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MULTIPHYSICS®

COMSOL Model Report B – Electrostatic Model of a Soluble Redox Couple with Ohmic Potential Drop Compensation

Report date	Dec 16, 2022 4:44:09 PM

Contents

1 Global Definitions

Date	Dec 16, 2022 4:10:09 PM

1.1 PARAMETERS

1.1.1 General System & Geometry

GENERAL SYSTEM & GEOMETRY

Name	Expression	Value	Description
epsilon_s	80	80	The relative dielectric constant of bulk water, assuming T = 293K
cAnion_b	cNO3b + cCounterIon0	1003 mol/m³	Bulk anion concentration of supporting electrolyte including counter ion of the redox couple
cCation_b	cKb	1000 mol/m³	Bulk cation concentration of supporting electrolyte
cKb	1[M]	1000 mol/m³	
cNO3b	cKb	1000 mol/m³	
D_K	2.0*10^ - 5 [cm^2/s]	2E−9 m²/s	Diffusion coefficient for K+ = 1.957
D_NO3	1.9*10^ - 5 [cm^2/s]	1.9E−9 m²/s	Diffusion coefficient for ClO4- = 1.902
D_Anion	D_NO3	1.9E−9 m²/s	
D_Cation	D_K	2E−9 m²/s	
L	0.25[cm]	0.0025 m	Length of domain/boundary
z_Anion	-1	−1	The electrostatic charge of supporting electrolyte anion

Name	Expression	Value	Description
z_Cation	+1	1	The electrostatic charge of supporting electrolyte cation
T	293.15 [K]	293.15 K	Temperature
conductivity	F_const*(F_RT*D_Cation*cCation_b + F_RT*D_Anion*cAnion_b + F_RT*DcOx*cOx0_dif)	14.92 S/m	
Resistance	L/conductivity	1.6756E−4 Ω·m²	
F_RT	(n*F_const)/(R_const*T)	39.586 1/V	
Kappa	e_const*sqrt((((z_Cation^2)*cCation_b + (z_Anion^2)*cAnion_b + cOx0_dif*(z_Ox_diff^2))*N_A_const)/(epsilon_s*epsilon0_const*k_B_const*T))	3.2938E9 1/m	Inverse Debye length
DebyeLength	1/Kappa	3.036E−10 m	Debye length

1.1.2 Stern Layer

Name	Expression	Value	Description
epsilon_1	6	6	The relative dielectric constant of the Stern layer
A	(1[mm])^2*pi	3.1416E−6 m²	Electrode area
d1	0.29 [nm]	2.9E−10 m	Stern layer thickness
d2	0.59 [nm]	5.9E−10 m	Stern layer thickness
epsilon_2	30	30	The relative dielectric constant of the Stern layer

1.1.3 Diffusing Redox Species

Name	Expression	Value	Description
DcOx	7.5*10^ - 6[cm^2/s]	7.5E−10 m²/s	Diffusion Coefficient Oxidised species
DcRed	DcOx/0.72	1.0417E−9 m²/s	Diffusion Coefficient reduced species
cOx0_dif	1 [mM]	1 mol/m³	Initial concentration of Ox species
k0_Dif	13.5 [cm/s]	0.135 m/s	Heterogeneous electron transfer rate constant (fast)
alpha_Dif	0.45	0.45	Transfer coefficient
n	z_Ox_diff - z_Red_diff	1	Number of electrons transferred

Name	Expression	Value	Description
E0_Dif	-0.173 [V]	−0.173 V	Standard redox potential for [Ru(NH3)6]+3/+2 Vs SCE
z_Red_diff	+2	2	The electrostatic charge of the reduced species
z_Ox_diff	+3	3	The electrostatic charge of the oxidised species
cCounterIon0	cOx0_dif*3	3 mol/m³	The concentration of the balancing counterion

1.1.4 CV Waveform

CV WAVEFORM

Name	Expression	Value	Description
E_Start	0 [V]	0 V	Starting potential applied to the working electrode
Start_Duration	(E_High - E_Start)/v	1E−4 s	Starting scan duration
ScanRange	abs(E_High - E_Low)	0.6 V	Absolute scan range
Segment_Duration	ScanRange/v	6E−4 s	Length of one sweep
v	1000 [V/s]	1000 V/s	Scan rate
sampling	1 [mV]	0.001 V	Potential step size of the CV
E_Low	-0.5 [V]	−0.5 V	Switching potential, the lowest potential applied to the working electrode
sampling_time	(2*Segment_Duration + Start_Duration)/(((abs(E_High - E_Low)*2 + (E_High - E_Start)))/(sampling))	1E−6 s	Corresponding sampling time interval for the potential step size at the specified scan rate
E_High	0.1 [V]	0.1 V	Switching potential, the highest potential applied to the

Name	Expression	Value	Description
			working electrode
Durr_Tot	(2*Segment_Duration + Start_Duration)	0.0013 s	

1.1.5 Ohmic drop compensation

OHMIC DROP COMPENSATION

Name	Expression	Value	Description
Gain	1e8	1E8	"Gain" in the ohmic drop 'compensation circuit' (proportional)
OhmicDropCompensation	95[%]	0.95	Amount of ohmic drop that is attempted to be corrected for

1.2 FUNCTIONS

1.2.1 Uncorrected potential

Function name	UncorrectedPotential
Function type	Piecewise

UncorrectedPotential(t) (V)
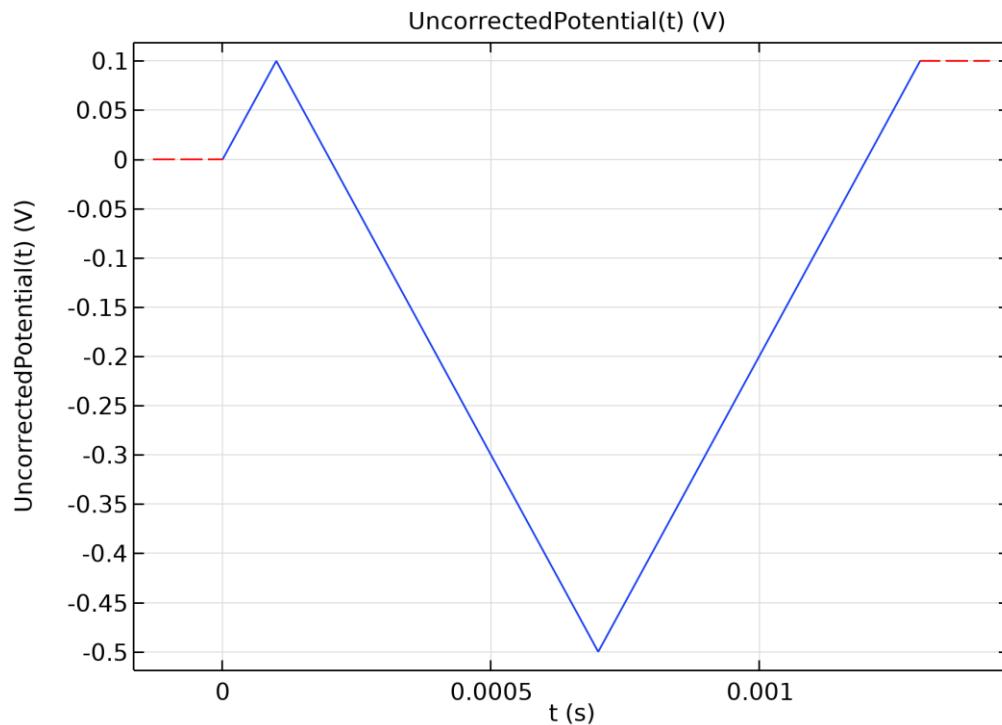
Uncorrected potential

DEFINITION

Description	Value
Argument	t
Extrapolation	Constant
Smoothing	No smoothing

DEFINITION

Start	End	Function
0	Start_Duration	E_Start+v*t
Start_Duration	Start_Duration+Segment_Duration	E_High-v*(t-Start_Duration)
Start_Duration+Segment_Duration	Start_Duration+2*Segment_Duration	E_Low+v*(t-Segment_Duration-Start_Duration)

UNITS

Description	Value
Arguments	s
Function	V

2 Component 1

Description	Value
Unit system	Same as global system (SI)

2.1 DEFINITIONS

2.1.1 Variables

ET kinetics

Geometric entity level	Entire model

Name	Expression	Unit	Description
kf	k0_Dif*exp((-alpha_Dif*F_RT*(CorrectedPotential - E0_Dif - intop2(Phi))))	m/s	
kb	k0_Dif*exp(((1 - alpha_Dif)*F_RT*(CorrectedPotential - E0_Dif - intop2(Phi))))	m/s	
CorrectedPotential	UncorrectedPotential(t) + comp2.IR*OhmicDropCompensation	V	Applied potential corrected for IR drop

2.1.2 Probes

Applied potential probe (uncorrected)

Probe type	Global variable probe

Description	Value
Expression	UncorrectedPotential(t)
Table and plot unit	V
Description	Applied potential Uncorrected

Description	Value
Output table	Probe Table
Plot window	Probe Plot 3

Applied potential probe (corrected)

Probe type	Global variable probe

Description	Value
Expression	CorrectedPotential
Table and plot unit	V
Description	Applied potential Corrected

TABLE AND WINDOW SETTINGS

Description	Value
Output table	Probe Table
Plot window	Probe Plot 3

Total current

Probe type	Point probe

SELECTION

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

$\times 10^{-4}$ m
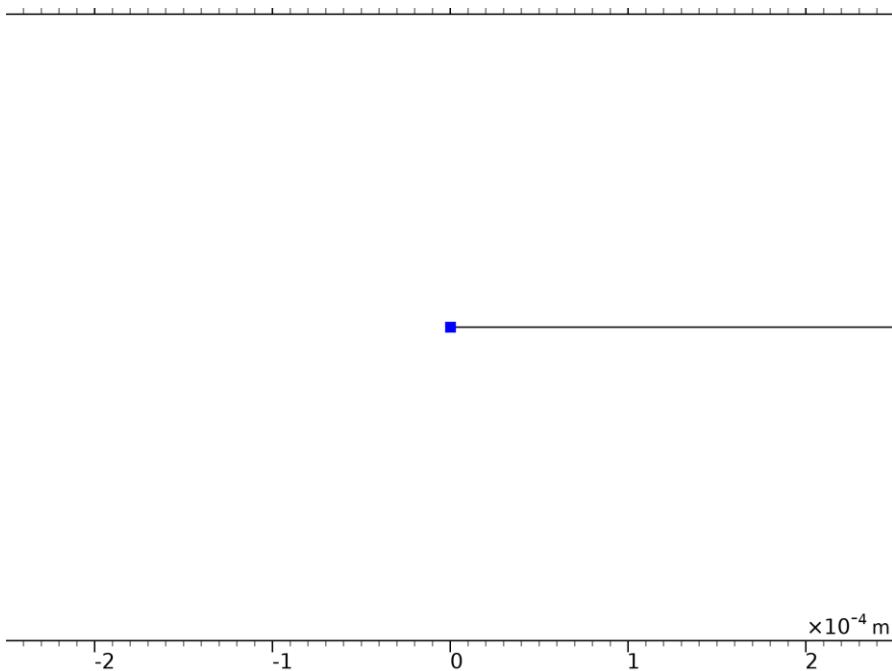
Selection

PROBE TYPE

Description	Value
Type	Integral

Description	Value
Expression	CurrentF + CurrentNF
Table and plot unit	A/m^2
Description	iTot

Description	Value
Output table	Probe Table
Plot window	Probe Plot 2

Faradaic current

Probe type	Point probe

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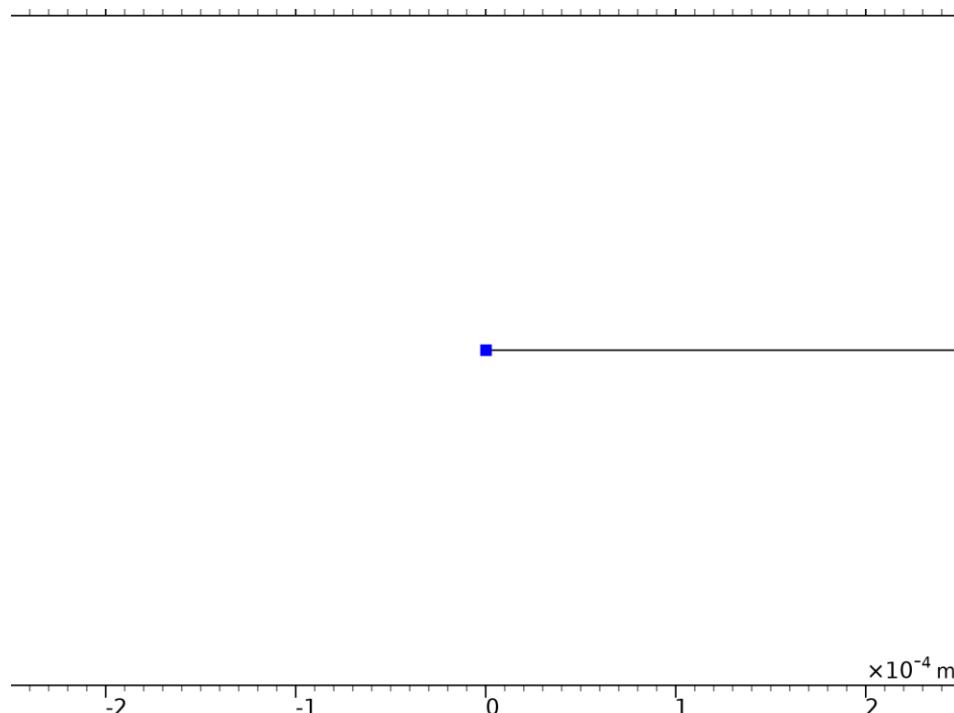
Selection

