Supporting information for

Quantification of the charge transport processes inside carbon nanopipettes

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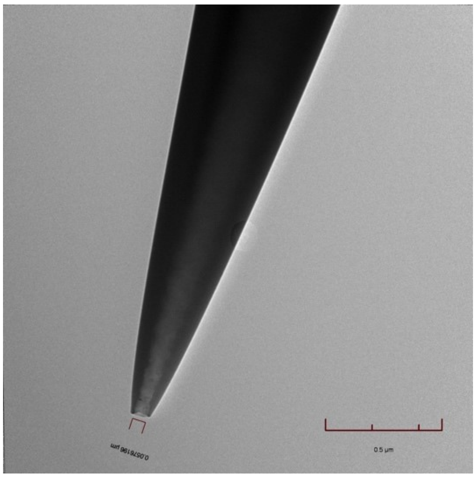


Figure S1. TEM image of prepared carbon nanopipettes. a = ~29 nm, half-cone angle (θ) is ~8°.

1. Calculation of the carbon nanopipette resistance.

The carbon nanopipette resistance can be calculated depends on the geometry of CNP according to the following equation[1]:

$$R = \frac{1}{4\kappa a} + \frac{1}{\kappa \pi a tan\theta} \quad \text{(S1)}$$

Where κ = 1.29 Ω^{-1} m^{-1} is the solution conductivity of 0.1 M KCl, a = 50 nm is the radius of CNPs, θ = 8° is the tip angle. So, the carbon nanopipette resistance (R) is 0.04 GΩ.

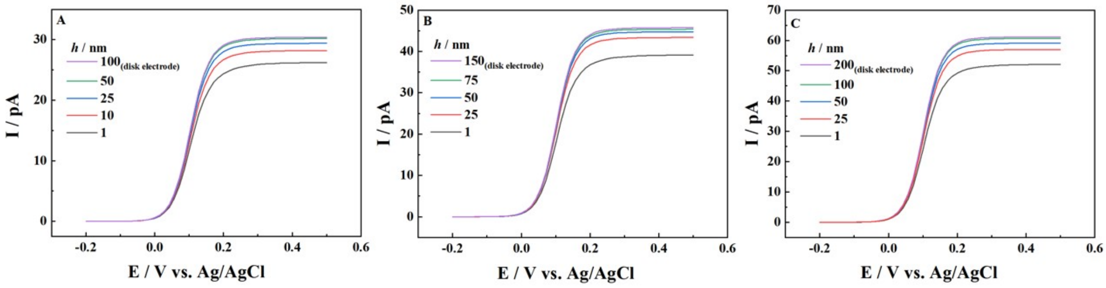


Figure S2 The simulated steady-state voltammograms of CNPs with various carbon layer thickness values in different-sized nanopipettes (A) a = 100 nm, (B) a = 150 nm and (C) a = 200 nm.

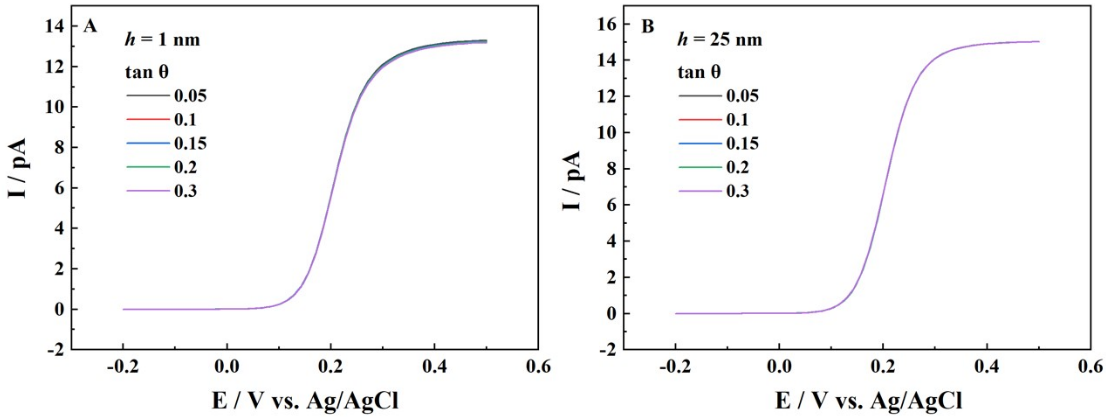


Figure S3 The half-cone angle effect on the steady-state voltammograms of carbon nanopipettes with carbon layer thickness of (A) h = 1 nm and (B) h =25 nm.

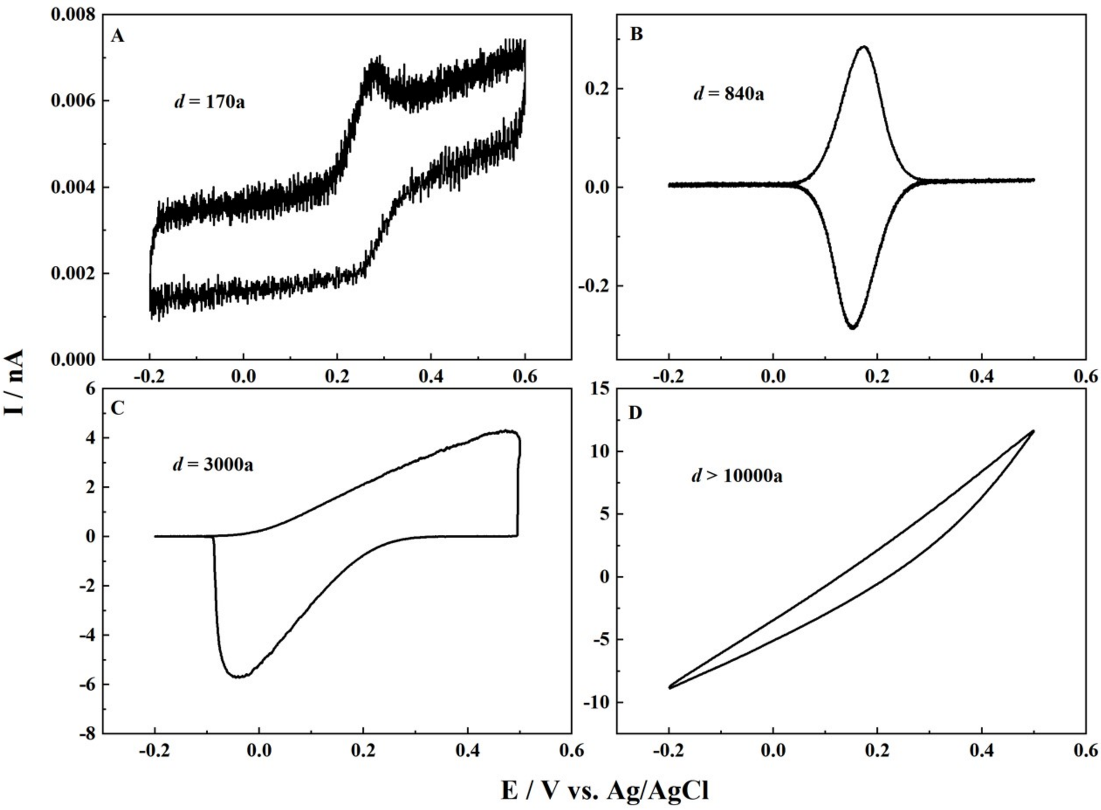


Figure S4 Experimental cyclic voltammograms from carbon nanopipettes with different solution depth roughly controlled by external pressure. a = 50 nm, tanθ = 0.2, v = 0.1 V/s and E^0 = 0.2 V.

