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

COMSOL report as annex to the supplementary information

Redox Titration of Gold and Platinum Surface Oxides at Porous Microelectrodes

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Contents

1 Global Definitions

Date	Jul 6, 2017 4:45:53 PM

GLOBAL SETTINGS

Name	2017 07 06 SI SECM Paper.mph
Path	
COMSOL version	COMSOL 5.3 (Build: 260)

USED PRODUCTS

COMSOL Multiphysics
Electrochemistry Module

1.1 PARAMETERS 1

PARAMETERS

Name	Expression	Value	Description
d	5[µm]	5E−6 m	Tip-Substrate distance
d_L	d/rt	0.2	
rt	25[µm]	2.5E−5 m	tip radius
st	25[µm]	2.5E−5 m	substrate radius
RG	3.5	3.5	
RG2	3.5	3.5	
BH	500	500	Box size
stz	8[µm]	8E−6 m	Cavity depth
pw	100[nm]	1E−7 m	Pore diameter
E01	0.0[V]	0 V	Standard pot. for tip reaction
k01	0.1[m*s^ - 1]	0.1 m/s	Tip Standard Electrochemical reaction constant
Do1	5.5e-10[m^2/s]	5.5E−10 m^2/s	Diffusion coefficient
Dr1	Do1	5.5E−10 m^2/s	
co1	10[mmol/L]	10 mol/m^3	Concentration of O species
T	298[K]	298 K	
R	R_const	8.3145 J/(mol·K)	
k_ox2	0.01[(m/s)]	0.01 m/s	Rate constant, mediator with oxide 2

Name	Expression	Value	Description
k_ox1	0.001[(m/s)]	0.001 m/s	Rate constant, mediator with oxide 1
q10	4.5[uC]	4.5E−6 C	Initial charge of Ox1
q20	1.6*q1ML	9.7625E−7 C	Initial charge of Ox2
cs10	q10/(A_sub*F)	2.9811E−4 mol/m²	surface conc. of Ox1
cs20	q20/(A_sub*F)	6.4673E−5 mol/m²	surface conc. of Ox2
F	F_const	96485 C/mol	Faraday constant
f	F/(R*T)	38.941 1/V	F/RT
n	1	1	number of electrons, tip reaction
a	0.50	0.5	symmetry factor
Cell_lim	BH*rt	0.0125 m	
D_L	6*sqrt(Dr1*abs(200[s]))	0.00199 m	diffusion layer size
ML_mol	ML/F_const	4.0421E−5 mol/m²	
ML	390[µC/cm^2]	3.9 C/m²	1 monolayer per surface area
q1ML	ML*A_sub	6.1016E−7 C	Charge of 1 Monolayer
A_sub	0.15645[mm^2]	1.5645E−7 m²	Substrate area
Theta_max	ML_mol	4.0421E−5 mol/m²	Maximut surface coverage
Sigma_cs1	1	1	
Sigma_cs2	1	1	
pore_num	st/(2*pw)	125	
Dcs1	100*Dr1	5.5E−8 m²/s	

2 Component 1

COMPONENT SETTINGS

Unit system	SI

2.1 DEFINITIONS

2.1.1 Variables

Tip

SELECTION

Geometric entity level	Boundary
Name	Tip
Selection	Boundary 4

Name	Expression	Unit	Description
kf1	k01*exp(-a*f*(E-E01))	m/s	Forward constant
kb1	k01*exp((1 - a)*f*(E-E01))	m/s	Backward constant
E	step1(t/(1[s]))*(-0.5[V])	V	
current	2*pi*F_const*intop1(Do1*o1z*r)	A	

Substrate

SELECTION

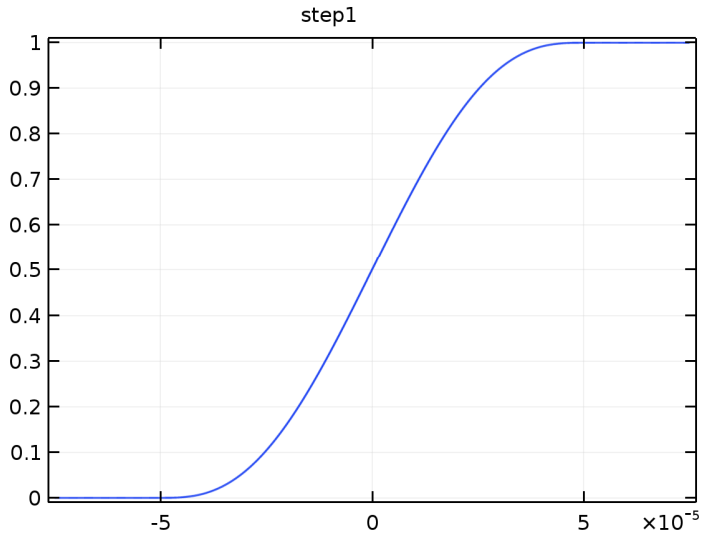
Geometric entity level	Boundary
Name	Substrate
Selection	Substrate21, 223, 225, 227, 229, 231, 233, 235, 237, 239, 241, 243, 245, 247, 249, 251, 253, 255, 257, 259, 261, 263, 265, 267, 269, 271, 273, 275, 277, 279, 281, 283, 285, 287, 289, 291, 293, 295, 297, 299, 301, 303, 305, 307, 309, 311, 313, 315, 317, 319, 321, 323, 325, 327, 329, 331, 333, 335, 337, 339, 341, 343, 345, 347, 349, 351, 353, 355, 357, 359, 361, 363, 365, 367, 369, 371, 373, 375, 377, 379, 381, 383, 385, 387, 389, 391, 393, 395, 397, 399, 401, 403, 405, 407, 409, 411, 413, 415, 417, 419, 421, 423, 425, 427, 429, 431, 433, 435, 437, 439, 441, 443, 445, 447, 449, 451, 453, 455, 457, 459, 461, 463, 465, 467, 469, 471, 473, 475, 477, 479, 481, 483, 485, 487, 489, 491, 493, 495, 497, 499, 501

Name	Expression	Unit	Description
eta2	E2 - E02		overpotential for tip reaction
theta1	max(eps, min(Sigma_cs1*cs1/Theta_max, 1))		Surface coverage Ox1
theta2	max(eps, min(Sigma_cs2*cs2/Theta_max, 1))		Surface coverage Ox2

2.1.2 Functions

Step 1

Function name	step1
Function type	Step



Step 1

PARAMETERS

Description	Value
Location	0
From	0
To	1

SMOOTHING

Description	Value
Size of transition zone	0.0001

2.1.3 Component Couplings

Integration 1

Coupling type	Integration
Operator name	intop1

SOURCE SELECTION

Geometric entity level	Boundary
Name	Tip

Selection	Boundary 4

Integration 2

Coupling type	Integration
Operator name	intop2

SOURCE SELECTION

Geometric entity level	Boundary
Name	Substrate
Selection	Substrate21, 223, 225, 227, 229, 231, 233, 235, 237, 239, 241, 243, 245, 247, 249, 251, 253, 255, 257, 259, 261, 263, 265, 267, 269, 271, 273, 275, 277, 279, 281, 283, 285, 287, 289, 291, 293, 295, 297, 299, 301, 303, 305, 307, 309, 311, 313, 315, 317, 319, 321, 323, 325, 327, 329, 331, 333, 335, 337, 339, 341, 343, 345, 347, 349, 351, 353, 355, 357, 359, 361, 363, 365, 367, 369, 371, 373, 375, 377, 379, 381, 383, 385, 387, 389, 391, 393, 395, 397, 399, 401, 403, 405, 407, 409, 411, 413, 415, 417, 419, 421, 423, 425, 427, 429, 431, 433, 435, 437, 439, 441, 443, 445, 447, 449, 451, 453, 455, 457, 459, 461, 463, 465, 467, 469, 471, 473, 475, 477, 479, 481, 483, 485, 487, 489, 491, 493, 495, 497, 499, 501

2.1.4 Selections

Tip

Selection type
Explicit

Selection
Boundary 4

Substrate

Selection type
Explicit

Selection
Substrate21, 223, 225, 227, 229, 231, 233, 235, 237, 239, 241, 243, 245, 247, 249, 251, 253, 255, 257, 259, 261, 263, 265, 267, 269, 271, 273, 275, 277, 279, 281, 283, 285, 287, 289, 291, 293, 295, 297, 299, 301, 303, 305, 307, 309, 311, 313, 315, 317, 319, 321, 323, 325, 327, 329, 331, 333, 335, 337, 339, 341, 343, 345, 347, 349, 351, 353, 355, 357, 359, 361, 363, 365, 367, 369, 371, 373, 375, 377, 379, 381, 383, 385, 387, 389, 391, 393, 395, 397, 399, 401, 403, 405, 407, 409, 411, 413, 415, 417, 419, 421, 423, 425, 427, 429, 431, 433, 435, 437, 439, 441, 443, 445, 447, 449, 451, 453, 455, 457, 459, 461, 463, 465, 467, 469, 471, 473, 475, 477, 479, 481, 483, 485, 487, 489, 491, 493, 495, 497, 499, 501