Description	Value
Type	Integral

EXPRESSION

Description	Value
Expression	(-kf*cOx + kb*cRed)*F_const*n
Table and plot unit	A/m^2
Description	iF

TABLE AND WINDOW SETTINGS

Description	Value
Output table	Probe Table
Plot window	Probe Plot 2

Non-faradaic current

Probe type	Point probe

SELECTION

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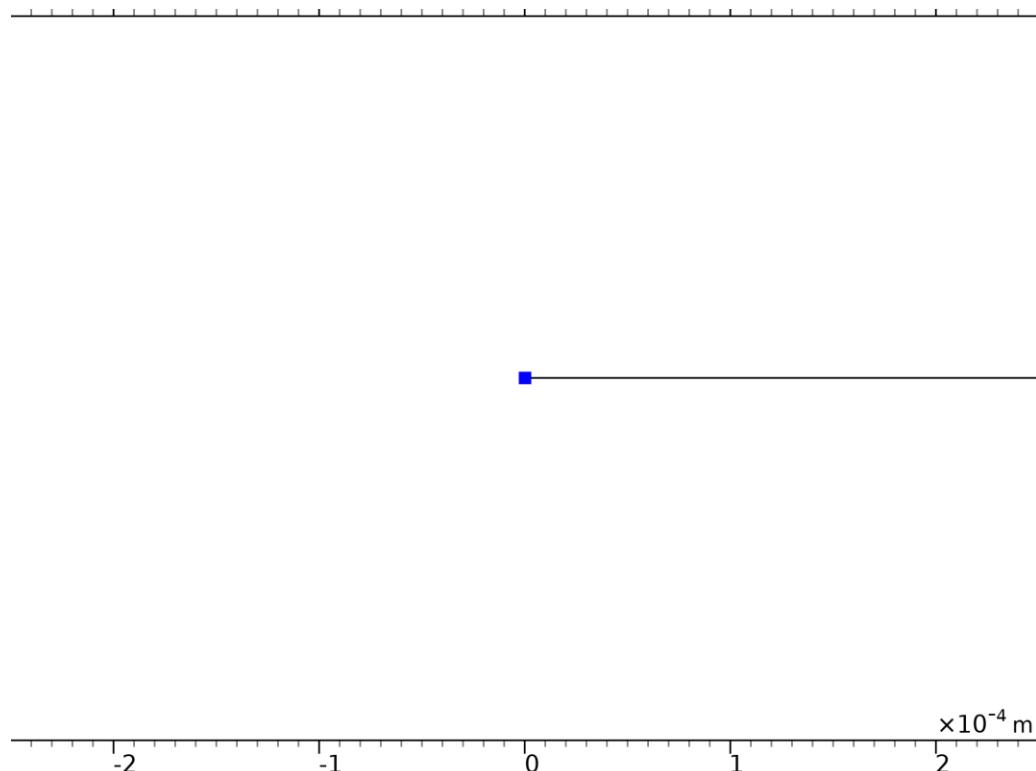
Selection

Description	Value
Type	Integral

EXPRESSION

Description	Value
Expression	intop1(d(es.nD, t))
Table and plot unit	A/m^2
Description	iNF

TABLE AND WINDOW SETTINGS

Description	Value
Output table	Probe Table
Plot window	Probe Plot 2

Ohmic drop (100%)

Probe type	Point probe

SELECTION

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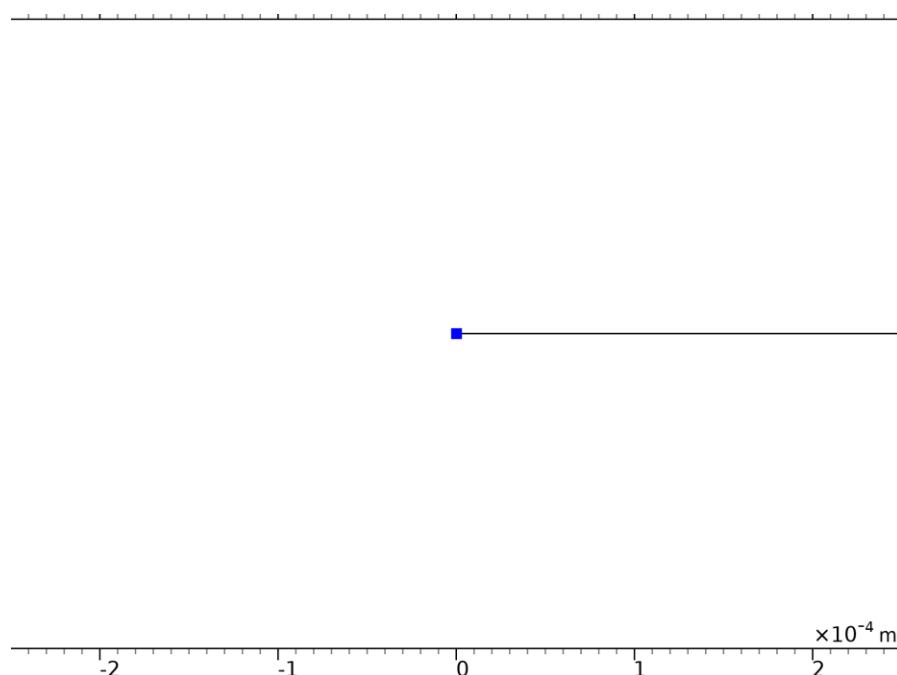
Selection

PROBE TYPE

Description	Value
Type	Integral

Description	Value
Expression	CurrentTot*Resistance
Table and plot unit	V
Description	IR

Description	Value
Output table	Probe Table
Plot window	Probe Plot 3

Domain Point Probe (potential just outside double layer)

Probe type	Domain point probe

2.1.3 Nonlocal Couplings

Electrode surface coupling

Coupling type	Integration
Operator name	intop1

Geometric entity level	Boundary
Selection	Geometry geom1: Dimension 0: Boundary 1
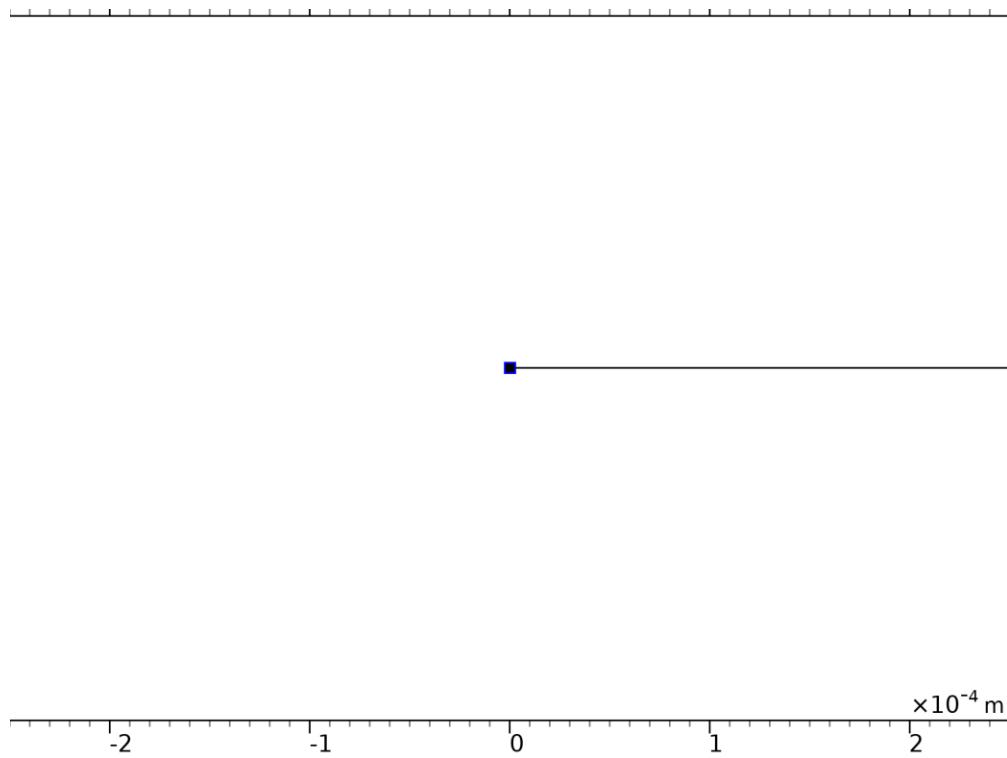
Selection

