SUPPORTING INFORMATION

Electrophoretic Migration and Particle Collisions in Scanning Electrochemical Microscopy

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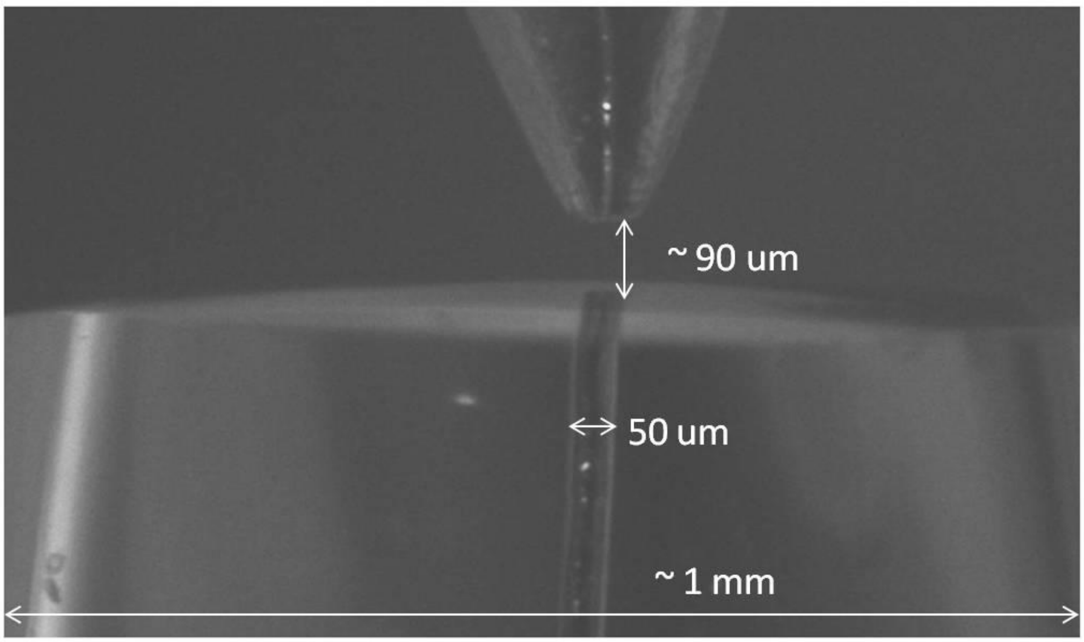


Scheme S1. Sample photograph of the gap between tip and substrate electrodes used in the SECM experiments.

Simulations of effect of migration under the conditions of SECM experiments

The model developed in the course of this work is similar to the previous one.[1] The initial conditions are exactly the same, while some of the boundaries conditions are different since another electrode is introduced into the system. These differences are discussed below.

At the surface of the substrate electrode, an inward current density condition is used (similar to the tip electrode surface):

$$-\bar{n}\cdot F\sum_i z_i J_i = z_{A^+}F\left(-D_{A^+}\frac{\partial C_{A^+}}{\partial z} - z_{A^+}u_{A^+}FC_{A^+}\frac{\partial \varphi}{\partial z}\right) \qquad \text{(S1)}$$

where u is the mobility of the ionic species indicated by the subscript and all other symbols have their usual meaning. One can see that this current density is proportional to the flux of the hydroxymethylferricinium ions (A^+).

For the concentration of the species at this boundary the following conditions were used:

$$C_A = C_b \qquad \text{(S2)}$$

where C_A is the concentration of ferrocenemethanol and C_b is the bulk concentration value.

$$C_{A^+} = 0 \qquad \text{(S3)}$$

where C_{A^+} is the concentration of hydroxymethylferricinium ions.

If the counter electrode is used instead, then the following equation is used for the electric potential at its surface:

$$\varphi = 0 \qquad \text{(S4)}$$

However, the boundary conditions for the concentrations of the species A and A^+ are the same as Eqs. S2 – S3.

All other boundary conditions, for the tip electrode surface, the surface of glass insulator and the bulk solution, are the same as published previously.

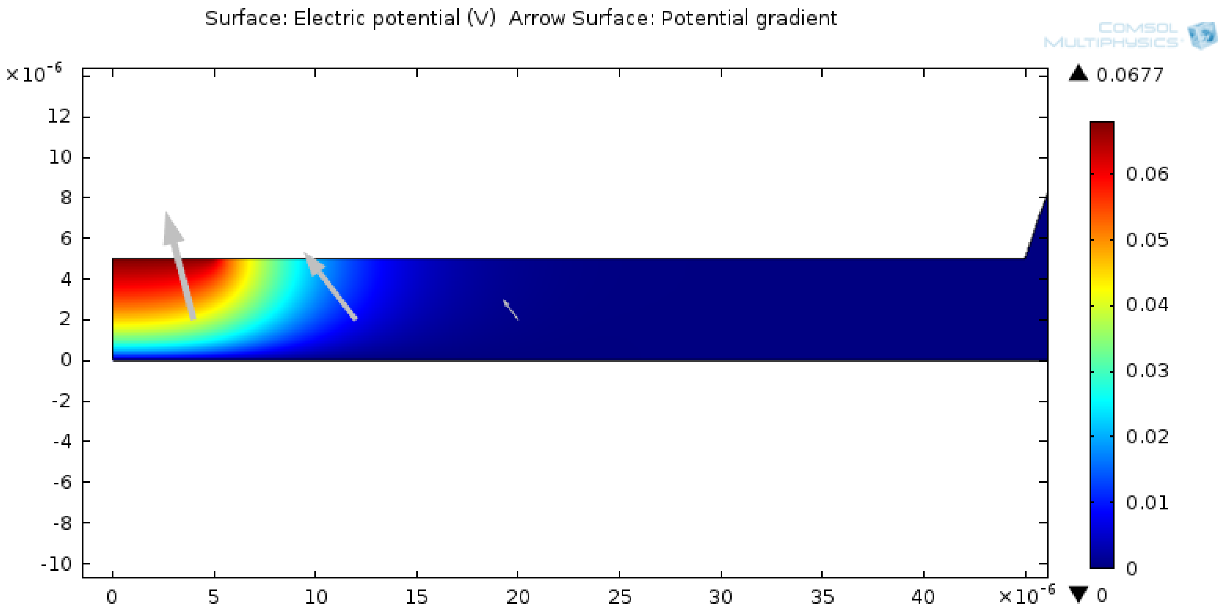


Figure S1. Electric potential distribution in solution with low supporting electrolyte concentration (0.1 mM) in a gap between the tip and counter electrodes. Tip radius, 5 μm (*RG* = 9), counter electrode disk radius, 25 μm; tip-to-counter separation 5 μm. Concentration of the redox species (FcMeOH), 3 mM. Tip is biased at a potential of mass transfer controlled oxidation of FcMeOH. Gray arrows indicate the direction of the electric potential gradient.

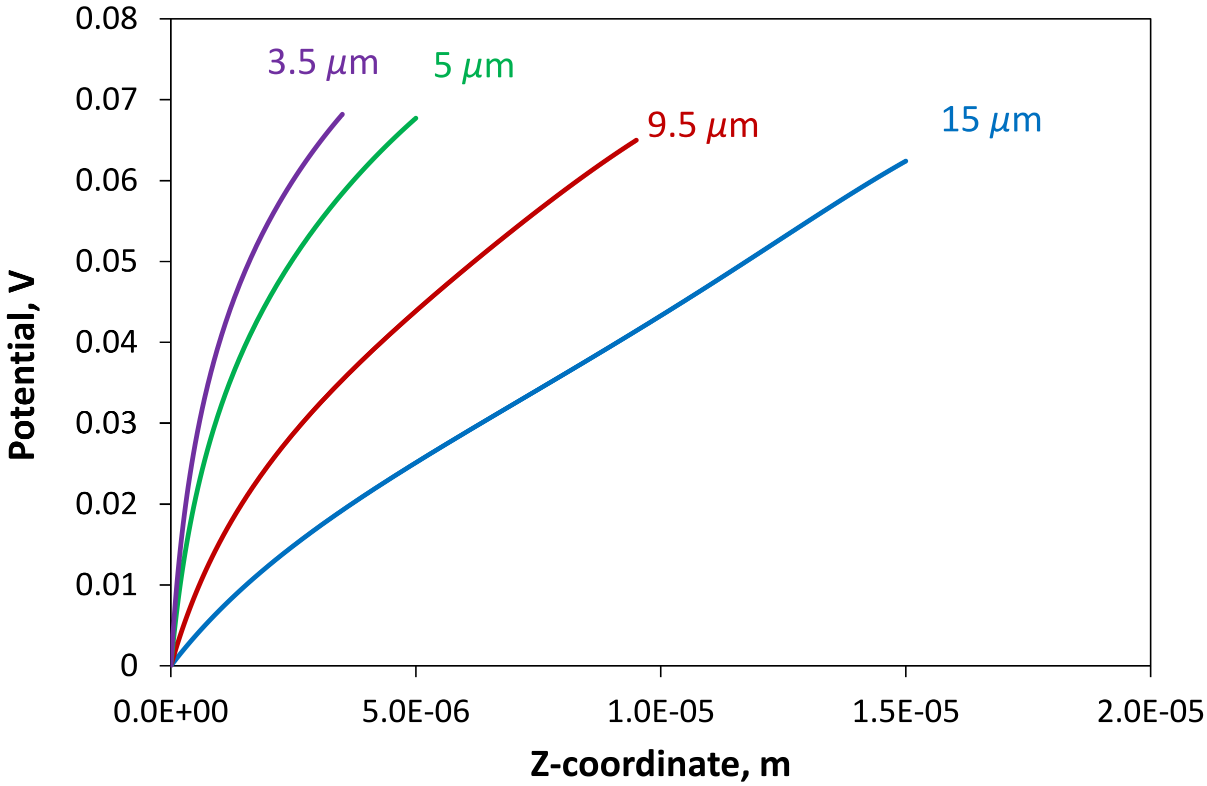


Figure S2. Electric potential distribution in solution with low supporting electrolyte concentration (0.1 mM) along a line going through the centers of the tip and counter electrodes (z-coordinate). Z = 0 corresponds to the surface of the counter electrode, while z = 3.5, 5, 9.5 or 15 μm corresponds to the surface of the tip. Tip radius, 5 μm (*RG* = 9), counter electrode disk radius, 25 μm; tip-to-counter separation between 3.5 μm and 15 μm (indicated beside each curve). Concentration of the redox species (FcMeOH) 3 mM. Tip is biased at a potential of mass transfer controlled oxidation of FcMeOH. Approximate electric field strengths (assuming linear potential profiles): 4.16 kV/m (15 μm), 6.84 kV/m (9.5 μm), 13.5 kV/m (5 μm), 19.5 kV/m (3.5 μm).

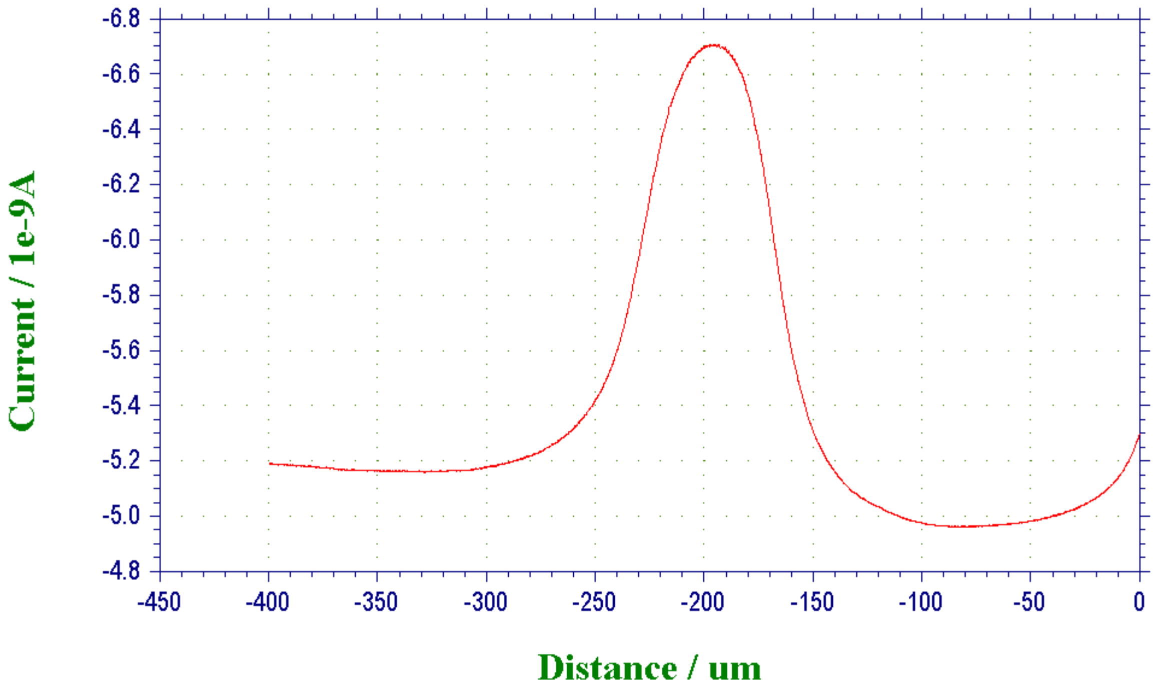


Figure S3. The scan in X-direction with a 10 µm Au tip electrode (RG = 9) over a 50 µm Au substrate electrode showing a positive feedback once the tip is over the substrate. The solution contains 4 mM FcMeOH. Tip was biased at a potential (0.1 V) corresponding to the steady-state oxidation of FcMeOH, substrate was biased at a potential (-0.4 V) corresponding to the mass transfer limited reduction of $FcMeOH^+$ produced at the tip. Reference electrode was mercury/mercurous sulfate in saturated potassium sulfate solution.

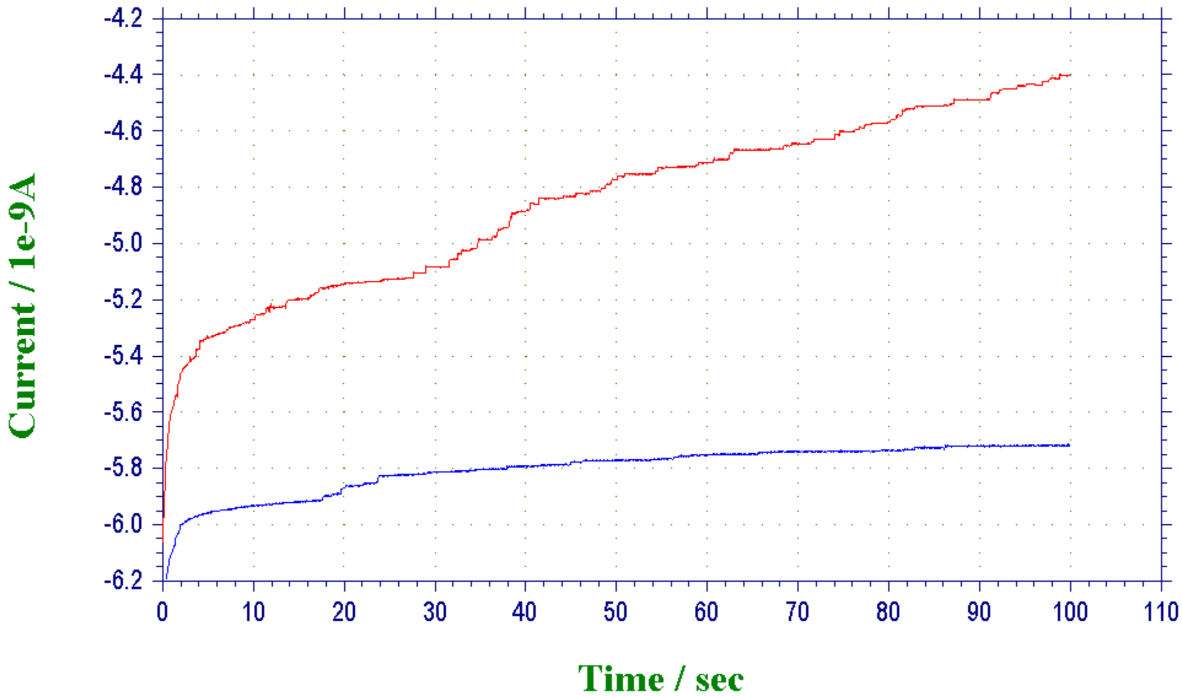


Figure S4. Two representative collision chronoamperograms recorded with a 10 µm Au tip electrode positioned above a 50 µm Au substrate at a distance 22 µm (red) and 6 µm (blue). The solution contains 4 mM FcMeOH and 87 fM polystyrene particles (1 µm in diam.). Tip was biased at a potential (0.1 V) corresponding to the steady-state oxidation of FcMeOH, substrate was biased at a potential (-0.4 V) corresponding to the mass transfer limited reduction of $FcMeOH^+$ produced at the tip. Reference electrode was mercury/mercurous sulfate in saturated potassium sulfate solution. Notice positive feedback for FcMeOH oxidation upon the decrease in the distance between the substrate and the tip electrodes (the current magnitude increases), yet the frequency of collisions decreases.

Comparison of travel times by diffusion and migration

A species such as an ion or a charged particle moves by diffusion the distance *d* in the following time:

$$t_d = d^2 / 2D \qquad \text{(S5)}$$

where *D* is the diffusion coefficient of the species.

