

RESIDUAL SCALING

Description	Value
Method	Manual

INITIAL VALUE CALCULATION CONSTANTS

Constant name	Initial value source
t	range(0,(2*SegmentDuration-0)/4000,2*SegmentDuration)
timestep	0.02[s]

Concentration (comp1.cOx) (comp1_cOx)

GENERAL

Description	Value
Field components	comp1.cOx
Internal variables	{comp1.uflux.cOx, comp1.dflux.cOx, comp1.tds.dt2Inv_cOx}

Concentration (comp1.cRed) (comp1_cRed)

GENERAL

Description	Value
Field components	comp1.cRed
Internal variables	{comp1.uflux.cRed, comp1.dflux.cRed, comp1.tds.dt2Inv_cRed}

Time-Dependent Solver 1 (t1)

GENERAL

Description	Value

Description	Value
Defined by study step	Time Dependent
Times	{0, 0.005, 0.01, 0.015, 0.02, 0.025, 0.03, 0.035, 0.04, 0.045, 0.05, 0.055, 0.06, 0.065, 0.07, 0.075, 0.08, 0.085, 0.09, 0.095, 0.1, 0.105, 0.11, 0.115, 0.12, 0.125, 0.13, 0.135, 0.14, 0.145, 0.15, 0.155, 0.16, 0.165, 0.17, 0.17500000000000002, 0.18, 0.185, 0.19, 0.195, 0.2, 0.20500000000000002, 0.21, 0.215, 0.22, 0.225, 0.23, 0.23500000000000001, 0.24, 0.245, 0.25, 0.255, 0.26, 0.265, 0.27, 0.275, 0.28, 0.28500000000000003, 0.29, 0.295, 0.3, 0.305, 0.31, 0.315, 0.32, 0.325, 0.33, 0.335, 0.34, 0.34500000000000003, 0.35000000000000003, 0.355, 0.36, 0.365, 0.37, 0.375, 0.38, 0.385, 0.39, 0.395, 0.4, 0.405, 0.41000000000000003, 0.41500000000000004, 0.42, 0.425, 0.43, 0.435, 0.44, 0.445, 0.45, 0.455, 0.46, 0.465, 0.47000000000000003, 0.47500000000000003, 0.48, 0.485, 0.49, 0.495, 0.5, 0.505, 0.51, 0.515, 0.52, 0.525, 0.53, 0.535, 0.54, 0.545, 0.55, 0.555, 0.56, 0.5650000000000001, 0.5700000000000001, 0.5750000000000001, 0.58, 0.585, 0.59, 0.595, 0.6, 0.605, 0.61, 0.615, 0.62, 0.625, 0.63, 0.635, 0.64, 0.645, 0.65, 0.655, 0.66, 0.665, 0.67, 0.675, 0.68, 0.685, 0.6900000000000001, 0.6950000000000001, 0.7000000000000001, 0.705, 0.71, 0.715, 0.72, 0.725, 0.73, 0.735, 0.74, 0.745, 0.75, 0.755, 0.76, 0.765, 0.77, 0.775, 0.78, 0.785, 0.79, 0.795, 0.8, 0.805, 0.81, 0.8150000000000001, 