PET coupling

Coupling type	Integration
Operator name	intop2

SELECTION

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

×10⁻⁴ m

-2	-1	0	1	2
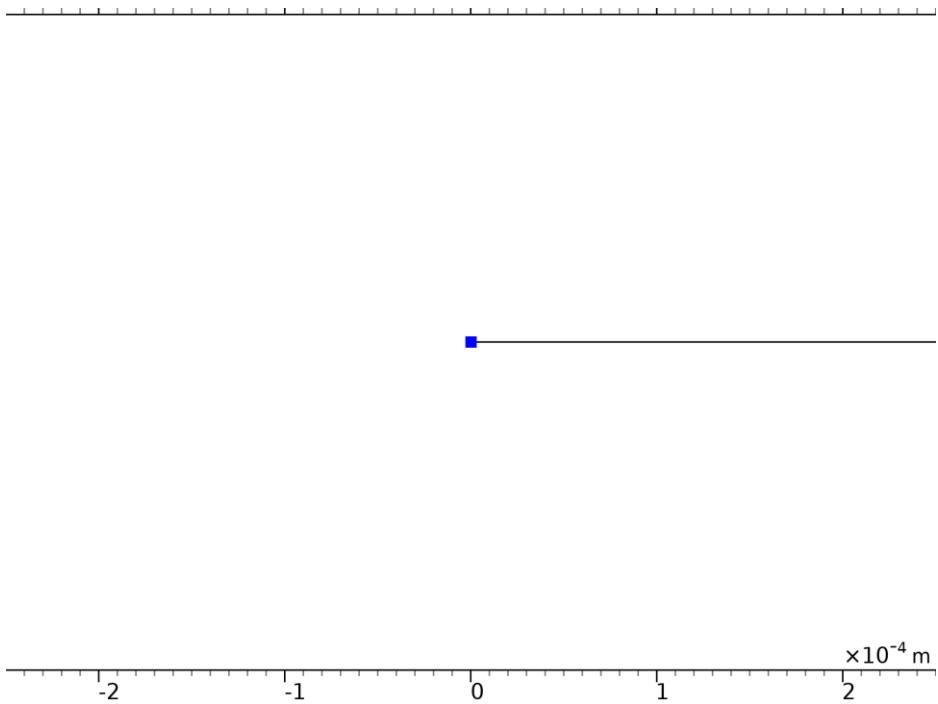
Selection

2.2 GEOMETRY 1

×10⁻⁴ m

0	5	10	15	20	25
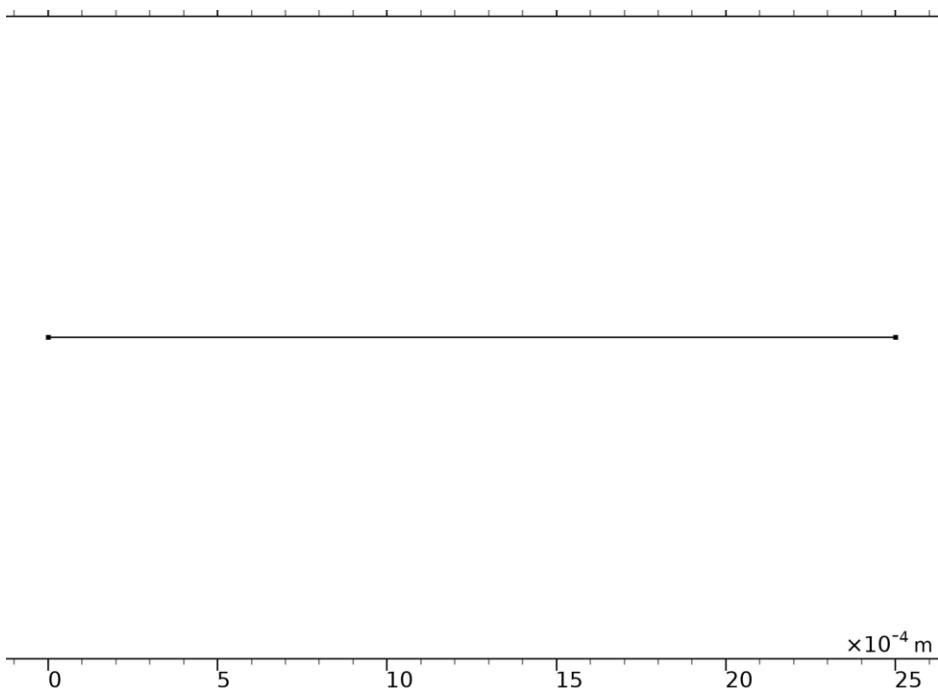
Geometry 1

UNITS

Length unit	m

Angular unit	deg

Description	Value
Space dimension	1
Number of domains	3
Number of boundaries	4

2.2.1 Interval 1 (i1)

INTERVAL

Coordinates (m)
0
L

2.2.2 Point 1 (pt1)

POINT

Description	Value
Point coordinate	5.9E-10

### 2.2.3 Point 2 (pt2)

POINT

Description	Value
Point coordinate	2.9E-10

2.3 TRANSPORT OF DILUTED SPECIES

USED PRODUCTS

COMSOL Multiphysics
Chemical Reaction Engineering Module

×10⁻⁴ m
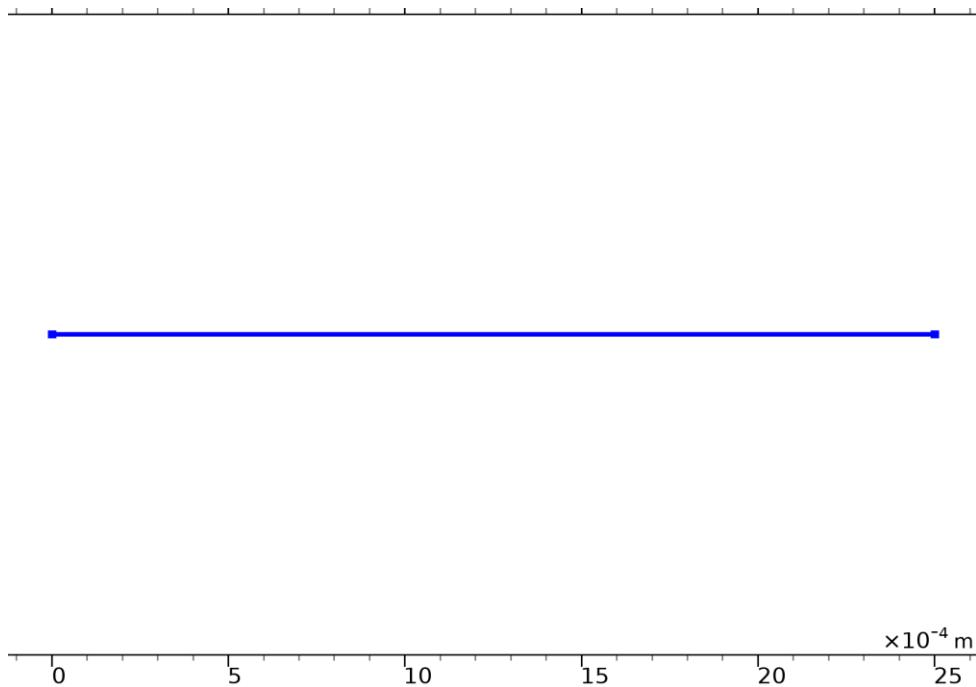
Transport of Diluted Species

SELECTION

Geometric entity level	Domain
Selection	Geometry geom1: Dimension 1: Domain 3

EQUATIONS

$$\frac{\partial c_i}{\partial t} + \nabla \cdot \mathbf{J}_i = R_i$$
$$\mathbf{J}_i = -D_i \nabla c_i - z_i u_{m,i} F c_i \nabla V$$

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

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Description	Value
Convection	Off
Migration in electric field	On
Mass transfer in porous media	Off

Advanced Settings

Description	Value
Convective term	Nonconservative form

2.3.2 Transport Properties 1

Transport Properties 1

Geometric entity level	Domain
Selection	Geometry geom1: Dimension 1: All domains

$$\nabla \cdot \mathbf{J}_i = R_i$$
$$\mathbf{J}_i = -D_i \nabla c_i - z_i u_{m,i} F c_i \nabla V$$

Diffusion

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Description	Value
Source	Material
Material	None
Diffusion coefficient	User defined
Diffusion coefficient	{{D_Cation, 0, 0}, {0, D_Cation, 0}, {0, 0, D_Cation}}
Diffusion coefficient	User defined
Diffusion coefficient	{{D_Anion, 0, 0}, {0, D_Anion, 0}, {0, 0, D_Anion}}

Migration in Electric Field

SETTINGS

| Description	Value
Electric potential	Electric potential (es)
Mobility	Nernst - Einstein relation
Charge number	{z_Cation, z_Anion}

Coordinate System Selection

SETTINGS

Description	Value
Coordinate system	Global coordinate system

Model Input

SETTINGS

Description	Value
Temperature	User defined
Temperature	T

2.3.3 No Flux 1
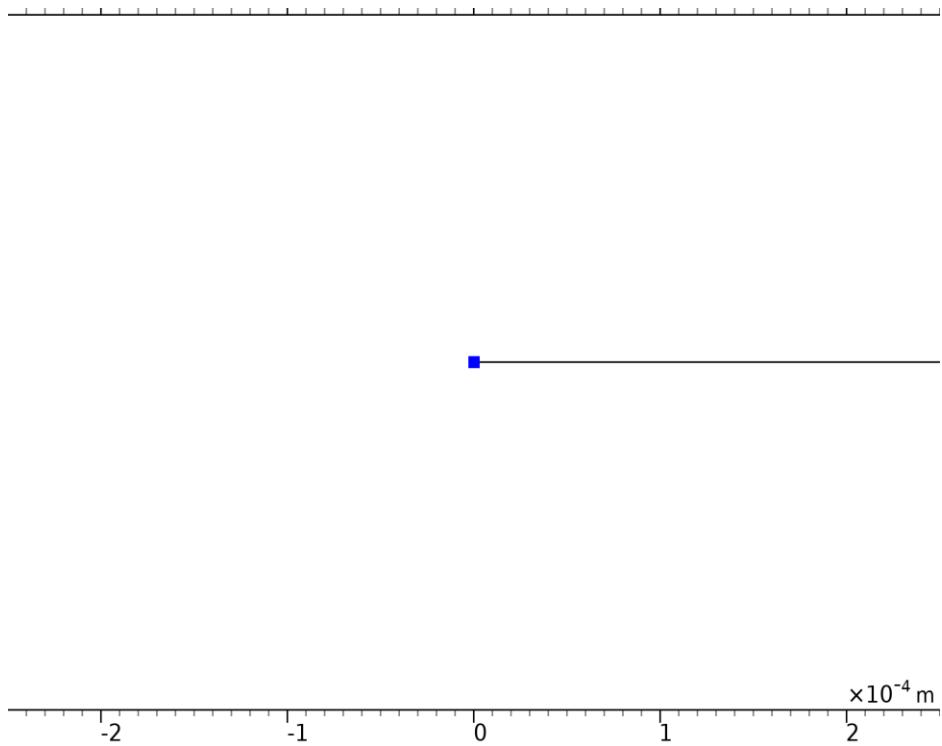
No Flux 1

SELECTION

Geometric entity level	Boundary
Selection	Geometry geom1: Dimension 0: All boundaries

EQUATIONS

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

2.3.4 Initial Values 1
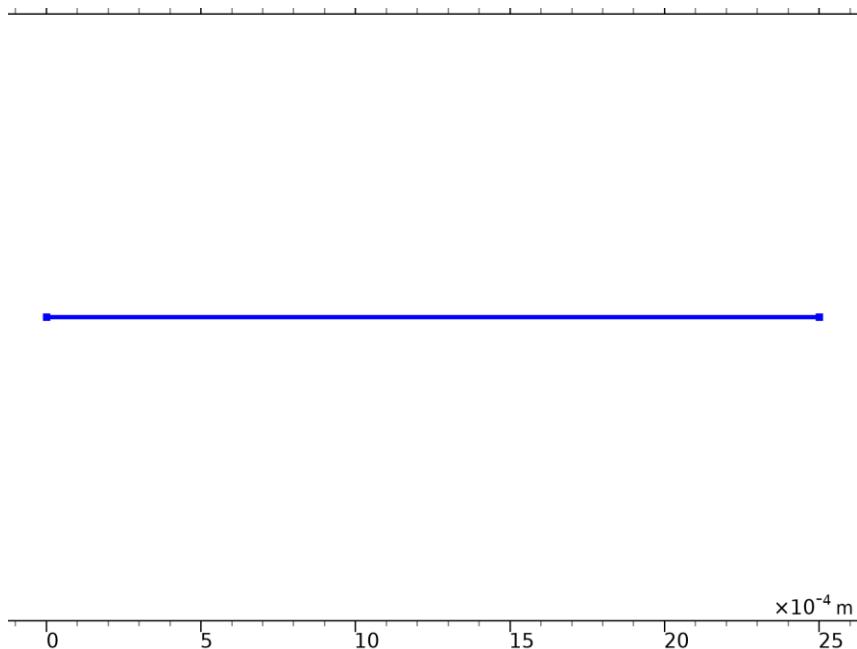
Initial Values 1

SELECTION

Geometric entity level	Domain
Selection	Geometry geom1: Dimension 1: All domains

Initial Values

SETTINGS

Description	Value
Concentration	{cCation_b, cAnion_b}

2.3.5 Concentration on bulk boundary
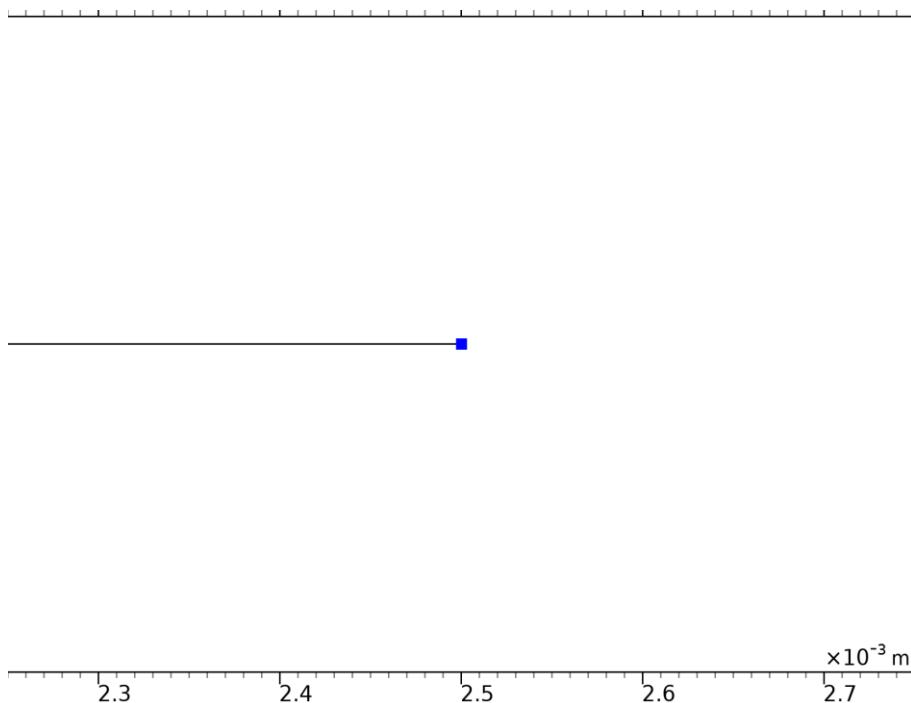
Concentration on bulk boundary

Geometric entity level	Boundary
Selection	Geometry geom1: Dimension 0: Boundary 4

EQUATIONS

$$c_i = c_{0,j}$$

Concentration

SETTINGS

Description	Value
Species cCation	On
Species cAnion	On
Concentration	{cCation_b, cAnion_b}

2.4 TRANSPORT OF DILUTED SPECIES 2

USED PRODUCTS

COMSOL Multiphysics
Chemical Reaction Engineering Module

$\times 10^{-4}$ m
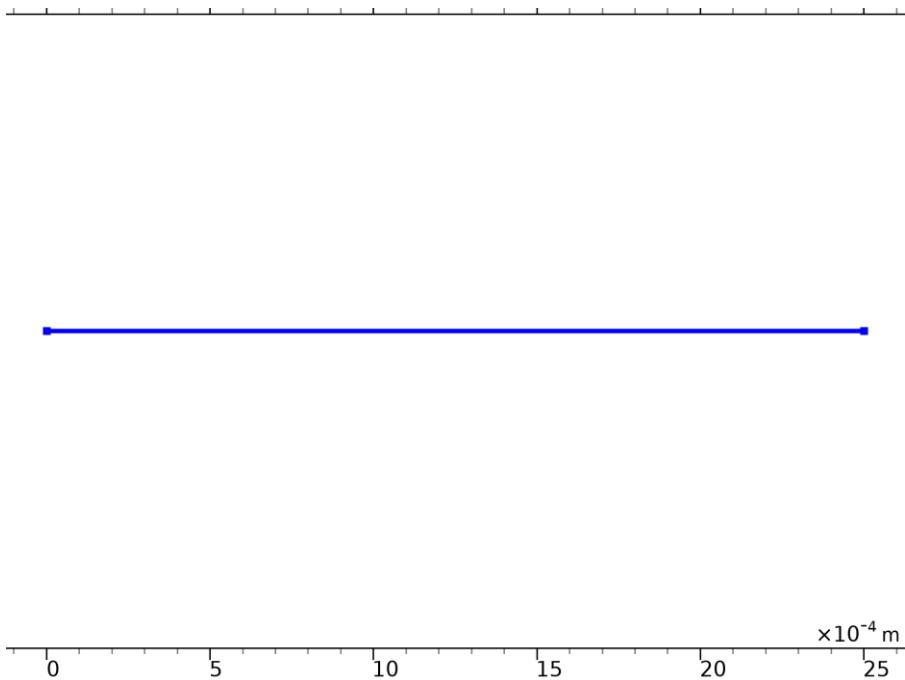
Transport of Diluted Species 2