2. Potential correction calculation of Ag/AgCl electrode

The potential of Ag/AgCl electrode depends on Cl^- concentration, which can be calculated by the Nernst equation.

$$E = E^{\ominus '} - \frac{RT}{nF} ln a_{cl^-} \quad (S2)$$

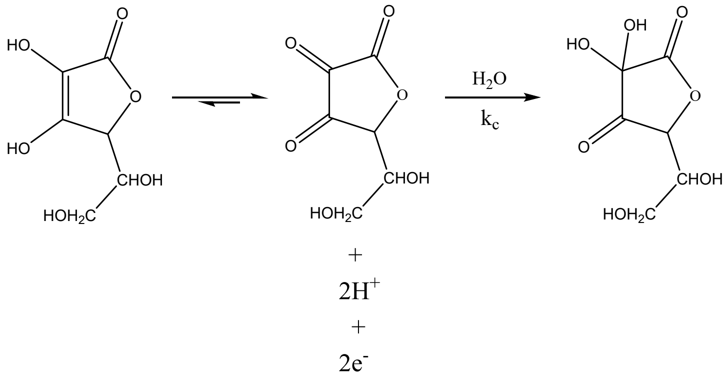
Where $E^{\ominus '}$ = 0.2224 V is the standard potential of Ag/AgCl, n = 1 is the number of transferred electrons for the Ag oxidation, F = 96485 C/mol is the Faraday constant, T = 298 K is the temperature. $a_{Cl^-} \approx c_{Cl^-}$ is the activity of Cl^-. The calculation results are shown in Table S1.

Table S1. The calculation results of $E_{Ag/AgCl}$ and $E_{Fe(CN)_6^{4-}}$ in different Cl^- concentration

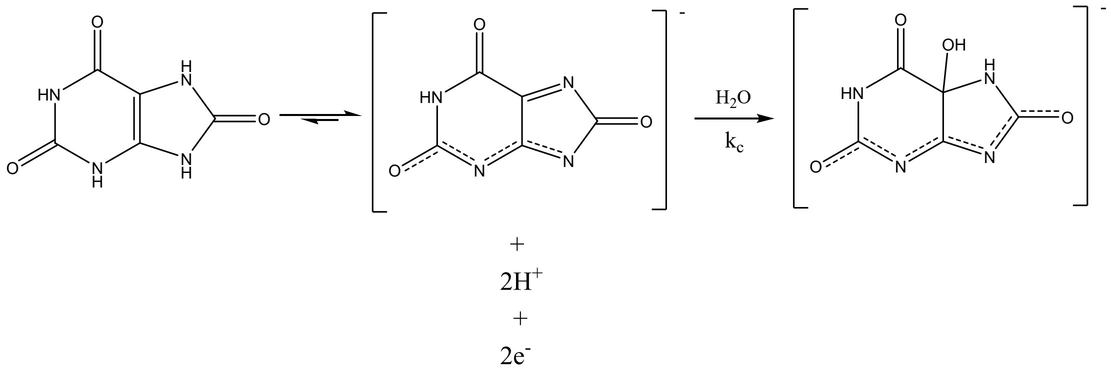
c_{Cl^-} / mM	10	50	100	500	1000
$E_{Ag/AgCl}$ / V vs. NHE	0.34	0.30	0.28	0.24	0.22
$E^0_{Fe(CN)_6^{4-}}$ / V vs. Ag/AgCl	0.12	0.18	0.24	0.26	0.29
$E^0_{Fe(CN)_6^{4-}}$ / V vs. NHE	0.46	0.48	0.52	0.50	0.51
$E^{\ominus}_{Fe(CN)_6^{4-}}$ / V vs. NHE[2]	0.49				

3. The irreversible EC mechanism of uric acid (UA) and ascorbic acid (AA).

The electro-oxidation products of UA and AA are very easily hydrolysed and go through an irreversible EC mechanism[3]. For AA:



For UA:



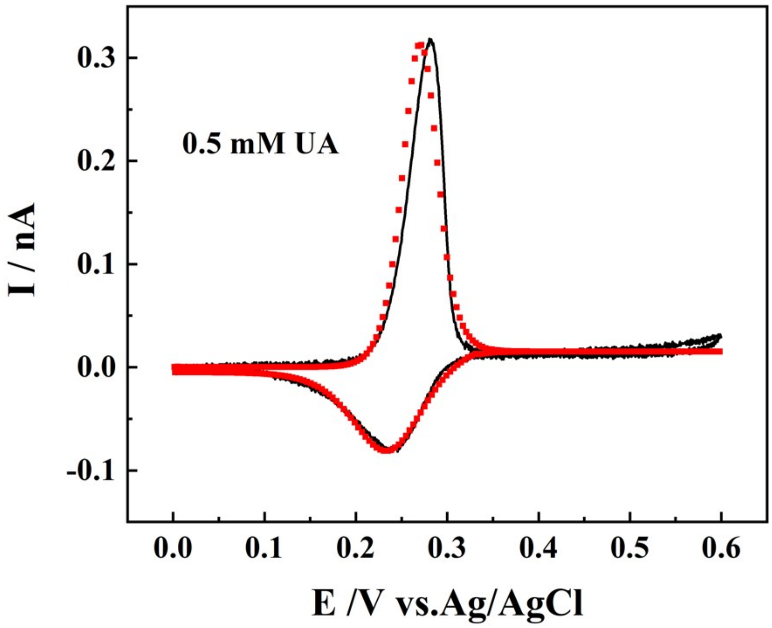


Figure S5 Experimental and simulated cyclic voltammograms of 0.5 mM UA in carbon nanopipettes. The oxidation peak is fitted by two-electron transfer process，while the reduction peak is fitted by one electron transfer process.

Reference:

1. Y. L. Ying, Y. X. Hu, R. Gao, R. J. Yu, Z. Gu, L. P. Lee and Y. T. Long, *J. Am. Chem. Soc.*, 2018, **140**, 5385-5392.
2. D. Polcari, P. Dauphin-Ducharme and J. J. C. R. Mauzeroll, *Chem. Rev.* 2016, **116**, 13234−13278.
3. L. Xiao, J. Chen and C. Cha, *J. Electroanal. Chem.*, 2000, **495**, 27-35..