The same distance will be covered by migration only in:

$$t_m = d / v_m \qquad \text{(S6)}$$

where v_m is the migrational velocity of the species.

v_m is given by the following equation:

$$v_m = |z| \left(F / RT \right) D E \qquad \text{(S7)}$$

where z is the charge of the species, E is the strength of the electric field and other symbols have their usual meaning.

As a result, combining Eqs. S5 – S7 one obtains Eq. 1 in the main text.

Investigation of the effect of the electric field in the interelectrode gap on mass transport of charged particles

The discussed experimental results (Figure 7 in the main text) were obtained in the following way. The experiment was done in a transparent cell which held 10 mL of solution, under microscopic observation. The representative image of the setup showing the alignment of the tip and substrate electrodes can be seen in Scheme 1 in the Supporting Information. The radius of the tip electrode was 5 μm, the radius of the substrate was 25 μm. Concentration of the redox species (FcMeOH) was 4 mM. Particle concentration (1 μm dia. polystyrene) was 87 fM. Tip was biased at a potential (0.1 V) corresponding to the steady-state oxidation of FcMeOH, substrate was biased at a potential (-0.4 V) corresponding to the mass transfer limited reduction of $FcMeOH^+$ produced at the tip. Reference electrode was mercury/mercurous sulfate in saturated potassium sulfate solution. Counter electrode was 1 mm dia. Pt wire. Both reference and counter electrodes were positioned in the bulk solution.

Before the beginning of the collision experiment, the tip and substrate electrodes were aligned (see Fig. S3 for positive feedback indication) and the separation between the two electrodes was confirmed microscopically (Scheme 1). After that the tip was retracted to the bulk of solution. Then the polystyrene particles were added and carefully dispersed throughout the solution to achieve the concentration mentioned above (87 fM). The injected volume of the stock particle solution was negligible compared to the volume of the solution in the cell.

During the collision experiment, the tip and substrate electrodes were biased at potentials indicated above. A chronoamperogram was recorded with the tip electrode for 100 s (see Fig. S4 for the representative data). After that the solution in the cell was carefully mixed with a Pasteur pipette to bring the concentrations of all species in the interelectrode gap to their bulk values, and the tip electrode was moved closer to the substrate. Then the next chronoamperogram was recorded corresponding to a new separation between the tip and substrate electrodes. In some cases at least three chronoamperograms were recorded at the same separation distance in order to calculate the variation of the collision frequency (error bars in Fig. 7). It should be stressed that the same tip electrode was used throughout all of the experiments presented in Fig. 7, i.e., the surface of the tip was not repolished or cleaned between the experiment. So, there was some variation in the background faradaic current due to the fact that polystyrene beads were stuck to its surface from the previous experimental runs, and also that some beads could have been dislodged during the mixing of the solution between the runs. For that reason, the normalized particle collision frequency was plotted in Fig. 7. The normalization was done with respect to the value of the average current recorded during the 100 s observation period, and thus the units of the normalized collision frequency were $s^{-1}nA^{-1}$. The average value of the current was determined as the charge divided by the time (100 s).

Dotted line in Fig. 7 represents the change in the normalized current at the tip due to negative feedback in SECM; it was calculated using an analytical expression for RG = 10 tip found in the reference,[2] p. 84:

$$I_T^{ins}(L) = \frac{1}{[A + B/L + C\exp(D/L)]} + \frac{E \times L}{(F + L)}$$

where A=0.4571825, B=1.4604238, C=0.4312735, D=-2.350667, E=-0.145437, F=5.5768952.

Model

Date	Oct 22, 2014 5:02:49 PM

Contents

1 Global Definitions

1.1 Parameters 1

Parameters

Name	Expression	Description
F	96485[C/mol]	Faraday constant
R	8.314[J/(mol*K)]	gas constant
T	298[K]	temperature
Cb	3[mol/m^3]	bulk conc of electroactive species
Cs	0.1[mol/m^3]	bulk conc of supp electrolyte
zA	0	Ox formal charge
zB	zA + 1	Red formal charge
zM	1	supp el cation formal charge
zX	-1	supp el anion formal charge
E0	0.28[V]	formal potential
a	0.5	alpha coefficient
k0	0.01[m/s]	standard rate constant
f	F/(R*T)	
eta	E-E0	overpotential
kf	k0*exp((1 - a)*f*eta)	forward process rate constant (oxidation)
kb	k0*exp((-a)*f*eta)	reverse process rate constant (reduction)
E	0.5[V]	tip electrode potential
Da	0.89e-9[m^2/s]	diffusion coefficient
Db	0.89e-9[m^2/s]	
Dm	1e-9[m^2/s]	
Dx	1e-9[m^2/s]	
uA	Da/(R*T)	mobility
uB	Db/(R*T)	
uM	Dm/(R*T)	
uX	Dx/(R*T)	
d	5 [um]	distance from tip to substrate
r_el	5[um]	radius of the tip electrode

Name	Expression	Description
Rg	9	Rg of a tip
r_co	25[um]	radius of a counter el
d_co_ins	1[mm]	thickness of counter insulation
l_co	1[mm]	length of a counter el
d_el	50e-4	length of the tip electrode
r_elcap	0.5e-3	radius of the tip electrode capillary
L	l_co + d_el + d	solution

2 Model 1 (mod1)

2.1 Definitions

2.1.1 Coordinate Systems

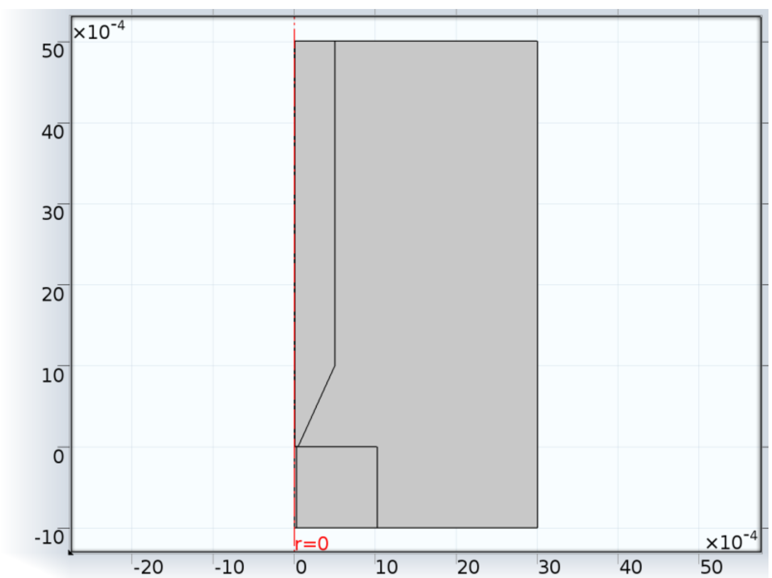
Boundary System 1

Coordinate system type	Boundary system
Identifier	sys1

Settings

Name	Value
Coordinate names	{t1, to, n}
Create first tangent direction from	Global Cartesian

2.2 Geometry 1



Geometry 1

Units

Length unit	m
Angular unit	deg

Geometry statistics

Property	Value
Space dimension	2

Property	Value
Number of domains	5
Number of boundaries	19

2.2.1 tip_electrode (r2)

Position

Name	Value
Position	{0, d}
Width	r_el
Height	d_el
Size	{r_el, d_el}

2.2.2 tip_el_capillary (pol1)

Selections of resulting entities

Name	Value
Data source	Table
Data points	{{r_el, d + d_el}, {r_elcap, d + d_el}, {r_elcap, d + 1[mm]}, {r_el*Rg, d}, {r_el, d}}

2.2.3 substrate_electrode (r4)

Position

Name	Value
Position	{0, -l_co}
Width	r_co
Height	l_co
Size	{r_co, l_co}

2.2.4 substrate insulation (r7)

Position

Name	Value
Position	{r_co, -l_co}
Width	d_co_ins
Height	l_co
Size	{d_co_ins, l_co}

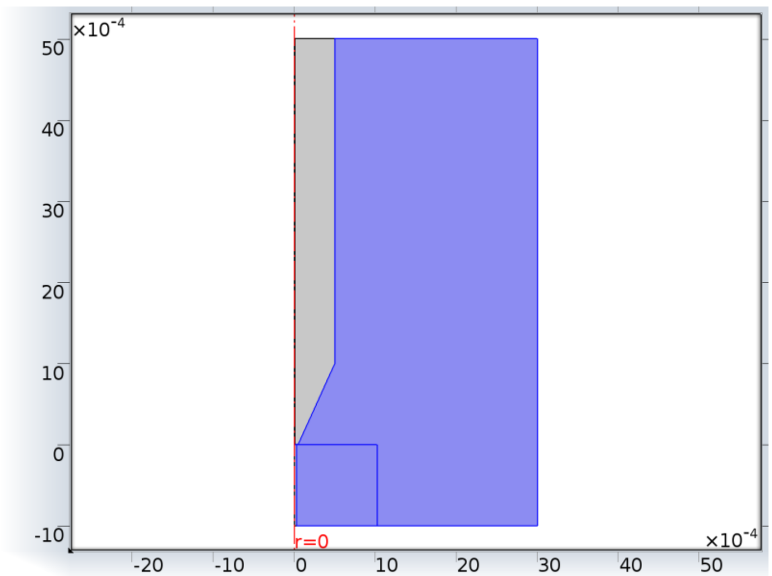
2.2.5 solution (r6)

Position

Name	Value
Position	{0, -l_co}
Width	L/2
Height	L
Size	{L/2, L}

2.3 Materials

2.3.1 Material 1



Material 1

Selection

Geometric entity level	Domain
Selection	Domains 2, 5

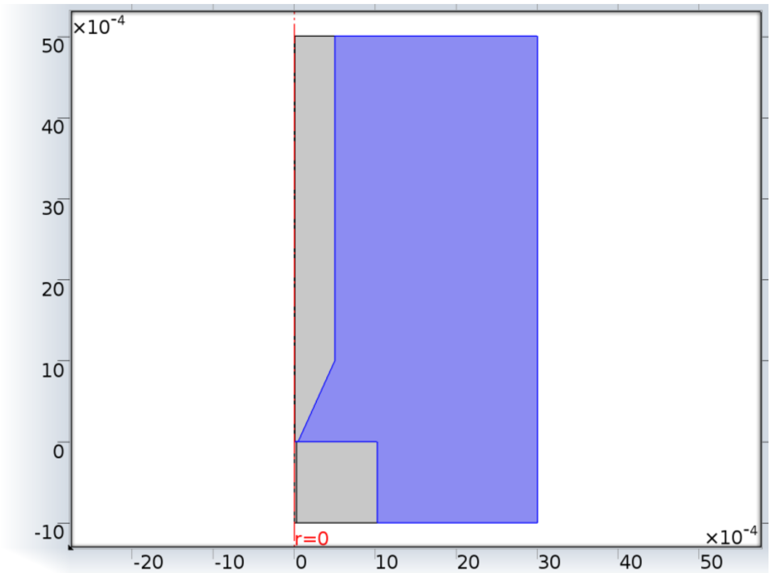
Material parameters

Name	Value	Unit

Basic Settings

Description	Value
Density	1000
Dynamic viscosity	0.001

2.4 Nernst-Planck Equations (chnp)



Nernst-Planck Equations

Selection

Geometric entity level	Domain
Selection	Domain 2

Equations

$$\frac{\partial c_i}{\partial t} + \nabla \cdot \left(-D_i \nabla c_i - z_i u_{m,i} F c_i \nabla V\right) + \mathbf{u} \cdot \nabla c_i = R_i$$

$$\nabla \cdot \mathbf{N}^V = F \sum_i z_i R_i$$

$$\sum_i z_i c_i = 0$$

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

$$\mathbf{N}^V = F \sum_i z_i (-D_i \nabla c_i - z_i u_{m,i} F c_i \nabla V)$$

Settings

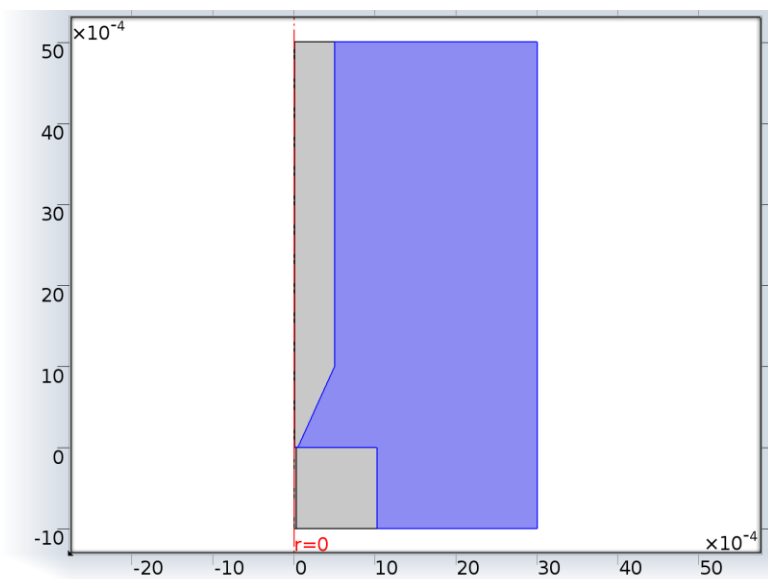
Description	Value
Concentration	Linear
Compute boundary fluxes	0
Electric potential	Linear
Compute boundary fluxes	0
Value type when using splitting of complex variables	{Real, Real}

Description	Value
Equation form	Study controlled
Convective term	Non - conservative form
From electroneutrality	c1
	{0, 1, 1, 1}
	{0, 0, 0, 0}
Equation residual	Approximate residual
Isotropic diffusion	0
Streamline diffusion	1
Crosswind diffusion	1
Lower gradient limit	0.1[mol/m^3]/chnp.helem
Tuning parameter	0.5
	1
Crosswind diffusion type	Codina
Show equation assuming	std1/time

Used products

COMSOL Multiphysics
Chemical Reaction Engineering Module

2.4.1 Convection, Diffusion, and Migration 1



Convection, Diffusion, and Migration 1

Selection

Geometric entity level	Domain
Selection	Domain 2

Equations

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

$$\nabla \cdot \mathbf{N}^V = F \sum_i z_i R_i$$

$$\sum_i z_i c_i = 0$$

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

$$\mathbf{N}^V = F \sum_i z_i(-D_i \nabla c_i - z_i u_{m,i} F c_i \nabla V)$$

Settings

Settings

Description	Value
Velocity field	User defined
Velocity field	{0, 0, 0}
Diffusion coefficient	User defined
Diffusion coefficient	{{Dx, 0, 0}, {0, Dx, 0}, {0, 0, Dx}}
Diffusion coefficient	User defined
Diffusion coefficient	{{Da, 0, 0}, {0, Da, 0}, {0, 0, Da}}
Diffusion coefficient	User defined
Diffusion coefficient	{{Db, 0, 0}, {0, Db, 0}, {0, 0, Db}}
Diffusion coefficient	User defined
Diffusion coefficient	{{Dm, 0, 0}, {0, Dm, 0}, {0, 0, Dm}}
Charge number	{zX, zA, zB, zM}
Mobility	{{{uX, 0, 0}, {0, uX, 0}, {0, 0, uX}}, {{uA, 0, 0}, {0, uA, 0}, {0, 0, uA}}, {{uB, 0, 0}, {0, uB, 0}, {0, 0, uB}}, {{uM, 0, 0}, {0, uM, 0}, {0, 0, uM}}}
Bulk material	None
Mobility	User defined

Variables

Name	Expression	Unit	Description	Selection

Name	Expression	Unit	Description	Selection
c1	(-c2*chnp.z_c2-c3*chnp.z_c3-c4*chnp.z_c4)/(chnp.z_c1+eps)	mol/m^3	Concentration	Domain 2
chnp.Drr_c1	Dx	m^2/s	Diffusion coefficient, rr component	Domain 2
chnp.Dphir_c1	0	m^2/s	Diffusion coefficient, phir component	Domain 2
chnp.Dzr_c1	0	m^2/s	Diffusion coefficient, zr component	Domain 2
chnp.Drphi_c1	0	m^2/s	Diffusion coefficient, rphi component	Domain 2
chnp.Dphiphi_c1	Dx	m^2/s	Diffusion coefficient, phiphi component	Domain 2
chnp.Dzphi_c1	0	m^2/s	Diffusion coefficient, zphi component	Domain 2
chnp.Drz_c1	0	m^2/s	Diffusion coefficient, rz component	Domain 2
chnp.Dphiz_c1	0	m^2/s	Diffusion coefficient, phiz component	Domain 2
chnp.Dzz_c1	Dx	m^2/s	Diffusion coefficient, zz component	Domain 2
chnp.Dav_c1	0.5*(chnp.Drr_c1+chnp.Dzz_c1)	m^2/s	Average diffusion coefficient	Domain 2
chnp.tfluxr_c1	-chnp.Drr_c1*d(c1,r)-chnp.Drz_c1*d(c1,z)+chnp.cfluxr_c1+chnp.mfluxr_c1	mol/(m^2*s)	Total flux, r component	Domain 2
chnp.tfluxphi_c1	-chnp.Dphir_c1*d(c1,r)-chnp.Dphiz_c1*d(c1,z)+chnp.cfluxphi_c1+chnp.mfluxphi_c1	mol/(m^2*s)	Total flux, phi component	Domain 2
chnp.tfluxz_c1	-chnp.Dzr_c1*d(c1,r)-chnp.Dzz_c1*d(c1,z)+chnp.cfluxz_c1+chnp.mfluxz_c1	mol/(m^2*s)	Total flux, z component	Domain 2
chnp.dfluxr_c1	-chnp.Drr_c1*d(c1,r)-chnp.Drz_c1*d(c1,z)	mol/(m^2*s)	Diffusive flux, r component	Domain 2