SELECTION

Geometric entity level	Domain
Selection	Geometry geom1: Dimension 1: Domain 3

EQUATIONS

$$\nabla \cdot \mathbf{J}_i = R_i$$
$$\mathbf{J}_i = -D_i \nabla c_i - z_i u_{m,i} F c_i \nabla V$$

2.4.1 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

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Description	Value
Migration in electric field	On
Mass transfer in porous media	Off

Advanced Settings

Description	Value
Convective term	Nonconservative form

2.4.2 Transport Properties 1
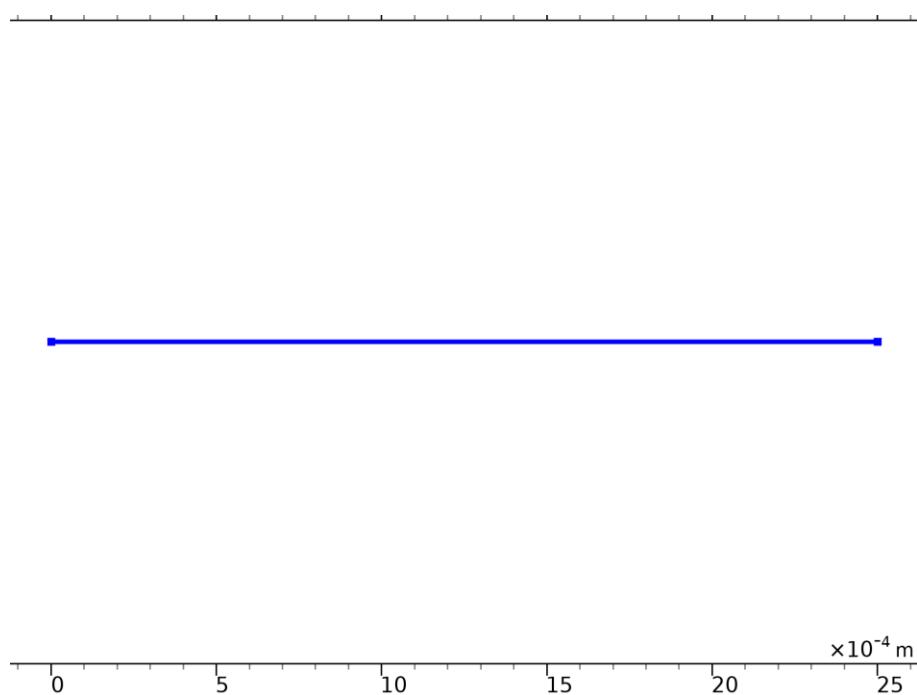
Transport Properties 1

SELECTION

Geometric entity level	Domain
Selection	Geometry geom1: Dimension 1: All domains

EQUATIONS

$$\nabla \cdot \mathbf{J}_i = R_i$$
$$\mathbf{J}_i = -D_i \nabla c_i - z_i u_{m,i} F c_i \nabla V$$

Diffusion

SETTINGS

Description	Value
Source	Material
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}}

Migration in Electric Field

SETTINGS

| Description	Value
Electric potential	Electric potential (es)
Mobility	Nernst - Einstein relation
Charge number	{z_Ox_diff, z_Red_diff}

Coordinate System Selection

SETTINGS

Description	Value
Coordinate system	Global coordinate system

Model Input

SETTINGS

| Description	Value
Temperature	User defined
Temperature	T

2.4.3 No Flux 1
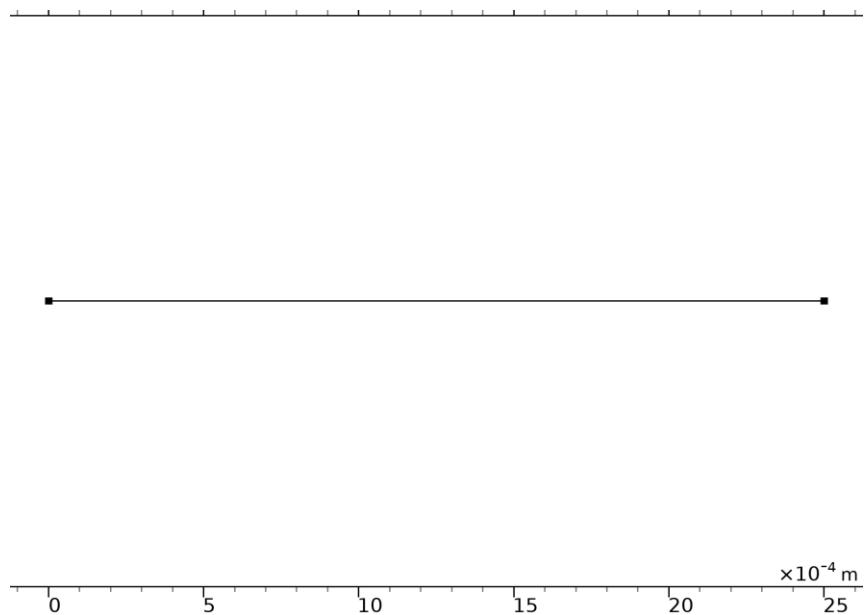
No Flux 1

Geometric entity level	Boundary
Selection	Geometry geom1: Dimension 0: All boundaries

EQUATIONS

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

2.4.4 Initial Values 1
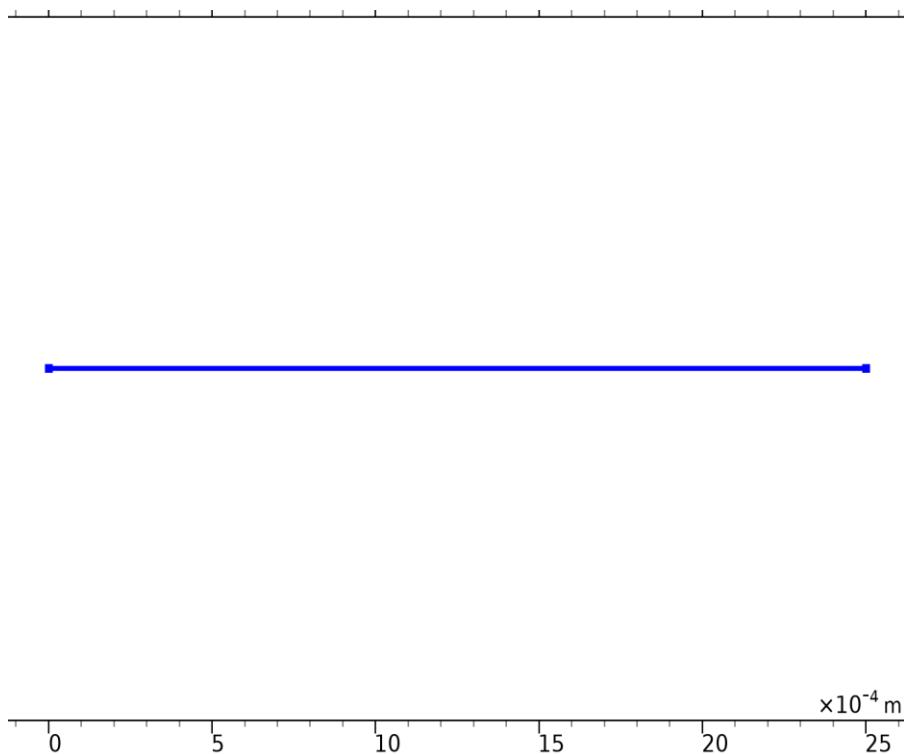
Initial Values 1

SELECTION

Geometric entity level	Domain
Selection	Geometry geom1: Dimension 1: All domains

Initial Values

SETTINGS

Description	Value
Concentration	{cOx0_dif, 0}

2.4.5 Concentration 1
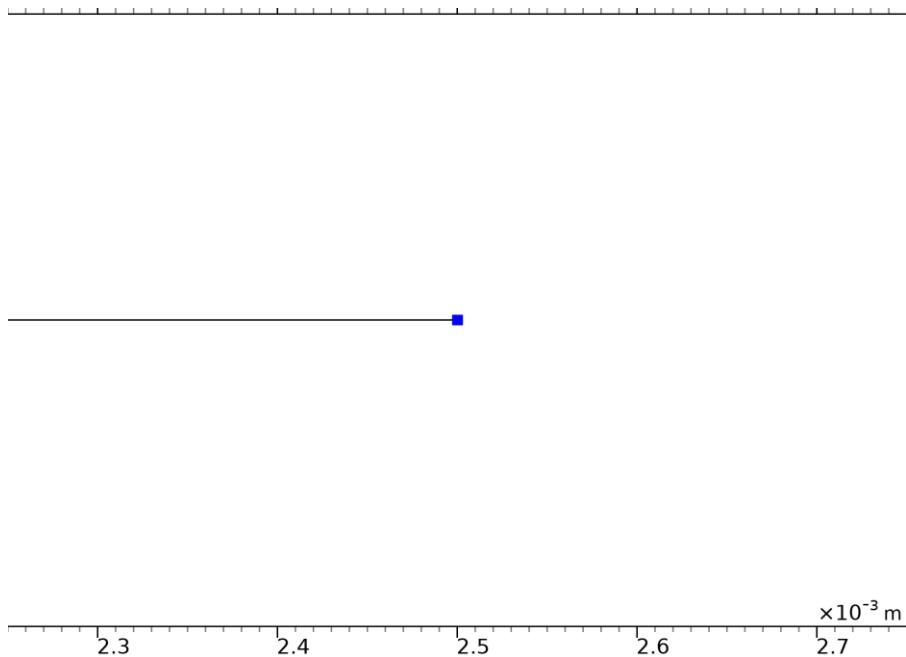
Concentration 1

SELECTION

Geometric entity level	Boundary
Selection	Geometry geom1: Dimension 0: Boundary 4

EQUATIONS

$$c_i = c_{0,i}$$

Concentration

SETTINGS

Description	Value
Species cOx	On
Species cRed	On
Concentration	{cOx0_dif, 0}

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2.4.6 Butler Volmer HET
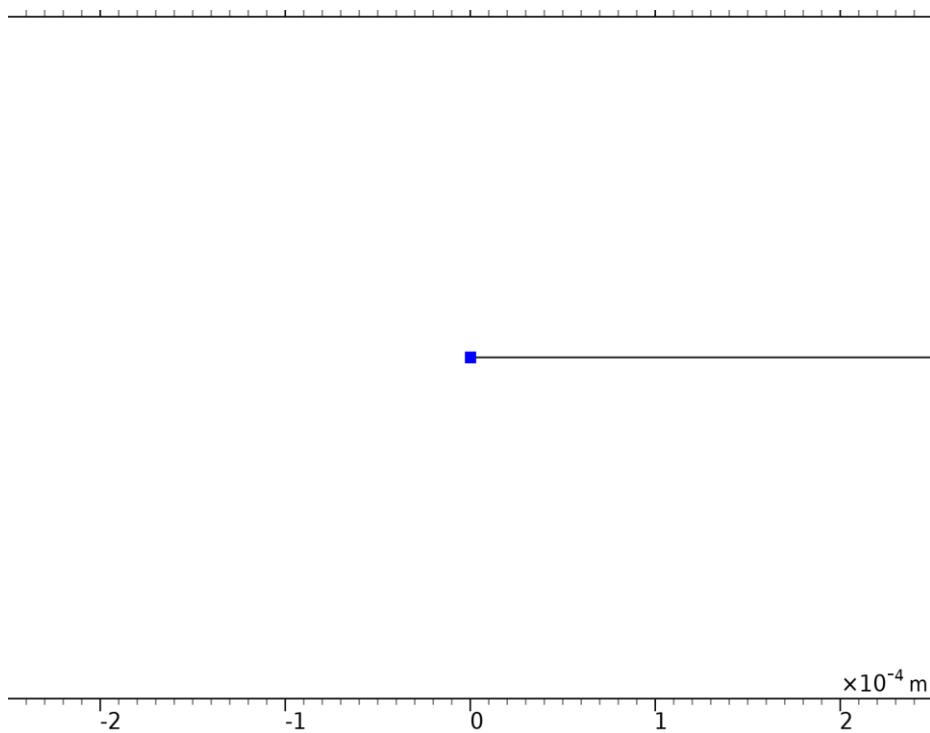
Butler Volmer HET

SELECTION

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

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
(-kf*cOx+kb*cRed)*test(cOx)	2	Spatial	Boundary 3
-(-kf*cOx+kb*cRed)*test(cRed)	2	Spatial	Boundary 3