0.8200000000000001, 0.8250000000000001, 0.8300000000000001, 0.835, 0.84, 0.845, 0.85, 0.855, 0.86, 0.865, 0.87, 0.875, 0.88, 0.885, 0.89, 0.895, 0.9, 0.905, 0.91, 0.915, 0.92, 0.925, 0.93, 0.935, 0.9400000000000001, 0.9450000000000001, 0.9500000000000001, 0.9550000000000001, 0.96, 0.965, 0.97, 0.975, 0.98, 0.985, 0.99, 0.995, 1, 1.0050000000000001, 1.01, 1.0150000000000001, 1.02, 1.025, 1.03, 1.035, 1.04, 1.045, 1.05, 1.055, 1.06, 1.065, 1.07, 1.075, 1.08, 1.085, 1.09, 1.095, 1.1, 1.105, 1.11, 1.115, 1.12, 1.125, 1.1300000000000001, 1.135, 1.1400000000000001, 1.145, 1.1500000000000001, 1.155, 1.16, 1.165, 1.17, 1.175, 1.18, 1.185, 1.19, 1.195, 1.2, 1.205, 1.21, 1.215, 1.22, 1.225, 1.23, 1.235, 1.24, 1.245, 1.25, 1.2550000000000001, 1.26, 1.2650000000000001, 1.27, 1.2750000000000001, 1.28, 1.285, 1.29, 1.295, 1.3, 1.305, 1.31, 1.315, 1.32, 1.325, 1.33, 1.335, 1.34, 1.345, 1.35, 1.355, 1.36, 1.365, 1.37, 1.375, 1.3800000000000001, 1.385, 1.3900000000000001, 1.395, 1.4000000000000001, 1.405, 1.41, 1.415, 1.42, 1.425, 1.43, 1.435, 1.44, 1.445, 1.45, 1.455, 1.46, 1.465, 1.47, 1.475, 1.48, 1.485, 1.49, 1.495, 1.5, 1.5050000000000001, 1.51, 1.5150000000000001, 1.52, 1.5250000000000001, 1.53, 1.5350000000000001, 1.54, 1.545, 1.55, 1.555, 1.56, 1.565, 1.57, 1.575, 1.58, 1.585, 1.59, 1.595, 1.6, 1.605, 1.61, 1.615, 1.62, 1.625, 1.6300000000000001, 1.635, 1.6400000000000001, 1.645, 1.6500000000000001, 1.655, 1.6600000000000001, 1.665, 1.67, 1.675, 1.68, 1.685, 1.69, 1.695, 1.7, 1.705, 1.71, 1.715, 1.72, 1.725, 1.73, 1.735, 1.74, 1.745, 1.75, 1.7550000000000001, 1.76, 1.7650000000000001, 1.77, 1.7750000000000001, 1.78, 1.7850000000000001, 1.79, 1.795, 1.8, 1.805, 1.81, 1.815, 1.82, 1.825, 1.83, 1.835, 1.84, 1.845, 1.85, 1.855, 1.86, 1.865, 1.87, 1.875, 1.8800000000000001, 1.885, 1.8900000000000001, 1.895, 1.9000000000000001, 1.905, 1.9100000000000001, 1.915, 1.92, 1.925, 1.93, 1.935, 1.94, 1.945, 1.95, 1.955, 1.96, 1.965, 1.97, 1.975, 1.98, 1.985, 1.99,

