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COMSOL Model Report A – Electrostatic Model of a Soluble Redox Couple

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1 Global Definitions

Date	Dec 7, 2022 2:31:44 PM

GLOBAL SETTINGS

Version	COMSOL Multiphysics 5.6 (Build: 280)

USED PRODUCTS

COMSOL Multiphysics
Chemical Reaction Engineering Module

COMPUTER INFORMATION

CPU	Intel64 Family 6 Model 158 Stepping 9, 4 cores
Operating system	Windows 10

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

Name	Expression	Value	Description
D_Anion	D_NO3	1.9E−9 m^2/s	
D_Cation	D_K	2E−9 m^2/s	
L	0.25[cm]	0.0025 m	Length of domain/boundary
z_Anion	-1	−1	The electrostatic charge of supporting electrolyte anion
z_Cation	+1	1	The electrostatic charge of supporting electrolyte cation
F_RT	(F_const)/(R_const*T)	39.586 1/V	Temperature
T	293.15[K]	293.15 K	
Kappa	e_const*sqrt(((cKb*(z_Cation^2) + cNO3b*(z_Anion^2) + (cOx0_dif)*(z_Ox_diff^2))*N_A_const)/(epsilon_s*epsilon0_const*k_B_const*T))	3.2913E9 1/m	Reciprocal of Debye length
DebyeLength	1/Kappa	3.0383E−10 m	Debye length

1.1.2 Compact Layers

COMPACT LAYERS

Name	Expression	Value	Description
epsilon_1	6	6	Dielectric constant of inner compact layer
epsilon_2	30	30	Dielectric constant of outer compact layer
d1	0.59 [nm]	5.9E−10 m	Distance from the electrode of OHP
d2	0.29 [nm]	2.9E−10 m	Distance from the electrode of IHP
A	(1[mm])^2*pi	3.1416E−6 m^2	Area of electrode (d = 2 mm)

1.1.3 Soluble Redox Species

SOLUBLE REDOX SPECIES

Name	Expression	Value	Description
DcOx	7.5*10^ - 6[cm^2/s]	7.5E−10 m^2/s	Diffusion Coefficient Oxidised species
DcRed	DcOx/0.72	1.0417E−9 m^2/s	Diffusion Coefficient reduced species
cOx0_dif	1 [mM]	1 mol/m^3	Initial concentration of Ox species
k0_Dif	13.5 [cm/s]	0.135 m/s	Rate constant (fast)

Name	Expression	Value	Description
alpha_Dif	0.45	0.45	Transfer coefficient
n_Dif	z_Ox_diff - z_Red_diff	1	Number of electrons transferred
E0_Dif	-0.173 [V]	−0.173 V	Standard redox potential for [Ru(NH3)6]+3/+2 Vs Ag/AgCl
z_Red_diff	+2	2	Electrostatic charge of reduced species
z_Ox_diff	+3	3	Electrostatic charge of oxidised species
cCounterIon0	cOx0_dif*3	3 mol/m³	Concentration of counter ions to the redox couple which is added to the concentration of the anion
n	1	1	Number of electrons transferred

1.1.4 CV Waveform

CV WAVEFORM

Name	Expression	Value	Description
v	1 [V/s]	1 V/s	Scan rate
E_Start	0 [V]	0 V	Starting potential applied to the working electrode
E_High	0.1 [V]	0.1 V	Switching potential, the highest potential applied to the working electrode
E_Low	-0.5 [V]	−0.5 V	Switching potential, the lowest potential applied to the working electrode
Start_Duration	(E_High - E_Start)/v	0.1 s	Starting scan duration
Segment_Duration	ScanRange/v	0.6 s	Length of one sweep

Name	Expression	Value	Description
ScanRange	abs(E_High - E_Low)	0.6 V	Absolute scan range
sampling	1 [mV]	0.001 V	Potential step size of the CV
sampling_time	(2*Segment_Duration + Start_Duration)/(((abs(E_High - E_Low)*2 + (E_High - E_Start)))/(sampling))	0.001 s	Corresponding sampling time interval for the potential step size at the specified scan rate

2 Component 1

SETTINGS

Description	Value
Unit system	Same as global system (SI)

2.1 DEFINITIONS

2.1.1 Variables

Butler-Volmer kinetics

SELECTION

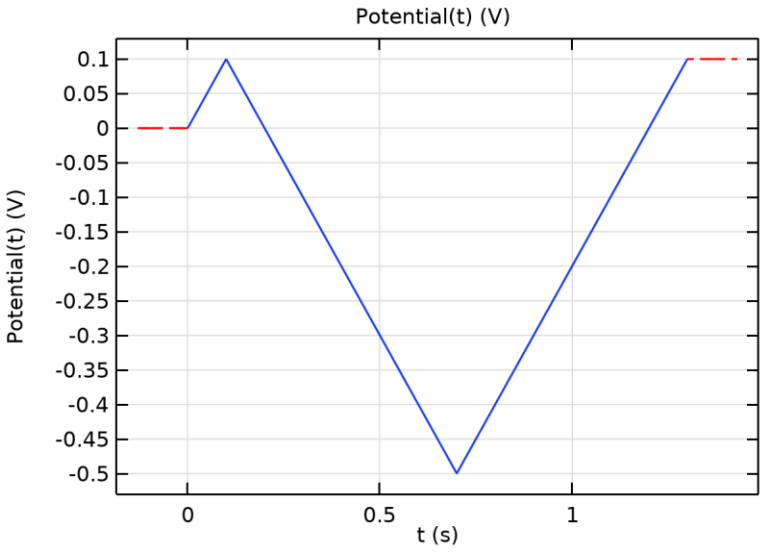
Geometric entity level	Boundary
Selection	Geometry geom1: Dimension 0: Boundary 3

Name	Expression	Unit	Description
kf_Dif	k0_Dif*exp((-alpha_Dif* F_RT *(Potential(t) - E0_Dif - Phi_PET)))	m/s	
kb_Dif	k0_Dif*exp(((1 - alpha_Dif)* F_RT *(Potential(t) - root.E0_Dif - Phi_PET)))	m/s	
Phi_PET	Phi	V	

2.1.2 Functions

Potential waveform function

Function name	Potential
Function type	Piecewise



Potential waveform function

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

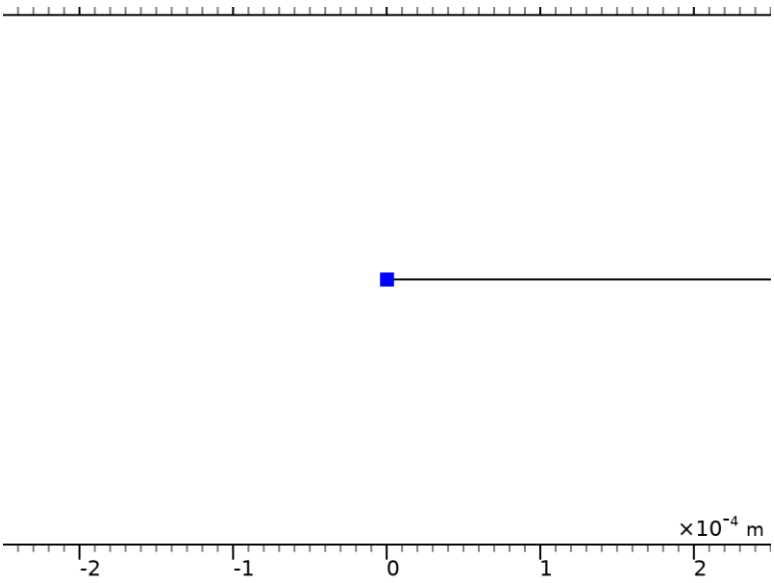
2.1.3 Probes

Total Current Probe

Probe type	Point probe

SELECTION

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



Selection

PROBE TYPE

Description	Value
Type	Integral

EXPRESSION

Description	Value
Expression	-(tds2.ntflux_cOx_dif)*F_const*root.n_Dif
Table and plot unit	A/m^2
Description	-(tds2.ntflux_cOx_dif)*F_const*root.n_Dif Normal total flux