Name	Expression	Unit	Description	Selection
chnp.dfluxphi_c1	-chnp.Dphir_c1*d(c1,r)-chnp.Dphiz_c1*d(c1,z)	mol/(m^2*s)	Diffusive flux, phi component	Domain 2
chnp.dfluxz_c1	-chnp.Dzr_c1*d(c1,r)-chnp.Dzz_c1*d(c1,z)	mol/(m^2*s)	Diffusive flux, z component	Domain 2
chnp.gradr_c1	d(c1,r)	mol/m^4	Concentration gradient, r component	Domain 2
chnp.gradphi_c1	0	mol/m^4	Concentration gradient, phi component	Domain 2
chnp.gradz_c1	d(c1,z)	mol/m^4	Concentration gradient, z component	Domain 2
chnp.ntflux_c1	(chnp.cfluxr_c1+chnp.mfluxr_c1)*chnp.nrc+(chnp.cfluxphi_c1+chnp.mfluxphi_c1)*chnp.nphic+(chnp.cfluxz_c1+chnp.mfluxz_c1)*chnp.nzc+chnp.ndflux_c1	mol/(m^2*s)	Normal total flux	Boundaries 3–4, 6, 9, 13–19
chnp.ndflux_c1	chnp.dfluxr_c1*chnp.nrc+chnp.dfluxphi_c1*chnp.nphic+chnp.dfluxz_c1*chnp.nzc	mol/(m^2*s)	Normal diffusive flux	Boundaries 3–4, 6, 9, 13–19
chnp.dfluxMag_c1	sqrt(chnp.dfluxr_c1^2+chnp.dfluxphi_c1^2+chnp.dfluxz_c1^2)	mol/(m^2*s)	Diffusive flux magnitude	Domain 2
chnp.tfluxMag_c1	sqrt(chnp.tfluxr_c1^2+chnp.tfluxphi_c1^2+chnp.tfluxz_c1^2)	mol/(m^2*s)	Total flux magnitude	Domain 2
chnp.Drr_c2	Da	m^2/s	Diffusion coefficient, rr component	Domain 2
chnp.Dphir_c2	0	m^2/s	Diffusion coefficient, phir component	Domain 2
chnp.Dzr_c2	0	m^2/s	Diffusion coefficient, zr component	Domain 2
chnp.Drphi_c2	0	m^2/s	Diffusion coefficient, rphi component	Domain 2

Name	Expression	Unit	Description	Selection
chnp.Dphiphi_c2	Da	m^2/s	Diffusion coefficient, phiphi component	Domain 2
chnp.Dzphi_c2	0	m^2/s	Diffusion coefficient, zphi component	Domain 2
chnp.Drz_c2	0	m^2/s	Diffusion coefficient, rz component	Domain 2
chnp.Dphiz_c2	0	m^2/s	Diffusion coefficient, phiz component	Domain 2
chnp.Dzz_c2	Da	m^2/s	Diffusion coefficient, zz component	Domain 2
chnp.Dav_c2	0.5*(chnp.Drr_c2+chnp.Dzz_c2)	m^2/s	Average diffusion coefficient	Domain 2
chnp.tfluxr_c2	-chnp.Drr_c2*c2r-chnp.Drz_c2*c2z+chnp.cfluxr_c2+chnp.mfluxr_c2	mol/(m^2*s)	Total flux, r component	Domain 2
chnp.tfluxphi_c2	-chnp.Dphir_c2*c2r-chnp.Dphiz_c2*c2z+chnp.cfluxphi_c2+chnp.mfluxphi_c2	mol/(m^2*s)	Total flux, phi component	Domain 2
chnp.tfluxz_c2	-chnp.Dzr_c2*c2r-chnp.Dzz_c2*c2z+chnp.cfluxz_c2+chnp.mfluxz_c2	mol/(m^2*s)	Total flux, z component	Domain 2
chnp.dfluxr_c2	-chnp.Drr_c2*c2r-chnp.Drz_c2*c2z	mol/(m^2*s)	Diffusive flux, r component	Domain 2
chnp.dfluxphi_c2	-chnp.Dphir_c2*c2r-chnp.Dphiz_c2*c2z	mol/(m^2*s)	Diffusive flux, phi component	Domain 2
chnp.dfluxz_c2	-chnp.Dzr_c2*c2r-chnp.Dzz_c2*c2z	mol/(m^2*s)	Diffusive flux, z component	Domain 2
chnp.gradr_c2	c2r	mol/m^4	Concentration gradient, r component	Domain 2
chnp.gradphi_c2	0	mol/m^4	Concentration gradient, phi component	Domain 2
chnp.gradz_c2	c2z	mol/m^4	Concentration gradient, z component	Domain 2

Name	Expression	Unit	Description	Selection
chnp.ntflux_c2	chnp.bndFlux_c2+chnp.cfluxr_c2*chnp.nrc+chnp.cfluxphi_c2*chnp.nphic+chnp.cfluxz_c2*chnp.nzc	mol/(m^2*s)	Normal total flux	Boundaries 3–4, 6, 9, 13–19
chnp.ndflux_c2	chnp.dfluxr_c2*chnp.nrc+chnp.dfluxphi_c2*chnp.nphic+chnp.dfluxz_c2*chnp.nzc	mol/(m^2*s)	Normal diffusive flux	Boundaries 3–4, 6, 9, 13–19
chnp.dfluxMag_c2	sqrt(chnp.dfluxr_c2^2+chnp.dfluxphi_c2^2+chnp.dfluxz_c2^2)	mol/(m^2*s)	Diffusive flux magnitude	Domain 2
chnp.tfluxMag_c2	sqrt(chnp.tfluxr_c2^2+chnp.tfluxphi_c2^2+chnp.tfluxz_c2^2)	mol/(m^2*s)	Total flux magnitude	Domain 2
chnp.Drr_c3	Db	m^2/s	Diffusion coefficient, rr component	Domain 2
chnp.Dphir_c3	0	m^2/s	Diffusion coefficient, phir component	Domain 2
chnp.Dzr_c3	0	m^2/s	Diffusion coefficient, zr component	Domain 2
chnp.Drphi_c3	0	m^2/s	Diffusion coefficient, rphi component	Domain 2
chnp.Dphiphi_c3	Db	m^2/s	Diffusion coefficient, phiphi component	Domain 2
chnp.Dzphi_c3	0	m^2/s	Diffusion coefficient, zphi component	Domain 2
chnp.Drz_c3	0	m^2/s	Diffusion coefficient, rz component	Domain 2
chnp.Dphiz_c3	0	m^2/s	Diffusion coefficient, phiz component	Domain 2
chnp.Dzz_c3	Db	m^2/s	Diffusion coefficient, zz component	Domain 2
chnp.Dav_c3	0.5*(chnp.Drr_c3+chnp.Dzz_c3)	m^2/s	Average diffusion coefficient	Domain 2
chnp.tfluxr_c3	-chnp.Drr_c3*c3r-chnp.Drz_c3*c3z+chnp.cfluxr_c3+chnp.mfluxr_c3	mol/(m^2*s)	Total flux, r component	Domain 2

Name	Expression	Unit	Description	Selection
chnp.tfluxphi_c3	-chnp.Dphir_c3*c3r-chnp.Dphiz_c3*c3z+chnp.cfluxphi_c3+chnp.mfluxphi_c3	mol/(m^2*s)	Total flux, phi component	Domain 2
chnp.tfluxz_c3	-chnp.Dzr_c3*c3r-chnp.Dzz_c3*c3z+chnp.cfluxz_c3+chnp.mfluxz_c3	mol/(m^2*s)	Total flux, z component	Domain 2
chnp.dfluxr_c3	-chnp.Drr_c3*c3r-chnp.Drz_c3*c3z	mol/(m^2*s)	Diffusive flux, r component	Domain 2
chnp.dfluxphi_c3	-chnp.Dphir_c3*c3r-chnp.Dphiz_c3*c3z	mol/(m^2*s)	Diffusive flux, phi component	Domain 2
chnp.dfluxz_c3	-chnp.Dzr_c3*c3r-chnp.Dzz_c3*c3z	mol/(m^2*s)	Diffusive flux, z component	Domain 2
chnp.gradr_c3	c3r	mol/m^4	Concentration gradient, r component	Domain 2
chnp.gradphi_c3	0	mol/m^4	Concentration gradient, phi component	Domain 2
chnp.gradz_c3	c3z	mol/m^4	Concentration gradient, z component	Domain 2
chnp.ntflux_c3	chnp.bndFlux_c3+chnp.cfluxr_c3*chnp.nrc+chnp.cfluxphi_c3*chnp.nphic+chnp.cfluxz_c3*chnp.nzc	mol/(m^2*s)	Normal total flux	Boundaries 3–4, 6, 9, 13–19
chnp.ndflux_c3	chnp.dfluxr_c3*chnp.nrc+chnp.dfluxphi_c3*chnp.nphic+chnp.dfluxz_c3*chnp.nzc	mol/(m^2*s)	Normal diffusive flux	Boundaries 3–4, 6, 9, 13–19
chnp.dfluxMag_c3	sqrt(chnp.dfluxr_c3^2+chnp.dfluxphi_c3^2+chnp.dfluxz_c3^2)	mol/(m^2*s)	Diffusive flux magnitude	Domain 2
chnp.tfluxMag_c3	sqrt(chnp.tfluxr_c3^2+chnp.tfluxphi_c3^2+chnp.tfluxz_c3^2)	mol/(m^2*s)	Total flux magnitude	Domain 2
chnp.Drr_c4	Dm	m^2/s	Diffusion coefficient, rr component	Domain 2

Name	Expression	Unit	Description	Selection
chnp.Dphir_c4	0	m^2/s	Diffusion coefficient, phir component	Domain 2
chnp.Dzr_c4	0	m^2/s	Diffusion coefficient, zr component	Domain 2
chnp.Drphi_c4	0	m^2/s	Diffusion coefficient, rphi component	Domain 2
chnp.Dphiphi_c4	Dm	m^2/s	Diffusion coefficient, phiphi component	Domain 2
chnp.Dzphi_c4	0	m^2/s	Diffusion coefficient, zphi component	Domain 2
chnp.Drz_c4	0	m^2/s	Diffusion coefficient, rz component	Domain 2
chnp.Dphiz_c4	0	m^2/s	Diffusion coefficient, phiz component	Domain 2
chnp.Dzz_c4	Dm	m^2/s	Diffusion coefficient, zz component	Domain 2
chnp.Dav_c4	0.5*(chnp.Drr_c4+chnp.Dzz_c4)	m^2/s	Average diffusion coefficient	Domain 2
chnp.tfluxr_c4	-chnp.Drr_c4*c4r-chnp.Drz_c4*c4z+chnp.cfluxr_c4+chnp.mfluxr_c4	mol/(m^2*s)	Total flux, r component	Domain 2
chnp.tfluxphi_c4	-chnp.Dphir_c4*c4r-chnp.Dphiz_c4*c4z+chnp.cfluxphi_c4+chnp.mfluxphi_c4	mol/(m^2*s)	Total flux, phi component	Domain 2
chnp.tfluxz_c4	-chnp.Dzr_c4*c4r-chnp.Dzz_c4*c4z+chnp.cfluxz_c4+chnp.mfluxz_c4	mol/(m^2*s)	Total flux, z component	Domain 2
chnp.dfluxr_c4	-chnp.Drr_c4*c4r-chnp.Drz_c4*c4z	mol/(m^2*s)	Diffusive flux, r component	Domain 2
chnp.dfluxphi_c4	-chnp.Dphir_c4*c4r-chnp.Dphiz_c4*c4z	mol/(m^2*s)	Diffusive flux, phi component	Domain 2
chnp.dfluxz_c4	-chnp.Dzr_c4*c4r-chnp.Dzz_c4*c4z	mol/(m^2*s)	Diffusive flux, z component	Domain 2
chnp.gradr_c4	c4r	mol/m^4	Concentration gradient, r	Domain 2

Name	Expression	Unit	Description	Selection
			component	
chnp.gradphi_c4	0	mol/m^4	Concentration gradient, phi component	Domain 2
chnp.gradz_c4	c4z	mol/m^4	Concentration gradient, z component	Domain 2
chnp.ntflux_c4	chnp.bndFlux_c4+chnp.cfluxr_c4*chnp.nrc+chnp.cfluxphi_c4*chnp.nphic+chnp.cfluxz_c4*chnp.nzc	mol/(m^2*s)	Normal total flux	Boundaries 3–4, 6, 9, 13–19
chnp.ndflux_c4	chnp.dfluxr_c4*chnp.nrc+chnp.dfluxphi_c4*chnp.nphic+chnp.dfluxz_c4*chnp.nzc	mol/(m^2*s)	Normal diffusive flux	Boundaries 3–4, 6, 9, 13–19
chnp.dfluxMag_c4	sqrt(chnp.dfluxr_c4^2+chnp.dfluxphi_c4^2+chnp.dfluxz_c4^2)	mol/(m^2*s)	Diffusive flux magnitude	Domain 2
chnp.tfluxMag_c4	sqrt(chnp.tfluxr_c4^2+chnp.tfluxphi_c4^2+chnp.tfluxz_c4^2)	mol/(m^2*s)	Total flux magnitude	Domain 2
chnp.u	model.input.u1	m/s	Velocity field, r component	Domain 2
chnp.v	model.input.u2	m/s	Velocity field, phi component	Domain 2
chnp.w	model.input.u3	m/s	Velocity field, z component	Domain 2
chnp.cfluxr_c1	c1*model.input.u1	mol/(m^2*s)	Convective flux, r component	Domain 2
chnp.cfluxphi_c1	c1*model.input.u2	mol/(m^2*s)	Convective flux, phi component	Domain 2
chnp.cfluxz_c1	c1*model.input.u3	mol/(m^2*s)	Convective flux, z component	Domain 2
chnp.cfluxMag_c1	sqrt(chnp.cfluxr_c1^2+chnp.cfluxphi_c1^2+chnp.cfluxz_c1^2)	mol/(m^2*s)	Convective flux magnitude	Domain 2
chnp.ncflux_c1	chnp.cfluxr_c1*chnp.nrc+chnp.cfluxphi_c1*c	mol/(m^2*s)	Normal convective flux	Boundaries 3–4, 6, 9, 13–

Name	Expression	Unit	Description	Selection
	hnp.nphic+chnp.cfluxz_c1*chnp.nzc			19
chnp.cfluxr_c2	c2*model.input.u1	mol/(m^2*s)	Convective flux, r component	Domain 2
chnp.cfluxphi_c2	c2*model.input.u2	mol/(m^2*s)	Convective flux, phi component	Domain 2
chnp.cfluxz_c2	c2*model.input.u3	mol/(m^2*s)	Convective flux, z component	Domain 2
chnp.cfluxMag_c2	sqrt(chnp.cfluxr_c2^2+chnp.cfluxphi_c2^2+chnp.cfluxz_c2^2)	mol/(m^2*s)	Convective flux magnitude	Domain 2
chnp.ncflux_c2	chnp.cfluxr_c2*chnp.nrc+chnp.cfluxphi_c2*chnp.nphic+chnp.cfluxz_c2*chnp.nzc	mol/(m^2*s)	Normal convective flux	Boundaries 3–4, 6, 9, 13–19
chnp.cbf_c2	0	mol/(m^2*s)	Convective boundary flux	Boundaries 3–4, 6, 9, 13–19
chnp.cfluxr_c3	c3*model.input.u1	mol/(m^2*s)	Convective flux, r component	Domain 2
chnp.cfluxphi_c3	c3*model.input.u2	mol/(m^2*s)	Convective flux, phi component	Domain 2
chnp.cfluxz_c3	c3*model.input.u3	mol/(m^2*s)	Convective flux, z component	Domain 2
chnp.cfluxMag_c3	sqrt(chnp.cfluxr_c3^2+chnp.cfluxphi_c3^2+chnp.cfluxz_c3^2)	mol/(m^2*s)	Convective flux magnitude	Domain 2
chnp.ncflux_c3	chnp.cfluxr_c3*chnp.nrc+chnp.cfluxphi_c3*chnp.nphic+chnp.cfluxz_c3*chnp.nzc	mol/(m^2*s)	Normal convective flux	Boundaries 3–4, 6, 9, 13–19
chnp.cbf_c3	0	mol/(m^2*s)	Convective boundary flux	Boundaries 3–4, 6, 9, 13–19
chnp.cfluxr_c4	c4*model.input.u1	mol/(m^2*s)	Convective flux, r component	Domain 2
chnp.cfluxphi_c4	c4*model.input.u2	mol/(m^2*s)	Convective flux, phi component	Domain 2