Description	Value
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Description	Value
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Description	Value
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Description	Value
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Description	Value
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Description	Value
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Relative tolerance	0.0001

ABSOLUTE TOLERANCE

Description	Value
Tolerance factor	0.001

TIME STEPPING

Description	Value
Steps taken by solver	Strict
Initial step	1E-3
Maximum BDF order	2

Fully Coupled 1 (fc1)

GENERAL

Description	Value
Linear solver	Direct 1

METHOD AND TERMINATION

Description	Value
Nonlinear method	Automatic (Newton)
Initial damping factor	0.9
Maximum number of iterations	8

Direct 1 (d1)

GENERAL

Description	Value
Solver	PARDISO

3.3.2 Parametric Solutions 1

R_U=0 (su1)

GENERAL

Description	Value
Solution	R_U=0

R_U=5000 (su2)

GENERAL

Description	Value
Solution	R_U=5000

R_U=50000 (su3)

GENERAL

Description	Value
Solution	R_U=50000

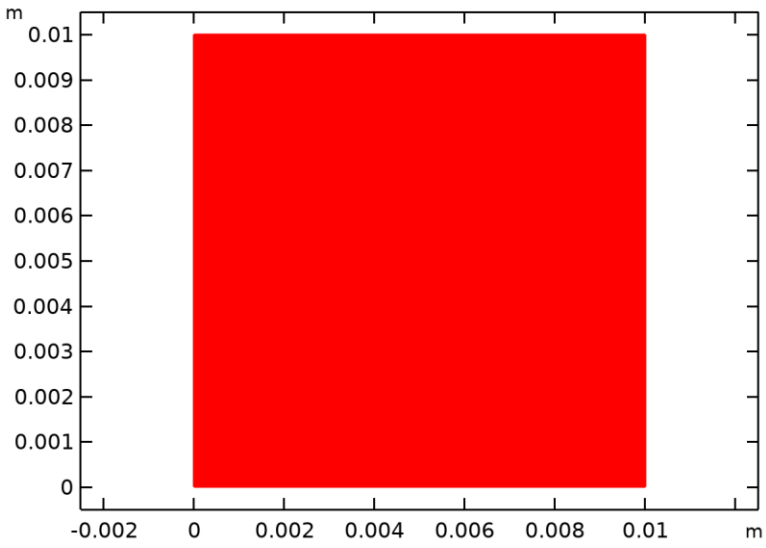
4 Results

4.1 DATA SETS

4.1.1 Study /Solution 7

SOLUTION

Description	Value
Solution	Solution 7
Component	Save Point Geometry 1



Dataset: Study /Solution 7

4.1.2 Study /Parametric Solutions 2

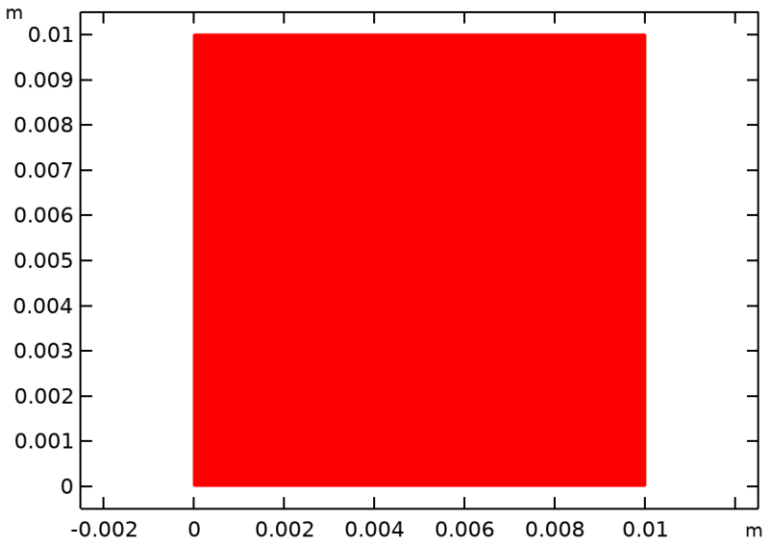
SOLUTION

Description	Value
Solution	Parametric Solutions 2
Component	Geometry 1

4.1.3 Probe Solution 5

SOLUTION

Description	Value
Solution	Solution 7
Component	Save Point Geometry 1
Frame	Mesh (Rm, PHIm, Zm)



Dataset: Probe Solution 5

4.1.4 Boundary Probe - Calculate Current (Method A)

SELECTION

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

DATA

Description	Value
Dataset	Probe Solution 5

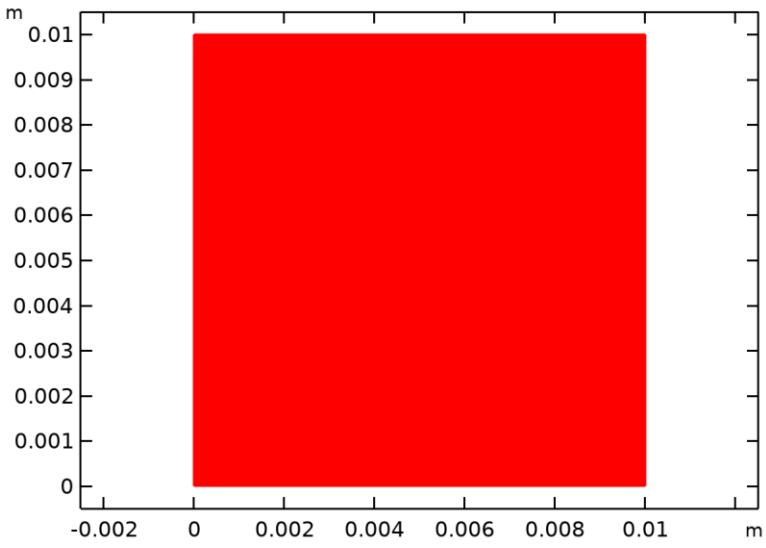
SETTINGS

Description	Value
Method	Integration
Integration order	2
Integration order	On

4.1.5 Study /Parametric Solutions 1

SOLUTION

Description	Value
Solution	Parametric Solutions 1
Component	Save Point Geometry 1