TABLE AND WINDOW SETTINGS

Description	Value
Output table	Probe Table 8
Plot window	Probe Plot 2

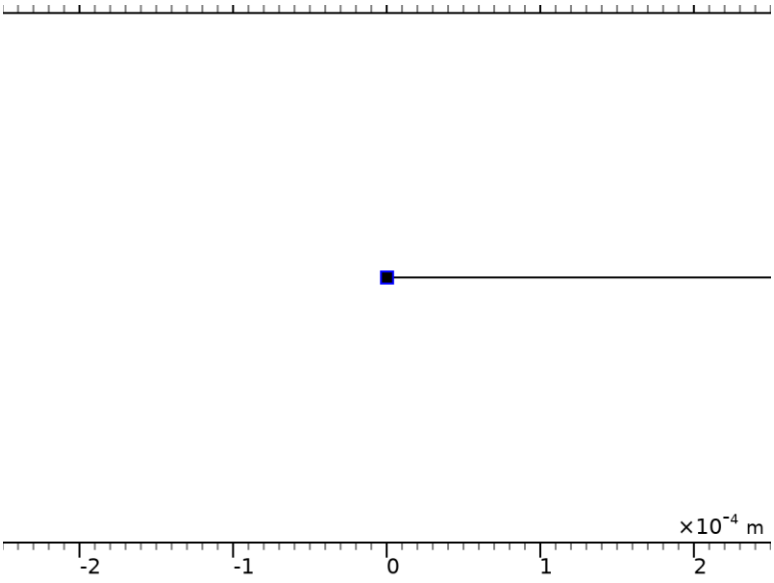
2.1.4 Nonlocal Couplings

Integration 1

Coupling type	Integration
Operator name	intop1

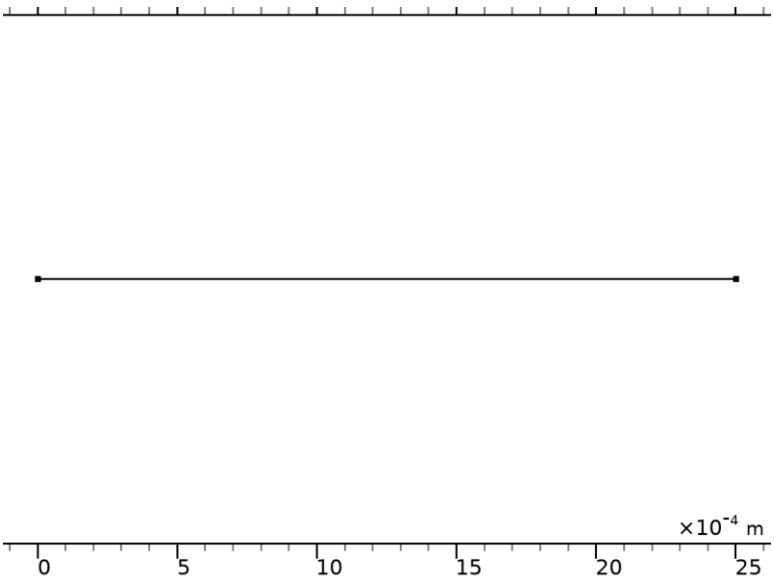
SELECTION

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



Selection

2.2 GEOMETRY 1



Geometry 1

UNITS

Length unit	m
Angular unit	deg

GEOMETRY STATISTICS

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 OHP (pt1)

POINT

Description	Value
Point coordinate	d2

2.2.3 IHP (pt2)

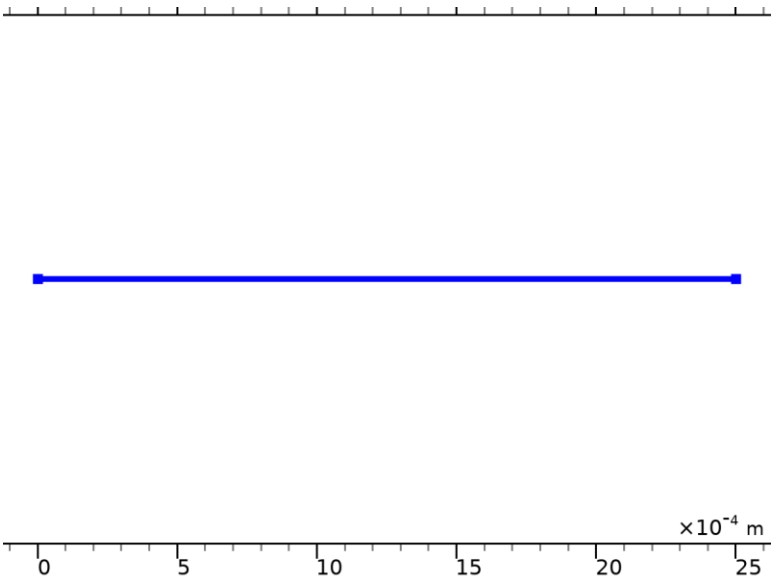
POINT

Description	Value
Point coordinate	d1

2.3 SUPPORTING ELECTROLYTE - TRANSPORT OF DILUTED SPECIES

USED PRODUCTS

COMSOL Multiphysics
Chemical Reaction Engineering Module



Supporting Electrolyte - 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

Description	Value
Convection	Off
Migration in electric field	On

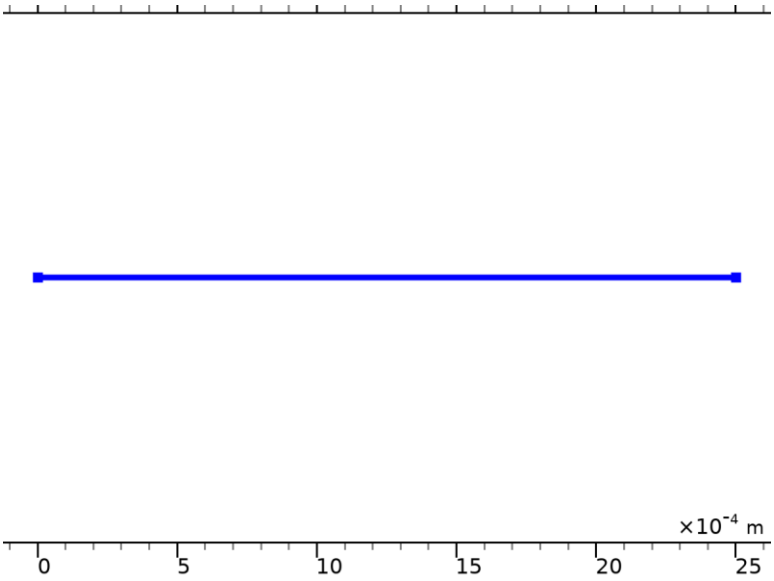
Description	Value
Mass transfer in porous media	Off

Advanced Settings

SETTINGS

Description	Value
Convective term	Nonconservative form

2.3.2 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

Description	Value
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	{root.z_Cation, root.z_Anion}

Coordinate System Selection

SETTINGS

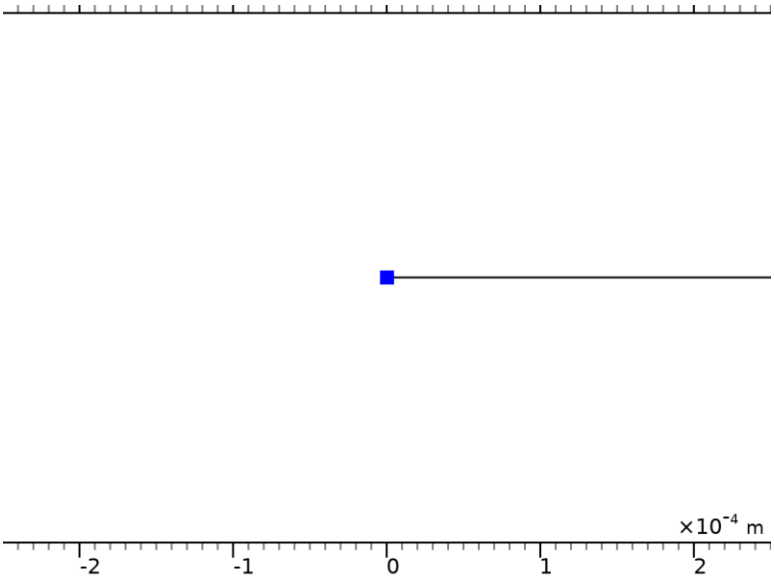
Description	Value
Coordinate system	Global coordinate system