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Report date Sep 22, 2021 11:12:40 AM

Contents

1 Global Definitions

Date Feb 22, 2021 3:15:53 PM

GLOBAL SETTINGS

Name	Depth-5000a.mph
Path	H:\simulation\20210222after\depth-5000a.mph
Version	COMSOL Multiphysics 5.4 (Build: 388)

USED PRODUCTS

COMSOL Multiphysics

Chemical Reaction Engineering Module

1.1 PARAMETERS

PARAMETERS 1

Name	Expression	Value	Description
a	50[nm]	5E−8 m	
depth	l*a	5E−5 m	
tan_theta	0.1	0.1	
thickness	5[nm]	5E−9 m	
k0	10[cm/s]	0.1 m/s	
E0	0.16[V]	0.16 V	
E1	0[V]	0 V	
F	96485[C/mol]	96485 C/mol	
v	1	1	
l	1000	1000	

2 Component 1

SETTINGS

Description	Value
Unit system	Same as global system

2.1 DEFINITIONS

2.1.1 Variables

Variables 1

SELECTION

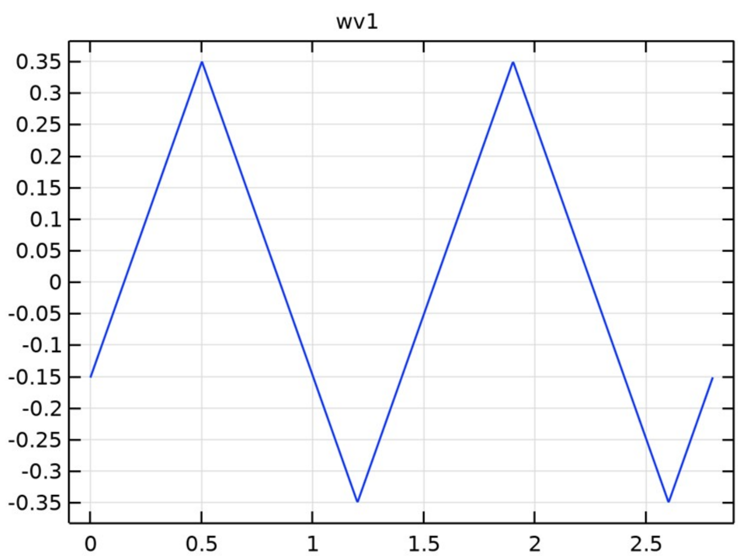
Geometric entity level	Entire model

Name	Expression	Unit	Description
E	1[V]*wv1(t/1[s]) + 0.15[V]	V	

2.1.2 Functions

Waveform 1

Function name	wv1
Function type	Waveform



Waveform 1

PARAMETERS

Description	Value

Description	Value
Type	Triangle
Size of transition zone	0.0001
Angular frequency	pi/0.7*v
Phase	-0.68
Amplitude	0.35

2.1.3 Coordinate Systems

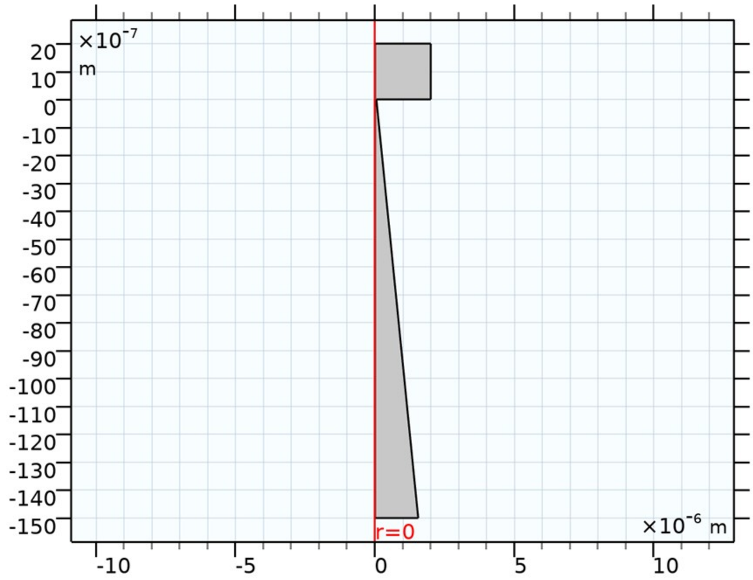
Boundary System 1

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

Description	Value
Number of boundaries	7
Number of vertices	7

2.2.1 Polygon 1 (pol1)

OBJECT TYPE

Description	Value
Type	Solid

COORDINATES

Description	Value
Data source	Table

COORDINATES

r (m)	z (m)
0	2e-6
2e-6	2e-6
2e-6	0
a	0
a+depth*tan_theta	-depth
0	-depth

2.2.2 Point 1 (pt1)

POINT

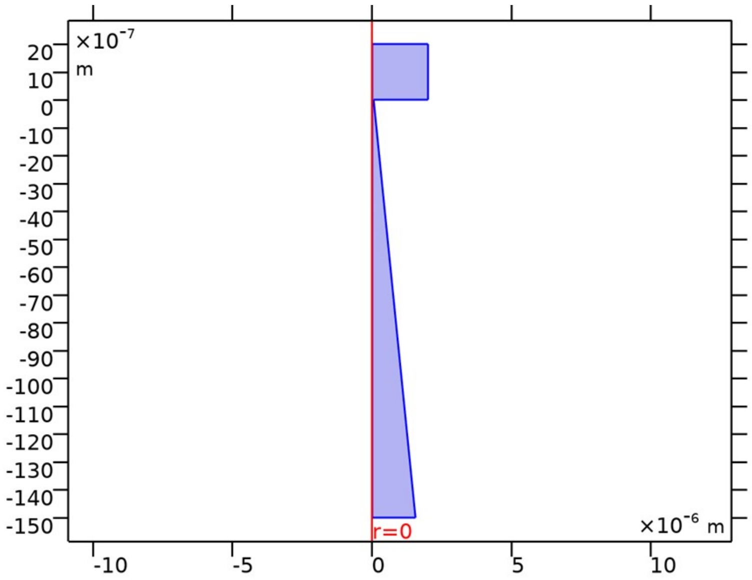
Description	Value
Point coordinate	{5.5E-8, 0}