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2.5 ELECTROSTATICS

COMSOL Multiphysics
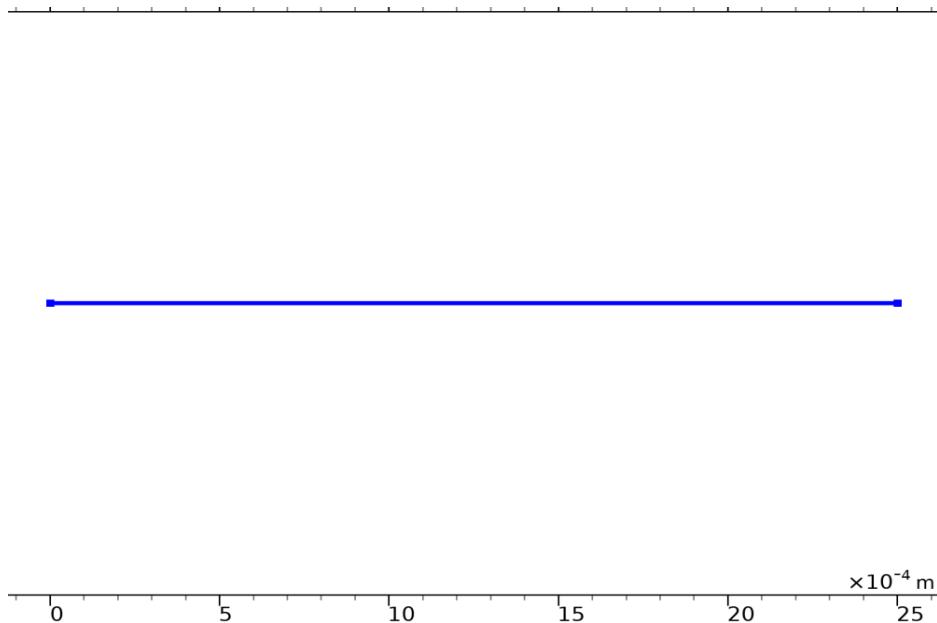
Electrostatics

SELECTION

Geometric entity level	Domain
Selection	Geometry geom1: Dimension 1: All domains

EQUATIONS

$$\nabla \cdot \mathbf{D} = \rho_v$$
$$\mathbf{E} = -\nabla V$$

2.5.1 Interface Settings

Discretization

SETTINGS

Description	Value
Electric potential	Linear
Value type when using splitting of complex variables	Complex

Manual Terminal Sweep Settings

SETTINGS

Description	Value
Use manual terminal sweep	Off
Reference impedance	50[ohm]

2.5.2 Charge Conservation - Inner Film
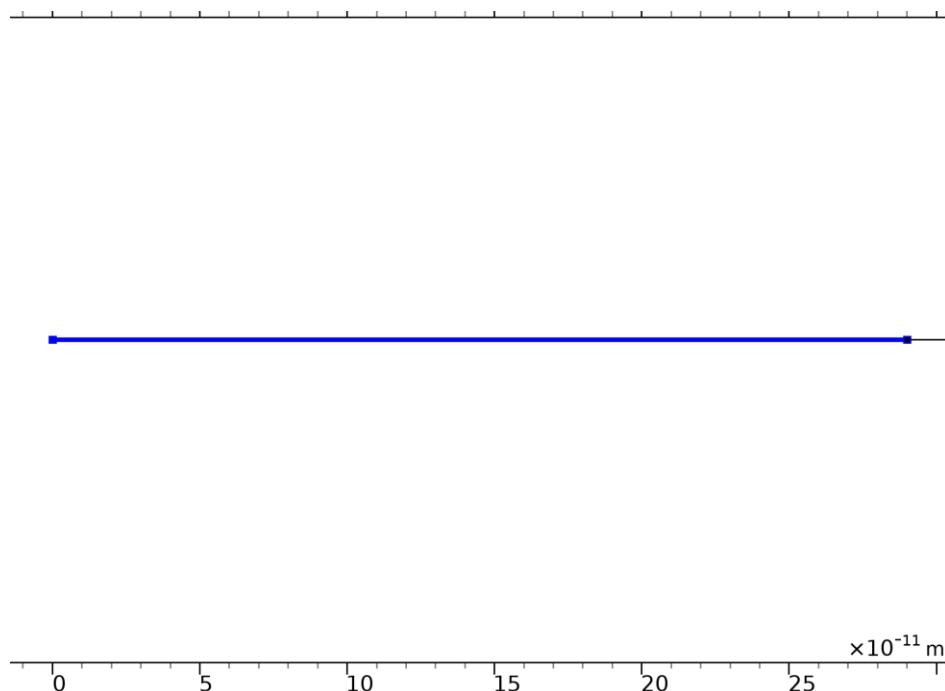
Charge Conservation - Inner Film

SELECTION

Geometric entity level	Domain
Selection	Geometry geom1: Dimension 1: All domains

EQUATIONS

$$\mathbf{E} = -\nabla V$$
$$\nabla \cdot (\epsilon_0 \epsilon_r \mathbf{E}) = \rho_v$$

Constitutive Relation D-E

SETTINGS

| Description	Value
Dielectric model	Relative permittivity
Relative permittivity	User defined
Relative permittivity	{{epsilon_1, 0, 0}, {0, epsilon_1, 0}, {0, 0, epsilon_1}}

Coordinate System Selection

Description	Value
Coordinate system	Global coordinate system

Model Input

Description	Value
Temperature	User defined
Temperature	T

## 2.5.3 Zero Charge 1
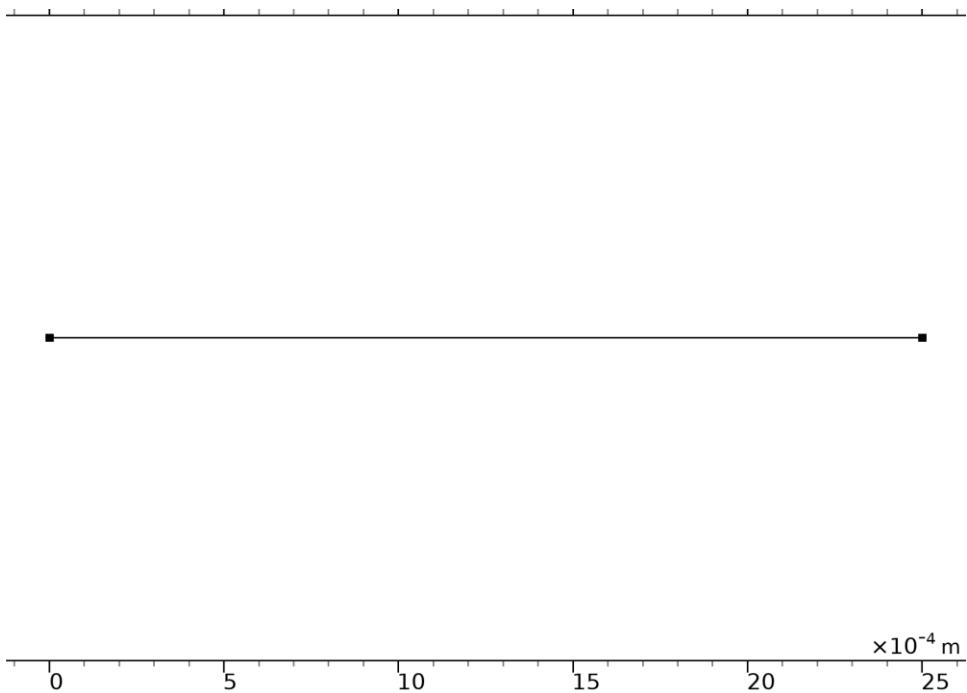
Zero Charge 1

Geometric entity level	Boundary
Selection	Geometry geom1: Dimension 0: All boundaries

$$\mathbf{n} \cdot \mathbf{D} = 0$$

2.5.4 Initial Values 1
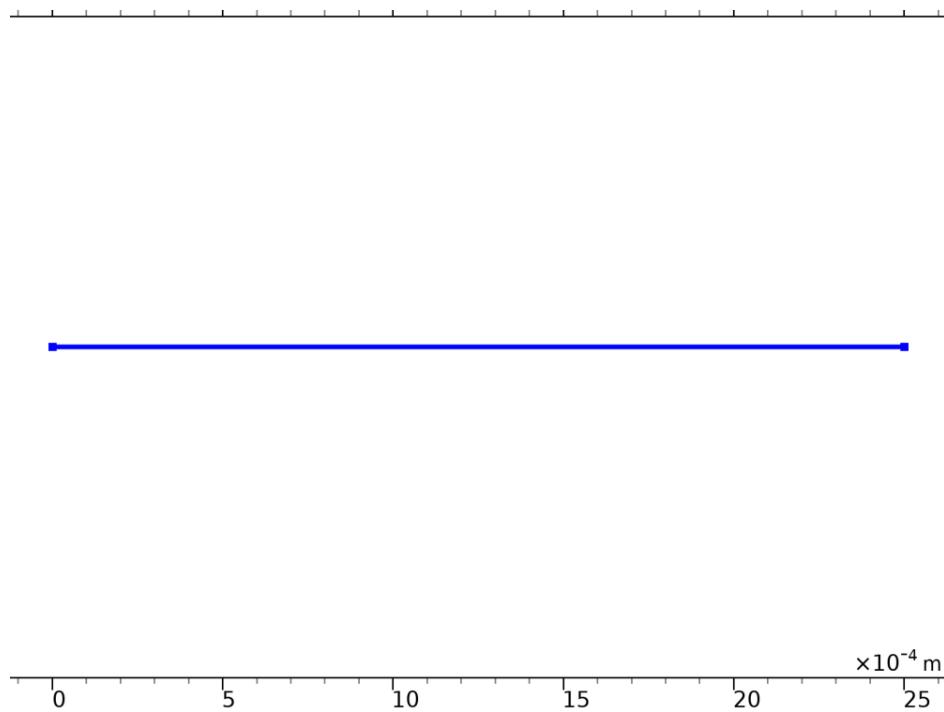
Initial Values 1

SELECTION

Geometric entity level	Domain
Selection	Geometry geom1: Dimension 1: All domains

SETTINGS

Description	Value
Electric potential	0

2.5.5 Charge Conservation - Solution
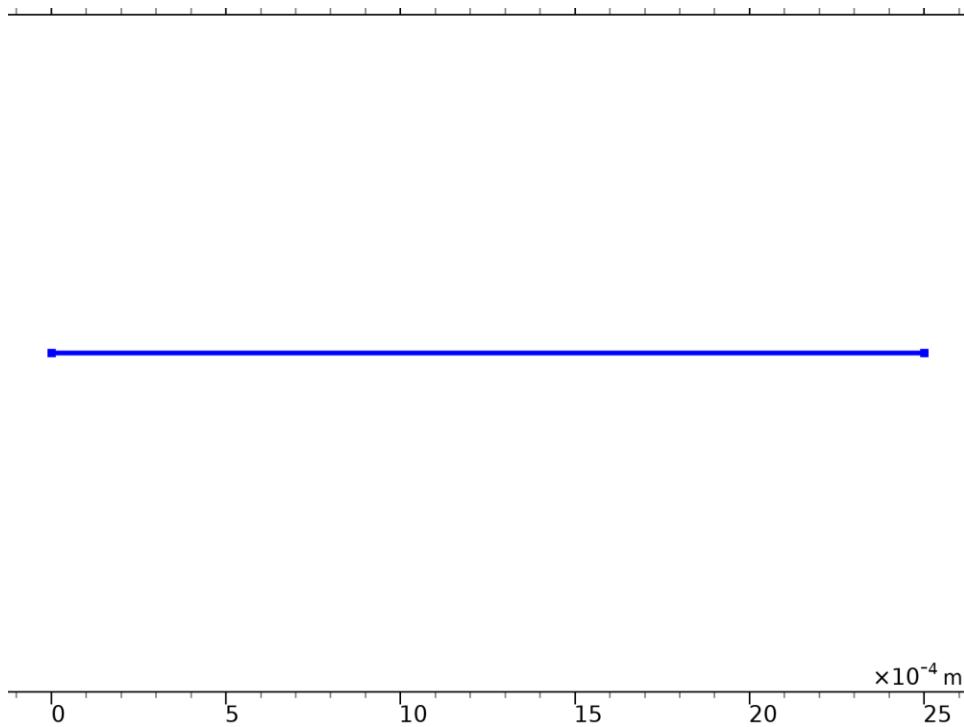
Charge Conservation - Solution

SELECTION

Geometric entity level	Domain
Selection	Geometry geom1: Dimension 1: Domain 3

EQUATIONS

$$\mathbf{E} = -\nabla V$$
$$\nabla \cdot (\epsilon_0 \epsilon_r \mathbf{E}) = \rho_v$$

Constitutive Relation D-E

SETTINGS

| Description	Value
Dielectric model	Relative permittivity
Relative permittivity	User defined
Relative permittivity	{{epsilon_s, 0, 0}, {0, epsilon_s, 0}, {0, 0, epsilon_s}}

Coordinate System Selection

SETTINGS

Description	Value
Coordinate system	Global coordinate system

Model Input

Description	Value
Temperature	User defined
Temperature	T

2.5.6 Ground – Ag/AgCl reference
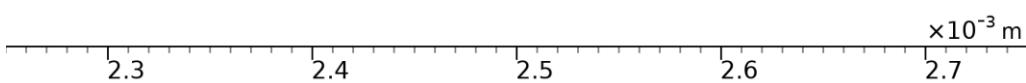
Ground - Ag|AgCl reference

SELECTION

Geometric entity level	Boundary
Selection	Geometry geom1: Dimension 0: Boundary 4