Model Input

SETTINGS

Description	Value
Temperature	User defined
Temperature	T

2.3.3 No Flux 1



No Flux 1

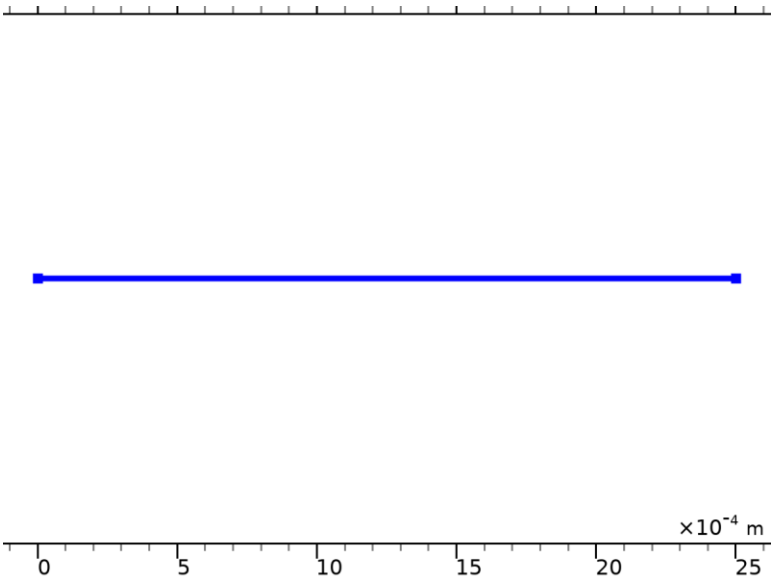
SELECTION

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

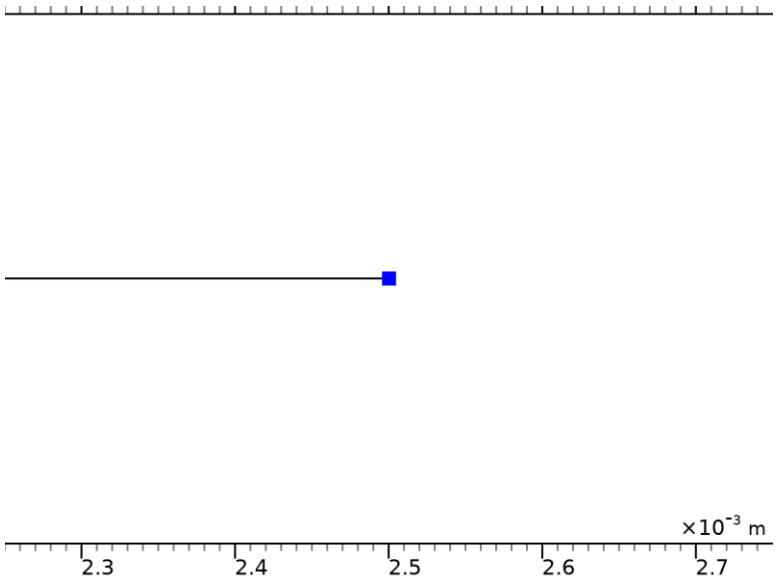
Geometric entity level	Domain
Selection	Geometry geom1: Dimension 1: All domains

Initial Values

SETTINGS

Description	Value
Concentration	{root.cCation_b, root.cAnion_b}

2.3.5 Concentration on BP 4



Concentration on BP 4

SELECTION

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

EQUATIONS

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

Concentration

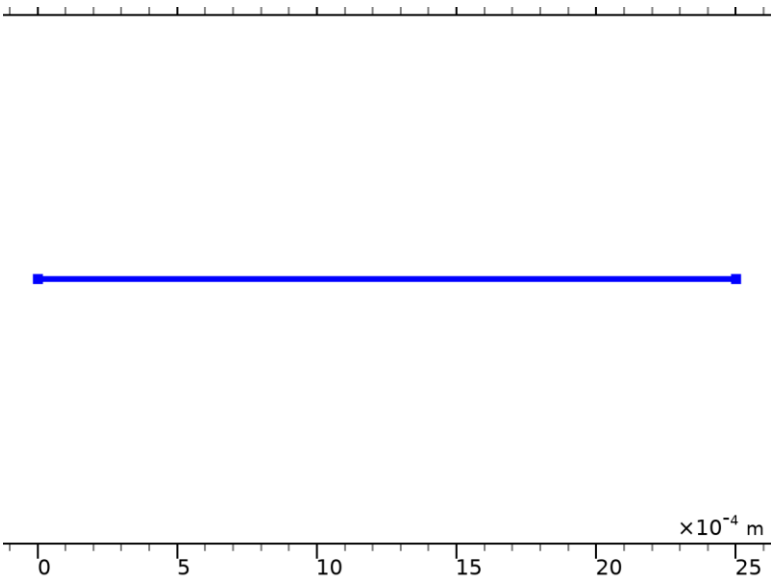
SETTINGS

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

2.4 SOLUBLE REDOX SPECIES - TRANSPORT OF DILUTED SPECIES 2

USED PRODUCTS

COMSOL Multiphysics
Chemical Reaction Engineering Module



Soluble Redox Species - 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

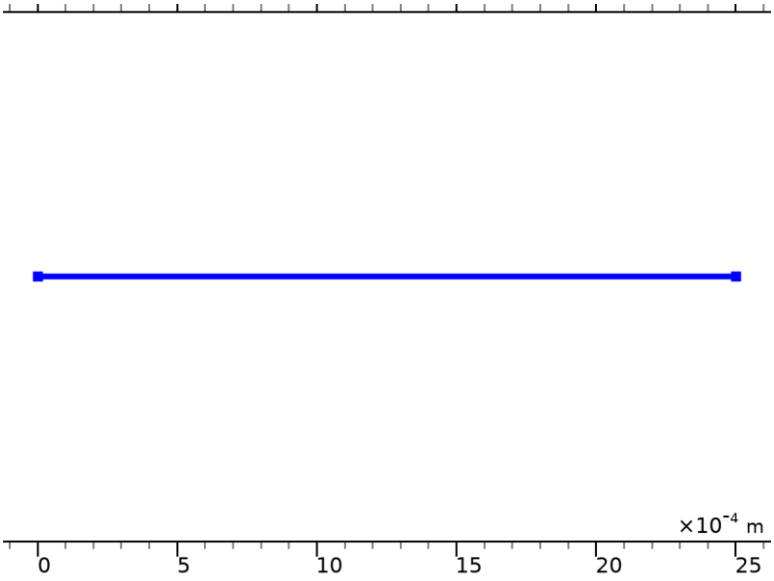
Description	Value
Convection	Off
Migration in electric field	On
Mass transfer in porous media	Off