2.3 TRANSPORT OF DILUTED SPECIES

USED PRODUCTS

COMSOL Multiphysics

Chemical Reaction Engineering Module



Transport of Diluted Species

SELECTION

Geometric entity level	Domain
Selection	Domain 1

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

Transport mechanisms

SETTINGS

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

2.3.2 Variables

Name	Expression	Unit	Description	Selection	Details

Name	Expression	Unit	Description	Selection	Details
tds.R_cO	0	mol/(m³·s)	Total rate expression	Domain 1	+ operation
tds.R_cR	0	mol/(m³·s)	Total rate expression	Domain 1	+ operation
tds.R_cK	0	mol/(m³·s)	Total rate expression	Domain 1	+ operation
tds.R_cCl	0	mol/(m³·s)	Total rate expression	Domain 1	+ operation
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 1–7	
tds.nphi	0	1	Normal vector, phi component	Boundaries 1–7	
tds.nz	dnz	1	Normal vector, z component	Boundaries 1–7	
tds.nrmesh	dnrmesh	1	Normal vector (mesh), r component	Boundaries 1–7	
tds.nphimesh	0	1	Normal vector (mesh), phi component	Boundaries 1–7	
tds.nzmesh	dnzmesh	1	Normal vector (mesh), z component	Boundaries 1–7	
tds.nrc	root.nrc/tds.ncLen	1	Normal vector, r component	Boundaries 1–7	
tds.nphic	0	1	Normal vector, phi component	Boundaries 1–7	
tds.nzc	root.nzc/tds.ncLen	1	Normal vector, z	Boundaries 1–7	

Name	Expression	Unit	Description	Selection	Details
			component		
tds.ncLen	sqrt(root.nrc^2+root.nzc^2+eps)	1	Help variable	Boundaries 1–7	

2.3.3 Transport Properties 1

Transport Properties 1

SELECTION

Geometric entity level	Domain
Selection	Domain 1

EQUATIONS

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

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

Diffusion

SETTINGS

Description	Value
Material	None
Diffusion coefficient	User defined
Diffusion coefficient	{{7.8e-10[m^2/s], 0, 0}, {0, 7.8e-10[m^2/s], 0}, {0, 0, 7.8e-10[m^2/s]}}
Diffusion coefficient	User defined
Diffusion coefficient	{{7.8e-10[m^2/s], 0, 0}, {0, 7.8e-10[m^2/s], 0}, {0, 0, 7.8e-10[m^2/s]}}
Diffusion coefficient	User defined
Diffusion coefficient	{{2e-9[m^2/s], 0, 0}, {0, 2e-9[m^2/s], 0}, {0, 0, 2e-9[m^2/s]}}

Description	Value
Diffusion coefficient	User defined
Diffusion coefficient	{{2e-9[m^2/s], 0, 0}, {0, 2e-9[m^2/s], 0}, {0, 0, 2e-9[m^2/s]}}

Migration in electric field

SETTINGS

Description	Value
Electric potential	Electric potential (ec)
Mobility	Nernst - Einstein relation
Charge number	{1, 0, 1, -1}

Coordinate system selection

SETTINGS

Description	Value
Coordinate system	Global coordinate system

Model input

SETTINGS

Description	Value
Temperature	Common model input

Shape functions

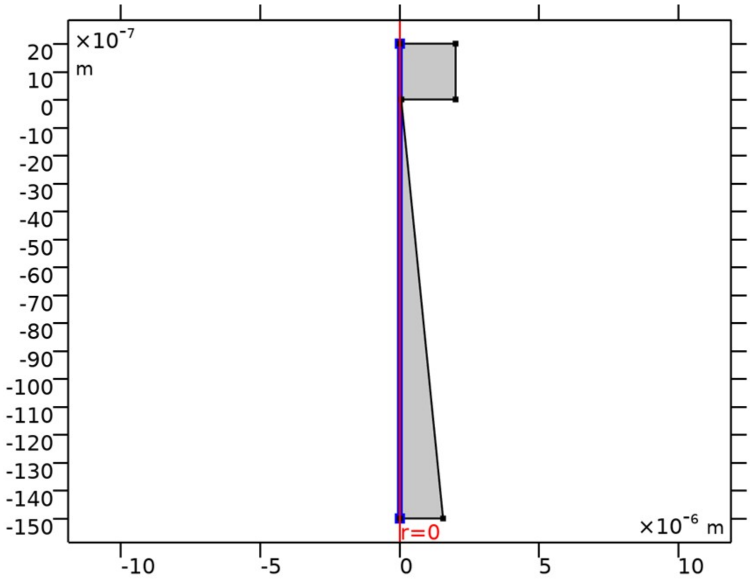
Name	Shape function	Unit	Description	Shape frame	Selection
cO	Lagrange (Linear)	mol/m³	Concentration	Spatial	Domain 1
cR	Lagrange (Linear)	mol/m³	Concentration	Spatial	Domain 1
cK	Lagrange (Linear)	mol/m³	Concentration	Spatial	Domain 1
cCl	Lagrange (Linear)	mol/m³	Concentration	Spatial	Domain 1

Weak expressions

Weak expression	Integration order	Integration frame	Selection
2*(-cOt*test(cO)+tds.dflux_cOr*test(cOr)+tds.dflux_cOz*test(cOz))*pi*r	2	Spatial	Domain 1
2*(-cRt*test(cR)+tds.dflux_cRr*test(cRr)+tds.dflux_cRz*test(cRz))*pi*r	2	Spatial	Domain 1
2*(-cKt*test(cK)+tds.dflux_cKr*test(cKr)+tds.dflux_cKz*test(cKz))*pi*r	2	Spatial	Domain 1
2*(-cClt*test(cCl)+tds.dflux_cClr*test(cClr)+tds.dflux_cClz*test(cClz))*p	2	Spatial	Domain 1

Weak expression	Integration order	Integration frame	Selection
i*r			
2*tds.z_cO*F_const*cO*((-tds.um_cOrr*d(tds.V,r)-tds.um_cOrz*d(tds.V,z))*test(cOr)+(-tds.um_cOzr*d(tds.V,r)-tds.um_cOzz*d(tds.V,z))*test(cOz))*pi*r	2	Spatial	Domain 1
2*tds.z_cR*F_const*cR*((-tds.um_cRrr*d(tds.V,r)-tds.um_cRrz*d(tds.V,z))*test(cRr)+(-tds.um_cRzr*d(tds.V,r)-tds.um_cRzz*d(tds.V,z))*test(cRz))*pi*r	2	Spatial	Domain 1
2*tds.z_cK*F_const*cK*((-tds.um_cKrr*d(tds.V,r)-tds.um_cKrz*d(tds.V,z))*test(cKr)+(-tds.um_cKzr*d(tds.V,r)-tds.um_cKzz*d(tds.V,z))*test(cKz))*pi*r	2	Spatial	Domain 1
2*tds.z_cCl*F_const*cCl*((-tds.um_cClrr*d(tds.V,r)-tds.um_cClrz*d(tds.V,z))*test(cClr)+(-tds.um_cClzr*d(tds.V,r)-tds.um_cClzz*d(tds.V,z))*test(cClz))*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