Electrodes

Selection type
Explicit

Selection
Boundaries 2, 4–502

Bulk Boundaries

Selection type
Explicit

Selection
No boundaries

Tip point

Selection type
Explicit

Selection
Point 503

Sub point

Selection type
Explicit

Selection
Point 502

Axis

Selection type
Box

Selection
Boundary 3

dL domain

Selection type
Box

Selection

Selection
Domain 1

2.1.5 Coordinate Systems

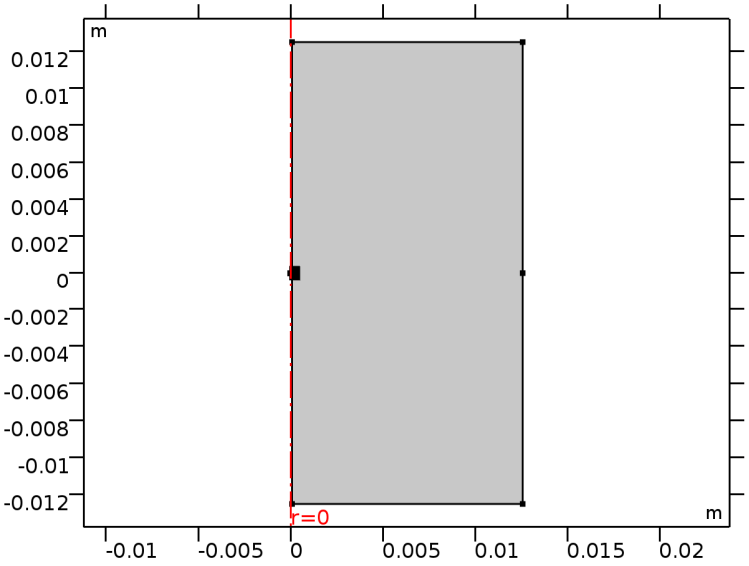
Boundary System 1

Coordinate system type	Boundary system
Tag	sys1

COORDINATE NAMES

First	Second	Third
t1	to	n

2.2 GEOMETRY 1



Geometry 1

UNITS

Length unit	m
Angular unit	deg

GEOMETRY STATISTICS

Description	Value
Space dimension	2
Number of domains	3
Number of boundaries	519
Number of vertices	517

2.2.1 Bézier Polygon 1 (b1)

POLYGON SEGMENTS

Description	Value
Control points	{{0, 0, pw, pw}, {0, -stz, -stz, 0}}
Degree	{1, 1, 1}
Weights	{1, 1, 1, 1, 1, 1}
Type	Solid

2.2.2 Array 1 (arr1)

SETTINGS

Description	Value
Size	125
Array type	Linear
Size	round(pore_num)
Displacement	{2*pw, 0}

2.2.3 Bulk Top (r1)

POSITION

Description	Value
Position	{rt*RG, d}

SIZE

Description	Value
Width	BH*rt
Height	BH*rt

2.2.4 Bulk Bottom (r2)

POSITION

Description	Value
Position	{st*RG2, -BH*rt}

SIZE

Description	Value
Width	rt*RG + BH*rt - (st*RG2)
Height	BH*rt

2.2.5 Bulk middle (r15)

POSITION

Description	Value
Position	{0, 0}

SIZE

Description	Value
Width	rt*RG + BH*rt
Height	d

2.2.6 Union 4 (uni4)

COMPOSE

Description	Value
Keep interior boundaries	Off

2.2.7 Rectangle 16 (r16)

POSITION

Description	Value
Position	{RG*rt, d/3}

SIZE

Description	Value
Width	(RG2*st) + (RG*rt + RG2*st + rt + d)
Height	(RG*rt + RG2*st + rt + st + d)

2.2.8 Rectangle 17 (r17)

POSITION

Description	Value
Position	{RG2*st, -(RG*rt + RG2*st + rt + st + d) + d/3}

SIZE

Description	Value
Width	(RG*rt) + (RG*rt + RG2*st + rt + d)
Height	(RG*rt + RG2*st + rt + st + d)

2.2.9 Union 1 (uni1)

COMPOSE

Description	Value

Description	Value
Keep interior boundaries	Off

2.2.10 Tip (pt1)

POINT

Description	Value
Point coordinate	{rt, d}

2.2.11 Sub (pt2)

POINT

Description	Value
Point coordinate	{st, 0}

2.2.12 Line Segment 1 (ls1)

SETTINGS

Description	Value
Specify	Coordinates
Coordinates	{0, 0}
Specify	Coordinates
Coordinates	{st, 0}

2.2.13 Form Union (fin)

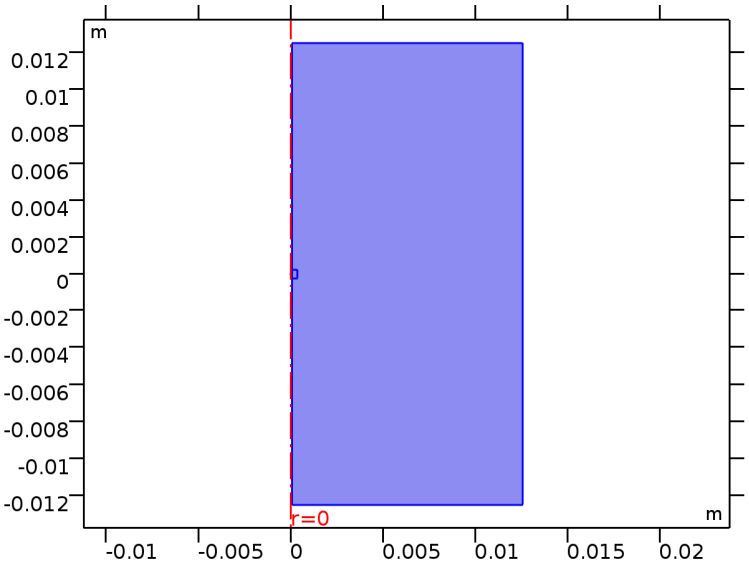
SETTINGS

Description	Value
Relative repair tolerance	1.0E-9

2.3 TRANSPORT OF DILUTED SPECIES

USED PRODUCTS

COMSOL Multiphysics
Electrochemistry Module



Transport of Diluted Species

SELECTION

Geometric entity level	Domain
Selection	Domains 1–3

EQUATIONS

$$\frac{\partial c_i}{\partial t} + \nabla \cdot (-D_i \nabla c_i) = R_i$$

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

SETTINGS

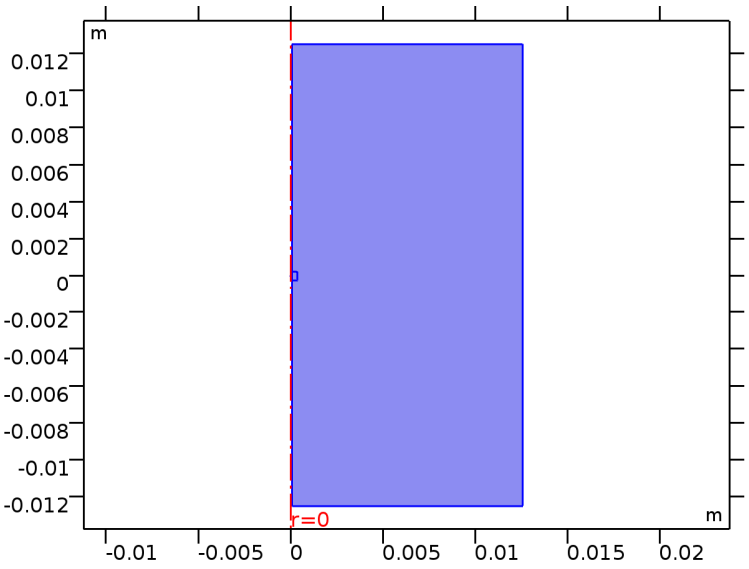
Description	Value
Concentration	Linear
Compute boundary fluxes	On
Apply smoothing to boundary fluxes	On
Value type when using splitting of complex variables	Real
Convection	Off
Migration in electric field	Off
Mass transfer in porous media	Off
Streamline diffusion	On
Crosswind diffusion	On
Equation residual	Approximate residual
Crosswind diffusion type for free flow	Do Carmo and Galeão
Convective term	Nonconservative form

VARIABLES

Name	Expression	Unit	Description	Selection
tds.R_o1	0	mol/(m³·s)	Total rate expression	Domains 1–3
tds.R_r1	0	mol/(m³·s)	Total rate expression	Domains 1–3
tds.epsilon_p	1	1	Porosity	Domains 1–3
tds.theta	tds.epsilon_p	1	Liquid volume fraction	Domains 1–3
tds.av	0	1	Gas volume fraction	Domains 1–3
tds.nr	nr	1	Normal vector, r component	Boundaries 508–510, 513, 515–516
tds.nphi	0	1	Normal vector, phi component	Boundaries 508–510, 513, 515–516
tds.nz	nz	1	Normal vector, z component	Boundaries 508–510, 513, 515–516
tds.nr	dnr	1	Normal vector, r component	Boundaries 1–507, 511–512, 514, 517–519
tds.nphi	0	1	Normal vector, phi component	Boundaries 1–507, 511–512, 514, 517–519
tds.nz	dnz	1	Normal vector, z component	Boundaries 1–507, 511–512, 514, 517–519
tds.nrmesh	root.nrmesh	1	Normal vector (mesh), r component	Boundaries 508–510, 513, 515–516
tds.nphimesh	0	1	Normal vector (mesh), phi component	Boundaries 508–510, 513, 515–516
tds.nzmesh	root.nzmesh	1	Normal vector (mesh), z component	Boundaries 508–510, 513, 515–516
tds.nrmesh	dnrmesh	1	Normal vector (mesh), r component	Boundaries 1–507, 511–512, 514, 517–519
tds.nphimesh	0	1	Normal vector (mesh), phi	Boundaries 1–507, 511–512,