Advanced Settings

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

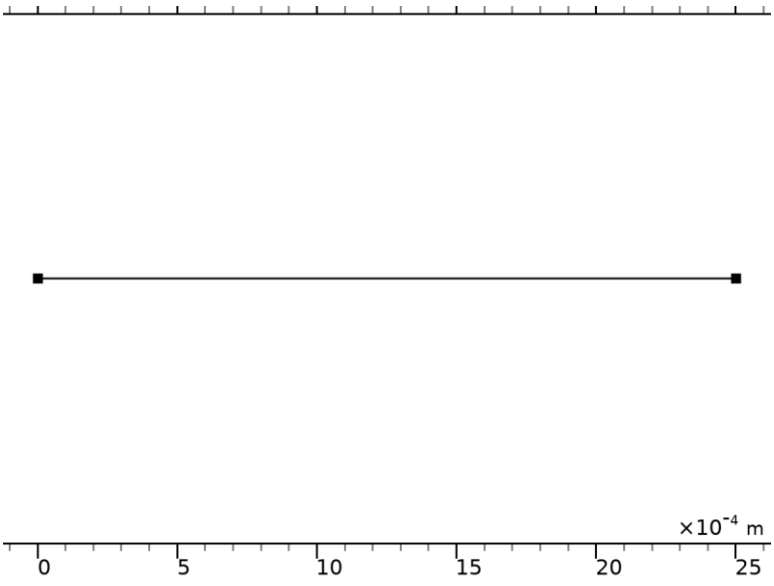
Description	Value
Coordinate system	Global coordinate system

Model Input

SETTINGS

Description	Value
Temperature	User defined
Temperature	T

2.4.3 No Flux 1



No Flux 1

SELECTION

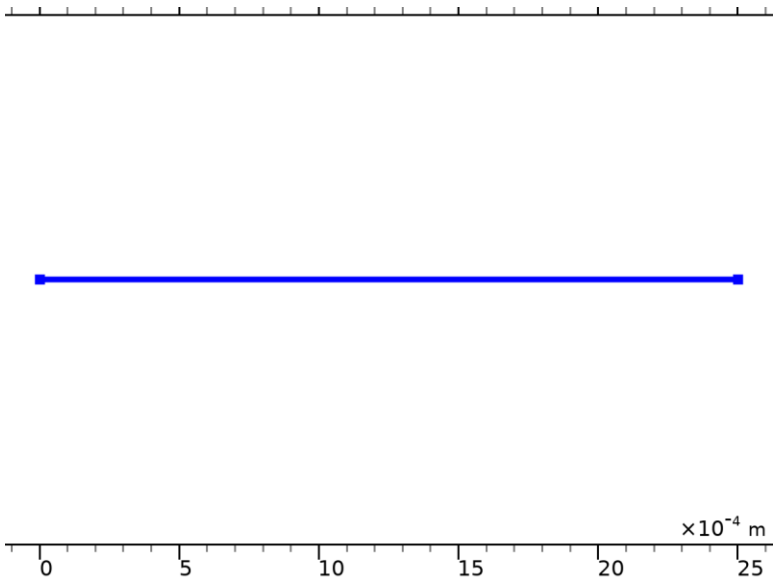
Geometric entity level	Boundary

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

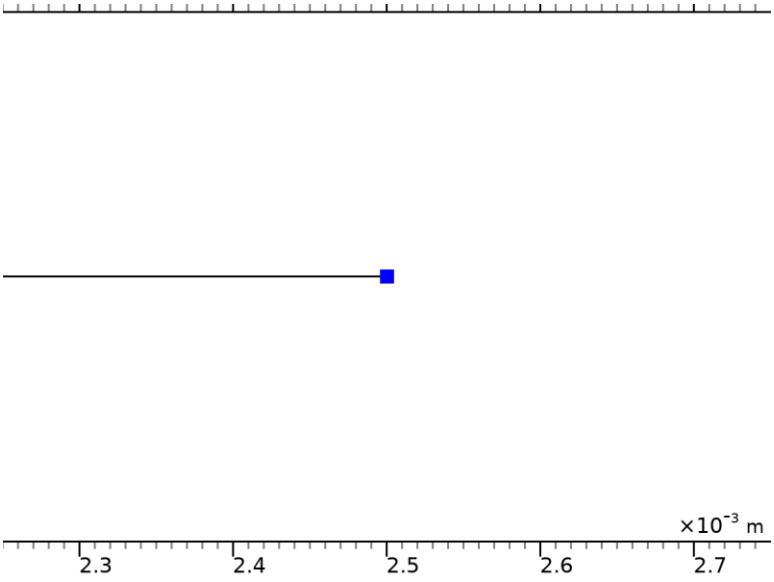
Geometric entity level	Domain
Selection	Geometry geom1: Dimension 1: All domains

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

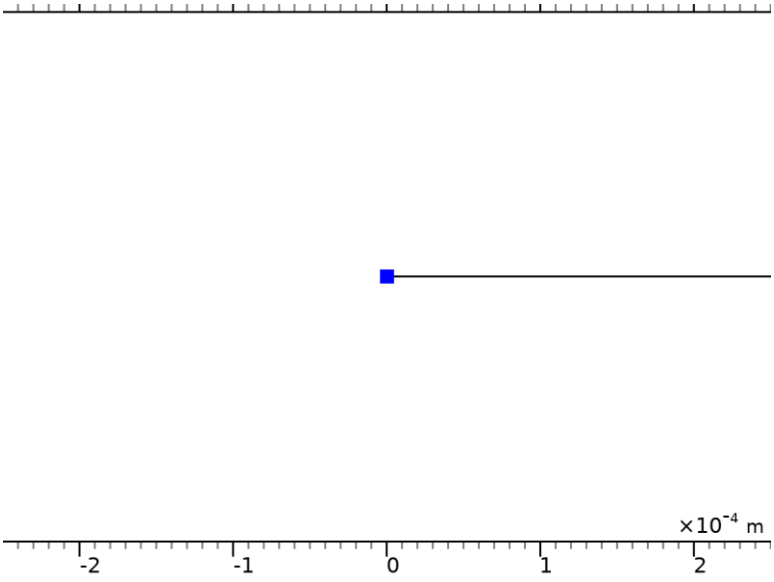
$c_i = c_{0,i}$

Concentration

SETTINGS

Description	Value
Species cOx_dif	On
Species cRed_dif	On
Concentration	{root.cOx0_dif, 0}

2.4.6 Butler-Volmer HET



Butler-Volmer HET

SELECTION

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

EQUATIONS

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

Inward Flux

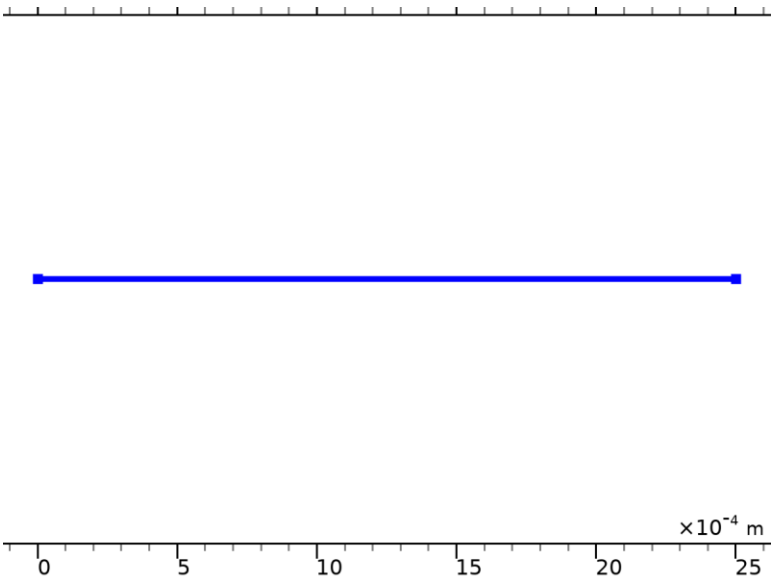
SETTINGS

Description	Value
Flux type	General inward flux
Species cOx_dif	On
Species cRed_dif	On
	{-kf_Dif*cOx_dif + kb_Dif*cRed_dif, -(-kf_Dif*cOx_dif + kb_Dif*cRed_dif)}