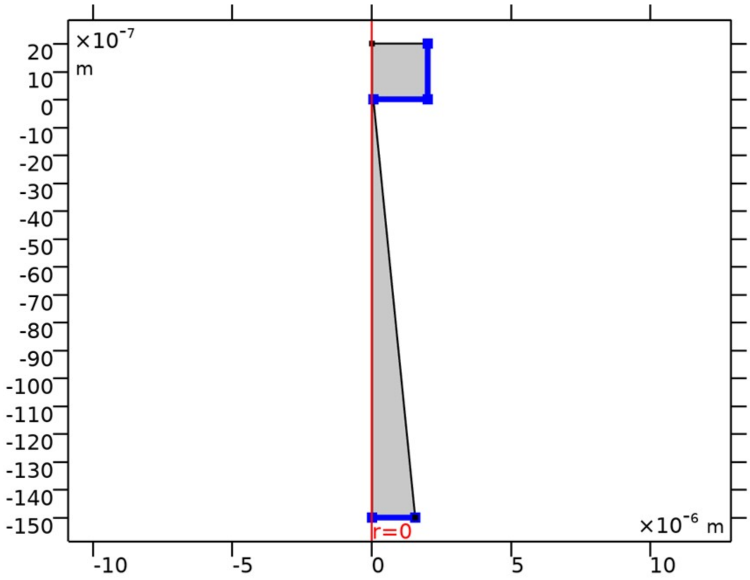


Axial Symmetry 1

SELECTION

Geometric entity level	Boundary
Selection	Boundary 1

2.3.5 No Flux 1



No Flux 1

SELECTION

Geometric entity level	Boundary
Selection	Boundaries 2, 6–7

EQUATIONS

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

2.3.6 Initial Values 1

Initial Values 1

SELECTION

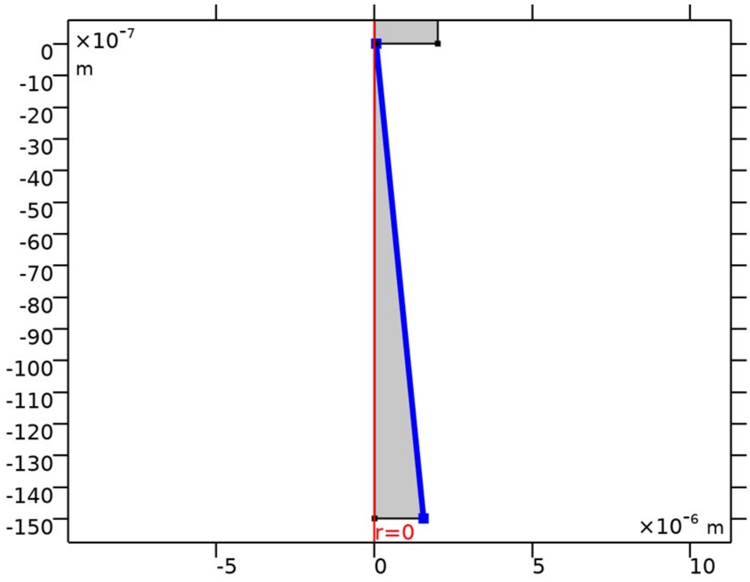
Geometric entity level	Domain
Selection	Domain 1

Initial values

SETTINGS

Description	Value
Concentration	{1, 0, 100, 100}

2.3.7 Flux 1



Flux 1

SELECTION

Geometric entity level	Boundary
Selection	Boundaries 4–5

EQUATIONS

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

Inward flux

SETTINGS

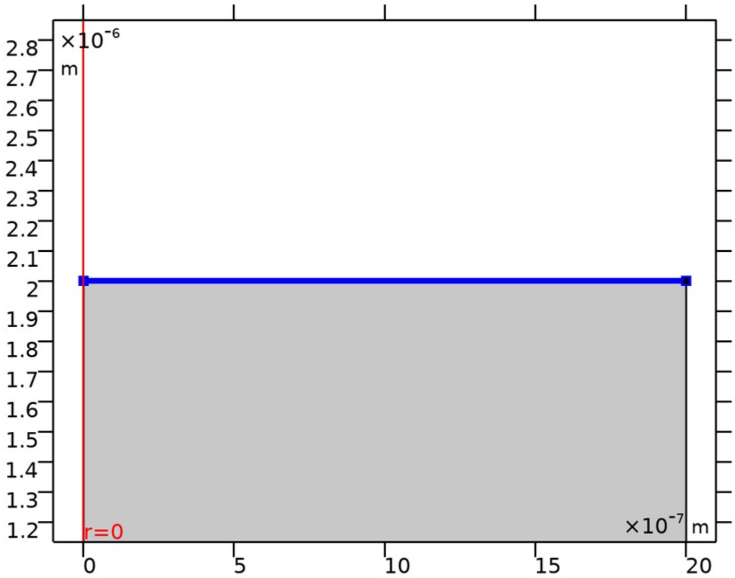
Description	Value
Flux type	General inward flux
Species cO	On
Species cR	On
Species cK	Off
Species cCl	Off
	{-k0*cO*exp(-0.5*38.9[1/V]*(E-E0 - V)) + k0*cR*exp(0.5*38.9[1/V]*(E-E0 - V)), k0*cO*exp(-0.5*38.9[1/V]*(E-E0 - V)) - k0*cR*exp(0.5*38.9[1/V]*(E-E0 - V)), 0, 0}

Weak expressions

Weak expression	Integration order	Integration frame	Selection
2*k0*(-cO*exp(-0.5*38.9[1/V]*(E-E0-V))+cR*exp(0.5*38.9[1/V]*(E-E0-V)))*test(cO)*pi*r	2	Spatial	Boundaries 4–5

Weak expression	Integration order	Integration frame	Selection
2*k0*(cO*exp(-0.5*38.9[1/V]*(E-E0-V))-cR*exp(0.5*38.9[1/V]*(E-E0-V)))*test(cR)*pi*r	2	Spatial	Boundaries 4–5
0	2	Spatial	Boundaries 4–5
0	2	Spatial	Boundaries 4–5

2.3.8 Concentration 1



Concentration 1

SELECTION

Geometric entity level	Boundary
Selection	Boundary 3

EQUATIONS

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

Concentration

SETTINGS

Description	Value
Species cO	On
Species cR	On
Species cK	On
Species cCl	On
Concentration	{1, 0, 100, 100}

Variables

Name	Expression	Unit	Description	Selection

Name	Expression	Unit	Description	Selection
tds.c0_cO	1	mol/m³	Concentration	Boundary 3
tds.c0_cR	0	mol/m³	Concentration	Boundary 3
tds.c0_cK	100	mol/m³	Concentration	Boundary 3
tds.c0_cCl	100	mol/m³	Concentration	Boundary 3

Constraints

Constraint	Constraint force	Shape function	Selection	Details
-cO+tds.c0_cO	test(-cO+tds.c0_cO)	Lagrange (Linear)	Boundary 3	Elemental
-cR+tds.c0_cR	test(-cR+tds.c0_cR)	Lagrange (Linear)	Boundary 3	Elemental
-cK+tds.c0_cK	test(-cK+tds.c0_cK)	Lagrange (Linear)	Boundary 3	Elemental
-cCl+tds.c0_cCl	test(-cCl+tds.c0_cCl)	Lagrange (Linear)	Boundary 3	Elemental