Name	Expression	Unit	Description	Selection
			component	514, 517–519
tds.nzmesh	dnzmesh	1	Normal vector (mesh), z component	Boundaries 1–507, 511–512, 514, 517–519
tds.nrc	root.nrc/sqrt(root.nrc^2+root.nzc^2+eps)	1	Normal vector, r component	Boundaries 1–519
tds.nphic	0	1	Normal vector, phi component	Boundaries 1–519
tds.nzc	root.nzc/sqrt(root.nrc^2+root.nzc^2+eps)	1	Normal vector, z component	Boundaries 1–519

2.3.1 Transport Properties 1



Transport Properties 1

SELECTION

Geometric entity level	Domain
Selection	Domains 1–3

EQUATIONS

$$\frac{\partial c_i}{\partial t} + \nabla \cdot (-D_i \nabla c_i) = R_i$$

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

SETTINGS

Description	Value
Material	None

Description	Value
Temperature	User defined
Temperature	T
Diffusion coefficient	User defined
Diffusion coefficient	{{Do1, 0, 0}, {0, Do1, 0}, {0, 0, Do1}}
Diffusion coefficient	User defined
Diffusion coefficient	{{Dr1, 0, 0}, {0, Dr1, 0}, {0, 0, Dr1}}

USED PRODUCTS

COMSOL Multiphysics

Variables

Name	Expression	Unit	Description	Selection
domflux.o1r	2*tds.dflux_o1r*pi*r	mol/(m·s)	Domain flux, r component	Domains 1–3
domflux.o1z	2*tds.dflux_o1z*pi*r	mol/(m·s)	Domain flux, z component	Domains 1–3
domflux.r1r	2*tds.dflux_r1r*pi*r	mol/(m·s)	Domain flux, r component	Domains 1–3
domflux.r1z	2*tds.dflux_r1z*pi*r	mol/(m·s)	Domain flux, z component	Domains 1–3
tds.ndflux_o1	tds.bndFlux_o1	mol/(m^2·s)	Normal diffusive flux	Boundaries 2, 4–519
tds.ndflux_r1	tds.bndFlux_r1	mol/(m^2·s)	Normal diffusive flux	Boundaries 2, 4–519
tds.ntflux_o1	tds.bndFlux_o1	mol/(m^2·s)	Normal total flux	Boundaries 2, 4–519
tds.ntflux_r1	tds.bndFlux_r1	mol/(m^2·s)	Normal total flux	Boundaries 2, 4–519
tds.D_o1rr	Do1	m^2/s	Diffusion coefficient, rr component	Domains 1–3
tds.D_o1phir	0	m^2/s	Diffusion coefficient, phir component	Domains 1–3
tds.D_o1zr	0	m^2/s	Diffusion coefficient, zr component	Domains 1–3
tds.D_o1rphi	0	m^2/s	Diffusion coefficient, rphi component	Domains 1–3

Name	Expression	Unit	Description	Selection
tds.D_o1phiphi	Do1	m^2/s	Diffusion coefficient, phiphi component	Domains 1–3
tds.D_o1zphi	0	m^2/s	Diffusion coefficient, zphi component	Domains 1–3
tds.D_o1rz	0	m^2/s	Diffusion coefficient, rz component	Domains 1–3
tds.D_o1phiz	0	m^2/s	Diffusion coefficient, phiz component	Domains 1–3
tds.D_o1zz	Do1	m^2/s	Diffusion coefficient, zz component	Domains 1–3
tds.D_r1rr	Dr1	m^2/s	Diffusion coefficient, rr component	Domains 1–3
tds.D_r1phir	0	m^2/s	Diffusion coefficient, phir component	Domains 1–3
tds.D_r1zr	0	m^2/s	Diffusion coefficient, zr component	Domains 1–3
tds.D_r1rphi	0	m^2/s	Diffusion coefficient, rphi component	Domains 1–3
tds.D_r1phiphi	Dr1	m^2/s	Diffusion coefficient, phiphi component	Domains 1–3
tds.D_r1zphi	0	m^2/s	Diffusion coefficient, zphi component	Domains 1–3
tds.D_r1rz	0	m^2/s	Diffusion coefficient, rz component	Domains 1–3
tds.D_r1phiz	0	m^2/s	Diffusion coefficient, phiz component	Domains 1–3
tds.D_r1zz	Dr1	m^2/s	Diffusion coefficient, zz component	Domains 1–3
tds.Dav_o1	0.5*(tds.D_o1rr+tds.D_o1zz)	m^2/s	Average diffusion	Domains 1–3

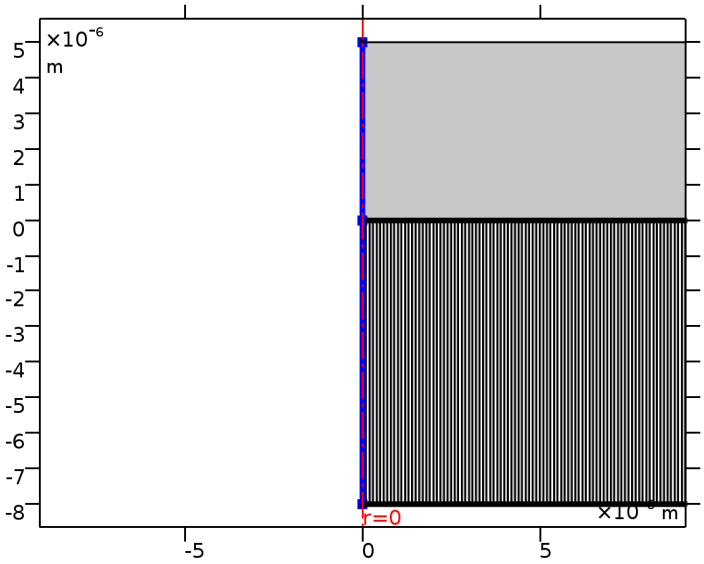
Name	Expression	Unit	Description	Selection
			coefficient	
tds.Dav_r1	0.5*(tds.D_r1rr+tds.D_r1zz)	m^2/s	Average diffusion coefficient	Domains 1–3
tds.tflux_o1r	tds.dflux_o1r	$mol/(m^2 \cdot s)$	Total flux, r component	Domains 1–3
tds.tflux_o1phi	tds.dflux_o1phi	$mol/(m^2 \cdot s)$	Total flux, phi component	Domains 1–3
tds.tflux_o1z	tds.dflux_o1z	$mol/(m^2 \cdot s)$	Total flux, z component	Domains 1–3
tds.tflux_r1r	tds.dflux_r1r	$mol/(m^2 \cdot s)$	Total flux, r component	Domains 1–3
tds.tflux_r1phi	tds.dflux_r1phi	$mol/(m^2 \cdot s)$	Total flux, phi component	Domains 1–3
tds.tflux_r1z	tds.dflux_r1z	$mol/(m^2 \cdot s)$	Total flux, z component	Domains 1–3
tds.dfluxMag_o1	sqrt(tds.dflux_o1r^2+tds.dflux_o1phi^2+tds.dflux_o1z^2)	$mol/(m^2 \cdot s)$	Diffusive flux magnitude	Domains 1–3
tds.dfluxMag_r1	sqrt(tds.dflux_r1r^2+tds.dflux_r1phi^2+tds.dflux_r1z^2)	$mol/(m^2 \cdot s)$	Diffusive flux magnitude	Domains 1–3
tds.tfluxMag_o1	sqrt(tds.tflux_o1r^2+tds.tflux_o1phi^2+tds.tflux_o1z^2)	$mol/(m^2 \cdot s)$	Total flux magnitude	Domains 1–3
tds.tfluxMag_r1	sqrt(tds.tflux_r1r^2+tds.tflux_r1phi^2+tds.tflux_r1z^2)	$mol/(m^2 \cdot s)$	Total flux magnitude	Domains 1–3
tds.dflux_o1r	-tds.D_o1rr*o1r-tds.D_o1rz*o1z	$mol/(m^2 \cdot s)$	Diffusive flux, r component	Domains 1–3
tds.dflux_o1phi	-tds.D_o1phir*o1r-tds.D_o1phiz*o1z	$mol/(m^2 \cdot s)$	Diffusive flux, phi component	Domains 1–3
tds.dflux_o1z	-tds.D_o1zr*o1r-tds.D_o1zz*o1z	$mol/(m^2 \cdot s)$	Diffusive flux, z component	Domains 1–3
tds.dflux_r1r	-tds.D_r1rr*r1r-tds.D_r1rz*r1z	$mol/(m^2 \cdot s)$	Diffusive flux, r component	Domains 1–3
tds.dflux_r1phi	-tds.D_r1phir*r1r-tds.D_r1phiz*r1z	$mol/(m^2 \cdot s)$	Diffusive flux, phi component	Domains 1–3
tds.dflux_r1z	-tds.D_r1zr*r1r-tds.D_r1zz*r1z	$mol/(m^2 \cdot s)$	Diffusive flux, z component	Domains 1–3
tds.grad_o1r	o1r	mol/m^4	Concentration gradient, r component	Domains 1–3
tds.grad_o1phi	0	mol/m^4	Concentration gradient, phi component	Domains 1–3