Dataset: Study /Parametric Solutions 1

4.1.6 Revolution 2D 5

DATA

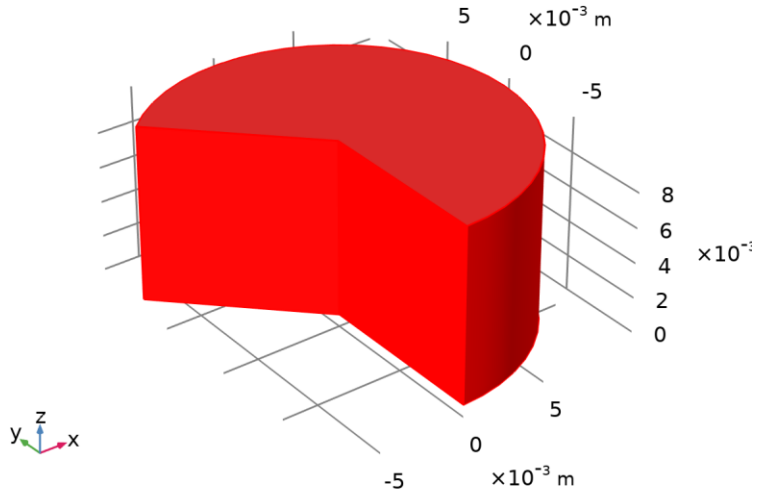
Description	Value
Dataset	Study /Parametric Solutions 1

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 5

4.2 DERIVED VALUES

4.2.1 Global Evaluation 1

OUTPUT

Evaluated in	Table 11

DATA

Description	Value
Dataset	Study /Parametric Solutions 1
Table columns	Outer solutions

EXPRESSIONS

Expression	Unit	Description
Potential(t)-E0	V	E-E0 /V
bnd1	A	Current calculated by boundary probe variable bnd1

4.2.2 Boundary Probe - Calculate Current

OUTPUT

Evaluated in	Probe Table 12

DATA

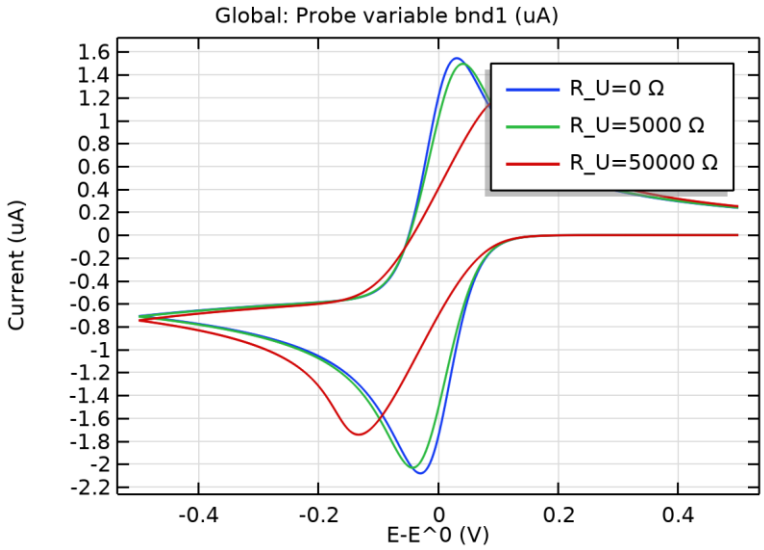
Description	Value
Dataset	Boundary Probe - Calculate Current