2.4 ELECTRIC CURRENTS

USED PRODUCTS

COMSOL Multiphysics

Electric Currents

SELECTION

Geometric entity level	Domain
Selection	Domain 1

EQUATIONS

$$\nabla \cdot \mathbf{J} = Q_{j,v}$$

$$\mathbf{J} = \sigma \mathbf{E} + \frac{\partial \mathbf{D}}{\partial t} + \mathbf{J}_e$$

$$\mathbf{E} = -\nabla V$$

2.4.1 Interface settings

Discretization

SETTINGS

Description	Value
Electric potential	Quadratic

Manual terminal sweep settings

SETTINGS

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

2.4.2 Current Conservation 1

Current Conservation 1

SELECTION

Geometric entity level	Domain
Selection	Domain 1

EQUATIONS

$$\nabla \cdot \mathbf{J} = Q_{\mathrm{j,v}}$$

$$\mathbf{J} = \sigma \mathbf{E} + \frac{\partial \mathbf{D}}{\partial t} + \mathbf{J}_{\mathrm{e}}$$

$$\mathbf{E} = -\nabla V$$

Conduction current

SETTINGS

Description	Value
Electrical conductivity	User defined
Electrical conductivity	{{1, 0, 0}, {0, 1, 0}, {0, 0, 1}}

Electric field

SETTINGS

Description	Value
Constitutive relation	Relative permittivity
Relative permittivity	User defined
Relative permittivity	{{80, 0, 0}, {0, 80, 0}, {0, 0, 80}}

Coordinate system selection

SETTINGS

Description	Value
Coordinate system	Global coordinate system

Variables

Shape functions

Name	Shape function	Unit	Description	Shape frame	Selection
V	Lagrange (Quadratic)	V	Electric potential	Spatial	Domain 1
V	Lagrange (Quadratic)	V	Electric potential	Material	Domain 1
V	Lagrange (Quadratic)	V	Electric potential	Geometry	Domain 1
V	Lagrange (Quadratic)	V	Electric potential	Mesh	Domain 1

Weak expressions

Weak expression	Integration order	Integration frame	Selection
2*(ec.Jr*test(Vr)+ec.Jz*test(Vz))*ec.d*pi*r	4	Spatial	Domain 1

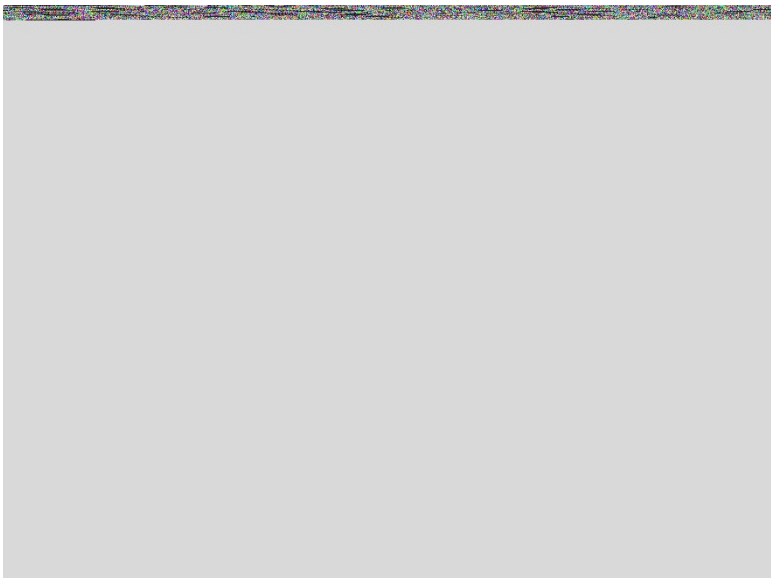
2.4.3 Axial Symmetry 1

Axial Symmetry 1

SELECTION

Geometric entity level	Boundary
Selection	Boundary 1

2.4.4 Electric Insulation 1



Electric Insulation 1

SELECTION

Geometric entity level	Boundary
Selection	Boundaries 2, 6–7

EQUATIONS

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

Variables

Name	Expression	Unit	Description	Selection	Details
ec.nJ	0	A/m²	Normal current density	Boundaries 2, 6–7	+ operation

Shape functions

Name	Shape function	Unit	Description	Shape frame	Selection	Details
V	Lagrange (Quadratic)	V	Electric potential	Spatial	No boundaries	Slit
V	Lagrange (Quadratic)	V	Electric potential	Material	No boundaries	Slit
V	Lagrange (Quadratic)	V	Electric potential	Geometry	No boundaries	Slit
V	Lagrange (Quadratic)	V	Electric potential	Mesh	No boundaries	Slit

2.4.5 Initial Values 1

Initial Values 1

SELECTION

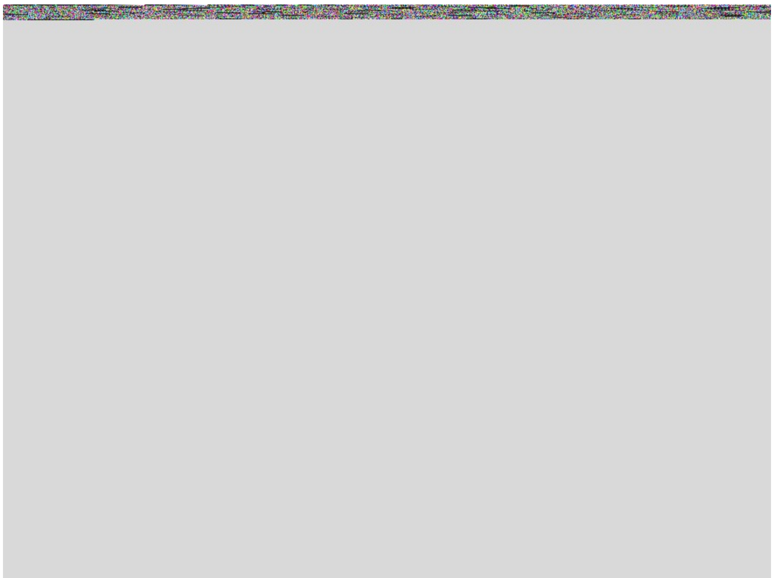
Geometric entity level	Domain
Selection	Domain 1

SETTINGS

Description	Value

Description	Value
Electric potential	0

2.4.6 Normal Current Density 1



Normal Current Density 1

SELECTION

Geometric entity level	Boundary
Selection	Boundaries 4–5

EQUATIONS

$$-\mathbf{n}\cdot\mathbf{J} = J_n$$

Normal current density

SETTINGS

Description	Value
Type	Inward current density
Normal current density	tds.ntflux_cR*F