EQUATIONS

$$V = 0$$

2.5.7 Electric Potential - Time Dependent
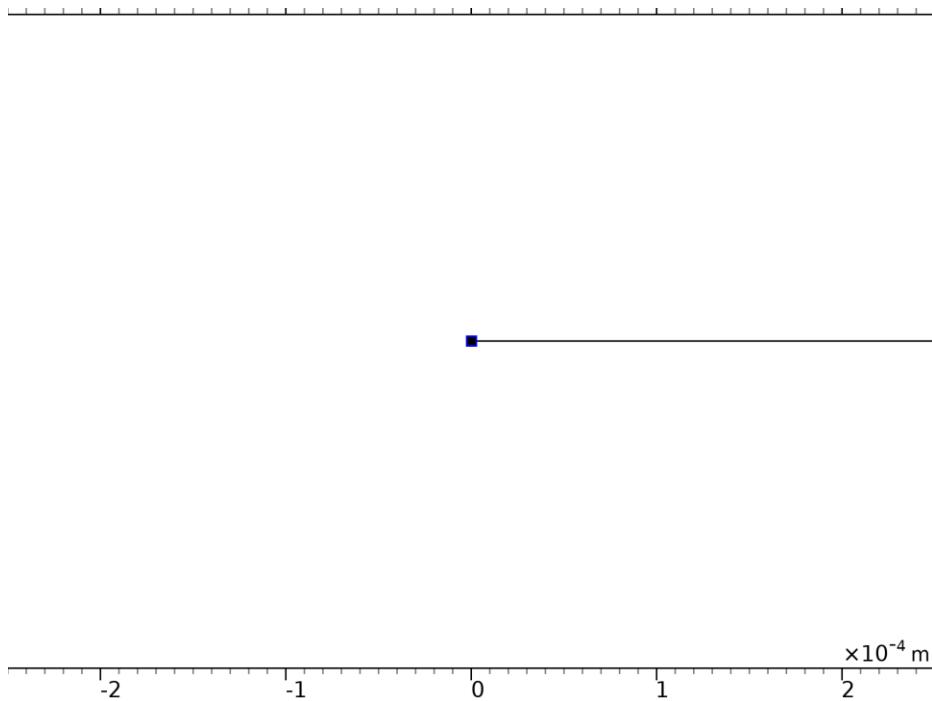
Electric Potential - Time Dependent

SELECTION

Geometric entity level	Boundary
Selection	Geometry geom1: Dimension 0: Boundary 1

EQUATIONS

$$V = V_0$$

Electric Potential

SETTINGS

Description	Value
Electric potential	CorrectedPotential

2.5.8 Space Charge Density - Multiphysics Coupling
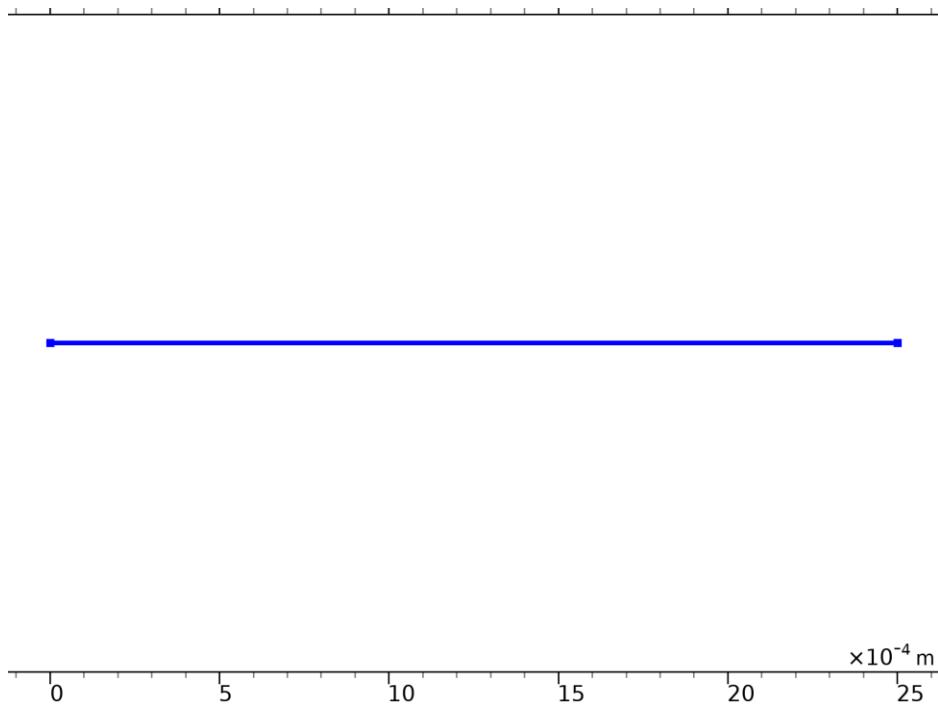
Space Charge Density - Multiphysics Coupling

SELECTION

Geometric entity level	Domain
Selection	Geometry geom1: Dimension 1: Domain 3

EQUATIONS

$$\nabla \cdot \mathbf{D} = \rho_v$$

Coordinate System Selection

SETTINGS

Description	Value
Coordinate system	Global coordinate system

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2.5.9 Charge Conservation - Solution 1
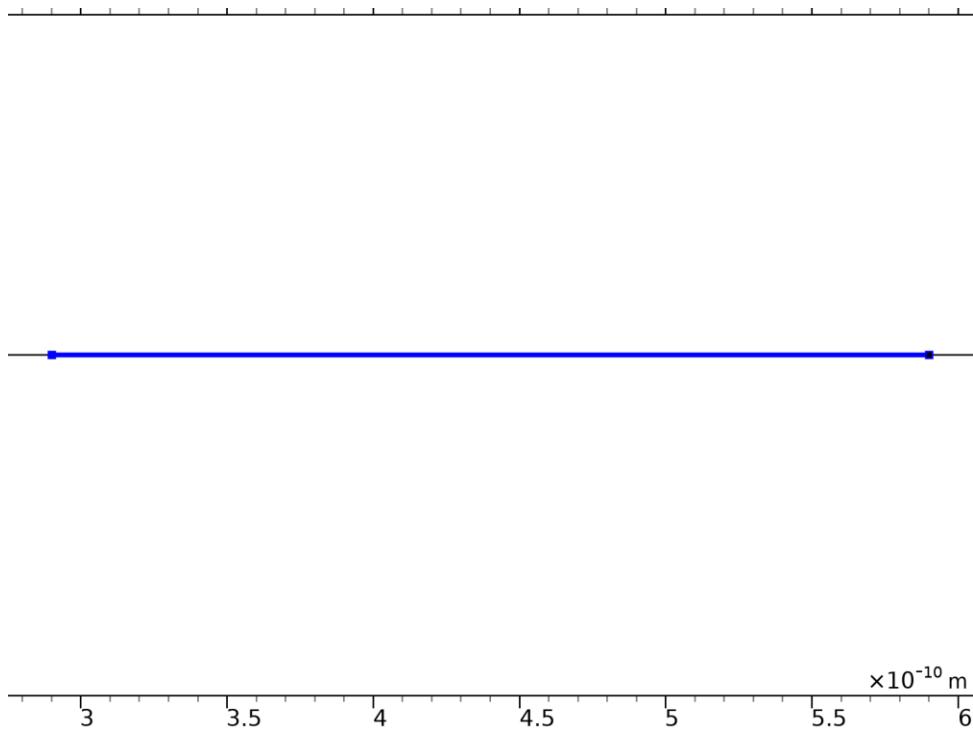
Charge Conservation - Solution 1

SELECTION

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

EQUATIONS

$$\mathbf{E} = -\nabla V$$
$$\nabla \cdot (\epsilon_0 \epsilon_r \mathbf{E}) = \rho_v$$

Constitutive Relation D-E

SETTINGS

| Description	Value
Dielectric model	Relative permittivity
Relative permittivity	User defined
Relative permittivity	{{epsilon_2, 0, 0}, {0, epsilon_2, 0}, {0, 0, epsilon_2}}

Coordinate System Selection

SETTINGS

Description	Value
Coordinate system	Global coordinate system

Model Input

Description	Value
Temperature	User defined
Temperature	T

2.6 MESH 1
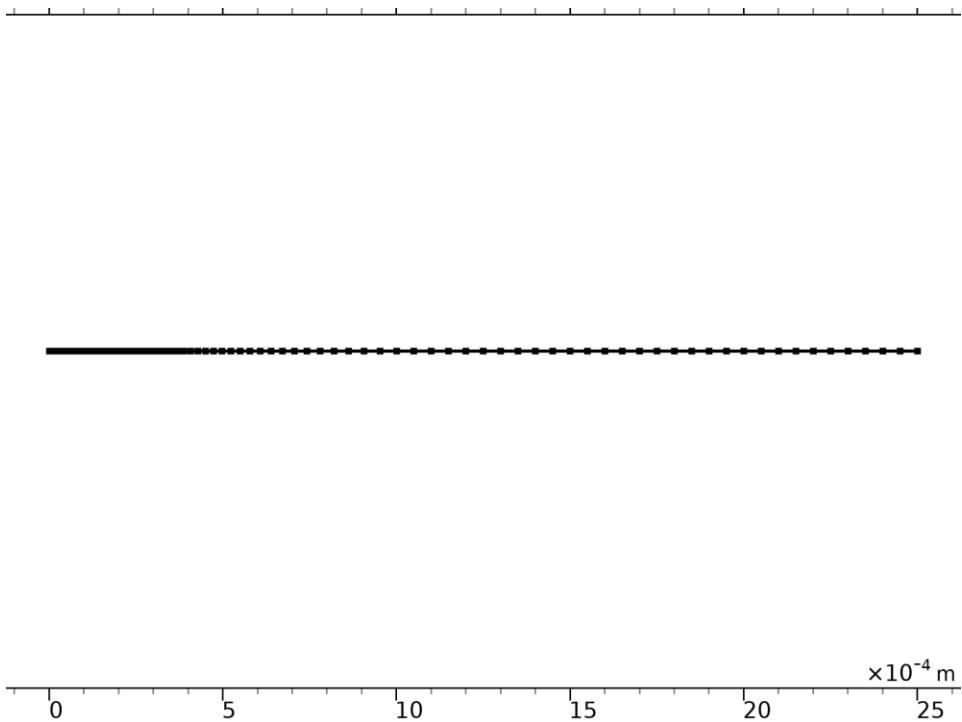
Mesh 1

2.6.1 Size (size)

Description	Value
Maximum element size	L/50
Minimum element size	3.0E-8
Curvature factor	0.3
Maximum element growth rate	1.3
Custom element size	Custom

2.6.2 Size 1 (size1)

Geometric entity level	Boundary

Selection	Geometry geom1: Dimension 0: Boundary 3
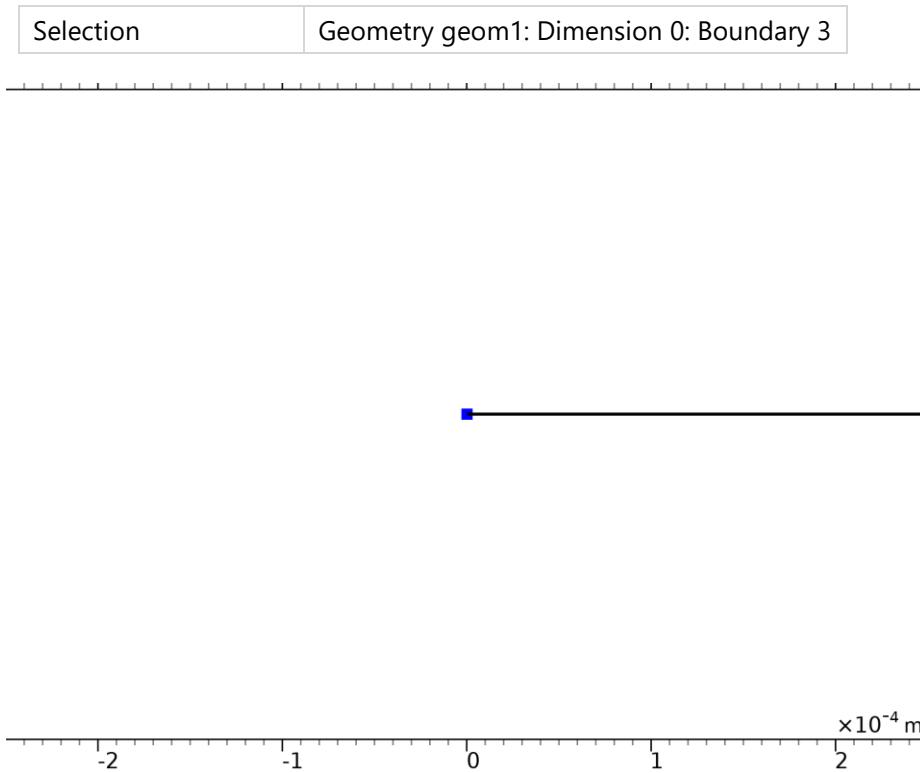
Size 1

Description	Value
Maximum element size	DebyeLength/20
Minimum element size	3.0E-8
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