Name	Expression	Unit	Description	Selection
tds.grad_o1z	o1z	mol/m^4	Concentration gradient, z component	Domains 1–3
tds.grad_r1r	r1r	mol/m^4	Concentration gradient, r component	Domains 1–3
tds.grad_r1phi	0	mol/m^4	Concentration gradient, phi component	Domains 1–3
tds.grad_r1z	r1z	mol/m^4	Concentration gradient, z component	Domains 1–3
tds.bndFlux_o1	if(r>0.001/sqrt(sqrt(mean(emetric2))),-0.5*dflux_spatial(o1)/(pi*r),NaN)	mol/(m^2·s)	Boundary flux	Boundaries 1–507, 511–512, 514, 517–519
tds.bndFlux_o1	if(r>0.001/sqrt(sqrt(mean(emetric2))),0.25*(uflux_spatial(o1)-dflux_spatial(o1))/(pi*r),NaN)	mol/(m^2·s)	Boundary flux	Boundaries 508–510, 513, 515–516
tds.bndFlux_r1	if(r>0.001/sqrt(sqrt(mean(emetric2))),-0.5*dflux_spatial(r1)/(pi*r),NaN)	mol/(m^2·s)	Boundary flux	Boundaries 1–507, 511–512, 514, 517–519
tds.bndFlux_r1	if(r>0.001/sqrt(sqrt(mean(emetric2))),0.25*(uflux_spatial(r1)-dflux_spatial(r1))/(pi*r),NaN)	mol/(m^2·s)	Boundary flux	Boundaries 508–510, 513, 515–516
tds.helem	h	m	Element size	Domains 1–3
tds.glim_mass	0.1[mol/m^3]/tds.helem	mol/m^4	Lower gradient limit	Domains 1–3
tds.Res_o1	o1t-tds.R_o1	mol/(m^3·s)	Equation residual	Domains 1–3
tds.Res_r1	r1t-tds.R_r1	mol/(m^3·s)	Equation residual	Domains 1–3

Shape functions

Name	Shape function	Unit	Description	Shape frame	Selection
o1	Lagrange (Linear)	mol/m^3	Concentration	Material	Domains 1–3
r1	Lagrange (Linear)	mol/m^3	Concentration	Material	Domains 1–3

2.3.2 Axial Symmetry 1



Axial Symmetry 1

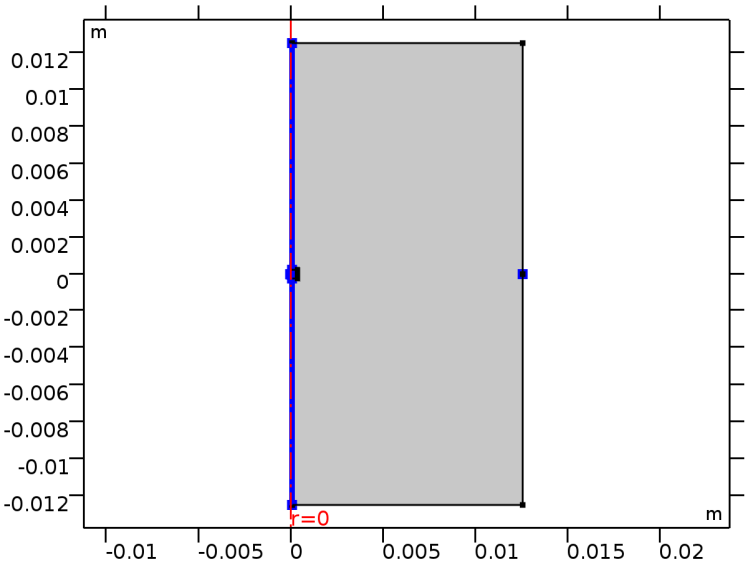
SELECTION

Geometric entity level	Boundary
Selection	Boundaries 1, 3

USED PRODUCTS

COMSOL Multiphysics

2.3.3 No Flux 1



No Flux 1

SELECTION

Geometric entity level	Boundary
Selection	Boundaries 2, 6, 8, 10, 12, 14, 16, 18, 20, 22, 24, 26, 28, 30, 32, 34, 36, 38, 40, 42, 44, 46, 48, 50, 52, 54, 56, 58, 60, 62, 64, 66, 68, 70, 72, 74, 76, 78, 80, 82, 84, 86, 88, 90, 92, 94, 96, 98, 100, 102, 104, 106, 108, 110, 112, 114, 116, 118, 120, 122, 124, 126, 128, 130, 132, 134, 136, 138, 140, 142, 144, 146, 148, 150, 152, 154, 156, 158, 160, 162, 164, 166, 168, 170, 172, 174, 176, 178, 180, 182, 184, 186, 188, 190, 192, 194, 196, 198, 200, 202, 204, 206, 208, 210, 212, 214, 216, 218, 220, 222, 224, 226, 228, 230, 232, 234, 236, 238, 240, 242, 244, 246, 248, 250, 252, 254, 256, 258, 260, 262, 264, 266, 268, 270, 272, 274, 276, 278, 280, 282, 284, 286, 288, 290, 292, 294, 296, 298, 300, 302, 304, 306, 308, 310, 312, 314, 316, 318, 320, 322, 324, 326, 328, 330, 332, 334, 336, 338, 340, 342, 344, 346, 348, 350, 352, 354, 356, 358, 360, 362, 364, 366, 368, 370, 372, 374, 376, 378, 380, 382, 384, 386, 388, 390, 392, 394, 396, 398, 400, 402, 404, 406, 408, 410, 412, 414, 416, 418, 420, 422, 424, 426, 428, 430, 432, 434, 436, 438, 440, 442, 444, 446, 448, 450, 452, 454, 456, 458, 460, 462, 464, 466, 468, 470, 472, 474, 476, 478, 480, 482, 484, 486, 488, 490, 492, 494, 496, 498, 500, 502–505, 507, 511–512, 518