Name	Expression	Unit	Description	Selection
chnp.cfluxz_c4	c4*model.input.u3	mol/(m^2*s)	Convective flux, z component	Domain 2
chnp.cfluxMag_c4	sqrt(chnp.cfluxr_c4^2+chnp.cfluxphi_c4^2+chnp.cfluxz_c4^2)	mol/(m^2*s)	Convective flux magnitude	Domain 2
chnp.ncflux_c4	chnp.cfluxr_c4*chnp.nrc+chnp.cfluxphi_c4*chnp.nphic+chnp.cfluxz_c4*chnp.nzc	mol/(m^2*s)	Normal convective flux	Boundaries 3–4, 6, 9, 13–19
chnp.cbf_c4	0	mol/(m^2*s)	Convective boundary flux	Boundaries 3–4, 6, 9, 13–19
chnp.V	model.input.V	V	Electric potential	Domain 2
chnp.z_c1	zX	1	Charge number	Domain 2
chnp.umrr_c1	uX	s*mol/kg	Mobility, rr component	Domain 2
chnp.umphir_c1	0	s*mol/kg	Mobility, phir component	Domain 2
chnp.umzr_c1	0	s*mol/kg	Mobility, zr component	Domain 2
chnp.umrphi_c1	0	s*mol/kg	Mobility, rphi component	Domain 2
chnp.umphiphi_c1	uX	s*mol/kg	Mobility, phiphi component	Domain 2
chnp.umzphi_c1	0	s*mol/kg	Mobility, zphi component	Domain 2
chnp.umrz_c1	0	s*mol/kg	Mobility, rz component	Domain 2
chnp.umphiz_c1	0	s*mol/kg	Mobility, phiz component	Domain 2
chnp.umzz_c1	uX	s*mol/kg	Mobility, zz component	Domain 2
chnp.mfluxr_c1	chnp.z_c1*F_const*c1*(-chnp.umrr_c1*d(chnp.V,r)-chnp.umrz_c1*d(chnp.V,z))	mol/(m^2*s)	Electrophoretic flux, r component	Domain 2

Name	Expression	Unit	Description	Selection
chnp.mfluxphi_c1	chnp.z_c1*F_const*c1*(-chnp.umphir_c1*d(chnp.V,r)-chnp.umphiz_c1*d(chnp.V,z))	mol/(m^2*s)	Electrophoretic flux, phi component	Domain 2
chnp.mfluxz_c1	chnp.z_c1*F_const*c1*(-chnp.umzr_c1*d(chnp.V,r)-chnp.umzz_c1*d(chnp.V,z))	mol/(m^2*s)	Electrophoretic flux, z component	Domain 2
chnp.nmflux_c1	chnp.mfluxr_c1*chnp.nrc+chnp.mfluxphi_c1*chnp.nphic+chnp.mfluxz_c1*chnp.nzc	mol/(m^2*s)	Normal electrophoretic flux	Boundaries 3–4, 6, 9, 13–19
chnp.z_c2	zA	1	Charge number	Domain 2
chnp.umrr_c2	uA	s*mol/kg	Mobility, rr component	Domain 2
chnp.umphir_c2	0	s*mol/kg	Mobility, phir component	Domain 2
chnp.umzr_c2	0	s*mol/kg	Mobility, zr component	Domain 2
chnp.umrphi_c2	0	s*mol/kg	Mobility, rphi component	Domain 2
chnp.umphiphi_c2	uA	s*mol/kg	Mobility, phiphi component	Domain 2
chnp.umzphi_c2	0	s*mol/kg	Mobility, zphi component	Domain 2
chnp.umrz_c2	0	s*mol/kg	Mobility, rz component	Domain 2
chnp.umphiz_c2	0	s*mol/kg	Mobility, phiz component	Domain 2
chnp.umzz_c2	uA	s*mol/kg	Mobility, zz component	Domain 2
chnp.mfluxr_c2	chnp.z_c2*F_const*c2*(-chnp.umrr_c2*d(chnp.V,r)-chnp.umrz_c2*d(chnp.	mol/(m^2*s)	Electrophoretic flux, r component	Domain 2

Name	Expression	Unit	Description	Selection
	V,z))			
chnp.mfluxphi_c2	chnp.z_c2*F_const*c2*(-chnp.umphir_c2*d(chnp.V,r)-chnp.umphiz_c2*d(chnp.V,z))	mol/(m^2*s)	Electrophoretic flux, phi component	Domain 2
chnp.mfluxz_c2	chnp.z_c2*F_const*c2*(-chnp.umzr_c2*d(chnp.V,r)-chnp.umzz_c2*d(chnp.V,z))	mol/(m^2*s)	Electrophoretic flux, z component	Domain 2
chnp.nmflux_c2	chnp.mfluxr_c2*chnp.nrc+chnp.mfluxphi_c2*chnp.nphic+chnp.mfluxz_c2*chnp.nzc	mol/(m^2*s)	Normal electrophoretic flux	Boundaries 3–4, 6, 9, 13–19
chnp.z_c3	zB	1	Charge number	Domain 2
chnp.umrr_c3	uB	s*mol/kg	Mobility, rr component	Domain 2
chnp.umphir_c3	0	s*mol/kg	Mobility, phir component	Domain 2
chnp.umzr_c3	0	s*mol/kg	Mobility, zr component	Domain 2
chnp.umrphi_c3	0	s*mol/kg	Mobility, rphi component	Domain 2
chnp.umphiphi_c3	uB	s*mol/kg	Mobility, phiphi component	Domain 2
chnp.umzphi_c3	0	s*mol/kg	Mobility, zphi component	Domain 2
chnp.umrz_c3	0	s*mol/kg	Mobility, rz component	Domain 2
chnp.umphiz_c3	0	s*mol/kg	Mobility, phiz component	Domain 2
chnp.umzz_c3	uB	s*mol/kg	Mobility, zz component	Domain 2
chnp.mfluxr_c3	chnp.z_c3*F_const*c3*(-chnp.umrr_c3*d(chnp.	mol/(m^2*s)	Electrophoretic flux, r component	Domain 2

Name	Expression	Unit	Description	Selection
	V,r)-chnp.umrz_c3*d(chnp.V,z))			
chnp.mfluxphi_c3	chnp.z_c3*F_const*c3*(-chnp.umphir_c3*d(chnp.V,r)-chnp.umphiz_c3*d(chnp.V,z))	mol/(m^2*s)	Electrophoretic flux, phi component	Domain 2
chnp.mfluxz_c3	chnp.z_c3*F_const*c3*(-chnp.umzr_c3*d(chnp.V,r)-chnp.umzz_c3*d(chnp.V,z))	mol/(m^2*s)	Electrophoretic flux, z component	Domain 2
chnp.nmflux_c3	chnp.mfluxr_c3*chnp.nrc+chnp.mfluxphi_c3*chnp.nphic+chnp.mfluxz_c3*chnp.nzc	mol/(m^2*s)	Normal electrophoretic flux	Boundaries 3–4, 6, 9, 13–19
chnp.z_c4	zM	1	Charge number	Domain 2
chnp.umrr_c4	uM	s*mol/kg	Mobility, rr component	Domain 2
chnp.umphir_c4	0	s*mol/kg	Mobility, phir component	Domain 2
chnp.umzr_c4	0	s*mol/kg	Mobility, zr component	Domain 2
chnp.umrphi_c4	0	s*mol/kg	Mobility, rphi component	Domain 2
chnp.umphiphi_c4	uM	s*mol/kg	Mobility, phiphi component	Domain 2
chnp.umzphi_c4	0	s*mol/kg	Mobility, zphi component	Domain 2
chnp.umrz_c4	0	s*mol/kg	Mobility, rz component	Domain 2
chnp.umphiz_c4	0	s*mol/kg	Mobility, phiz component	Domain 2
chnp.umzz_c4	uM	s*mol/kg	Mobility, zz component	Domain 2
chnp.mfluxr_c4	chnp.z_c4*F_const*c4	mol/(m^2*s)	Electrophoretic flux,	Domain 2

Name	Expression	Unit	Description	Selection
	*(-chnp.umrr_c4*d(chnp.V,r)-chnp.umrz_c4*d(chnp.V,z))		r component	
chnp.mfluxphi_c4	chnp.z_c4*F_const*c4*(-chnp.umphir_c4*d(chnp.V,r)-chnp.umphiz_c4*d(chnp.V,z))	mol/(m^2*s)	Electrophoretic flux, phi component	Domain 2
chnp.mfluxz_c4	chnp.z_c4*F_const*c4*(-chnp.umzr_c4*d(chnp.V,r)-chnp.umzz_c4*d(chnp.V,z))	mol/(m^2*s)	Electrophoretic flux, z component	Domain 2
chnp.nmflux_c4	chnp.mfluxr_c4*chnp.nrc+chnp.mfluxphi_c4*chnp.nphic+chnp.mfluxz_c4*chnp.nzc	mol/(m^2*s)	Normal electrophoretic flux	Boundaries 3–4, 6, 9, 13–19
chnp.kapparr	(c1*chnp.z_c1^2*chnp.umrr_c1+c2*chnp.z_c2^2*chnp.umrr_c2+c3*chnp.z_c3^2*chnp.umrr_c3+c4*chnp.z_c4^2*chnp.umrr_c4)*F_const^2	S/m	Electrolyte conductivity, rr component	Domain 2
chnp.kappaphir	(c1*chnp.z_c1^2*chnp.umphir_c1+c2*chnp.z_c2^2*chnp.umphir_c2+c3*chnp.z_c3^2*chnp.umphir_c3+c4*chnp.z_c4^2*chnp.umphir_c4)*F_const^2	S/m	Electrolyte conductivity, phir component	Domain 2
chnp.kappazr	(c1*chnp.z_c1^2*chnp.umzr_c1+c2*chnp.z_c2^2*chnp.umzr_c2+c3*chnp.z_c3^2*chnp.umzr_c3+c4*chnp.z_c4^2*chnp.umzr_c4)*F_const^2	S/m	Electrolyte conductivity, zr component	Domain 2

Name	Expression	Unit	Description	Selection
chnp.kapparphi	(c1*chnp.z_c1^2*chnp.umrphi_c1+c2*chnp.z_c2^2*chnp.umrphi_c2+c3*chnp.z_c3^2*chnp.umrphi_c3+c4*chnp.z_c4^2*chnp.umrphi_c4)*F_const^2	S/m	Electrolyte conductivity, rphi component	Domain 2
chnp.kappaphiphi	(c1*chnp.z_c1^2*chnp.umphiphi_c1+c2*chnp.z_c2^2*chnp.umphiphi_c2+c3*chnp.z_c3^2*chnp.umphiphi_c3+c4*chnp.z_c4^2*chnp.umphiphi_c4)*F_const^2	S/m	Electrolyte conductivity, phiphi component	Domain 2
chnp.kappazphi	(c1*chnp.z_c1^2*chnp.umzphi_c1+c2*chnp.z_c2^2*chnp.umzphi_c2+c3*chnp.z_c3^2*chnp.umzphi_c3+c4*chnp.z_c4^2*chnp.umzphi_c4)*F_const^2	S/m	Electrolyte conductivity, zphi component	Domain 2
chnp.kapparz	(c1*chnp.z_c1^2*chnp.umrz_c1+c2*chnp.z_c2^2*chnp.umrz_c2+c3*chnp.z_c3^2*chnp.umrz_c3+c4*chnp.z_c4^2*chnp.umrz_c4)*F_const^2	S/m	Electrolyte conductivity, rz component	Domain 2
chnp.kappaphiz	(c1*chnp.z_c1^2*chnp.umphiz_c1+c2*chnp.z_c2^2*chnp.umphiz_c2+c3*chnp.z_c3^2*chnp.umphiz_c3+c4*chnp.z_c4^2*chnp.umphiz_c4)*F_const^2	S/m	Electrolyte conductivity, phiz component	Domain 2
chnp.kappazz	(c1*chnp.z_c1^2*chnp.umzz_c1+c2*chnp.z_c2^2*chnp.umzz_c2+c3*chnp.z_c3^2*chnp.umzz_c3+c4*chnp.z_c4^2*chnp.umzz_c4)*F_const^2	S/m	Electrolyte conductivity, zz component	Domain 2
chnp.Jr	F_const*(chnp.z_c1*(-	A/m^2	Current density, r	Domain 2

Name	Expression	Unit	Description	Selection
	chnp.Drr_c1*d(c1,r)-chnp.Drz_c1*d(c1,z)-chnp.z_c1*chnp.umrr_c1*F_const*c1*Vr-chnp.z_c1*chnp.umrz_c1*F_const*c1*Vz)+chnp.z_c2*(-chnp.Drr_c2*c2r-chnp.Drz_c2*c2z-chnp.z_c2*chnp.umrr_c2*F_const*c2*Vr-chnp.z_c2*chnp.umrz_c2*F_const*c2*Vz)+chnp.z_c3*(-chnp.Drr_c3*c3r-chnp.Drz_c3*c3z-chnp.z_c3*chnp.umrr_c3*F_const*c3*Vr-chnp.z_c3*chnp.umrz_c3*F_const*c3*Vz)+chnp.z_c4*(-chnp.Drr_c4*c4r-chnp.Drz_c4*c4z-chnp.z_c4*chnp.umrr_c4*F_const*c4*Vr-chnp.z_c4*chnp.umrz_c4*F_const*c4*Vz))		component	
chnp.Jphi	F_const*(chnp.z_c1*(-chnp.Dphir_c1*d(c1,r)-chnp.Dphiz_c1*d(c1,z)-chnp.z_c1*chnp.umphir_c1*F_const*c1*Vr-chnp.z_c1*chnp.umphiz_c1*F_const*c1*Vz)+chnp.z_c2*(-chnp.Dphir_c2*c2r-chnp.Dphiz_c2*c2z-chnp.z_c2*chnp.umphir_c2*F_const*c2*Vr-chnp.z_c2*chnp.umphiz_c2*F_const*c2*Vz)+chnp.z_c3*(-chnp.Dphir_c3*c3r-chnp.Dphiz_c3*c3z-chnp.z_c3*chnp.umphir_c3*F_const*c3*Vr-	A/m^2	Current density, phi component	Domain 2

Name	Expression	Unit	Description	Selection
	chnp.z_c3*chnp.umphiz_c3*F_const*c3*Vz)+chnp.z_c4*(-chnp.Dphir_c4*c4r-chnp.Dphiz_c4*c4z-chnp.z_c4*chnp.umphir_c4*F_const*c4*Vr-chnp.z_c4*chnp.umphiz_c4*F_const*c4*Vz))			
chnp.Jz	F_const*(chnp.z_c1*(-chnp.Dzr_c1*d(c1,r)-chnp.Dzz_c1*d(c1,z)-chnp.z_c1*chnp.umzr_c1*F_const*c1*Vr-chnp.z_c1*chnp.umzz_c1*F_const*c1*Vz)+chnp.z_c2*(-chnp.Dzr_c2*c2r-chnp.Dzz_c2*c2z-chnp.z_c2*chnp.umzr_c2*F_const*c2*Vr-chnp.z_c2*chnp.umzz_c2*F_const*c2*Vz)+chnp.z_c3*(-chnp.Dzr_c3*c3r-chnp.Dzz_c3*c3z-chnp.z_c3*chnp.umzr_c3*F_const*c3*Vr-chnp.z_c3*chnp.umzz_c3*F_const*c3*Vz)+chnp.z_c4*(-chnp.Dzr_c4*c4r-chnp.Dzz_c4*c4z-chnp.z_c4*chnp.umzr_c4*F_const*c4*Vr-chnp.z_c4*chnp.umzz_c4*F_const*c4*Vz))	A/m^2	Current density, z component	Domain 2
chnp.helem	h	m	Element size	Domain 2
chnp.glim_mass	0.1[mol/m^3]/chnp.helem	mol/m^4	Lower gradient limit	Domain 2
chnp.Ck_mass	0.5	1	Tuning parameter	Domain 2
chnp.Res_c2	d(c2*chnp.z_c2*F_const*(-chnp.umrr_c2*d(chnp.	mol/(m^3*s)	Equation residual	Domain 2

Name	Expression	Unit	Description	Selection
	V,r)-chnp.umrz_c2*d(chnp.V,z)),r)+if(abs(r)<0.0010*h,d(c2*chnp.z_c2*F_const*(-chnp.umrr_c2*d(chnp.V,r)-chnp.umrz_c2*d(chnp.V,z)),r),c2*chnp.z_c2*F_const*(-chnp.umrr_c2*d(chnp.V,r)-chnp.umrz_c2*d(chnp.V,z))/r)+d(c2*chnp.z_c2*F_const*(-chnp.umzr_c2*d(chnp.V,r)-chnp.umzz_c2*d(chnp.V,z)),z)+chnp.u*c2r+chnp.w*c2z-chnp.R_c2			
chnp.Res_c3	d(c3*chnp.z_c3*F_const*(-chnp.umrr_c3*d(chnp.V,r)-chnp.umrz_c3*d(chnp.V,z)),r)+if(abs(r)<0.0010*h,d(c3*chnp.z_c3*F_const*(-chnp.umrr_c3*d(chnp.V,r)-chnp.umrz_c3*d(chnp.V,z)),r),c3*chnp.z_c3*F_const*(-chnp.umrr_c3*d(chnp.V,r)-chnp.umrz_c3*d(chnp.V,z))/r)+d(c3*chnp.z_c3*F_const*(-chnp.umzr_c3*d(chnp.V,r)-chnp.umzz_c3*d(chnp.V,z)),z)+chnp.u*c3r+chnp.w*c3z-chnp.R_c3	mol/(m^3*s)	Equation residual	Domain 2
chnp.Res_c4	d(c4*chnp.z_c4*F_const*(-	mol/(m^3*s)	Equation residual	Domain 2