EXPRESSIONS

Expression	Unit	Description
-(tds.ntflux_cOx)*F_const*n	A	

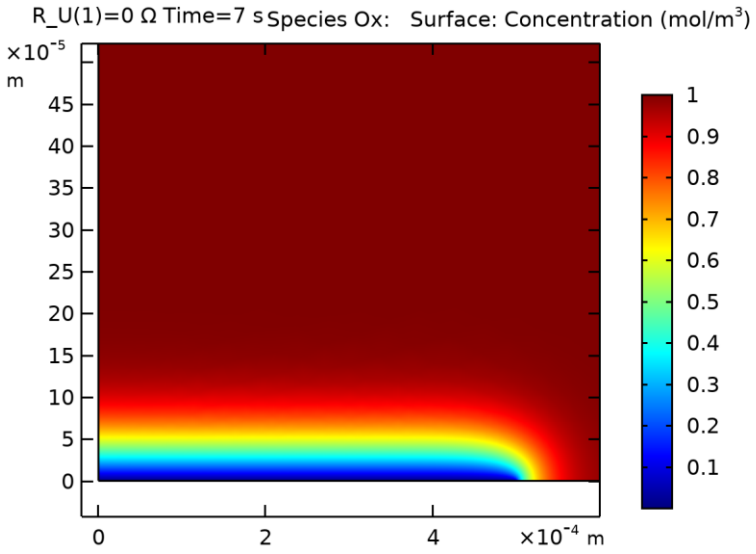
4.3 PLOT GROUPS

4.3.1 Cyclic Voltammetry from bnd1



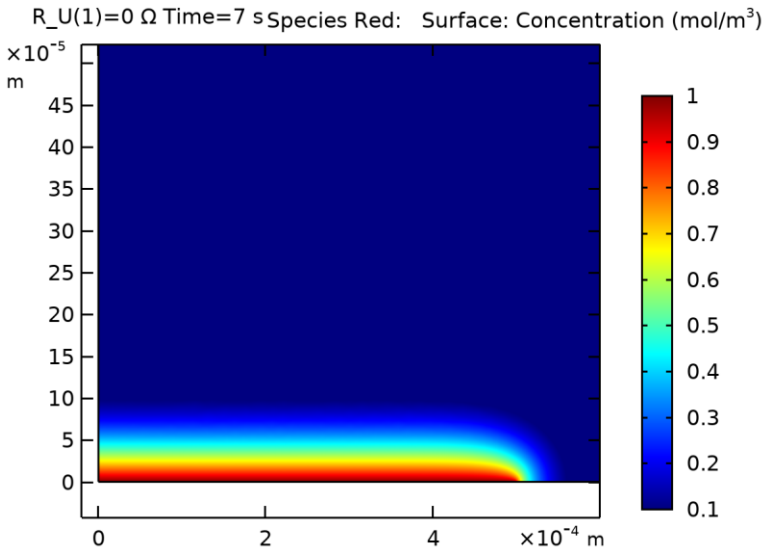
Global: Probe variable bnd1 (uA)

4.3.2 Concentration, Ox (tds)



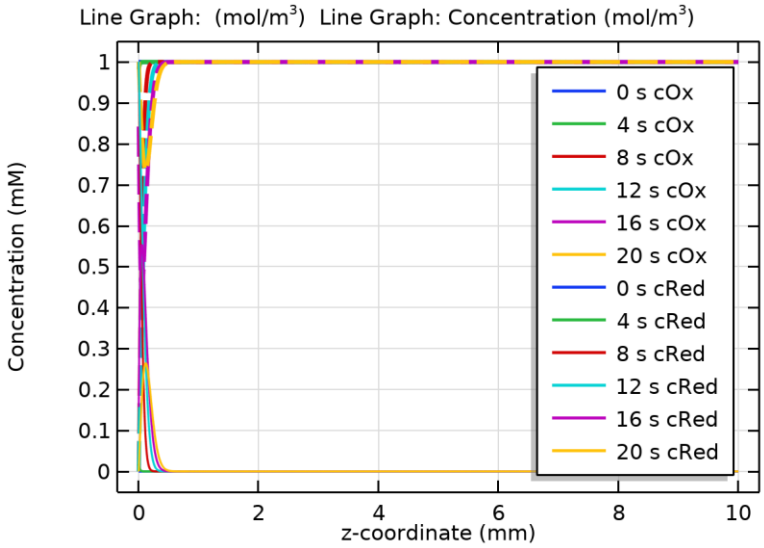
Species Ox: Surface: Concentration (mol/m³)

4.3.3 Concentration, Red (tds)



Species Red: Surface: Concentration (mol/m³)

4.3.4 Concentration z axis



Line Graph: (mol/m³) Line Graph: Concentration (mol/m³)