2.6.3 Size 2 (size2)

SELECTION

Geometric entity level	Domain
Selection	Geometry geom1: Dimension 1: Domains 1–2
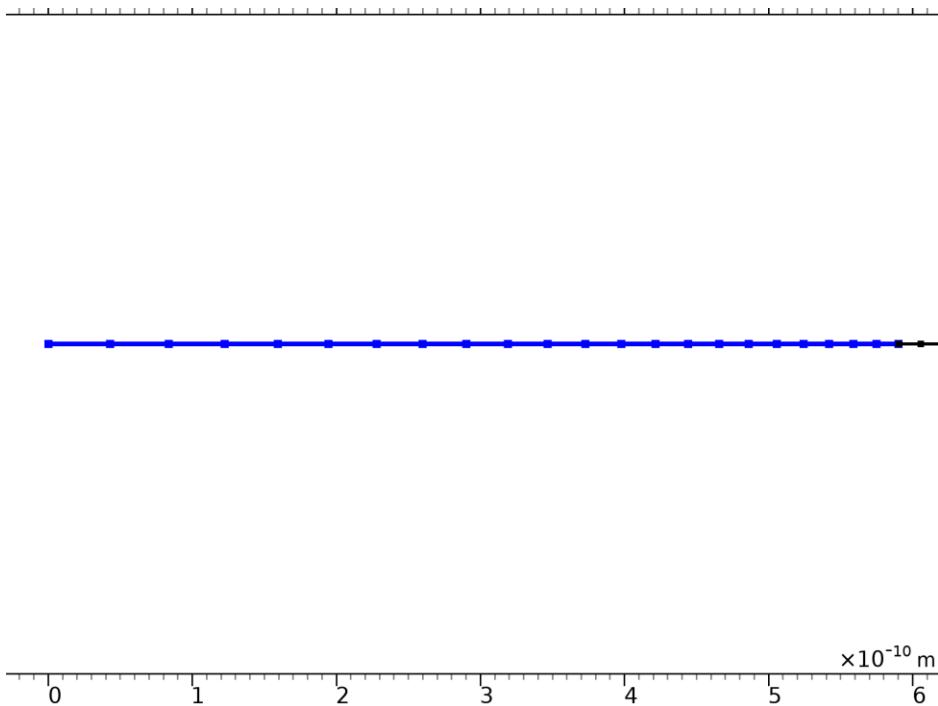
Size 2

SETTINGS

Description	Value
Maximum element size	1E-10
Minimum element size	3.0E-8
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

2.6.4 Edge 1 (edg1)

SELECTION

Geometric entity level	Domain
Selection	Geometry geom1: Dimension 1: Domains 1–3

×10⁻⁴ m

0   5   10   15   20   25
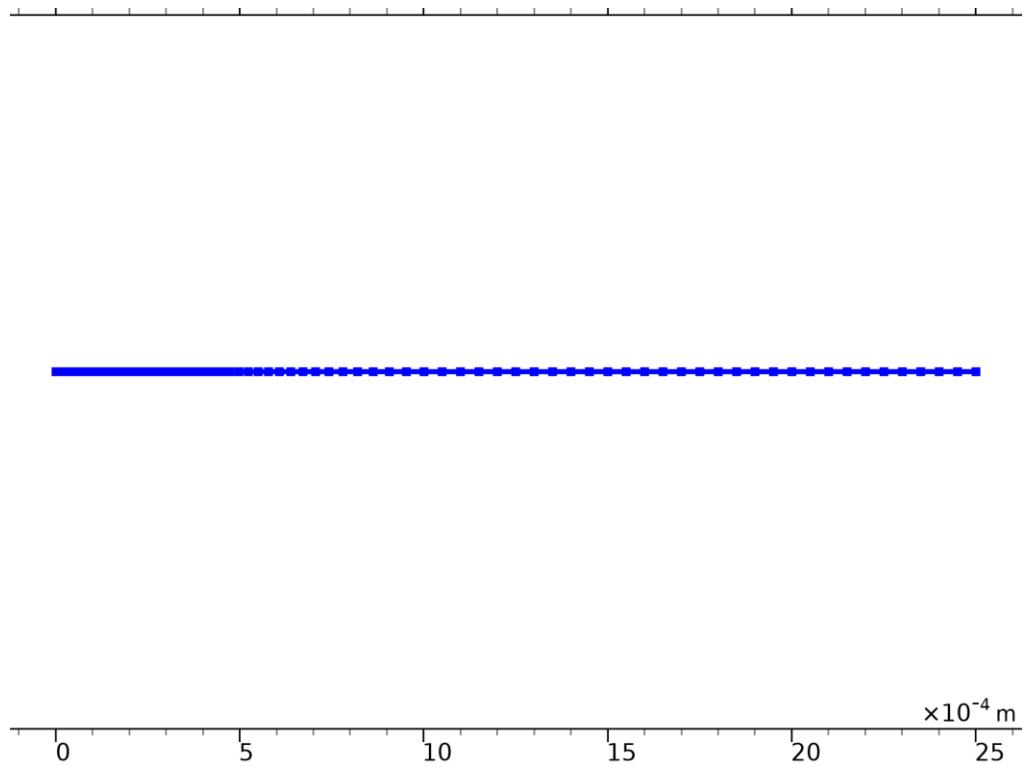
Edge 1

3 Component (IR drop compensation)

Description	Value
Unit system	Same as global system (SI)

3.1 DEFINITIONS

3.1.1 Probes

Ohmic drop (from gain) probe

Probe type	Global variable probe

EXPRESSION

Description	Value
Expression	IR
Table and plot unit	V
Description	Ohmic drop as determined by 'gain circuit'

TABLE AND WINDOW SETTINGS

Description	Value
Output table	Probe Table
Plot window	Probe Plot 3

3.2 GLOBAL ODES AND DAES

USED PRODUCTS

COMSOL Multiphysics

SELECTION

Geometric entity level	Entire model

3.2.1 Global Equations

SELECTION

Geometric entity level	Entire model

Global Equations

Name	f(u,ut,utt,t)	Initial value (u_0)	Initial value (u_t0)	Description
IR	IRt+Gain[1/s]*(IR-comp1.CurrentTot*Resistance)	0	0	Ohmic drop as determined by 'gain circuit'

Discretization

SETTINGS

Description	Value
Value type when using splitting of complex variables	Complex

Units

Dependent variable quantity	Unit
Custom unit	V

Source term quantity	Unit
Custom unit	V/s

Shape functions

Name	Shape function	Unit	Description	Shape frame	Selection
IR	ODE	V	Ohmic drop as determined by 'gain circuit'		Global

4 Study (time-dependent)

Computation time	1 min 4 s

4.1 PARAMETRIC SWEEP

Parameter name	Parameter value list	Parameter unit
z_Red_diff	+2	
z_Ox_diff	+3	
OhmicDropCompensation	0.95	1

STUDY SETTINGS

Description	Value
Sweep type	All combinations
Parameter name	{z_Red_diff, z_Ox_diff, OhmicDropCompensation}
Unit	{, , 1}

PARAMETERS

Parameter name	Parameter value list	Parameter unit
z_Red_diff	+2	
z_Ox_diff	+3	
OhmicDropCompensation (Amount of ohmic drop that is attempted to be corrected for)	0.95	1

4.2 STATIONARY

STUDY SETTINGS

Description	Value
Include geometric nonlinearity	Off

VALUES OF DEPENDENT VARIABLES

Description	Value
Settings	User controlled

PHYSICS AND VARIABLES SELECTION

Physics interface	Discretization
Transport of Diluted Species (tds)	physics
Transport of Diluted Species 2 (tds2)	physics
Electrostatics (es)	physics

MESH SELECTION

Geometry	Mesh
Geometry 1 (geom1)	mesh1

4.3 TIME DEPENDENT

Times	Unit
range(0, sampling_time, 2*Segment_Duration+Start_Duration)	s

Description	Value
Include geometric nonlinearity	Off

Physics interface	Discretization
Transport of Diluted Species (tds)	physics
Transport of Diluted Species 2 (tds2)	physics
Electrostatics (es)	physics
Events (ev)	physics
Global ODEs and DAEs (ge)	physics

Geometry	Mesh
Geometry 1 (geom1)	mesh1

4.4 SOLVER CONFIGURATIONS

4.4.1 Solution 2

Compile Equations: Stationary (st1)

Description	Value
Use study	Study (time-dependent)
Use study step	Stationary

Dependent Variables 1 (v1)

Description	Value
Defined by study step	Stationary

Constant name	Initial value source
timestep	1.3E-6[s]

Concentration (comp1.cAnion) (comp1_cAnion)

GENERAL

Description	Value
Field components	comp1.cAnion
Internal variables	{comp1.uflux.cAnion, comp1.dflux.cAnion}

Concentration (comp1.cCation) (comp1_cCation)

GENERAL

Description	Value
Field components	comp1.cCation
Internal variables	{comp1.uflux.cCation, comp1.dflux.cCation}

Concentration (comp1.cOx) (comp1_cOx)

GENERAL

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

Concentration (comp1.cRed) (comp1_cRed)

GENERAL

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

Electric potential (comp1.Phi) (comp1_Phi)

GENERAL

Description	Value
Field components	comp1.Phi

Ohmic drop as determined by 'gain circuit' (comp2.ODE1) (comp2_ODE1)

GENERAL

Description	Value
State components	comp2.IR
Solve for this state	Off

Stationary Solver 1 (s1)

GENERAL

Description	Value
Defined by study step	Stationary
Relative tolerance	1E-4

RESULTS WHILE SOLVING

Description	Value
Probes	None

Advanced (aDef)

ASSEMBLY SETTINGS

Description	Value
Reuse sparsity pattern	On

Fully Coupled 1 (fc1)

GENERAL

Description	Value
Linear solver	Direct 1

METHOD AND TERMINATION

Description	Value
Initial damping factor	0.01
Minimum damping factor	1.0E-6
Maximum number of iterations	50

Direct 1 (d1)

GENERAL

Description	Value
Solver	PARDISO
Pivoting perturbation	1.0E-13

Solution Store 1 (su1)

GENERAL

Description	Value
Solution	Solution Store 1

Compile Equations: Time Dependent (st2)

STUDY AND STEP

Description	Value
Use study	Study (time-dependent)
Use study step	Time Dependent

Dependent Variables 2 (v2)

GENERAL

Description	Value
Defined by study step	Time Dependent

INITIAL VALUES OF VARIABLES SOLVED FOR

Description	Value
Method	Solution
Solution	Solution 2

RESIDUAL SCALING

Description	Value
Method	Manual

VALUES OF VARIABLES NOT SOLVED FOR

Description	Value
Method	Solution
Solution	Solution 2

INITIAL VALUE CALCULATION CONSTANTS

Constant name	Initial value source
t	range(0, sampling_time, 2*Segment_Duration+Start_Duration)
timestep	1.3E-6[s]

Concentration (comp1.cAnion) (comp1_cAnion)

GENERAL

Description	Value
Field components	comp1.cAnion
Internal variables	{comp1.uflux.cAnion, comp1.dflux.cAnion, comp1.tds.dt2Inv_cAnion}

Concentration (comp1.cCation) (comp1_cCation)

GENERAL

Description	Value
Field components	comp1.cCation
Internal variables	{comp1.uflux.cCation, comp1.dflux.cCation, comp1.tds.dt2Inv_cCation}

Concentration (comp1.cOx) (comp1_cOx)

GENERAL

Description	Value
Field components	comp1.cOx
Internal variables	{comp1.uflux.cOx, comp1.dflux.cOx, comp1.tds2.dt2Inv_cOx}

Concentration (comp1.cRed) (comp1_cRed)

GENERAL

Description	Value
Field components	comp1.cRed
Internal variables	{comp1.uflux.cRed, comp1.dflux.cRed, comp1.tds2.dt2Inv_cRed}

Electric potential (comp1.Phi) (comp1_Phi)

GENERAL

Description	Value
Field components	comp1.Phi

Ohmic drop as determined by 'gain circuit' (comp2.ODE1) (comp2_ODE1)

GENERAL

Description	Value
State components	comp2.IR

Time-Dependent Solver 1 (t1)

TIME STEPPING

Description	Value
Steps taken by solver	Strict
Initial step	1E-9
Maximum BDF order	2
Nonlinear controller	On

Advanced (aDef)

ASSEMBLY SETTINGS

Description	Value
Reuse sparsity pattern	On

Fully Coupled 1 (fc1)

GENERAL

Description	Value
Linear solver	Direct 1

Description	Value
Nonlinear method	Automatic (Newton)
Restriction for step-size update	5
Maximum number of iterations	100

Direct 1 (d1)