Name	Expression	Unit	Description	Selection
	chnp.umrr_c4*d(chnp.V,r)-chnp.umrz_c4*d(chnp.V,z)),r)+if(abs(r)<0.0010*h,d(c4*chnp.z_c4*F_const*(-chnp.umrr_c4*d(chnp.V,r)-chnp.umrz_c4*d(chnp.V,z)),r),c4*chnp.z_c4*F_const*(-chnp.umrr_c4*d(chnp.V,r)-chnp.umrz_c4*d(chnp.V,z))/r)+d(c4*chnp.z_c4*F_const*(-chnp.umzr_c4*d(chnp.V,r)-chnp.umzz_c4*d(chnp.V,z)),z)+chnp.u*c4r+chnp.w*c4z-chnp.R_c4			
chnp.cellPe_c1	h*sqrt((chnp.u-chnp.z_c1*chnp.umrr_c1*F_const*Vr-chnp.z_c1*chnp.umrz_c1*F_const*Vz)^2+(chnp.v-chnp.z_c1*chnp.umphir_c1*F_const*Vr-chnp.z_c1*chnp.umphiz_c1*F_const*Vz)^2+(chnp.w-chnp.z_c1*chnp.umzr_c1*F_const*Vr-chnp.z_c1*chnp.umzz_c1*F_const*Vz)^2)*(sqrt((chnp.u-chnp.z_c1*chnp.umrr_c1*F_const*Vr-chnp.z_c1*chnp.umrz_c1*F_const*Vz)^2+(chnp.v-chnp.z_c1*chnp.umphir_c1*F_const*Vr-chnp.z_c1*chnp.umphiz_c1*F_const*Vz)^2+(c	1	Cell Péclet number	Domain 2

Name	Expression	Unit	Description	Selection
	hnp.w-chnp.z_c1*chnp.umzr_c1*F_const*Vr-chnp.z_c1*chnp.umzz_c1*F_const*Vz)^2)+eps)/(((chnp.u-chnp.z_c1*chnp.umrr_c1*F_const*Vr-chnp.z_c1*chnp.umrz_c1*F_const*Vz)*chnp.Drr_c1+(chnp.v-chnp.z_c1*chnp.umphir_c1*F_const*Vr-chnp.z_c1*chnp.umphiz_c1*F_const*Vz)*chnp.Dphir_c1+(chnp.w-chnp.z_c1*chnp.umzr_c1*F_const*Vr-chnp.z_c1*chnp.umzz_c1*F_const*Vz)*chnp.Dzr_c1)*(chnp.u-chnp.z_c1*chnp.umrr_c1*F_const*Vr-chnp.z_c1*chnp.umrz_c1*F_const*Vz)+((chnp.u-chnp.z_c1*chnp.umrr_c1*F_const*Vr-chnp.z_c1*chnp.umrz_c1*F_const*Vz)*chnp.Drphi_c1+(chnp.v-chnp.z_c1*chnp.umphir_c1*F_const*Vr-chnp.z_c1*chnp.umphiz_c1*F_const*Vz)*chnp.Dphiphi_c1+(chnp.w-chnp.z_c1*chnp.umzr_c1*F_const*Vr-chnp.z_c1*chnp.umzz_c1*F_const*Vz)*chnp.Dzphi_c1)*(chnp.v-chnp.z_c1*chnp.umphir_c1*F_const*Vr-chnp.z_c1*chnp.umphiz_c1*F_const*Vz)+((chnp.u-			

Name	Expression	Unit	Description	Selection
	chnp.z_c1*chnp.umrr_c1*F_const*Vr-chnp.z_c1*chnp.umrz_c1*F_const*Vz)*chnp.Drz_c1+(chnp.v-chnp.z_c1*chnp.umphir_c1*F_const*Vr-chnp.z_c1*chnp.umphiz_c1*F_const*Vz)*chnp.Dphiz_c1+(chnp.w-chnp.z_c1*chnp.umzr_c1*F_const*Vr-chnp.z_c1*chnp.umzz_c1*F_const*Vz)*chnp.Dzz_c1)*(chnp.w-chnp.z_c1*chnp.umzr_c1*F_const*Vr-chnp.z_c1*chnp.umzz_c1*F_const*Vz))			
chnp.cellPe_c2	h*sqrt((chnp.u-chnp.z_c2*chnp.umrr_c2*F_const*Vr-chnp.z_c2*chnp.umrz_c2*F_const*Vz)^2+(chnp.v-chnp.z_c2*chnp.umphir_c2*F_const*Vr-chnp.z_c2*chnp.umphiz_c2*F_const*Vz)^2+(chnp.w-chnp.z_c2*chnp.umzr_c2*F_const*Vr-chnp.z_c2*chnp.umzz_c2*F_const*Vz)^2)*(sqrt((chnp.u-chnp.z_c2*chnp.umrr_c2*F_const*Vr-chnp.z_c2*chnp.umrz_c2*F_const*Vz)^2+(chnp.v-chnp.z_c2*chnp.umphir_c2*F_const*Vr-chnp.z_c2*chnp.umphiz_c2*F_const*Vz)^2+(chnp.w-chnp.z_c2*chnp.umzr_	1	Cell Péclet number	Domain 2

Name	Expression	Unit	Description	Selection
	c2*F_const*Vr-chnp.z_c2*chnp.umzz_c2*F_const*Vz)^2)+eps)/(((chnp.u-chnp.z_c2*chnp.umrr_c2*F_const*Vr-chnp.z_c2*chnp.umrz_c2*F_const*Vz)*chnp.Drr_c2+(chnp.v-chnp.z_c2*chnp.umphir_c2*F_const*Vr-chnp.z_c2*chnp.umphiz_c2*F_const*Vz)*chnp.Dphir_c2+(chnp.w-chnp.z_c2*chnp.umzr_c2*F_const*Vr-chnp.z_c2*chnp.umzz_c2*F_const*Vz)*chnp.Dzr_c2)*(chnp.u-chnp.z_c2*chnp.umrr_c2*F_const*Vr-chnp.z_c2*chnp.umrz_c2*F_const*Vz)+((chnp.u-chnp.z_c2*chnp.umrr_c2*F_const*Vr-chnp.z_c2*chnp.umrz_c2*F_const*Vz)*chnp.Drphi_c2+(chnp.v-chnp.z_c2*chnp.umphir_c2*F_const*Vr-chnp.z_c2*chnp.umphiz_c2*F_const*Vz)*chnp.Dphiphi_c2+(chnp.w-chnp.z_c2*chnp.umzr_c2*F_const*Vr-chnp.z_c2*chnp.umzz_c2*F_const*Vz)*chnp.Dzphi_c2)*(chnp.v-chnp.z_c2*chnp.umphir_c2*F_const*Vr-chnp.z_c2*chnp.umphiz_c2*F_const*Vz)+((chnp.u-chnp.z_c2*chnp.umrr_c2*F_const*Vr-			

Name	Expression	Unit	Description	Selection
	chnp.z_c2*chnp.umrz_c2*F_const*Vz)*chnp.Drz_c2+(chnp.v-chnp.z_c2*chnp.umphir_c2*F_const*Vr-chnp.z_c2*chnp.umphiz_c2*F_const*Vz)*chnp.Dphiz_c2+(chnp.w-chnp.z_c2*chnp.umzr_c2*F_const*Vr-chnp.z_c2*chnp.umzz_c2*F_const*Vz)*chnp.Dzz_c2)*(chnp.w-chnp.z_c2*chnp.umzr_c2*F_const*Vr-chnp.z_c2*chnp.umzz_c2*F_const*Vz))			
chnp.cellPe_c3	h*sqrt((chnp.u-chnp.z_c3*chnp.umrr_c3*F_const*Vr-chnp.z_c3*chnp.umrz_c3*F_const*Vz)^2+(chnp.v-chnp.z_c3*chnp.umphir_c3*F_const*Vr-chnp.z_c3*chnp.umphiz_c3*F_const*Vz)^2+(chnp.w-chnp.z_c3*chnp.umzr_c3*F_const*Vr-chnp.z_c3*chnp.umzz_c3*F_const*Vz)^2)*(sqrt((chnp.u-chnp.z_c3*chnp.umrr_c3*F_const*Vr-chnp.z_c3*chnp.umrz_c3*F_const*Vz)^2+(chnp.v-chnp.z_c3*chnp.umphir_c3*F_const*Vr-chnp.z_c3*chnp.umphiz_c3*F_const*Vz)^2+(chnp.w-chnp.z_c3*chnp.umzr_c3*F_const*Vr-chnp.z_c3*chnp.umzz_	1	Cell Péclet number	Domain 2

Name	Expression	Unit	Description	Selection
	c3*F_const*Vz)^2)+eps)/(((chnp.u-chnp.z_c3*chnp.umrr_c3*F_const*Vr-chnp.z_c3*chnp.umrz_c3*F_const*Vz)*chnp.Drr_c3+(chnp.v-chnp.z_c3*chnp.umphir_c3*F_const*Vr-chnp.z_c3*chnp.umphiz_c3*F_const*Vz)*chnp.Dphir_c3+(chnp.w-chnp.z_c3*chnp.umzr_c3*F_const*Vr-chnp.z_c3*chnp.umzz_c3*F_const*Vz)*chnp.Dzr_c3)*(chnp.u-chnp.z_c3*chnp.umrr_c3*F_const*Vr-chnp.z_c3*chnp.umrz_c3*F_const*Vz)+((chnp.u-chnp.z_c3*chnp.umrr_c3*F_const*Vr-chnp.z_c3*chnp.umrz_c3*F_const*Vz)*chnp.Drphi_c3+(chnp.v-chnp.z_c3*chnp.umphir_c3*F_const*Vr-chnp.z_c3*chnp.umphiz_c3*F_const*Vz)*chnp.Dphiphi_c3+(chnp.w-chnp.z_c3*chnp.umzr_c3*F_const*Vr-chnp.z_c3*chnp.umzz_c3*F_const*Vz)*chnp.Dzphi_c3)*(chnp.v-chnp.z_c3*chnp.umphir_c3*F_const*Vr-chnp.z_c3*chnp.umphiz_c3*F_const*Vz)+((chnp.u-chnp.z_c3*chnp.umrr_c3*F_const*Vr-chnp.z_c3*chnp.umrz_c3*F_const*Vz)*chnp.			

Name	Expression	Unit	Description	Selection
	Drz_c3+(chnp.v-chnp.z_c3*chnp.umphir_c3*F_const*Vr-chnp.z_c3*chnp.umphiz_c3*F_const*Vz)*chnp.Dphiz_c3+(chnp.w-chnp.z_c3*chnp.umzr_c3*F_const*Vr-chnp.z_c3*chnp.umzz_c3*F_const*Vz)*chnp.Dzz_c3)*(chnp.w-chnp.z_c3*chnp.umzr_c3*F_const*Vr-chnp.z_c3*chnp.umzz_c3*F_const*Vz))			
chnp.cellPe_c4	h*sqrt((chnp.u-chnp.z_c4*chnp.umrr_c4*F_const*Vr-chnp.z_c4*chnp.umrz_c4*F_const*Vz)^2+(chnp.v-chnp.z_c4*chnp.umphir_c4*F_const*Vr-chnp.z_c4*chnp.umphiz_c4*F_const*Vz)^2+(chnp.w-chnp.z_c4*chnp.umzr_c4*F_const*Vr-chnp.z_c4*chnp.umzz_c4*F_const*Vz)^2)*(sqrt((chnp.u-chnp.z_c4*chnp.umrr_c4*F_const*Vr-chnp.z_c4*chnp.umrz_c4*F_const*Vz)^2+(chnp.v-chnp.z_c4*chnp.umphir_c4*F_const*Vr-chnp.z_c4*chnp.umphiz_c4*F_const*Vz)^2+(chnp.w-chnp.z_c4*chnp.umzr_c4*F_const*Vr-chnp.z_c4*chnp.umzz_c4*F_const*Vz)^2)+eps)/(((chnp.u-	1	Cell Péclet number	Domain 2

Name	Expression	Unit	Description	Selection
	chnp.z_c4*chnp.umrr_c4*F_const*Vr-chnp.z_c4*chnp.umrz_c4*F_const*Vz)*chnp.Drr_c4+(chnp.v-chnp.z_c4*chnp.umphir_c4*F_const*Vr-chnp.z_c4*chnp.umphiz_c4*F_const*Vz)*chnp.Dphir_c4+(chnp.w-chnp.z_c4*chnp.umzr_c4*F_const*Vr-chnp.z_c4*chnp.umzz_c4*F_const*Vz)*chnp.Dzr_c4)*(chnp.u-chnp.z_c4*chnp.umrr_c4*F_const*Vr-chnp.z_c4*chnp.umrz_c4*F_const*Vz)+((chnp.u-chnp.z_c4*chnp.umrr_c4*F_const*Vr-chnp.z_c4*chnp.umrz_c4*F_const*Vz)*chnp.Drphi_c4+(chnp.v-chnp.z_c4*chnp.umphir_c4*F_const*Vr-chnp.z_c4*chnp.umphiz_c4*F_const*Vz)*chnp.Dphiphi_c4+(chnp.w-chnp.z_c4*chnp.umzr_c4*F_const*Vr-chnp.z_c4*chnp.umzz_c4*F_const*Vz)*chnp.Dzphi_c4)*(chnp.v-chnp.z_c4*chnp.umphir_c4*F_const*Vr-chnp.z_c4*chnp.umphiz_c4*F_const*Vz)+((chnp.u-chnp.z_c4*chnp.umrr_c4*F_const*Vr-chnp.z_c4*chnp.umrz_c4*F_const*Vz)*chnp.Drz_c4+(chnp.v-chnp.z_c4*chnp.umphi			

Name	Expression	Unit	Description	Selection
	r_c4*F_const*Vr-chnp.z_c4*chnp.umphiz_c4*F_const*Vz)*chnp.Dphiz_c4+(chnp.w-chnp.z_c4*chnp.umzr_c4*F_const*Vr-chnp.z_c4*chnp.umzz_c4*F_const*Vz)*chnp.Dzz_c4)*(chnp.w-chnp.z_c4*chnp.umzr_c4*F_const*Vr-chnp.z_c4*chnp.umzz_c4*F_const*Vz))			
chnp.gradVr	Vr	V/m	Potential gradient, r component	Domain 2
chnp.gradVphi	0	V/m	Potential gradient, phi component	Domain 2
chnp.gradVz	Vz	V/m	Potential gradient, z component	Domain 2
domflux.c1r	chnp.dfluxr_c1+chnp.mfluxr_c1	mol/(m^2*s)	Domain flux	Domain 2
domflux.c1z	chnp.dfluxphi_c1+chnp.mfluxphi_c1	mol/(m^2*s)	Domain flux	Domain 2
domflux.c2r	chnp.dfluxr_c2+chnp.mfluxr_c2	mol/(m^2*s)	Domain flux	Domain 2
domflux.c2z	chnp.dfluxphi_c2+chnp.mfluxphi_c2	mol/(m^2*s)	Domain flux	Domain 2
domflux.c3r	chnp.dfluxr_c3+chnp.mfluxr_c3	mol/(m^2*s)	Domain flux	Domain 2
domflux.c3z	chnp.dfluxphi_c3+chnp.mfluxphi_c3	mol/(m^2*s)	Domain flux	Domain 2
domflux.c4r	chnp.dfluxr_c4+chnp.mfluxr_c4	mol/(m^2*s)	Domain flux	Domain 2
domflux.c4z	chnp.dfluxphi_c4+chnp.mfluxphi_c4	mol/(m^2*s)	Domain flux	Domain 2
chnp.nrc	root.nrc/sqrt(root.nrc^2+root.nzc^2+eps)		Normal vector, r component	Boundaries 3–4, 6, 9, 13–19
chnp.nphic	0		Normal vector, phi	Boundaries 3–4, 6, 9, 13–

Name	Expression	Unit	Description	Selection
			component	19
chnp.nzc	root.nzc/sqrt(root.nrc^2+root.nzc^2+eps)		Normal vector, z component	Boundaries 3–4, 6, 9, 13–19
chnp.bndFlux_c2	-uflux_spatial(c2)	mol/(m^2*s)	Boundary flux	Boundaries 4, 6, 9, 13–15, 17
chnp.bndFlux_c2	if(r>0.0010/sqrt(sqrt(mean(emetric2))),-0.5*dflux_spatial(c2)/(r*pi),NaN)	mol/(m^2*s)	Boundary flux	Boundaries 3, 16, 18–19
chnp.bndFlux_c3	-uflux_spatial(c3)	mol/(m^2*s)	Boundary flux	Boundaries 4, 6, 9, 13–15, 17
chnp.bndFlux_c3	if(r>0.0010/sqrt(sqrt(mean(emetric2))),-0.5*dflux_spatial(c3)/(r*pi),NaN)	mol/(m^2*s)	Boundary flux	Boundaries 3, 16, 18–19
chnp.bndFlux_c4	-uflux_spatial(c4)	mol/(m^2*s)	Boundary flux	Boundaries 4, 6, 9, 13–15, 17
chnp.bndFlux_c4	if(r>0.0010/sqrt(sqrt(mean(emetric2))),-0.5*dflux_spatial(c4)/(r*pi),NaN)	mol/(m^2*s)	Boundary flux	Boundaries 3, 16, 18–19