2.5 ELECTROSTATICS

USED PRODUCTS

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

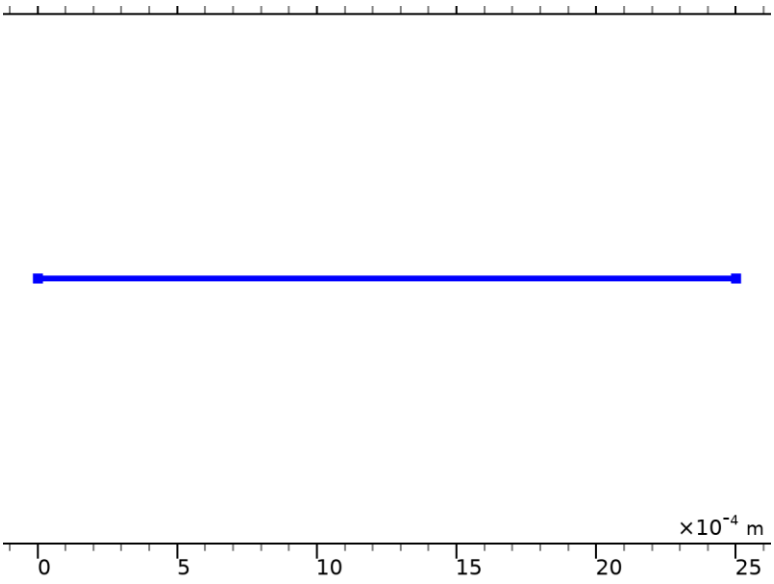
Description	Value
Electric potential	Linear
Value type when using splitting of complex variables	Complex

Manual Terminal Sweep Settings

SETTINGS

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

2.5.2 Charge Conservation - Solution



Charge Conservation - Solution

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	{{root.epsilon_s, 0, 0}, {0, root.epsilon_s, 0}, {0, 0, root.epsilon_s}}

Coordinate System Selection

SETTINGS

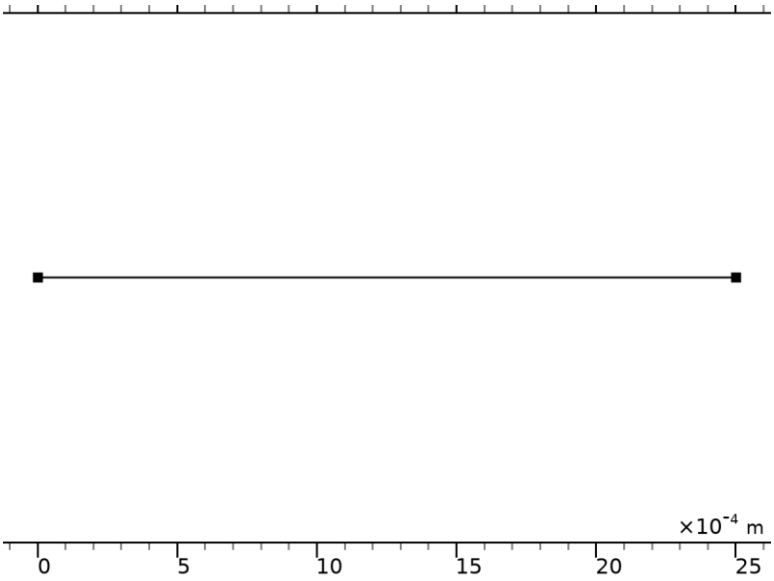
Description	Value
Coordinate system	Global coordinate system

Model Input

SETTINGS

Description	Value
Temperature	User defined
Temperature	T

2.5.3 Zero Charge 1



Zero Charge 1

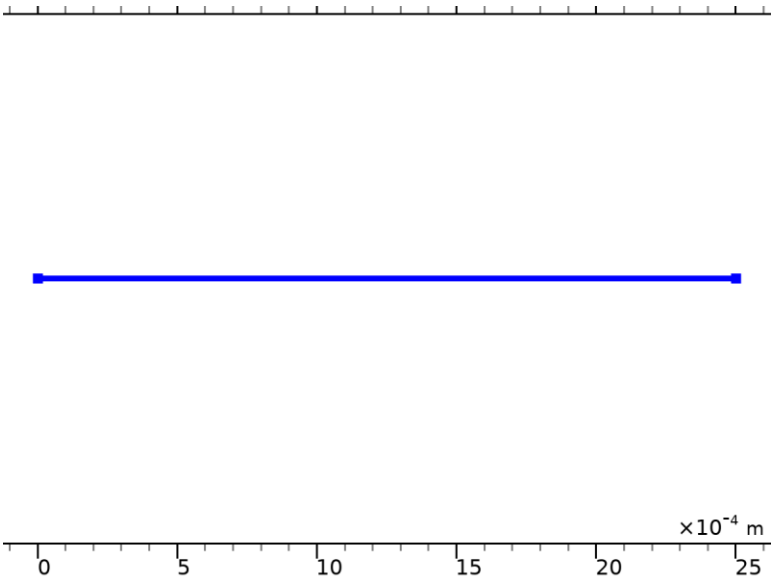
SELECTION

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

EQUATIONS

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

2.5.4 Initial Values 1



Initial Values 1

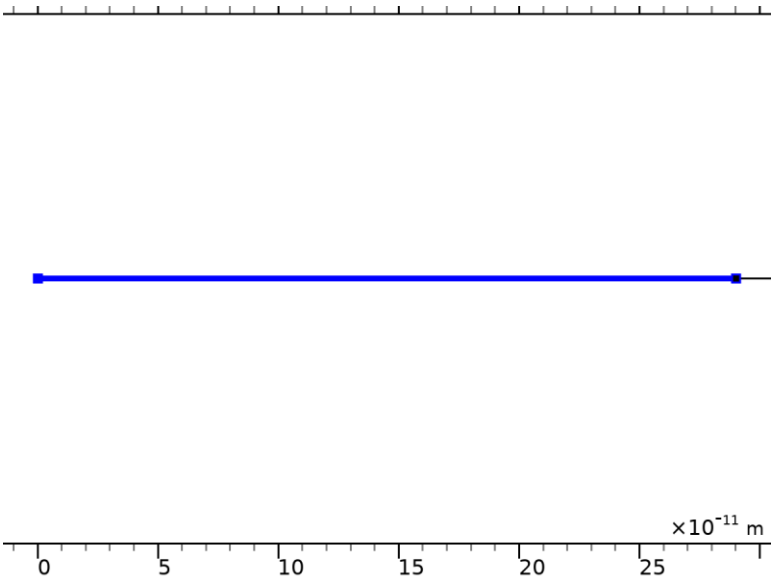
SELECTION

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

SETTINGS

Description	Value
Electric potential	0

2.5.5 Charge Conservation - Inner Film



Charge Conservation - Inner Film

SELECTION

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

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

SETTINGS

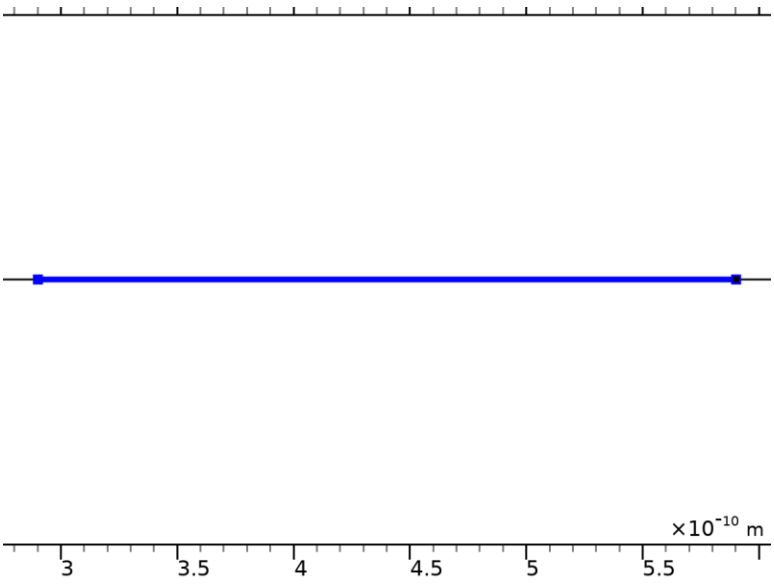
Description	Value
Coordinate system	Global coordinate system