GENERAL

Description	Value
Solver	PARDISO
Pivoting perturbation	1.0E-13

4.4.2 Parametric Solutions 1

**z_Red_diff=2, z_Ox_diff=3, OhmicDropCompensation=0.95 (su1)**

GENERAL

Description	Value
Solution	z_Red_diff=2, z_Ox_diff=3, OhmicDropCompensation=0.95

5   Results

5.1   PLOT GROUPS

5.1.1   Current Density
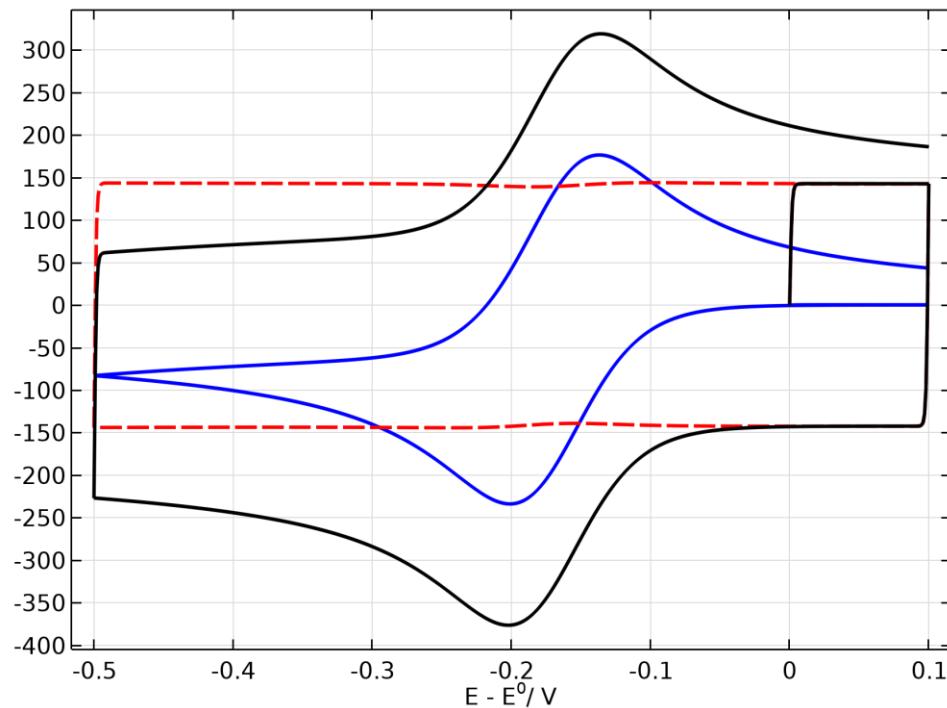
### 5.1.2 Surface Species Concentration - Time Dependent
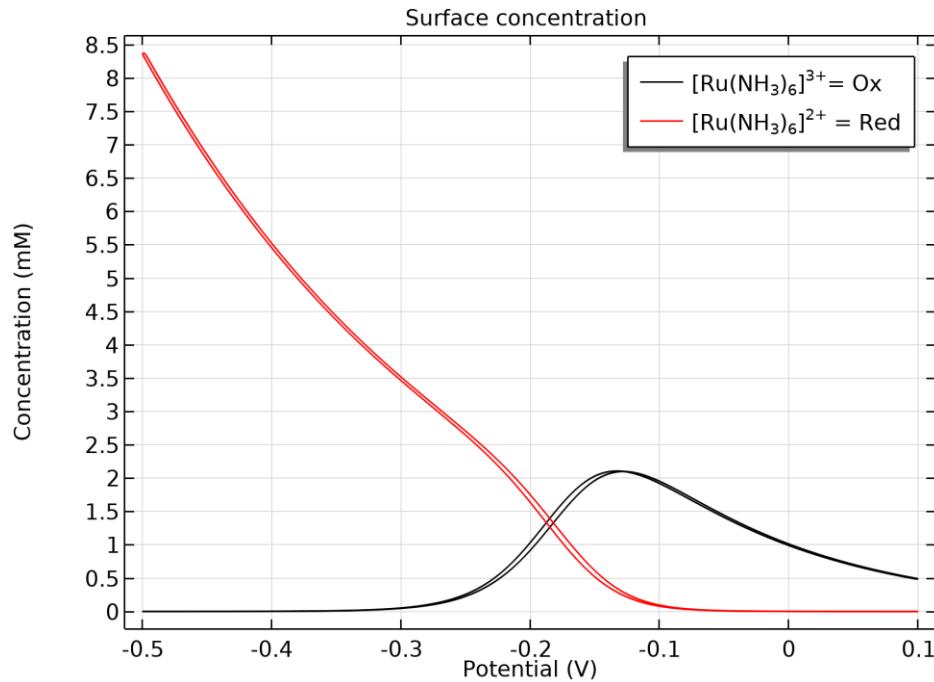
Surface concentration

### 5.1.3 Applied potential vs time (corrected & uncorrected)
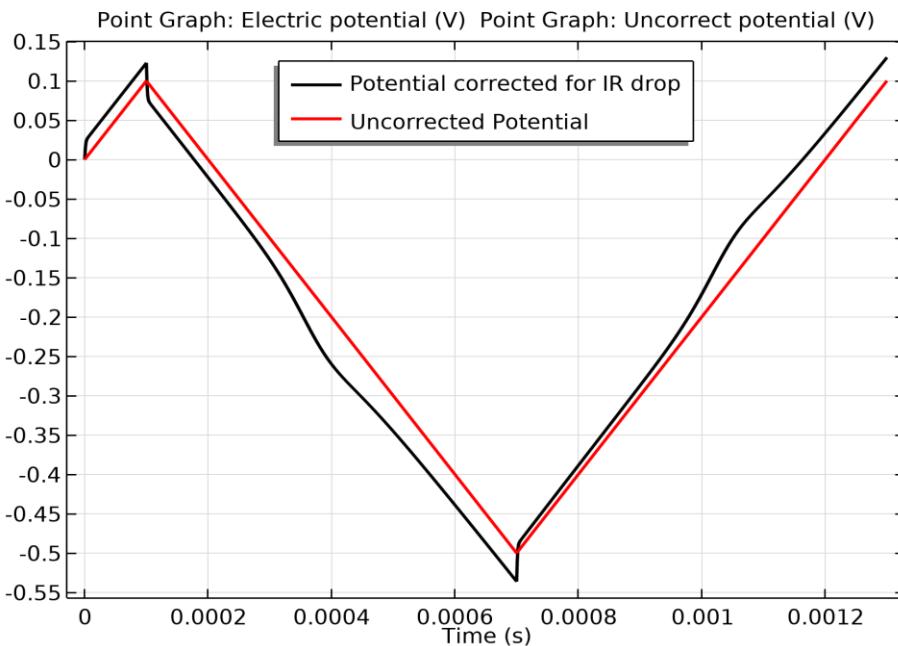
*Point Graph: Electric potential (V) Point Graph: Uncorrected potential (V)*

### 5.1.4 Electric Potential across Solution - Time Dependent

Uncorrected potential = -0.284 V, corrected potential = -0.33112 V
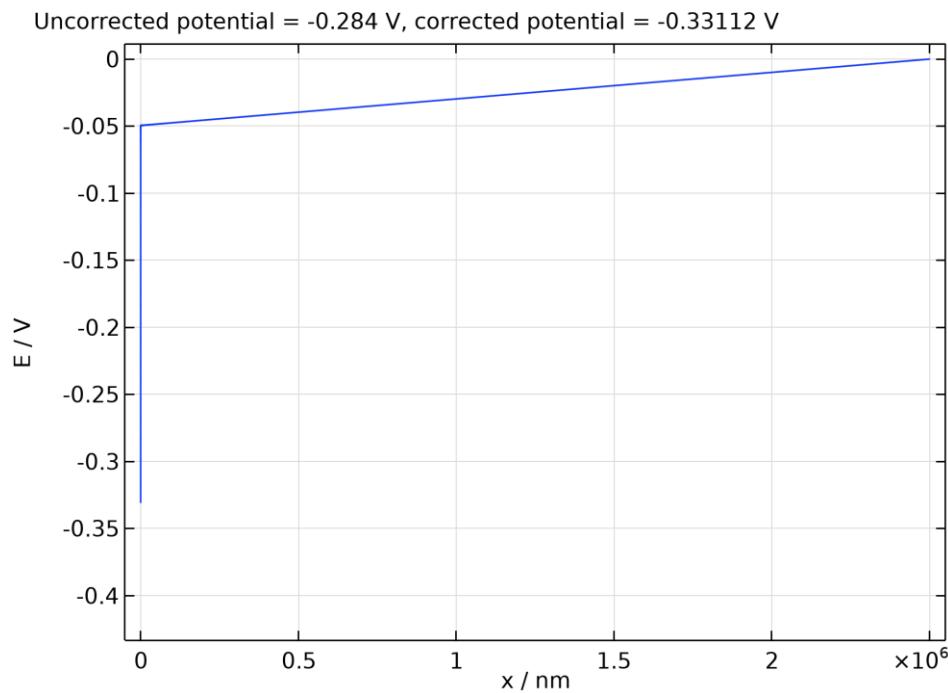
5.1.5 Probe Plot (current components vs time)
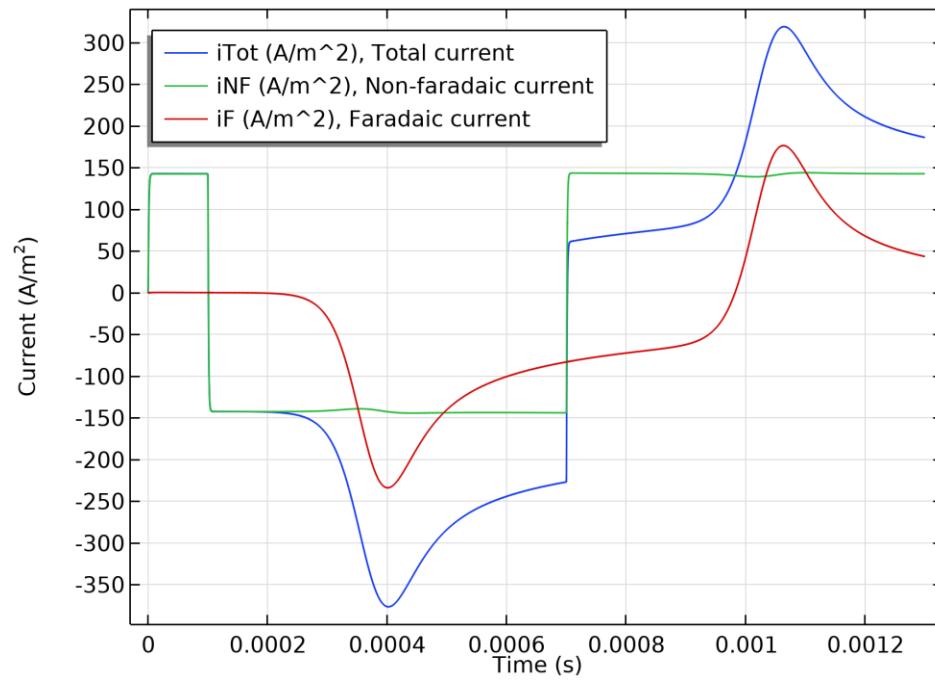
5.1.6 IR drop
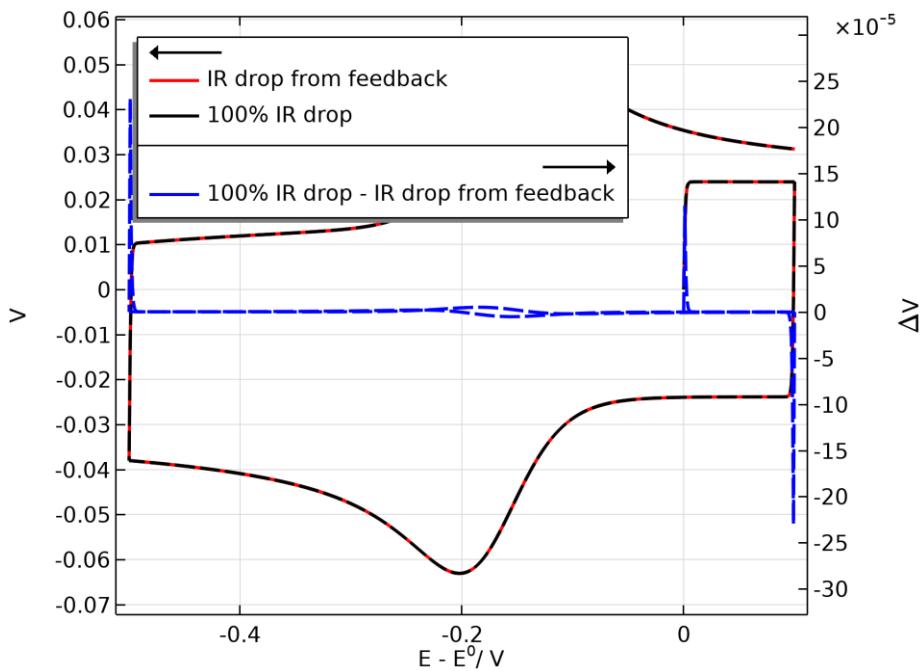
5.1.7 Probe (potentials vs time)
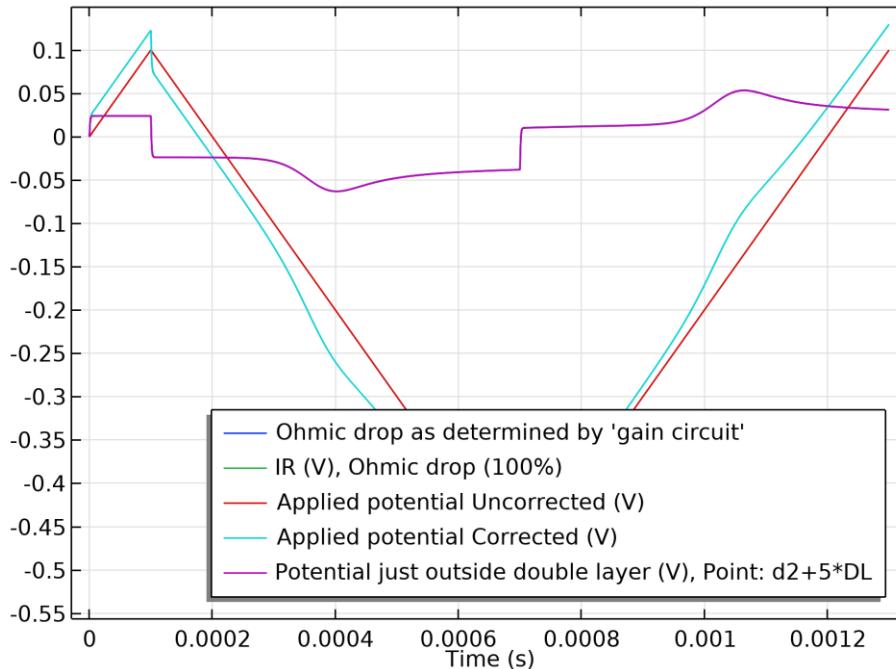
5.1.8 Probe - potential at positions

Point Graph: Phi (V)

5.1.9 Scan rate (dE_corr/dt)