Shape functions

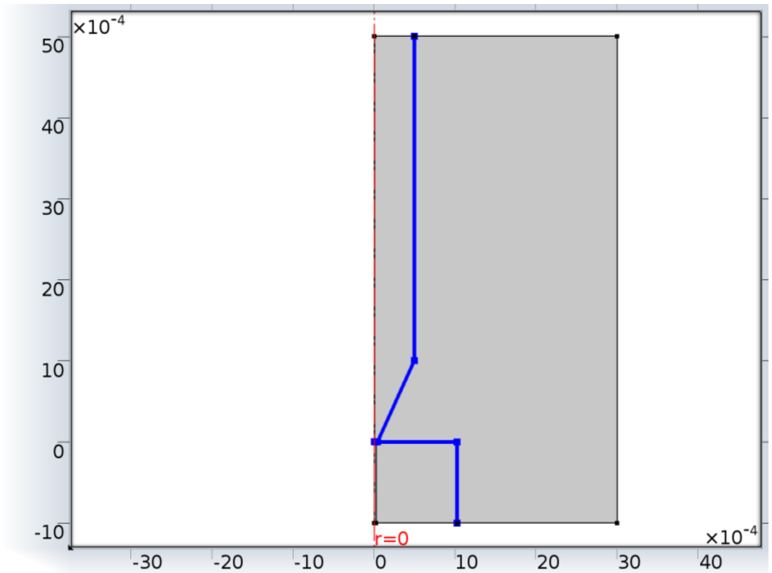
Name	Shape function	Unit	Description	Shape frame	Selection
c2	Lagrange (Linear)	mol/m^3	Concentration	Material	Domain 2
c3	Lagrange (Linear)	mol/m^3	Concentration	Material	Domain 2
c4	Lagrange (Linear)	mol/m^3	Concentration	Material	Domain 2
V	Lagrange (Linear)	V	Electric potential	Material	Domain 2

Weak expressions

Weak expression	Integration frame	Selection
2*(-d(c2,t)*test(c2)-(chnp.Drr_c2*c2r+chnp.Drz_c2*c2z)*test(c2r)-(chnp.Dzr_c2*c2r+chnp.Dzz_c2*c2z)*test(c2z))*pi*r	Material	Domain 2

Weak expression	Integration frame	Selection
2*(-d(c3,t)*test(c3)-(chnp.Drr_c3*c3r+chnp.Drz_c3*c3z)*test(c3r)-(chnp.Dzr_c3*c3r+chnp.Dzz_c3*c3z)*test(c3z))*pi*r	Material	Domain 2
2*(-d(c4,t)*test(c4)-(chnp.Drr_c4*c4r+chnp.Drz_c4*c4z)*test(c4r)-(chnp.Dzr_c4*c4r+chnp.Dzz_c4*c4z)*test(c4z))*pi*r	Material	Domain 2
2*(-chnp.u*c2r-chnp.w*c2z)*test(c2)*pi*r	Material	Domain 2
2*chnp.cbf_c2*test(c2)*pi*r	Material	Boundaries 3–4, 6, 9, 13–19
2*(-chnp.u*c3r-chnp.w*c3z)*test(c3)*pi*r	Material	Domain 2
2*chnp.cbf_c3*test(c3)*pi*r	Material	Boundaries 3–4, 6, 9, 13–19
2*(-chnp.u*c4r-chnp.w*c4z)*test(c4)*pi*r	Material	Domain 2
2*chnp.cbf_c4*test(c4)*pi*r	Material	Boundaries 3–4, 6, 9, 13–19
2*chnp.z_c2*F_const*c2*(-(chnp.umrr_c2*d(chnp.V,r)+chnp.umrz_c2*d(chnp.V,z))*test(c2r)-(chnp.umzr_c2*d(chnp.V,r)+chnp.umzz_c2*d(chnp.V,z))*test(c2z))*pi*r	Material	Domain 2
2*chnp.z_c3*F_const*c3*(-(chnp.umrr_c3*d(chnp.V,r)+chnp.umrz_c3*d(chnp.V,z))*test(c3r)-(chnp.umzr_c3*d(chnp.V,r)+chnp.umzz_c3*d(chnp.V,z))*test(c3z))*pi*r	Material	Domain 2
2*chnp.z_c4*F_const*c4*(-(chnp.umrr_c4*d(chnp.V,r)+chnp.umrz_c4*d(chnp.V,z))*test(c4r)-(chnp.umzr_c4*d(chnp.V,r)+chnp.umzz_c4*d(chnp.V,z))*test(c4z))*pi*r	Material	Domain 2
2*(chnp.Jr*test(Vr)+chnp.Jz*test(Vz))*pi*r	Material	Domain 2
2*chnp.streamline*pi*r	Material	Domain 2
2*chnp.crosswind*pi*r	Material	Domain 2

2.4.2 Electric Insulation 1



Electric Insulation 1

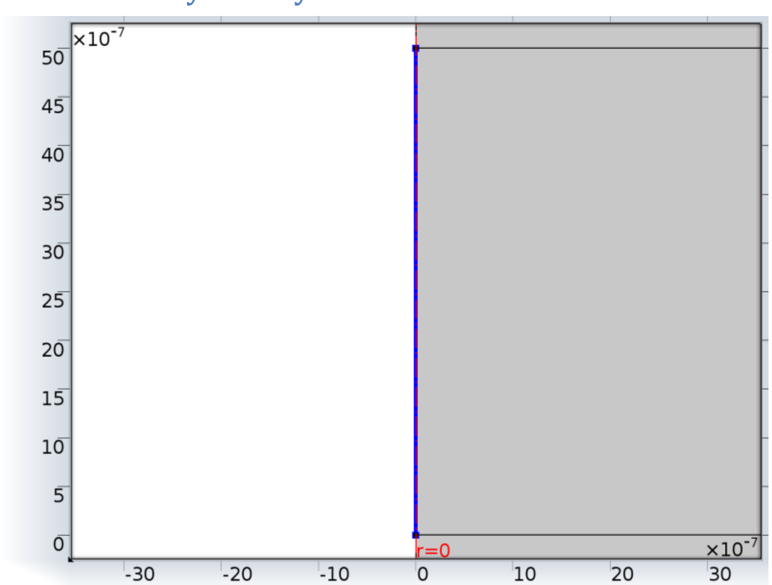
Selection

Geometric entity level	Boundary
Selection	Boundaries 9, 13–15, 17

Equations

$$-n \cdot \mathbf{N}^{V} = 0$$

2.4.3 Axial Symmetry 1

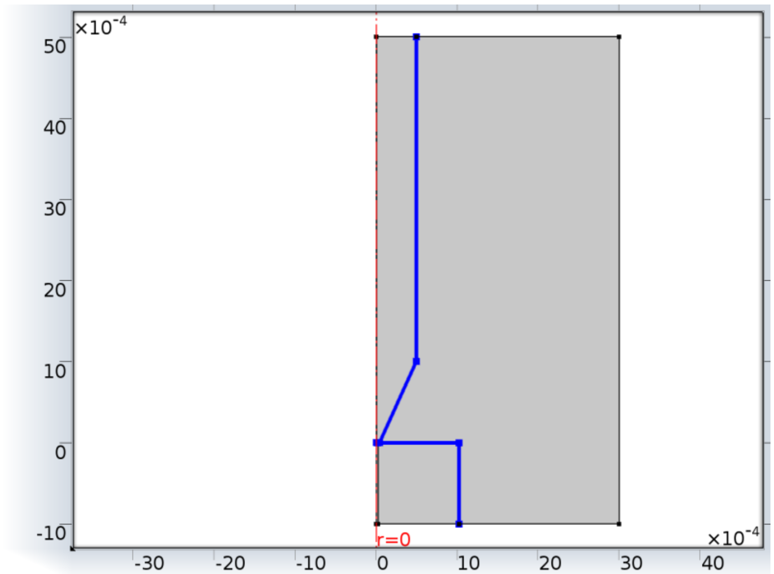


Axial Symmetry 1

Selection

Geometric entity level	Boundary
Selection	Boundary 3

2.4.4 No Flux 1



No Flux 1

Selection

Geometric entity level	Boundary
Selection	Boundaries 9, 13–15, 17

Equations

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

Settings

Settings

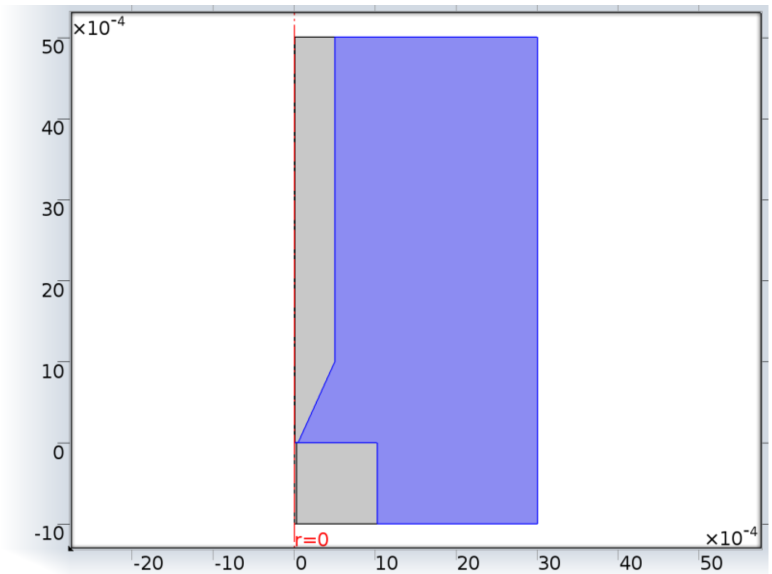
Description	**Value**
Apply for all species	Apply for all species

Variables

Name	**Expression**	**Unit**	**Description**	**Selection**
chnp.cbf_c2	c2*(chnp.u*chnp.nrmesh+chnp.v*chnp.nphimesh+chnp.w*chnp.nzmesh)	mol/(m^2*s)	Convective boundary flux	Boundaries 9, 13–15, 17
chnp.cbf_c3	c3*(chnp.u*chnp.nrmesh+chnp.v*chnp.nphimesh+chnp.w*chnp.nz	mol/(m^2*s)	Convective	Boundaries 9,

Name	Expression	Unit	Description	Selection
	mesh)		boundary flux	13–15, 17
chnp.cbf_c4	c4*(chnp.u*chnp.nrmesh+chnp.v *chnp.nphimesh+chnp.w*chnp.nz mesh)	mol/(m^2*s)	Convective boundary flux	Boundaries 9, 13–15, 17

2.4.5 Initial Values 1



Initial Values 1

Selection

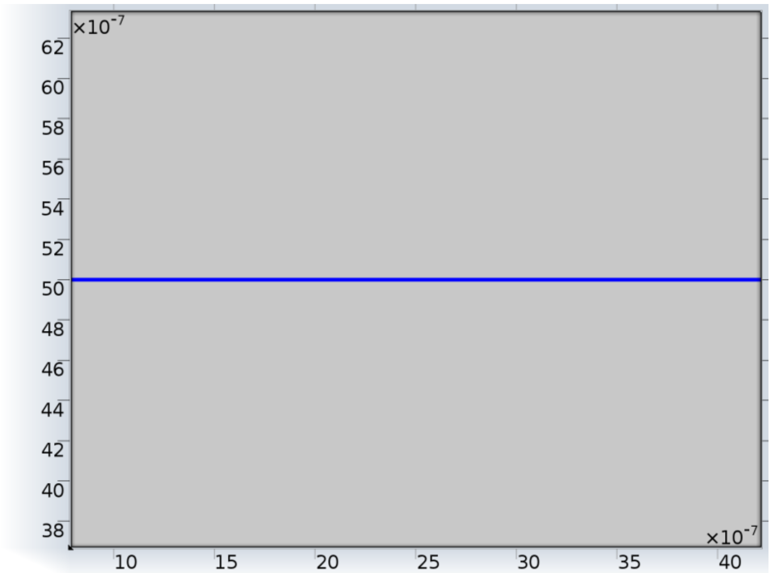
Geometric entity level	Domain
Selection	Domain 2

Settings

Settings

Description	Value
Concentration	Cb
Concentration	0
Concentration	Cs
Electric potential	0

2.4.6 Current Density 2



Current Density 2

Selection

Geometric entity level	Boundary
Selection	Boundary 6

Equations

$$-n \cdot \mathbf{N}^{V} = i_0$$

Settings

Settings

Description	Value
Inward current density	-(zA*F*(-Da*c2z - zA*uA*F*c2*Vz) + zB*F*(-Db*c3z - zB*uB*F*c3*Vz))

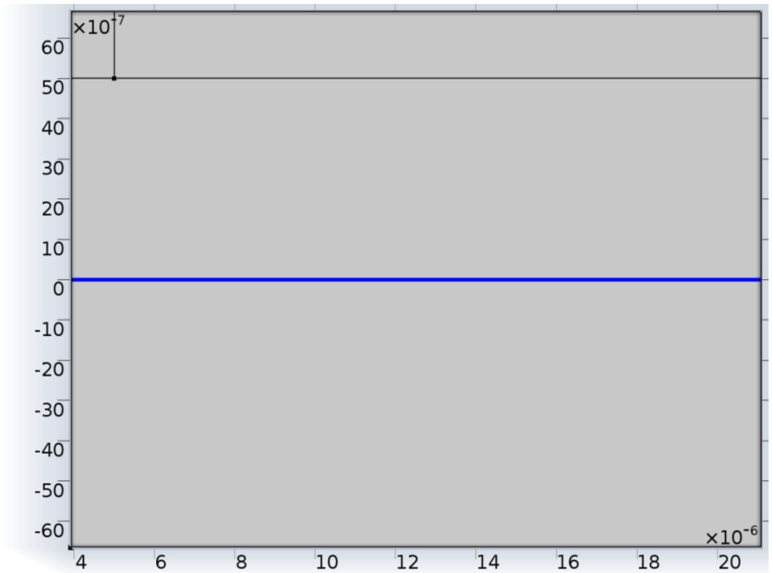
Variables

Name	Expression	Unit	Description	Selection
chnp.i0_cdens2	F*(-zA*(-Da*c2z-zA*uA*F*c2*Vz)-zB*(-Db*c3z-zB*uB*F*c3*Vz))	A/m^2	Inward current density	Boundary 6

Weak expressions

Weak expression	Integration frame	Selection
2*chnp.i0_cdens2*test(V)*pi*r	Material	Boundary 6

2.4.7 Current Density 3



Current Density 3

Selection

Geometric entity level	Boundary
Selection	Boundary 4

Equations

$$-n \cdot \mathbf{N}^V = i_0$$

Settings

Settings

Description	**Value**
Inward current density	(zA*F*(-Da*c2z - zA*uA*F*c2*Vz) + zB*F*(-Db*c3z - zB*uB*F*c3*Vz))

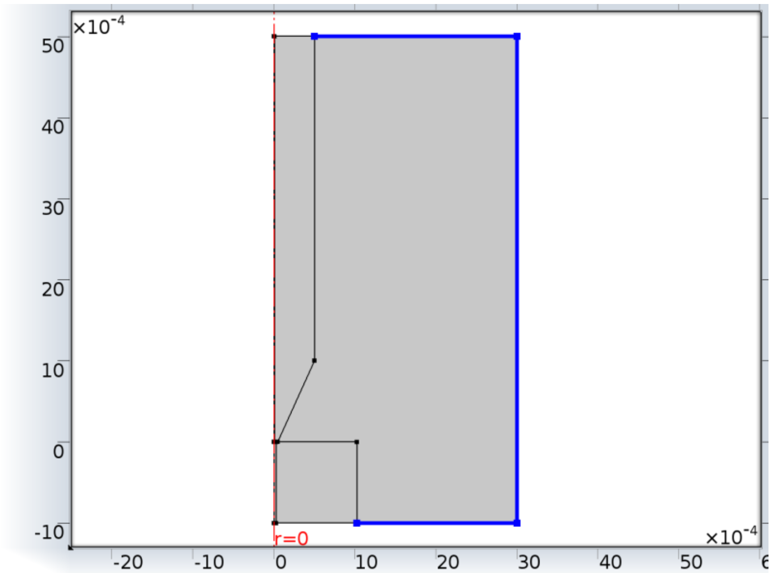
Variables

Name	**Expression**	**Unit**	**Description**	**Selection**
chnp.i0_cdens3	F*(zA*(-Da*c2z-zA*uA*F*c2*Vz)+zB*(-Db*c3z-zB*uB*F*c3*Vz))	A/m^2	Inward current density	Boundary 4

Weak expressions

Weak expression	**Integration frame**	**Selection**
2*chnp.i0_cdens3*test(V)*pi*r	Material	Boundary 4

2.4.8 Electric Potential 1



Electric Potential 1

Selection

Geometric entity level	Boundary
Selection	Boundaries 16, 18–19

Equations

$$V = V_0$$

Settings

Settings

Description	Value
Electric potential	0
Apply reaction terms on	All physics (symmetric)
Use weak constraints	0