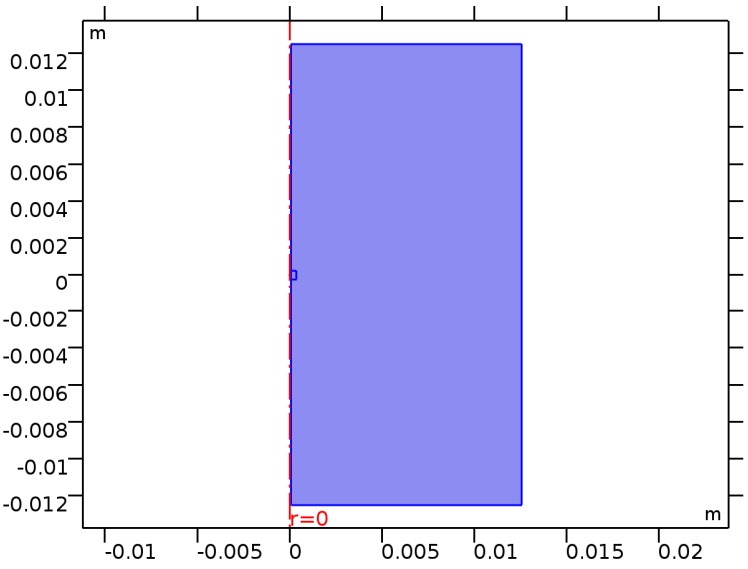
EQUATIONS

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

USED PRODUCTS

COMSOL Multiphysics

2.3.4 Initial Values 1



Initial Values 1

SELECTION

Geometric entity level	Domain
Selection	Domains 1–3

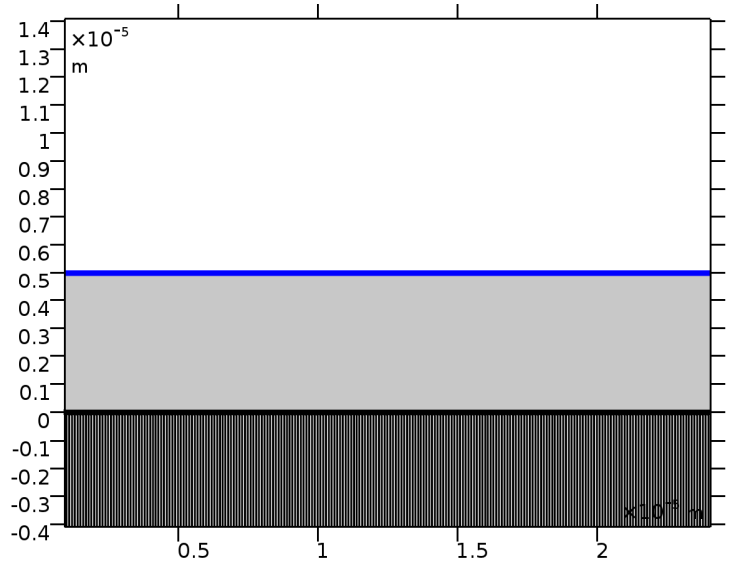
SETTINGS

Description	Value
Concentration	{co1, eps[mmol/L]}

USED PRODUCTS

COMSOL Multiphysics

2.3.5 Tip



Tip

SELECTION

Geometric entity level	Boundary
Name	Tip
Selection	Boundary 4

EQUATIONS

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

SETTINGS

Description	Value
Flux type	General inward flux
Species o1	On
Species r1	On

Description	Value
Inward flux	{(-kf1*o1 + kb1*r1), -(-kf1*o1 + kb1*r1)}

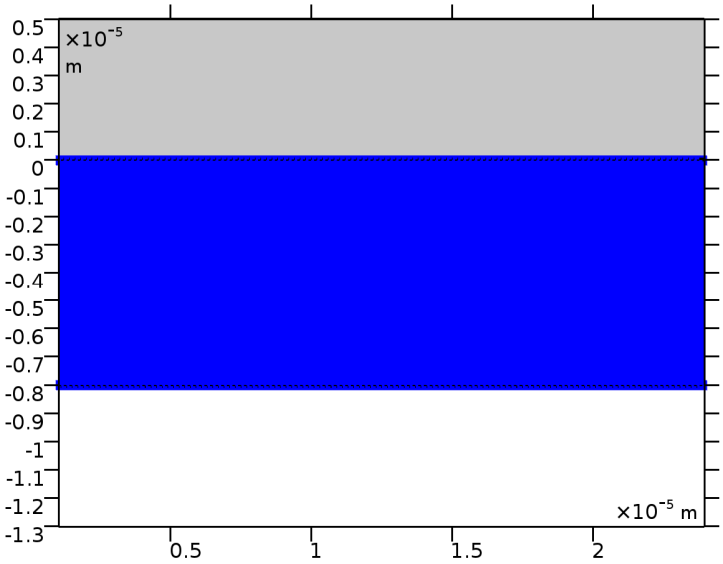
USED PRODUCTS

COMSOL Multiphysics

Weak expressions

Weak expression	Integration order	Integration frame	Selection
2*(-kf1*o1+kb1*r1)*test(o1)*pi*r	2	Material	Boundary 4
-2*(-kf1*o1+kb1*r1)*test(r1)*pi*r	2	Material	Boundary 4

2.3.6 Substrate Feedback Ads



Substrate Feedback Ads

SELECTION

Geometric entity level	Boundary
Name	Substrate
Selection	Boundaries 5, 7, 9, 11, 13, 15, 17, 19, 21, 23, 25, 27, 29, 31, 33, 35, 37, 39, 41, 43, 45, 47, 49, 51, 53, 55, 57, 59, 61, 63, 65, 67, 69, 71, 73, 75, 77, 79, 81, 83, 85, 87, 89, 91, 93, 95, 97, 99, 101, 103, 105, 107, 109, 111, 113, 115, 117, 119, 121, 123, 125, 127, 129, 131, 133, 135, 137, 139, 141, 143, 145, 147, 149, 151, 153, 155, 157, 159, 161, 163, 165, 167, 169, 171, 173, 175, 177, 179, 181, 183, 185, 187, 189, 191, 193, 195, 197, 199, 201, 203, 205, 207, 209, 211, 213, 215, 217, 219, 221, 223, 225, 227, 229, 231, 233, 235, 237, 239, 241, 243, 245, 247, 249, 251, 253, 255, 257, 259, 261, 263, 265, 267, 269, 271, 273, 275, 277, 279, 281, 283, 285, 287, 289, 291, 293, 295, 297, 299, 301, 303, 305, 307, 309, 311, 313, 315, 317, 319, 321, 323, 325, 327, 329, 331, 333, 335, 337, 339, 341, 343, 345, 347, 349, 351, 353, 355,

	357, 359, 361, 363, 365, 367, 369, 371, 373, 375, 377, 379, 381, 383, 385, 387, 389, 391, 393, 395, 397, 399, 401, 403, 405, 407, 409, 411, 413, 415, 417, 419, 421, 423, 425, 427, 429, 431, 433, 435, 437, 439, 441, 443, 445, 447, 449, 451, 453, 455, 457, 459, 461, 463, 465, 467, 469, 471, 473, 475, 477, 479, 481, 483, 485, 487, 489, 491, 493, 495, 497, 499, 501

EQUATIONS

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

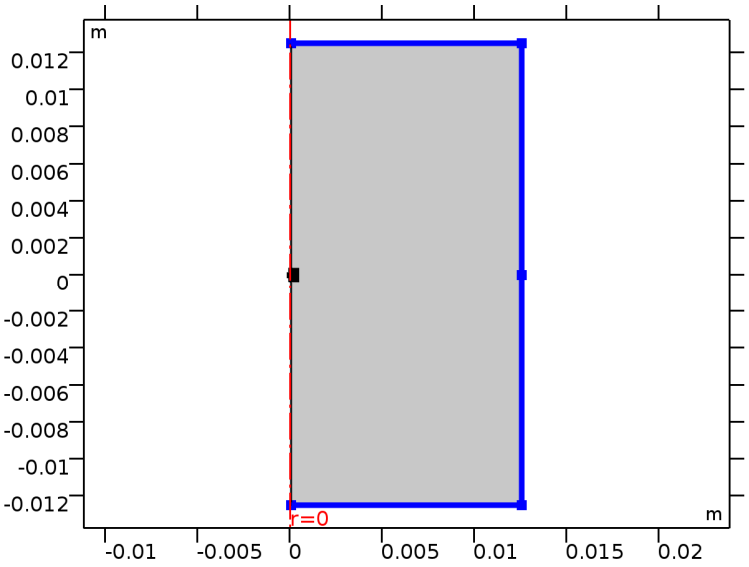
SETTINGS

Description	Value
Flux type	General inward flux
Species o1	On
Species r1	On
Inward flux	{((theta1 - theta2)*k_ox1*r1 + (theta2)*k_ox2*r1)*2, (-((theta1 - theta2)*k_ox1*r1 + (theta2)*k_ox2*r1))*2}

USED PRODUCTS

COMSOL Multiphysics

2.3.7 Concentration 1



Concentration 1

SELECTION

Geometric entity level	Boundary
Selection	Boundaries 506, 514, 517, 519

EQUATIONS

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

SETTINGS

Description	Value
Species o1	On
Species r1	On
Concentration	{co1, eps[mmol/L]}
Apply reaction terms on	All physics (symmetric)
Use weak constraints	Off
Constraint method	Elemental

USED PRODUCTS

COMSOL Multiphysics

Variables

Name	Expression	Unit	Description	Selection
tds.c0_o1	co1	mol/m³	Concentration	Boundaries 506, 514, 517, 519
tds.c0_r1	eps[mmol/L]	mol/m³	Concentration	Boundaries 506, 514, 517, 519

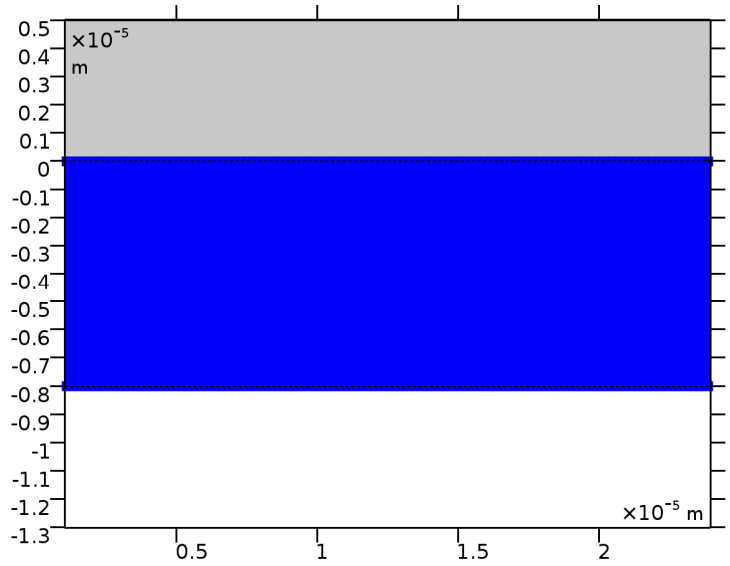
Shape functions

Constraint	Constraint force	Shape function	Selection
-o1+tds.c0_o1	test(-o1+tds.c0_o1)	Lagrange (Linear)	Boundaries 506, 514, 517, 519
-r1+tds.c0_r1	test(-r1+tds.c0_r1)	Lagrange (Linear)	Boundaries 506, 514, 517, 519