Coordinate system selection

SETTINGS

Description	Value
Coordinate system	Global coordinate system

Variables

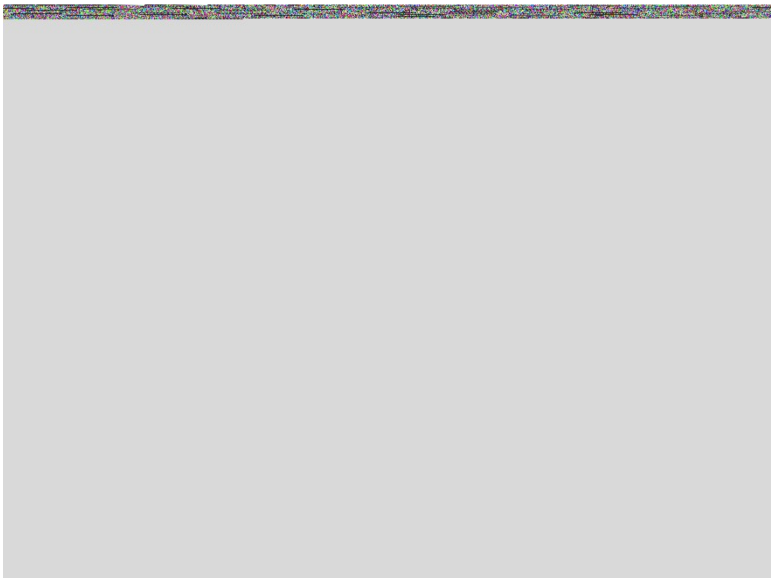
Name	Expression	Unit	Description	Selection	Details
ec.nJ	ec.ncd1.nJ	A/m^2	Normal current density	Boundaries 4–5	+ operation

Name	Expression	Unit	Description	Selection	Details
ec.ncd1.nJ	tds.ntflux_cR*F	A/m²	Normal current density	Boundaries 4–5	

Weak expressions

Weak expression	Integration order	Integration frame	Selection
2*ec.d*ec.ncd1.nJ*test(V)*pi*r	4	Spatial	Boundaries 4–5

2.4.7 Ground 1



Ground 1

SELECTION

Geometric entity level	Boundary
Selection	Boundary 3

EQUATIONS

$$V = 0$$

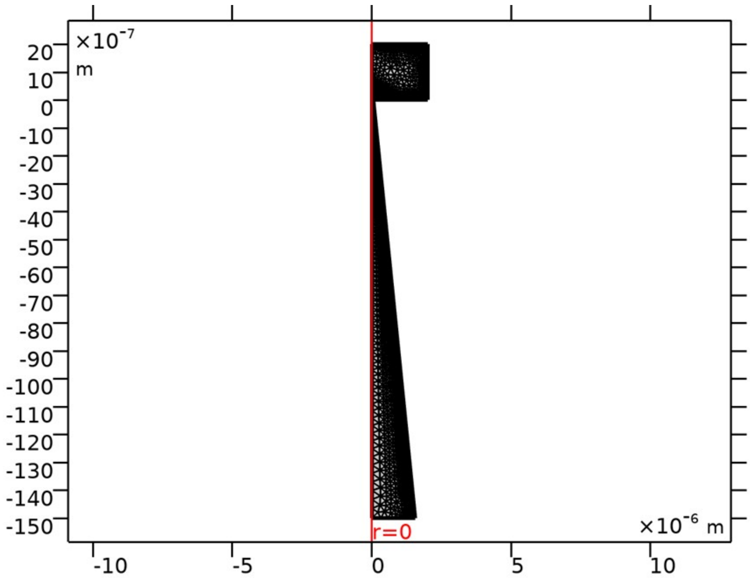
Variables

Name	Expression	Unit	Description	Selection	Details
ec.nJ	ec.unr*down(ec.Jr)+ec.unphi*down(ec.Jphi)+ec.unz*down(ec.Jz)	A/m²	Normal current density	Boundary 3	+ operation
ec.V0	0	V	Electric potential	Boundary 3	

Constraints

Constraint	Constraint force	Shape function	Selection	Details
ec.V0-V	test(ec.V0-V)	Lagrange (Quadratic)	Boundary 3	Elemental

2.5 MESH 1



Mesh 1

2.5.1 Size (size)

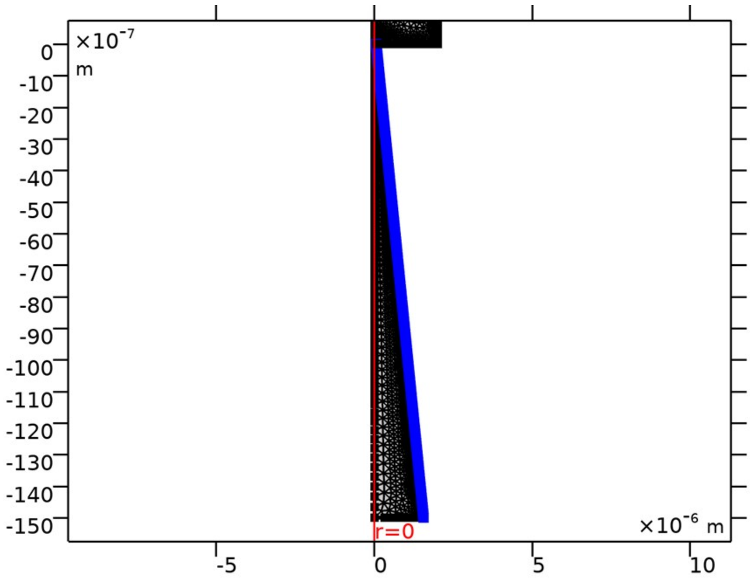
SETTINGS

Description	Value
Maximum element size	3.4E-7
Minimum element size	1.28E-9
Curvature factor	0.25
Maximum element growth rate	1.2
Predefined size	Extra fine

2.5.2 Size 1 (size1)

SELECTION

Geometric entity level	Boundary
Selection	Boundaries 4–5



Size 1

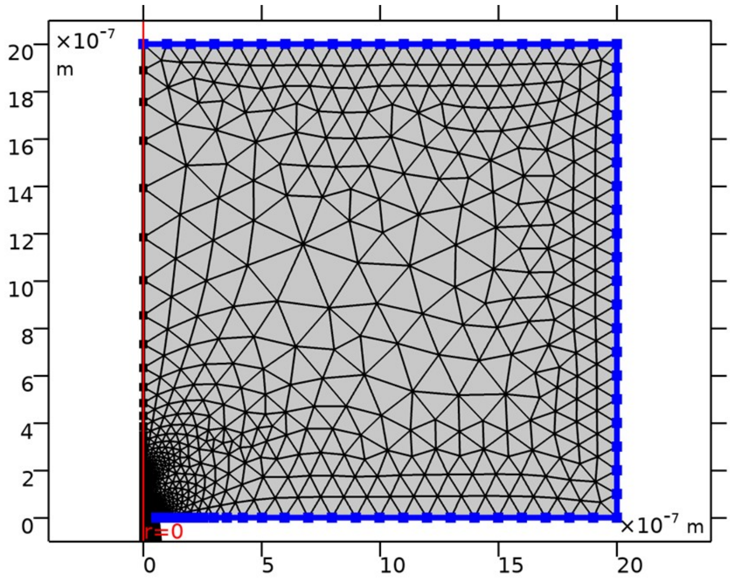
SETTINGS

Description	Value
Maximum element size	30[nm]
Minimum element size	1.56E-8
Minimum element size	Off
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