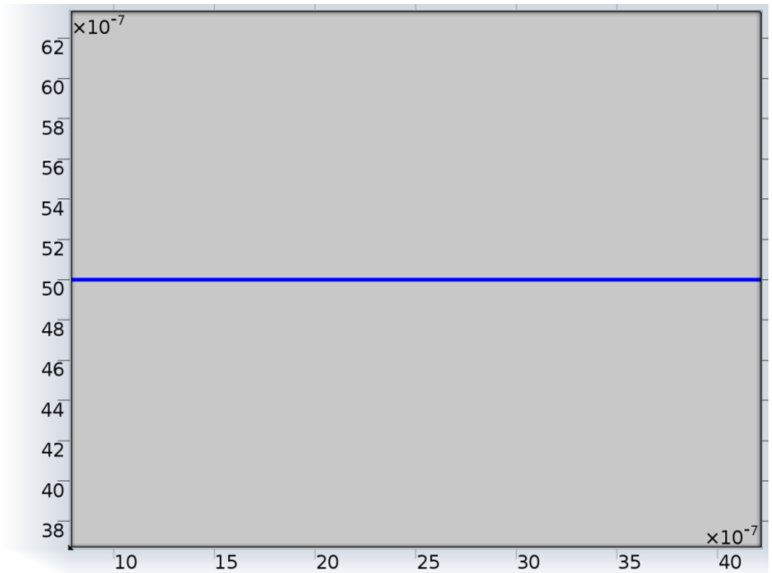
Variables

Name	Expression	Unit	Description	Selection
chnp.V0	0	V	Electric potential	Boundaries 16, 18–19

Constraints

Constraint	Constraint force	Shape function	Selection
chnp.V0-V	test(chnp.V0-V)	Lagrange (Linear)	Boundaries 16, 18–19

2.4.9 Flux 1



Flux 1

Selection

Geometric entity level	Boundary
Selection	Boundary 6

Equations

$$-\mathbf{n}\cdot\mathbf{N}_i = N_{0,i}$$

Settings

Settings

Description	Value
Species c1	0
Species c2	1
Species c3	1
Species c4	1
Inward flux	{0, -(kf*c2 - kb*c3), (kf*c2 - kb*c3), 0}
Flux type	General inward flux

Variables

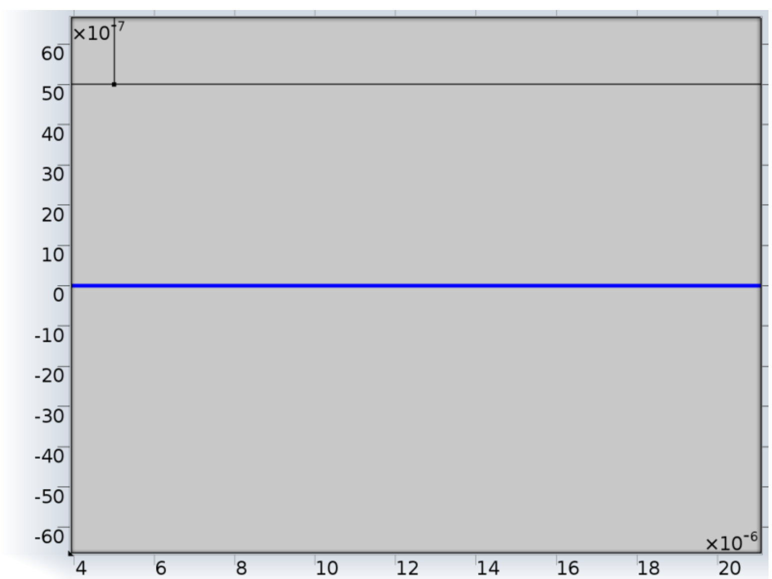
Name	Expression	Unit	Description	Selection
chnp.cbf_c2	c2*(chnp.u*chnp.nrmesh+chnp.v *chnp.nphimesh+chnp.w*chnp.nz	mol/(m^2*s)	Convective boundary flux	Boundary 6

Name	Expression	Unit	Description	Selection
	mesh)			
chnp.cbf_c3	c3*(chnp.u*chnp.nrmesh+chnp.v*chnp.nphimesh+chnp.w*chnp.nzmesh)	mol/(m^2*s)	Convective boundary flux	Boundary 6
chnp.cbf_c4	c4*(chnp.u*chnp.nrmesh+chnp.v*chnp.nphimesh+chnp.w*chnp.nzmesh)	mol/(m^2*s)	Convective boundary flux	Boundary 6

Weak expressions

Weak expression	Integration frame	Selection
-2*(kf*c2-kb*c3)*test(c2)*pi*r	Material	Boundary 6
2*(kf*c2-kb*c3)*test(c3)*pi*r	Material	Boundary 6
0	Material	Boundary 6

2.4.10 Concentration 1



Concentration 1

Selection

Geometric entity level	Boundary
Selection	Boundary 4

Equations

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

Settings

Settings

Description	Value
Concentration	{0, Cb, 0, Cs}
Species c1	0
Species c2	1
Species c3	1
Species c4	0
Apply reaction terms on	All physics (symmetric)
Use weak constraints	0

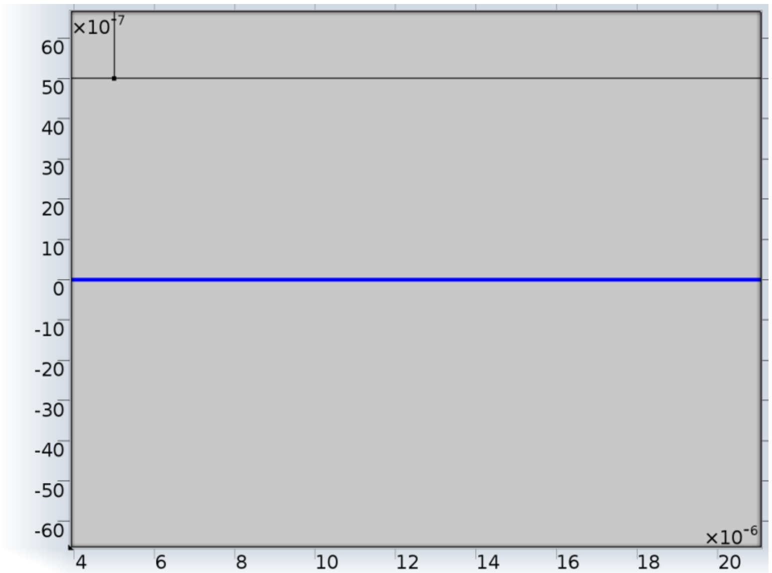
Variables

Name	Expression	Unit	Description	Selection
chnp.c0_c2	Cb	mol/m^3	Concentration	Boundary 4
chnp.c0_c3	0	mol/m^3	Concentration	Boundary 4
chnp.c0_c4	Cs	mol/m^3	Concentration	Boundary 4

Constraints

Constraint	Constraint force	Shape function	Selection
-c2+chnp.c0_c2	test(-c2+chnp.c0_c2)	Lagrange (Linear)	Boundary 4
-c3+chnp.c0_c3	test(-c3+chnp.c0_c3)	Lagrange (Linear)	Boundary 4

2.4.11 Flux 2



Flux 2

Selection

Geometric entity level	Boundary
Selection	Boundary 4

Equations

$$-\mathbf{n}\cdot\mathbf{N}_i = N_{0,i}$$

Settings

Settings

Description	Value
Species c1	0
Species c2	0
Species c3	0
Species c4	1
Inward flux	{0, 0, 0, 0}
Flux type	General inward flux

Variables

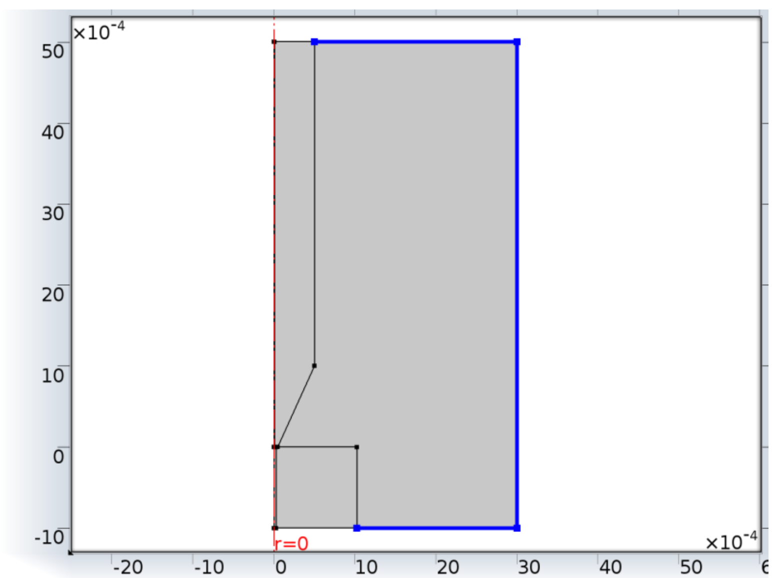
Name	Expression	Unit	Description	Selection
chnp.cbf_c2	c2*(chnp.u*chnp.nrmesh+chnp.v *chnp.nphimesh+chnp.w*chnp.nz	mol/(m^2*s)	Convective boundary flux	Boundary 4

Name	Expression	Unit	Description	Selection
	mesh)			
chnp.cbf_c3	c3*(chnp.u*chnp.nrmesh+chnp.v*chnp.nphimesh+chnp.w*chnp.nzmesh)	mol/(m^2*s)	Convective boundary flux	Boundary 4
chnp.cbf_c4	c4*(chnp.u*chnp.nrmesh+chnp.v*chnp.nphimesh+chnp.w*chnp.nzmesh)	mol/(m^2*s)	Convective boundary flux	Boundary 4

Weak expressions

Weak expression	Integration frame	Selection
0	Material	Boundary 4

2.4.12 Concentration 2



Concentration 2

Selection

Geometric entity level	Boundary
Selection	Boundaries 16, 18–19

Equations

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

Settings

Settings

Description	Value
Concentration	{0, Cb, 0, Cs}
Species c1	0
Species c2	1
Species c3	1
Species c4	1
Apply reaction terms on	All physics (symmetric)
Use weak constraints	0

Variables

Name	Expression	Unit	Description	Selection
chnp.c0_c2	Cb	mol/m^3	Concentration	Boundaries 16, 18–19
chnp.c0_c3	0	mol/m^3	Concentration	Boundaries 16, 18–19
chnp.c0_c4	Cs	mol/m^3	Concentration	Boundaries 16, 18–19

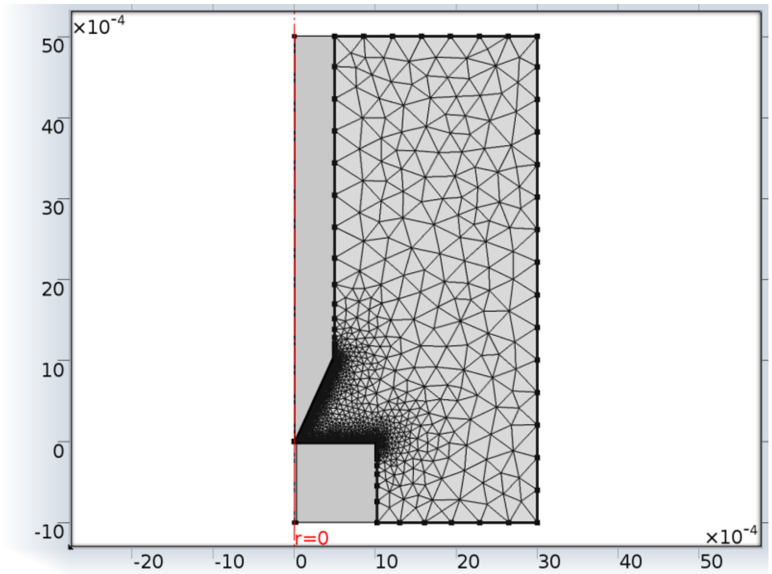
Constraints

Constraint	Constraint force	Shape function	Selection
-c2+chnp.c0_c2	test(-c2+chnp.c0_c2)	Lagrange (Linear)	Boundaries 16, 18–19
-c3+chnp.c0_c3	test(-c3+chnp.c0_c3)	Lagrange (Linear)	Boundaries 16, 18–19
-c4+chnp.c0_c4	test(-c4+chnp.c0_c4)	Lagrange (Linear)	Boundaries 16, 18–19

2.5 Mesh 1

Mesh statistics

Property	Value
Minimum element quality	0.02416
Average element quality	0.9223
Triangular elements	439414
Quadrilateral elements	0
Edge elements	9100
Vertex elements	11



Mesh 1

2.5.1 Size (size)

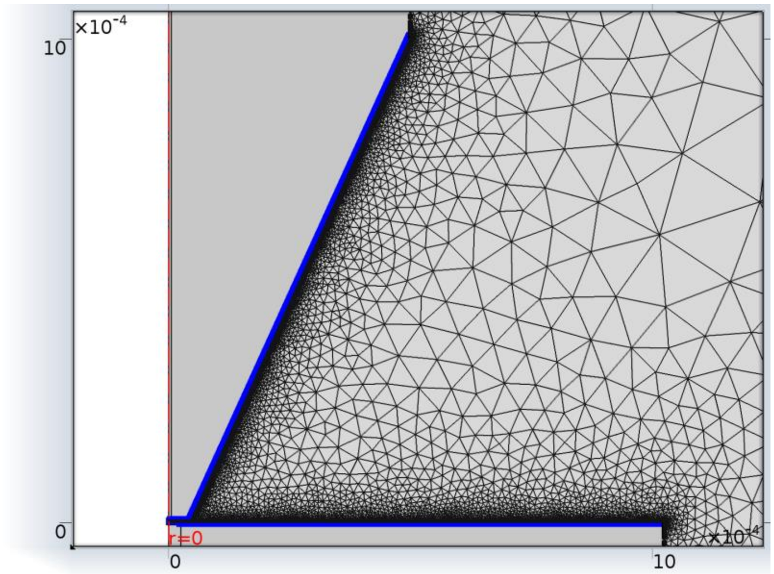
Settings

Name	Value
Maximum element size	4.02E-4
Minimum element size	1.8E-6
Resolution of curvature	0.3
Maximum element growth rate	1.3

2.5.2 Edge 1 (edg1)

Selection

Geometric entity level	Boundary
Selection	Boundaries 9, 13–14

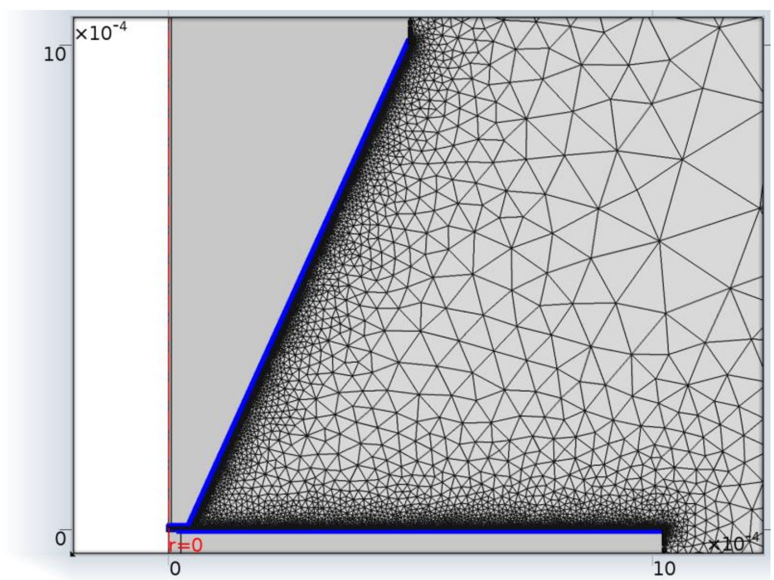


Edge 1

Size 1 (size1)

Selection

Geometric entity level	Boundary
Selection	Boundaries 9, 13–14



Size 1

Settings

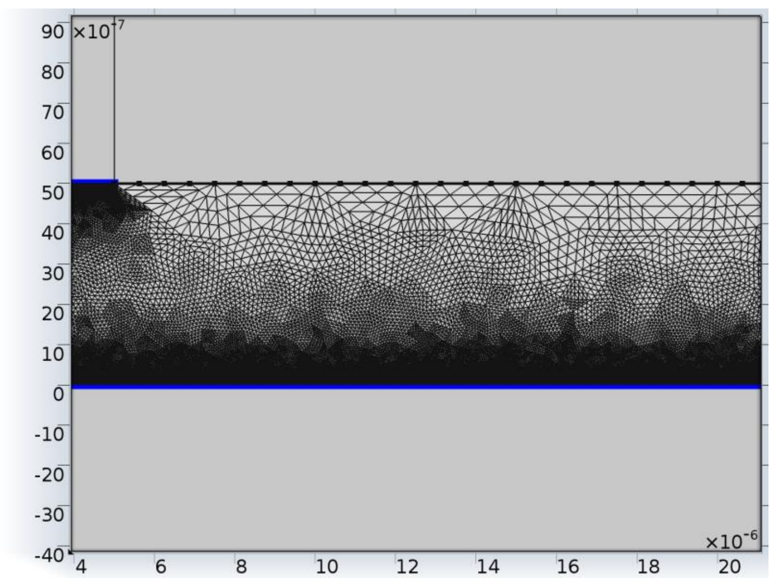
Name	Value

Name	Value
Maximum element size	r_elcap/200
Minimum element size	1.05E-5
Minimum element size	Off
Resolution of curvature	0.3
Resolution of curvature	Off
Resolution of narrow regions	Off
Maximum element growth rate	1.3
Maximum element growth rate	Off
Custom element size	Custom