2.4 SURFACE REACTIONS

USED PRODUCTS

COMSOL Multiphysics
Electrochemistry Module



Surface Reactions

SELECTION

Geometric entity level	Boundary
Name	Substrate
Selection	Substrate

EQUATIONS

$$\frac{\partial c_{s,j}}{\partial t} + \nabla_t \cdot (-D_i \nabla_t c_{s,j}) = R_{s,j}$$

$$\mathbf{N}_{s,j} = -D_i \nabla_t c_{s,j}$$

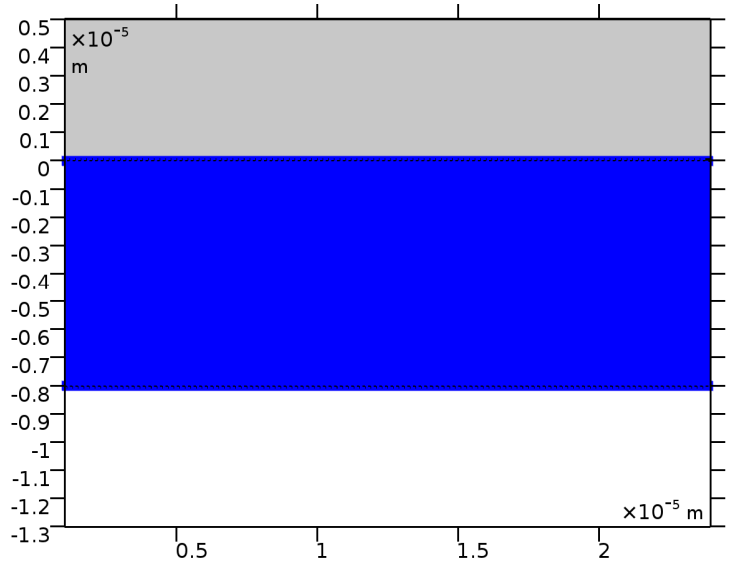
$$\theta_i = \frac{c_{s,j} \sigma_i}{\Gamma_s}$$

$$\frac{\partial c_{b,j}}{\partial t} = R_{b,j}$$

SETTINGS

Description	Value
Surface concentration	Linear
Bulk concentration	Linear
Value type when using splitting of complex variables	{Real, Real}

2.4.1 Surface Properties 1



Surface Properties 1

SELECTION

Geometric entity level	Boundary
Selection	Substrate

EQUATIONS

$$\frac{\partial c_{s,j}}{\partial t} + \nabla_t \cdot (-D_i \nabla_t c_{s,j}) = R_{s,j}$$

$$\mathbf{N}_{s,j} = -D_i \nabla_t c_{s,j}$$

$$\theta_i = \frac{c_{s,j}\sigma_i}{\Gamma_s}$$

SETTINGS

Description	Value
Density of sites	ML_mol
Site occupancy number	{Sigma_cs1, Sigma_cs2}
Surface material	None
Diffusion coefficient	User defined
Diffusion coefficient	{{Dcs1, 0, 0}, {0, Dcs1, 0}, {0, 0, Dcs1}}
Diffusion coefficient	User defined
Diffusion coefficient	{{Dcs1, 0, 0}, {0, Dcs1, 0}, {0, 0, Dcs1}}

Variables

Name	Expression	Unit	Description	Selection

Name	Expression	Unit	Description	Selection
sr.Rs_cs1	0	mol/(m²·s)	Reaction rate for surface species	Substrate
sr.Rs_cs2	0	mol/(m²·s)	Reaction rate for surface species	Substrate
sr.Dav_cs1	0.5*(sr.D_cs1rr+sr.D_cs1zz)	m²/s	Average diffusion coefficient	Substrate
sr.Dav_cs2	0.5*(sr.D_cs2rr+sr.D_cs2zz)	m²/s	Average diffusion coefficient	Substrate
sr.Gamma	ML_mol	mol/m²	Density of sites	Substrate
sr.Sigma_cs1	Sigma_cs1	1	Site occupancy number	Substrate
sr.Sigma_cs2	Sigma_cs2	1	Site occupancy number	Substrate
sr.D_cs1rr	Dcs1	m²/s	Diffusion coefficient, rr component	Substrate
sr.D_cs1phir	0	m²/s	Diffusion coefficient, phir component	Substrate
sr.D_cs1zr	0	m²/s	Diffusion coefficient, zr component	Substrate
sr.D_cs1rphi	0	m²/s	Diffusion coefficient, rphi component	Substrate
sr.D_cs1phiphi	Dcs1	m²/s	Diffusion coefficient, phiphi component	Substrate
sr.D_cs1zphi	0	m²/s	Diffusion coefficient, zphi component	Substrate
sr.D_cs1rz	0	m²/s	Diffusion coefficient, rz component	Substrate
sr.D_cs1phiz	0	m²/s	Diffusion coefficient, phiz component	Substrate
sr.D_cs1zz	Dcs1	m²/s	Diffusion coefficient, zz component	Substrate
sr.D_cs2rr	Dcs1	m²/s	Diffusion coefficient, rr	Substrate

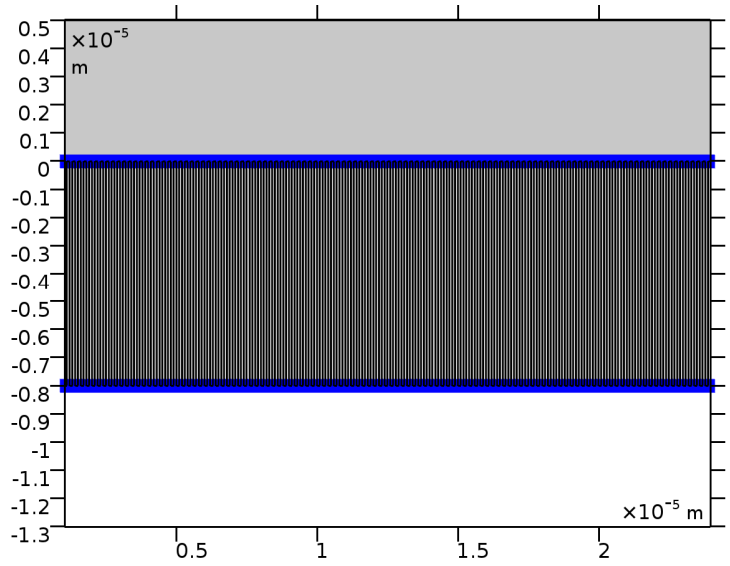
Name	Expression	Unit	Description	Selection
			component	
sr.D_cs2phir	0	m^2/s	Diffusion coefficient, phir component	Substrate
sr.D_cs2zr	0	m^2/s	Diffusion coefficient, zr component	Substrate
sr.D_cs2rphi	0	m^2/s	Diffusion coefficient, rphi component	Substrate
sr.D_cs2phiphi	Dcs1	m^2/s	Diffusion coefficient, phiphi component	Substrate
sr.D_cs2zphi	0	m^2/s	Diffusion coefficient, zphi component	Substrate
sr.D_cs2rz	0	m^2/s	Diffusion coefficient, rz component	Substrate
sr.D_cs2phiz	0	m^2/s	Diffusion coefficient, phiz component	Substrate
sr.D_cs2zz	Dcs1	m^2/s	Diffusion coefficient, zz component	Substrate
sr.theta_i_cs1	max(eps^2,sr.Sigma_cs1*cs1/sr.Gamma)	1	Surface coverage	Substrate
sr.theta_i_cs2	max(eps^2,sr.Sigma_cs2*cs2/sr.Gamma)	1	Surface coverage	Substrate
sr.theta_i0	sr.theta_i_cs1+sr.theta_i_cs2	1	Surface coverage	Substrate
sr.dflux_cs1r	-(sr.D_cs1rr*cs1Tr+sr.D_cs1rz*cs1Tz)*sr.Gamma/sr.Sigma_cs1	$mol^2/(m^3 \cdot s)$	Diffusive flux, r component	Substrate
sr.dflux_cs1phi	-(sr.D_cs1phir*cs1Tr+sr.D_cs1phiz*cs1Tz)*sr.Gamma/sr.Sigma_cs1	$mol^2/(m^3 \cdot s)$	Diffusive flux, phi component	Substrate
sr.dflux_cs1z	-(sr.D_cs1zr*cs1Tr+sr.D_cs1zz*cs1Tz)*sr.Gamma/sr.Sigma_cs1	$mol^2/(m^3 \cdot s)$	Diffusive flux, z component	Substrate
sr.dflux_cs2r	-(sr.D_cs2rr*cs2Tr+sr.D_cs2rz*cs2	$mol^2/(m^3 \cdot s)$	Diffusive flux, r component	Substrate