Model Input

SETTINGS

Description	Value
Temperature	User defined
Temperature	T

2.5.6 Charge Conservation - Outer Film



Charge Conservation - Outer Film

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

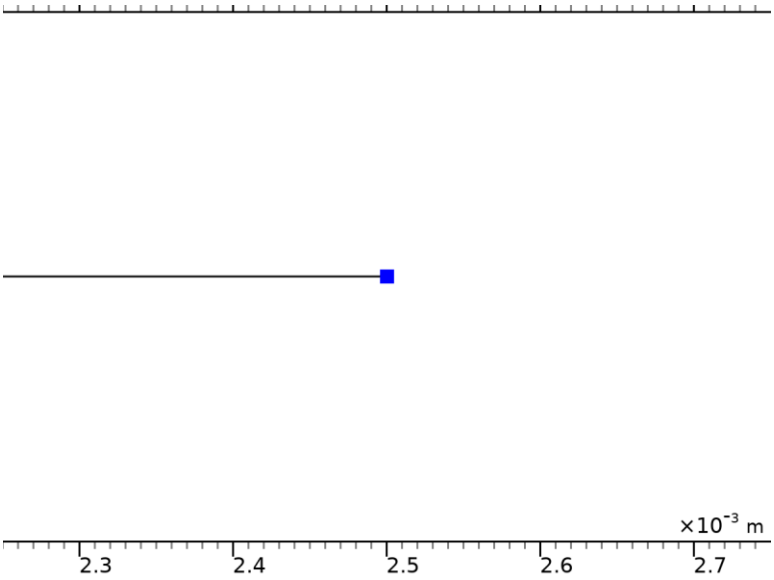
Description	Value
Coordinate system	Global coordinate system

Model Input

SETTINGS

Description	Value
Temperature	User defined
Temperature	T

2.5.7 Ground



Ground

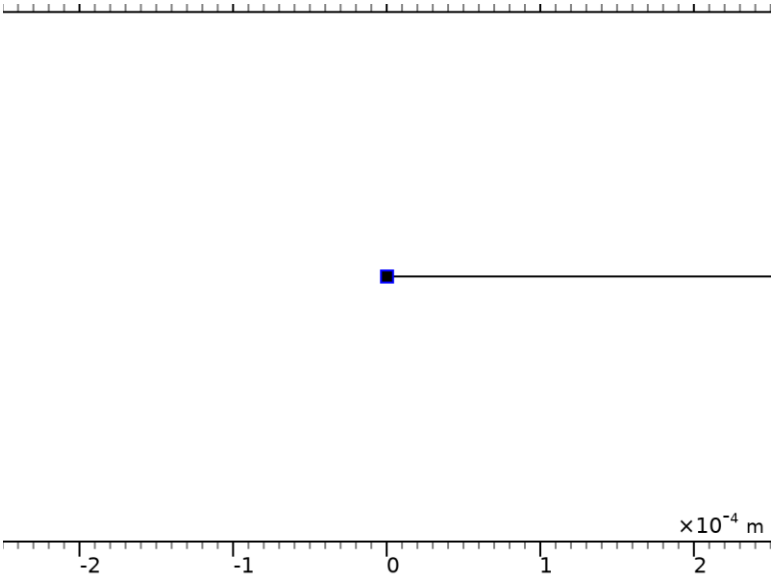
SELECTION

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

EQUATIONS

$V = 0$

2.5.8 Electric Potential - Time Dependent



Electric Potential - Time Dependent

SELECTION

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

EQUATIONS

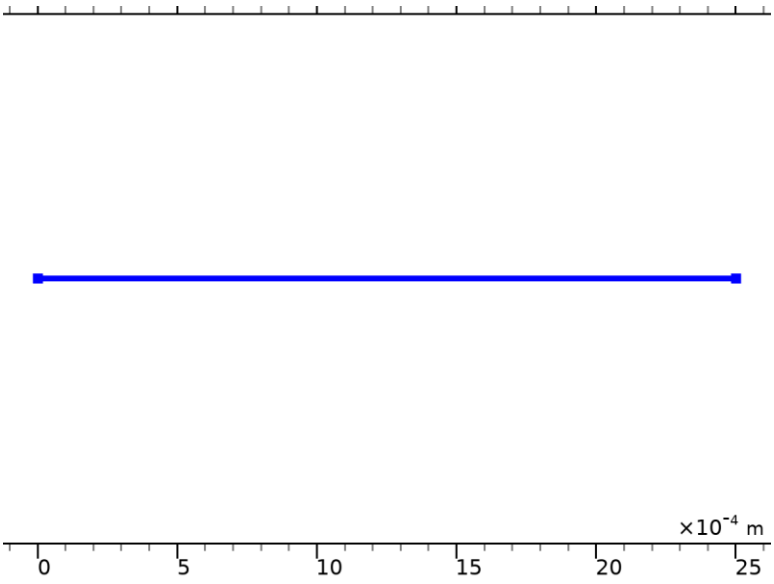
$$V = V_0$$

Electric Potential

SETTINGS

Description	Value
Electric potential	Potential(t)

2.5.9 Space Charge Density - Multiphysics Coupling



Space Charge Density - Multiphysics Coupling

SELECTION

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

EQUATIONS

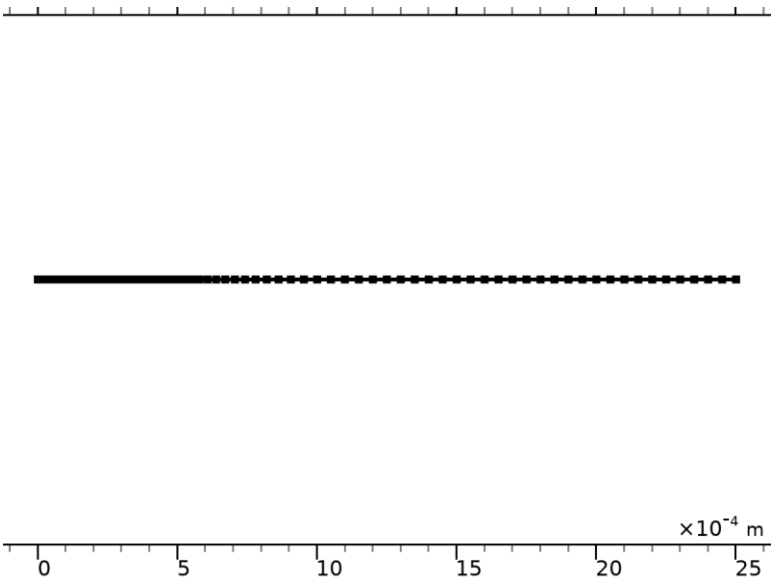
$$\nabla \cdot \mathbf{D} = \underset{\cdots}{\rho_v}$$

Coordinate System Selection

SETTINGS

Description	Value
Coordinate system	Global coordinate system

2.6 MESH 1



Mesh 1

2.6.1 Size (size)

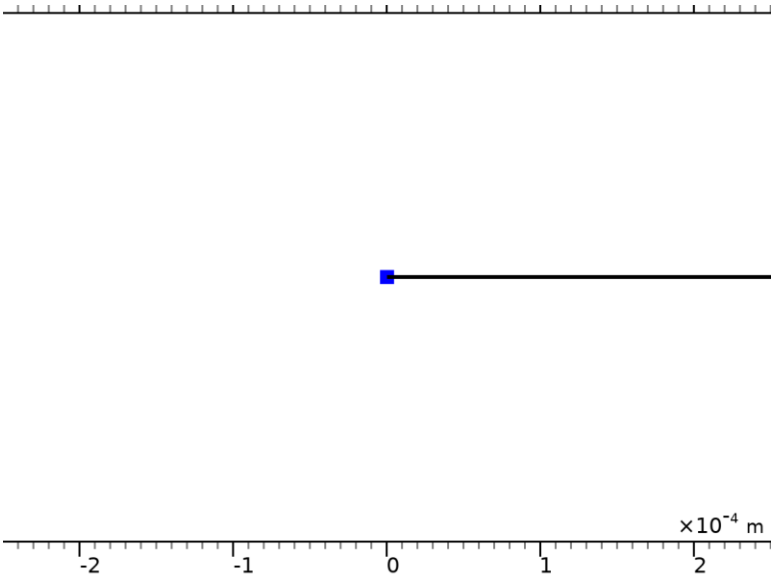
SETTINGS

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)