2.5.3 Size 2 (size2)

SELECTION

Geometric entity level	Boundary
Selection	Boundaries 3, 6–7



Size 2

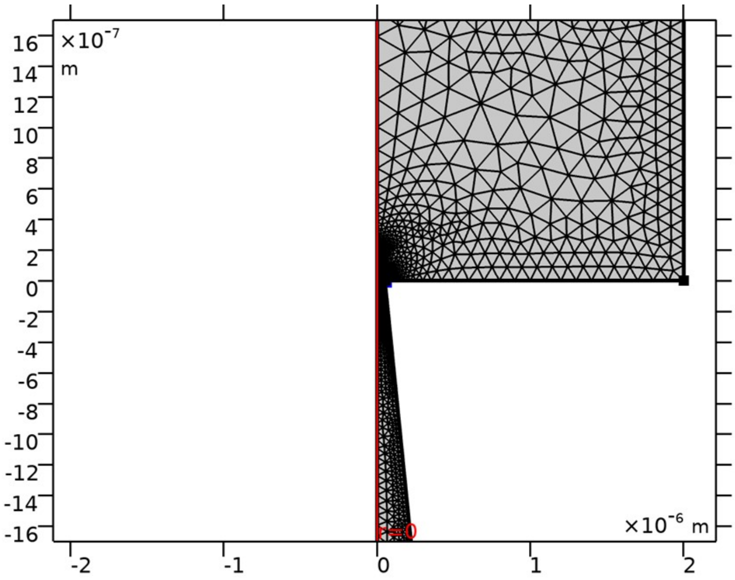
SETTINGS

Description	Value
Maximum element size	1e-7
Minimum element size	1.56E-8
Minimum element size	Off
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

2.5.4 Size 3 (size3)

SELECTION

Geometric entity level	Point
Selection	Point 3



Size 3

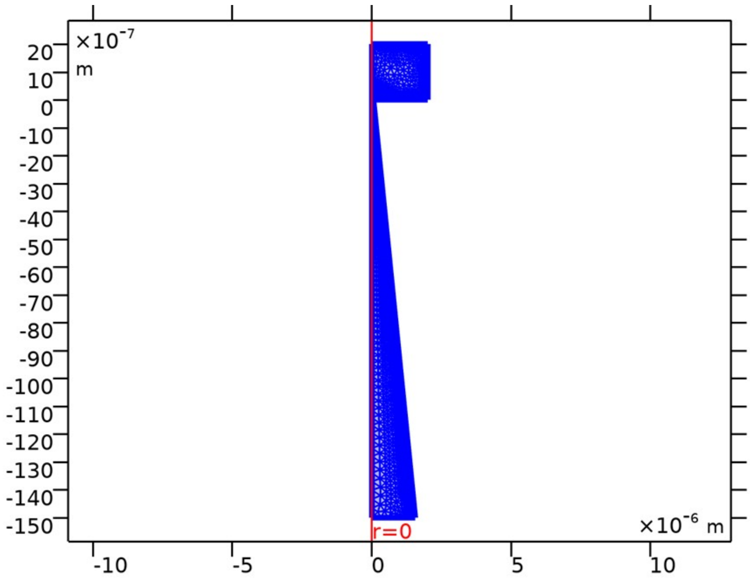
SETTINGS

Description	Value
Maximum element size	1e-10
Minimum element size	1.56E-8
Minimum element size	Off
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

2.5.5 Free Triangular 1 (ftri1)

SELECTION

Geometric entity level	Domain
Selection	Remaining



Free Triangular 1

3 Study 2

COMPUTATION INFORMATION

Computation time	9 min 28 s
CPU	Intel64 Family 6 Model 158 Stepping 10, 6 cores
Operating system	Windows 10

3.1 PARAMETRIC SWEEP

Parameter name	Parameter value list
l	300

STUDY SETTINGS

Description	Value
Sweep type	Specified combinations
Parameter name	l
Unit	

PARAMETERS

Parameter name	Parameter value list	Parameter unit
l	300	

3.2 TIME DEPENDENT

Times	Unit
range(0,2.8/799,2.8)	s

STUDY SETTINGS

Description	Value
Include geometric nonlinearity	Off

MESH SELECTION

Geometry	Mesh
mesh1	mesh1

PHYSICS AND VARIABLES SELECTION

Physics interface	Discretization
Transport of Diluted Species (tds)	physics
Electric Currents (ec)	physics

MESH SELECTION

Geometry	Mesh
Geometry 1 (geom1)	mesh1

3.3 SOLVER CONFIGURATIONS

3.3.1 Solution 1

Compile Equations: Time Dependent (st1)

STUDY AND STEP

Description	Value
Use study	Study 2
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(0,2.8/799,2.8)
timestep	0.0028[s]

Concentration (comp1.cCl) (comp1_cCl)

GENERAL

Description	Value
Field components	comp1.cCl

Concentration (comp1.cK) (comp1_cK)

GENERAL

Description	Value
Field components	comp1.cK

Concentration (comp1.cO) (comp1_cO)

GENERAL

Description	Value
Field components	comp1.cO

Concentration (comp1.cR) (comp1_cR)

GENERAL

Description	Value
Field components	comp1.cR

Electric potential (comp1.V) (comp1_V)

GENERAL

Description	Value
Field components	comp1.V

Time-Dependent Solver 1 (t1)

GENERAL

TIME STEPPING

Description	Value
Steps taken by solver	Intermediate
Maximum BDF order	2

Fully Coupled 1 (fc1)

GENERAL

Description	Value
Linear solver	Direct 1

METHOD AND TERMINATION

Description	Value
Damping factor	0.9
Jacobian update	Once per time step
Maximum number of iterations	8
Stabilization and acceleration	Anderson acceleration
Dimension of iteration space	5

3.3.2 Parametric Solutions 2

l=300 (su1)

GENERAL

Description	Value
Solution	l=300

4 Results

4.1 DERIVED VALUES

4.1.1 Line Integration 1

OUTPUT

Evaluated in Table 4

DATA

Description	Value
Data set	Study 2/Parametric Solutions 2

EXPRESSIONS

Expression	Unit	Description
tds.ntflux_cR*F	A	

INTEGRATION SETTINGS

Description	Value
Integration order	4
Compute surface integral	On

4.1.2 Line Average 1

OUTPUT

Evaluated in Table 3

DATA

Description	Value
Data set	Study 2/Parametric Solutions 2

EXPRESSIONS

Expression	Unit	Description
E	V	

INTEGRATION SETTINGS

Description	Value
Integration order	4
Compute surface integral	On