Name	Expression	Unit	Description	Selection
	Tz)*sr.Gamma/sr.Sigma_cs2			
sr.dflux_cs2phi	-(sr.D_cs2phir*cs2Tr+sr.D_cs2phiz*cs2Tz)*sr.Gamma/sr.Sigma_cs2	$mol^2/(m^3 \cdot s)$	Diffusive flux, phi component	Substrate
sr.dflux_cs2z	-(sr.D_cs2zr*cs2Tr+sr.D_cs2zz*cs2Tz)*sr.Gamma/sr.Sigma_cs2	$mol^2/(m^3 \cdot s)$	Diffusive flux, z component	Substrate
sr.grad_cs1r	cs1Tr	mol/m^3	Concentration gradient, r component	Substrate
sr.grad_cs1phi	0	mol/m^3	Concentration gradient, phi component	Substrate
sr.grad_cs1z	cs1Tz	mol/m^3	Concentration gradient, z component	Substrate
sr.grad_cs2r	cs2Tr	mol/m^3	Concentration gradient, r component	Substrate
sr.grad_cs2phi	0	mol/m^3	Concentration gradient, phi component	Substrate
sr.grad_cs2z	cs2Tz	mol/m^3	Concentration gradient, z component	Substrate
sr.tflux_cs1r	-(sr.D_cs1rr*cs1Tr+sr.D_cs1rz*cs1Tz)*sr.Gamma/sr.Sigma_cs1	$mol^2/(m^3 \cdot s)$	Total flux, r component	Substrate
sr.tflux_cs1phi	-(sr.D_cs1phir*cs1Tr+sr.D_cs1phiz*cs1Tz)*sr.Gamma/sr.Sigma_cs1	$mol^2/(m^3 \cdot s)$	Total flux, phi component	Substrate
sr.tflux_cs1z	-(sr.D_cs1zr*cs1Tr+sr.D_cs1zz*cs1Tz)*sr.Gamma/sr.Sigma_cs1	$mol^2/(m^3 \cdot s)$	Total flux, z component	Substrate
sr.tflux_cs2r	-(sr.D_cs2rr*cs2Tr+sr.D_cs2rz*cs2Tz)*sr.Gamma/sr.Sigma_cs2	$mol^2/(m^3 \cdot s)$	Total flux, r component	Substrate
sr.tflux_cs2phi	-(sr.D_cs2phir*cs2Tr+sr.D_cs2phiz*cs2Tz)*sr.Gamma/sr.Sigma_cs2	$mol^2/(m^3 \cdot s)$	Total flux, phi component	Substrate

Name	Expression	Unit	Description	Selection
sr.tflux_cs2z	-(sr.D_cs2zr*cs2Tr+sr.D_cs2zz*cs2Tz)*sr.Gamma/sr.Sigma_cs2	mol²/(m³·s)	Total flux, z component	Substrate
sr.dfluxMag_cs1	sqrt(sr.dflux_cs1r^2+sr.dflux_cs1phi^2+sr.dflux_cs1z^2)	mol²/(m³·s)	Diffusive flux magnitude	Substrate
sr.dfluxMag_cs2	sqrt(sr.dflux_cs2r^2+sr.dflux_cs2phi^2+sr.dflux_cs2z^2)	mol²/(m³·s)	Diffusive flux magnitude	Substrate
sr.tfluxMag_cs1	sqrt(sr.tflux_cs1r^2+sr.tflux_cs1phi^2+sr.tflux_cs1z^2)	mol²/(m³·s)	Total flux magnitude	Substrate
sr.tfluxMag_cs2	sqrt(sr.tflux_cs2r^2+sr.tflux_cs2phi^2+sr.tflux_cs2z^2)	mol²/(m³·s)	Total flux magnitude	Substrate
sr.theta_free	max(eps^2,min(1,1-sr.theta_i0))	1	Fraction of free sites	Substrate

Shape functions

2.4.2 No Flux 1



No Flux 1

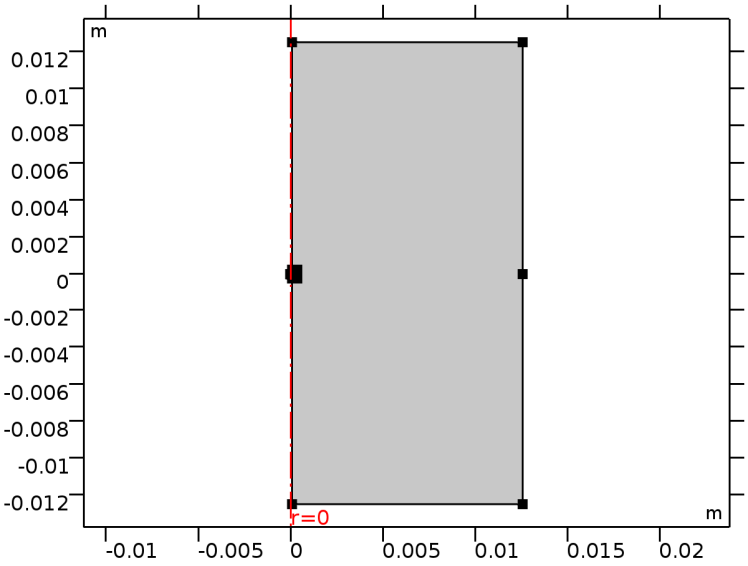
SELECTION

Geometric entity level	Point
Selection	Points 4–501

EQUATIONS

$$-\mathbf{n}\cdot\mathbf{N}_{s,i}=0$$

2.4.3 Axial Symmetry 1

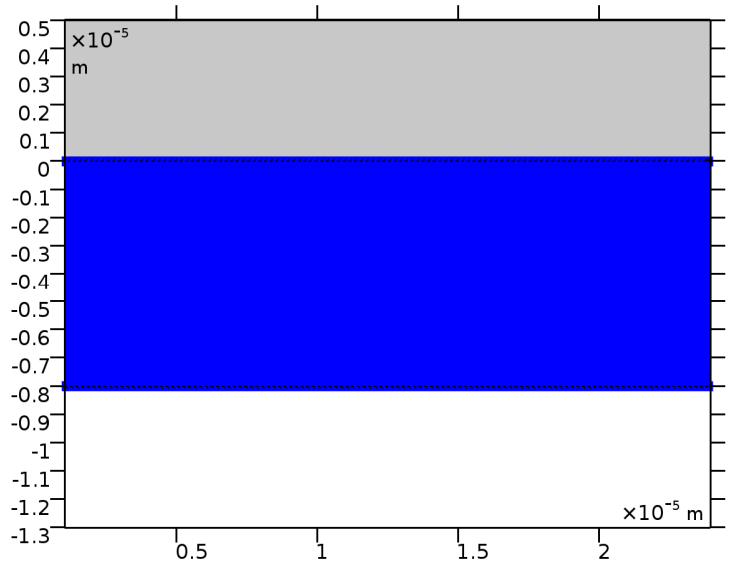


Axial Symmetry 1

SELECTION

Geometric entity level	Point
Selection	No points

2.4.4 Initial Values 1



Initial Values 1

SELECTION

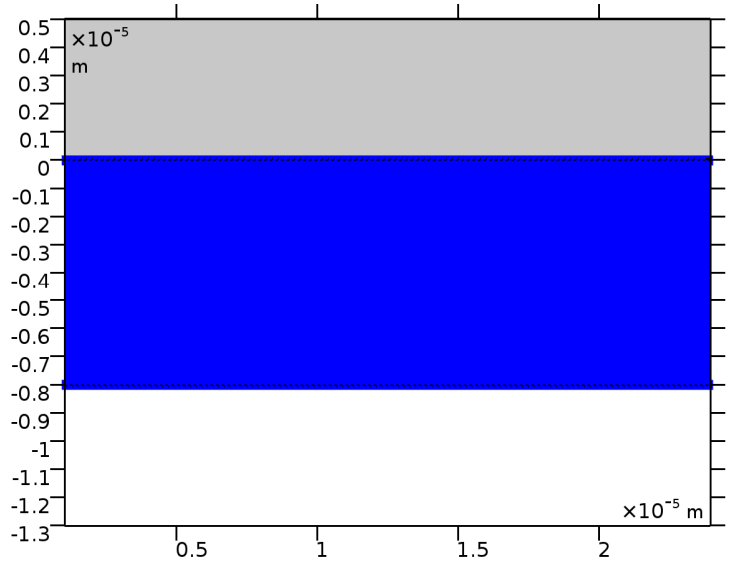
Geometric entity level	Boundary

Selection	Substrate

SETTINGS

Description	Value
Surface concentration	{cs10, cs20}

2.4.5 Reactions 1



Reactions 1

SELECTION

Geometric entity level	Boundary
Name	Substrate
Selection	Substrate

EQUATIONS

$$\frac{\partial c_{s,j}}{\partial t} + \nabla_t \cdot (-D_i \nabla_t c_{s,j}) = R_{s,j}$$

SETTINGS

Description	Value
Reaction rate for surface species	User defined
Reaction rate for surface species	-(theta1 - theta2)*k_ox1*r1
Reaction rate for surface species	User defined
Reaction rate for surface species	-(theta2)*k_ox2*r1

Variables

Name	Expression	Unit	Description	Selection

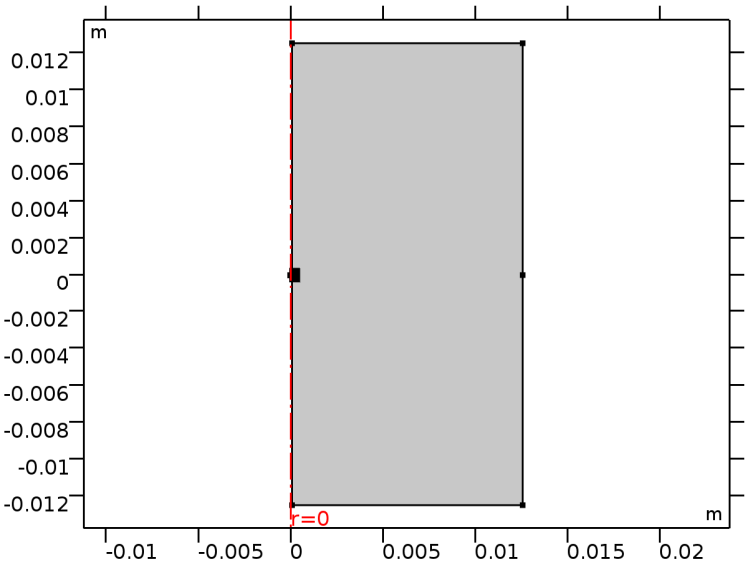
Name	Expression	Unit	Description	Selection
sr.Rs_cs1	model.input.Rs_cs1	mol/(m²·s)	Reaction rate for surface species	Substrate
sr.Rs_cs2	model.input.Rs_cs2	mol/(m²·s)	Reaction rate for surface species	Substrate