SELECTION

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



Size 1

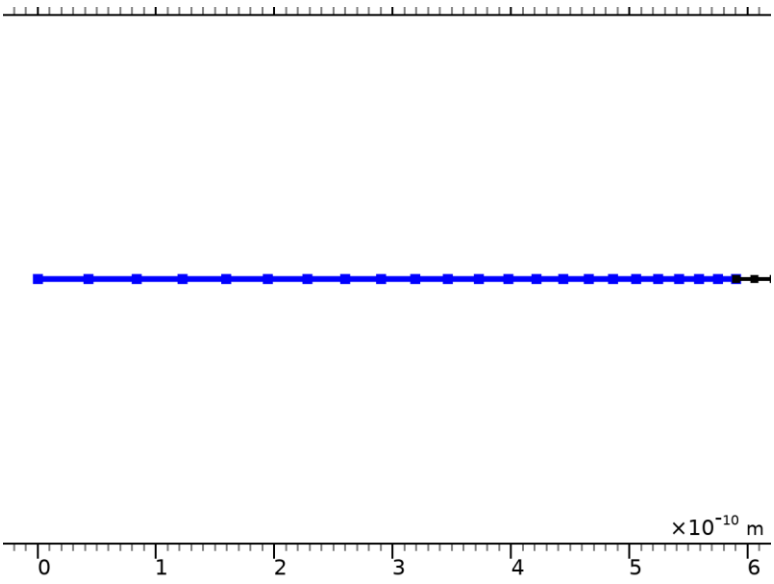
SETTINGS

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

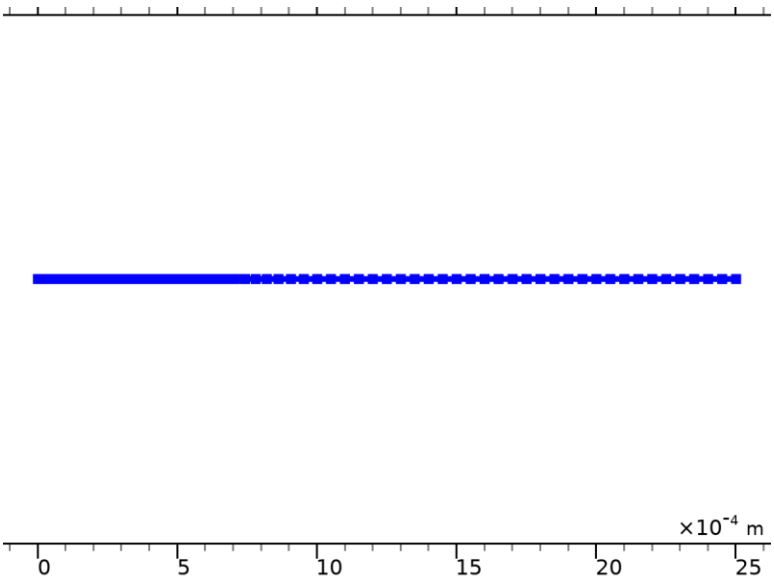
SETTINGS

Description	Value
Maximum element size	0.1 [nm]
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



Edge 1

3 Study 1

COMPUTATION INFORMATION

Computation time	5 min 31 s

3.1 PARAMETRIC SWEEP

Parameter name	Parameter value list	Parameter unit
v	1	V/s

STUDY SETTINGS

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

PARAMETERS

Parameter name	Parameter value list	Parameter unit
v (Scan rate)	1	V/s

3.2 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
Supporting Electrolyte - Transport of Diluted Species (tds)	physics
Soluble Redox Species - Transport of Diluted Species 2 (tds2)	physics
Electrostatics (es)	physics

MESH SELECTION

Geometry	Mesh
Geometry 1 (geom1)	mesh1

3.3 TIME DEPENDENT

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

STUDY SETTINGS

Description	Value
Include geometric nonlinearity	Off

VALUES OF DEPENDENT VARIABLES

Description	Value
Settings	User controlled
Method	Solution
Study	Study 1

PHYSICS AND VARIABLES SELECTION

Physics interface	Discretization
Supporting Electrolyte - Transport of Diluted Species (tds)	physics
Soluble Redox Species - Transport of Diluted Species 2 (tds2)	physics
Electrostatics (es)	physics

MESH SELECTION

Geometry	Mesh
Geometry 1 (geom1)	mesh1

3.4 SOLVER CONFIGURATIONS

3.4.1 Solution 2

Compile Equations: Stationary (st1)

STUDY AND STEP

Description	Value
Use study	Study 1
Use study step	Stationary

Dependent Variables 1 (v1)

GENERAL

Description	Value
Defined by study step	Stationary

INITIAL VALUE CALCULATION CONSTANTS

Constant name	Initial value source
t	0
timestep	0.0013000000000000002[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}

Electric potential (comp1.Phi) (comp1_Phi)

GENERAL

Description	Value
Field components	comp1.Phi

Concentration (comp1.cOx_dif) (comp1_cOx_dif)

GENERAL

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

Concentration (comp1.cRed_dif) (comp1_cRed_dif)

GENERAL

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

Stationary Solver 1 (s1)

GENERAL

Description	Value
Defined by study step	Stationary

RESULTS WHILE SOLVING

Description	Value
Probes	None

CONSTANTS

Constant name	Constant value
t	0

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 1

Description	Value
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	0.0013000000000000002[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}

Electric potential (comp1.Phi) (comp1_Phi)

GENERAL

Description	Value
Field components	comp1.Phi

Concentration (comp1.cOx_dif) (comp1_cOx_dif)

GENERAL

Description	Value
Field components	comp1.cOx_dif
Internal variables	{comp1.uflux.cOx_dif, comp1.dflux.cOx_dif, comp1.tds2.dt2Inv_cOx_dif}

Concentration (comp1.cRed_dif) (comp1_cRed_dif)

GENERAL

Description	Value
Field components	comp1.cRed_dif
Internal variables	{comp1.uflux.cRed_dif, comp1.dflux.cRed_dif, comp1.tds2.dt2Inv_cRed_dif}

Time-Dependent Solver 1 (t1)

TIME STEPPING

Description	Value
Steps taken by solver	Strict
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

METHOD AND TERMINATION

Description	Value
Nonlinear method	Automatic (Newton)
Maximum number of iterations	8

Direct 1 (d1)

GENERAL

Description	Value
Solver	PARDISO
Pivoting perturbation	1.0E-13

3.4.2 Parametric Solutions 1

v=1 (su1)