2.5.3 Edge 2 (edg2)

Selection

Geometric entity level	Boundary
Selection	Boundaries 4, 6

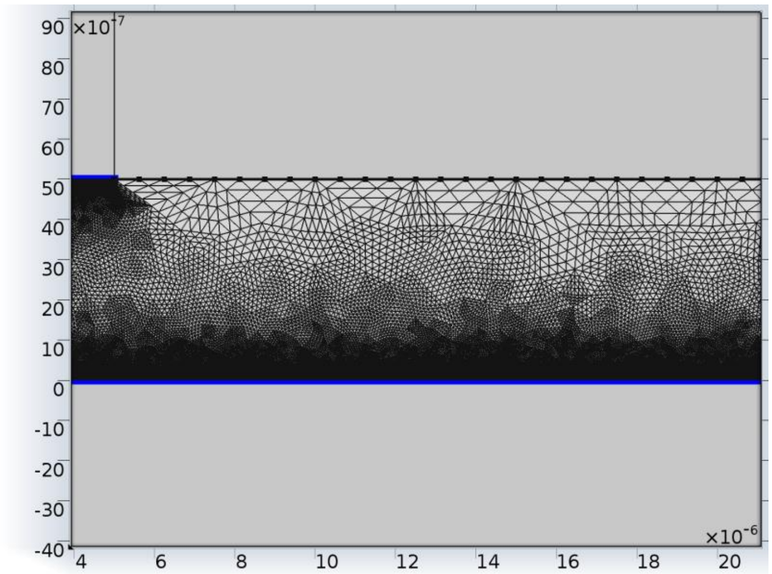


Edge 2

Size 1 (size1)

Selection

Geometric entity level	Boundary
Selection	Boundaries 4, 6



Size 1

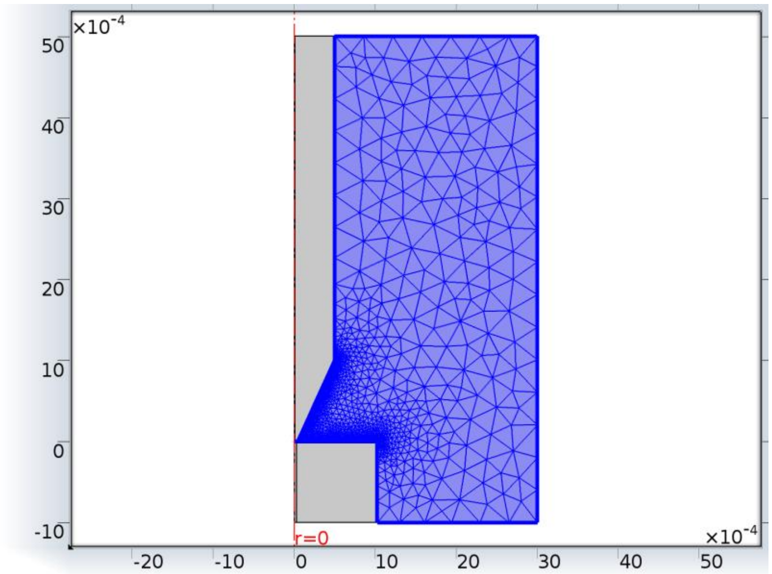
Settings

Name	Value
Maximum element size	r_el/335
Minimum element size	4.8E-6
Minimum element size	Off
Resolution of curvature	0.3
Resolution of curvature	Off
Resolution of narrow regions	Off
Maximum element growth rate	1.3
Maximum element growth rate	Off
Custom element size	Custom

2.5.4 Free Triangular 1 (ftri1)

Selection

Geometric entity level	Domain
Selection	Domain 2

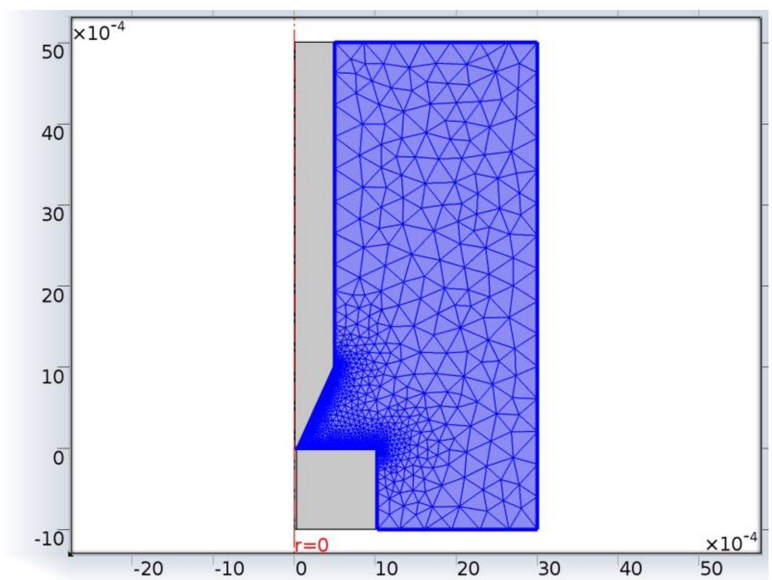


Free Triangular 1

Size 1 (size1)

Selection

Geometric entity level	Domain
Selection	Domain 2



Size 1

Settings

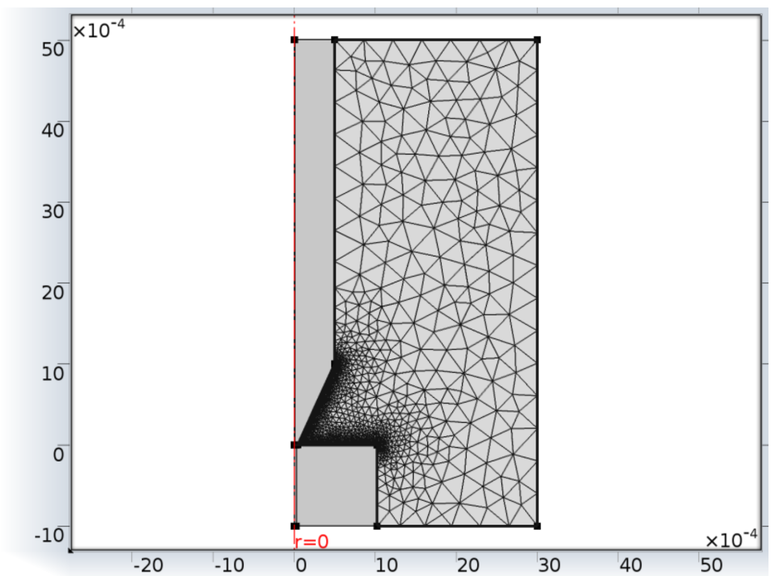
Name	Value

Name	Value
Maximum element size	4.02E-4
Minimum element size	1.8E-6
Resolution of curvature	0.3
Maximum element growth rate	1.3

2.5.5 Refine 1 (ref1)

Selection

Geometric entity level	Domain
Selection	Geometry geom1



Refine 1

Settings

Name	Value
Specify bounding box	Use bounding box
xmax	r_co
ymax	2*d
Number of refinements	2

3 Study 1

3.1 Parametric Sweep

Parameter name: d

Parameters:

3.2 Stationary

Study settings

Property	Value
Include geometric nonlinearity	Off

Mesh selection

Geometry	Mesh
Geometry 1 (geom1)	mesh1

Physics selection

Physics	Discretization
Nernst-Planck Equations (chnp)	physics

3.3 Time Dependent

Study settings

Property	Value
Include geometric nonlinearity	Off

Times: range(0,0.1,10)

Mesh selection

Geometry	Mesh
Geometry 1 (geom1)	mesh1

Physics selection

Physics	Discretization
Nernst-Planck Equations (chnp)	physics

3.4 Solver Configurations

3.4.1 Solver 1

Compile Equations: Stationary (st1)

Study and step

Name	Value
Use study	Study 1
Use study step	Stationary

Dependent Variables 1 (v1)

General

Name	Value
Defined by study step	Stationary

Initial values of variables solved for

Name	Value
Solution	Zero

Values of variables not solved for

Name	Value
Solution	Zero

Electric potential (mod1.V) (mod1_V)

General

Name	Value
Field components	mod1.V

Concentration (mod1.c4) (mod1_c4)

General

Name	Value
Field components	mod1.c4

Concentration (mod1.c3) (mod1_c3)

General

Name	Value
Field components	mod1.c3

Concentration (mod1.c2) (mod1_c2)

General

Name	Value
Field components	mod1.c2

Stationary Solver 1 (s1)

General

Name	Value
Defined by study step	Stationary

Log

```
Stationary Solver 1 in Solver 1 started at 22-Oct-2014 17:00:29.
Nonlinear solver
Number of degrees of freedom solved for: 897032.
Nonsymmetric matrix found.
Scales for dependent variables:
Electric potential (mod1.V): 0.00053
Concentration (mod1.c4): 3
Concentration (mod1.c3): 0.11
Concentration (mod1.c2): 0.73
Iter      ErrEst      Damping    Stepsize #Res #Jac #Sol
   1         6.5    0.0100000         6.6    2    1    2
   2         2.8    0.0749763         3.2    3    2    4
   3        0.52    0.2505018        0.72    4    3    6
   4       0.021    1.0000000         2.9    5    4    8
   5     0.00026    1.0000000       0.059    6    5   10
Stationary Solver 1 in Solver 1: Solution time: 81 s (1 minute, 21 seconds)
                                 Physical memory: 3.55 GB
                                 Virtual memory: 3.87 GB
```

Fully Coupled 1 (fc1)

General

Name	Value
Linear solver	Direct 1

Direct 1 (d1)

General

Name	Value
Solver	PARDISO

4 Results

4.1 Data Sets

4.1.1 Solution 1

Selection

Geometric entity level	Domain
Selection	Geometry geom1

Solution

Name	Value
Solution	Solver 1
Model	Save Point Geometry 1

4.1.2 Revolution 2D 1

Data

Name	Value
Data set	Solution 1

Revolution layers

Name	Value
Start angle	-90
Revolution angle	225

4.2 Derived Values

4.2.1 Line Integration 1

Selection

Geometric entity level	Boundary
Selection	No boundaries

Data

Name	Value
Data set	Solution 1

Expression

Name	Value
Expression	c1

Name	Value
Unit	mol/m^2
Description	Concentration

4.3 Tables

4.3.1 Table 1

Line Integration 1 (chnp.tfluxMag_c2*F)

Table 1

chnp.tfluxMag_c2*F (A)
8.08729e-9

4.3.2 Table 2

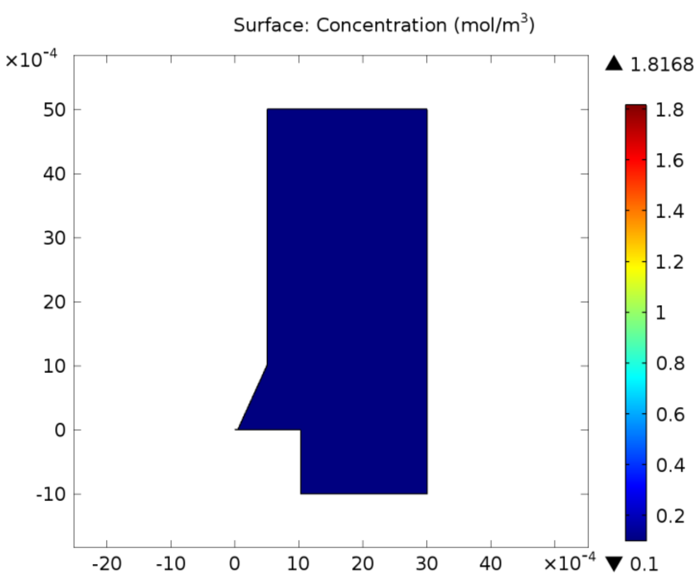
Line Integration 2 (chnp.tfluxMag_c3*F)

Table 2

chnp.tfluxMag_c3*F (A)
8.36378e-9

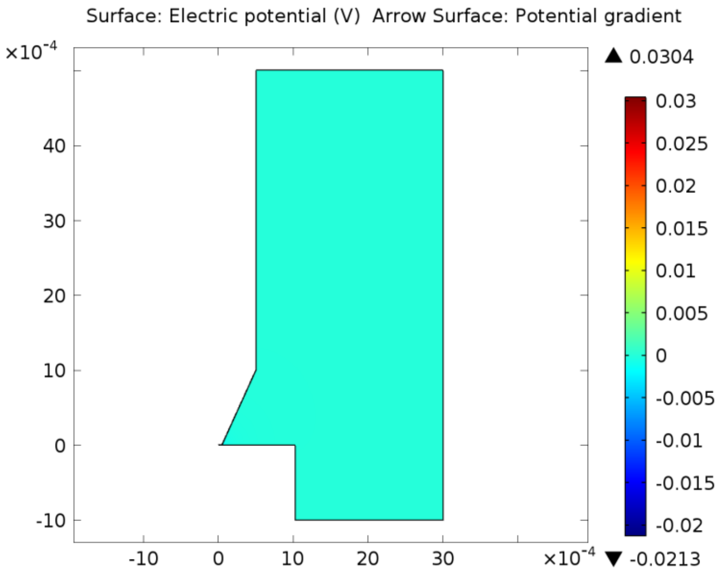
4.4 Plot Groups

4.4.1 Concentration (chnp)



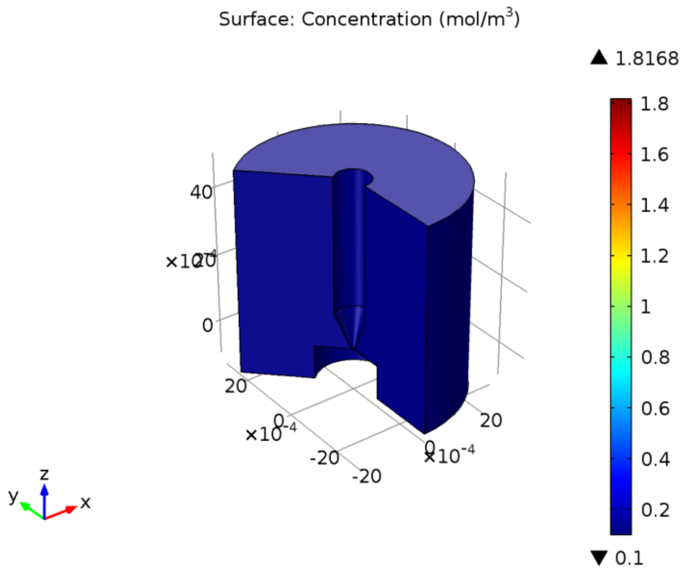
Surface: Concentration (mol/m^3)

4.4.2 Electric Potential (chnp)



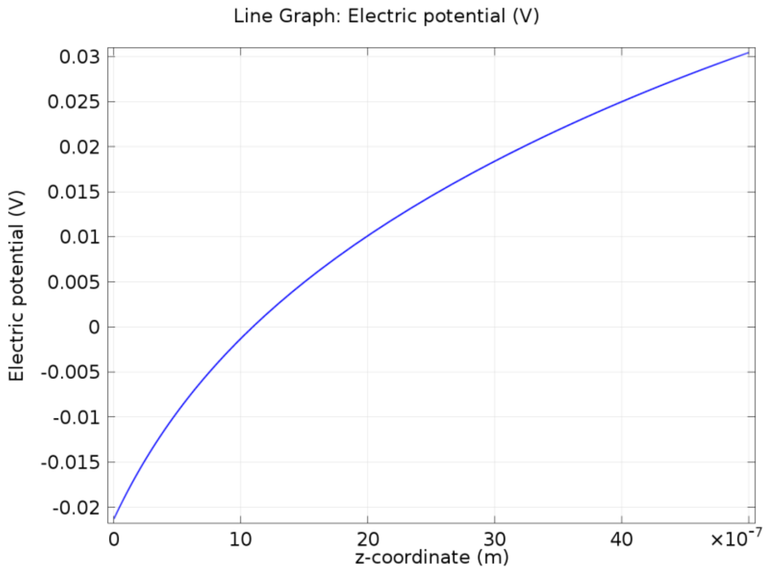
Surface: Electric potential (V) Arrow Surface: Potential gradient

4.4.3 Concentration, 3D (chnp)



Surface: Concentration (mol/m^3)

4.4.4 1D Plot Group 4



Line Graph: Electric potential (V)

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[1] Boika, A.; Thorgaard, S. N.; Bard, A. J. 2013. Monitoring the Electrophoretic Migration and Adsorption of Single Insulating Nanoparticles at Ultramicroelectrodes. *J. Phys. Chem. B* 117(16): 4371-80.
[2] Bard, A. J.; Mirkin, M. V. Scanning Electrochemical Microscopy, 2nd ed.; Taylor & Francis: Boca Raton, 2012.