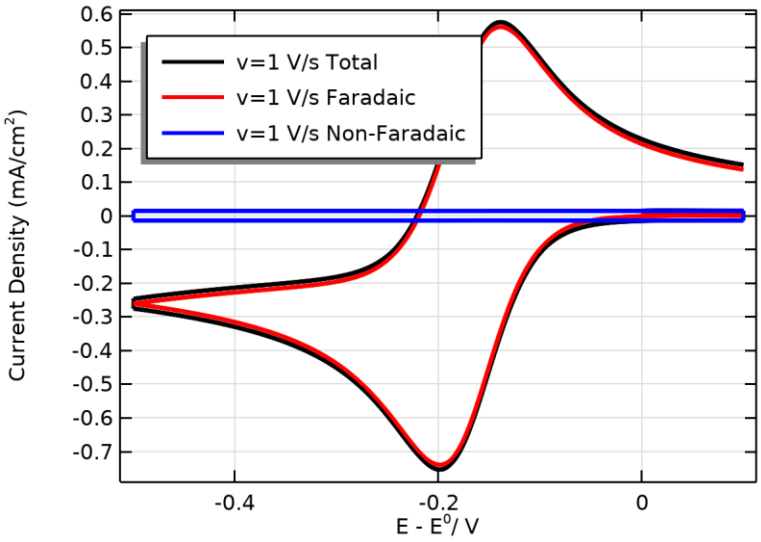
GENERAL

Description	Value
Solution	v=1

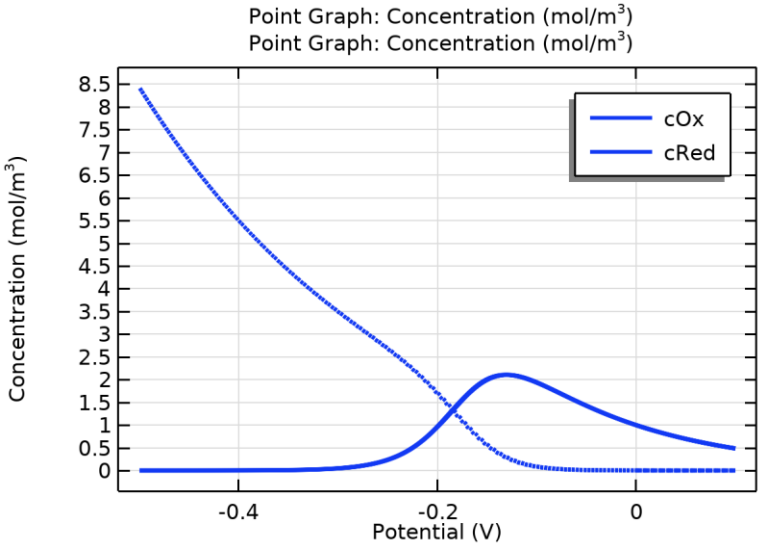
4 Results

4.1 PLOT GROUPS

4.1.1 Current Density

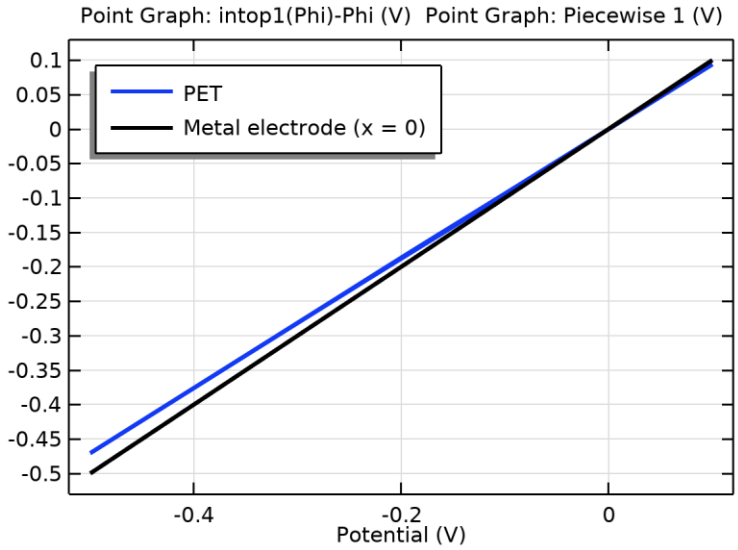


4.1.2 Surface Species Concentration - Time Dependent



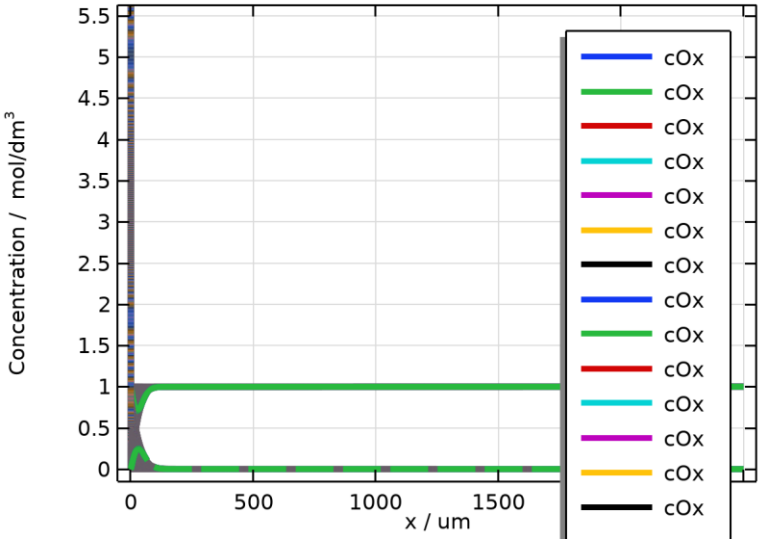
Point Graph: Concentration (mol/m³) Point Graph: Concentration (mol/m³)

4.1.3 Interfacial Potential

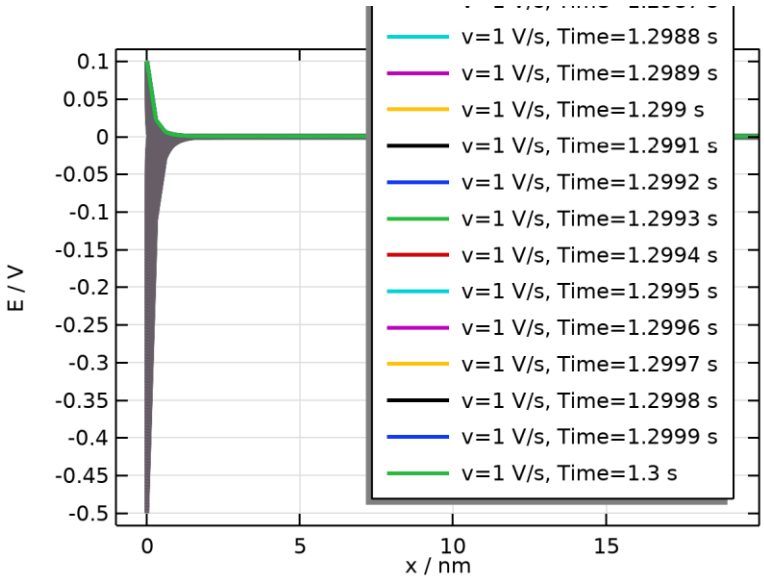
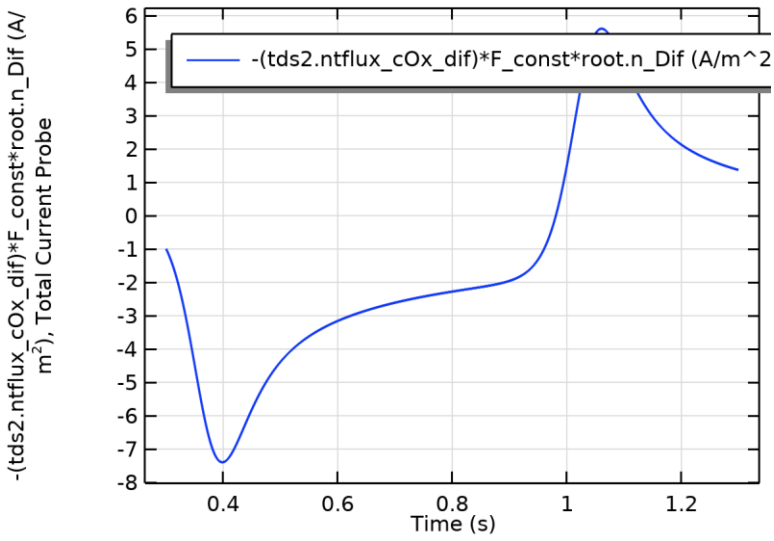


Point Graph: intop1(Phi)-Phi (V) Point Graph: Piecewise 1 (V)

4.1.4 Concentrations Ox/Red



4.1.5 Electric Potential across solution - Time Dependent



4.1.6 Probe Plot Group 26