Weak expressions

Weak expression	Integration order	Integration frame	Selection
2*model.input.Rs_cs1*test(cs1)*pi*r	2	Material	Substrate
2*model.input.Rs_cs2*test(cs2)*pi*r	2	Material	Substrate

2.5 MESHES

2.5.1 Mesh 1



Mesh 1

Size (size)

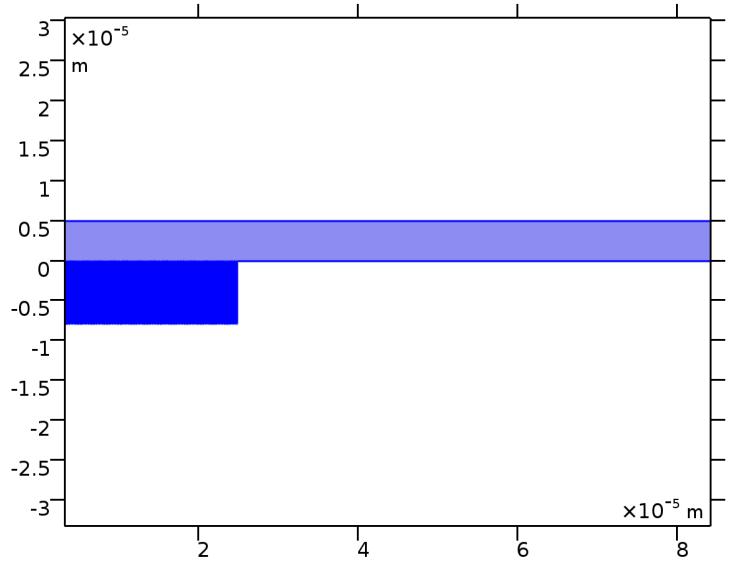
SETTINGS

Description	Value
Maximum element size	0.00168
Minimum element size	7.5E-6
Curvature factor	0.3
Maximum element growth rate	1.3

Mapped 1 (map1)

SELECTION

Geometric entity level	Domain
Name	dL domain
Selection	Domain 1

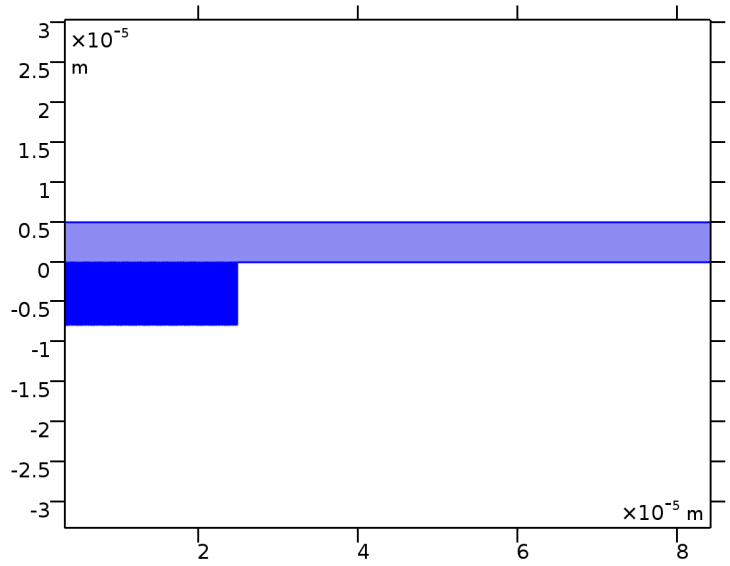


Mapped 1

Size 1 (size1)

SELECTION

Geometric entity level	Domain
Name	dL domain
Selection	Domain 1



Size 1

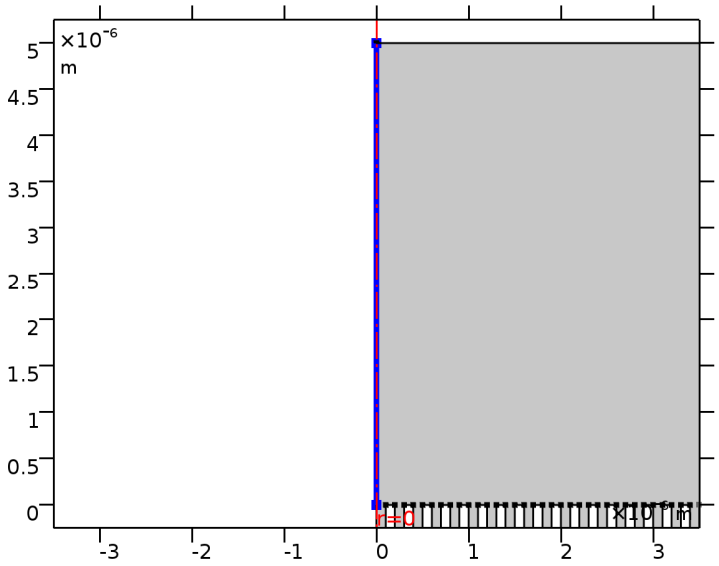
SETTINGS

Description	Value
Maximum element size	0.001/10000
Minimum element size	1E-8
Curvature factor	0.3
Maximum element growth rate	1.2
Custom element size	Custom

Distribution 1 (dis1)

SELECTION

Geometric entity level	Boundary
Name	Axis
Selection	Boundary 3



Distribution 1

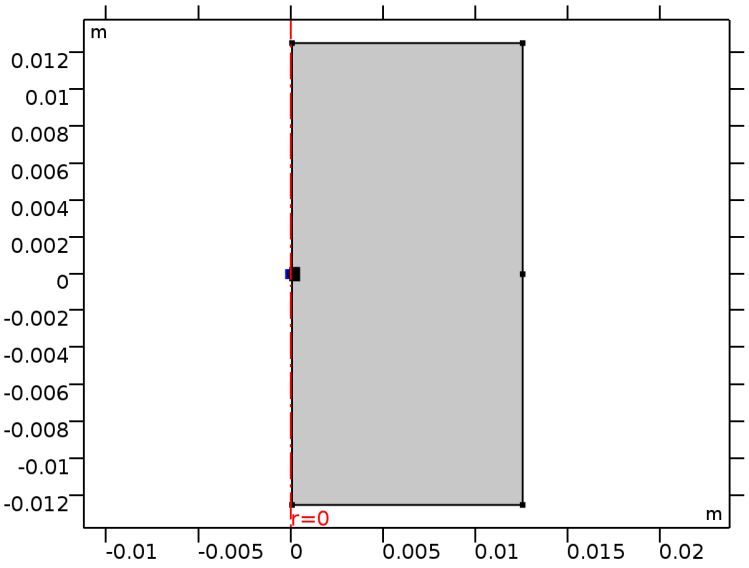
SETTINGS

Description	Value
Distribution properties	Predefined distribution type
Number of elements	20
Element ratio	10
Symmetric distribution	On

Free Triangular 1 (ftri1)

SELECTION

Geometric entity level	Remaining

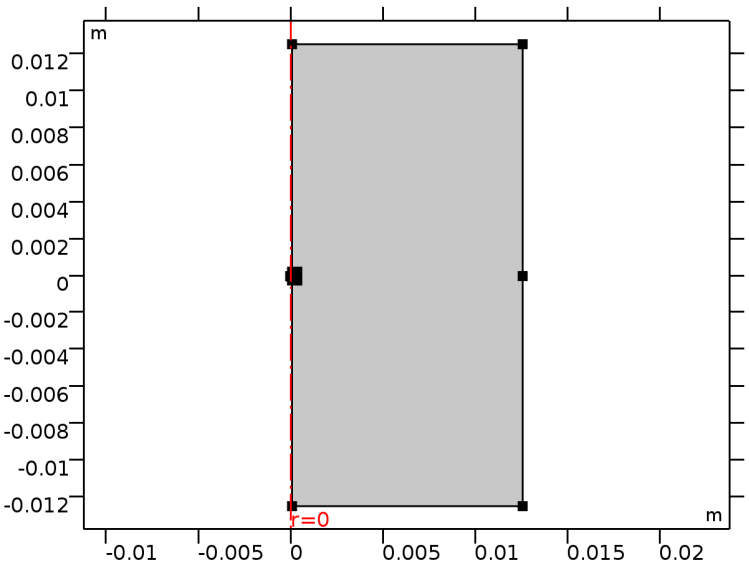


Free Triangular 1

Size 1 (size1)

SELECTION

Geometric entity level	Domain
Selection	Geometry geom1



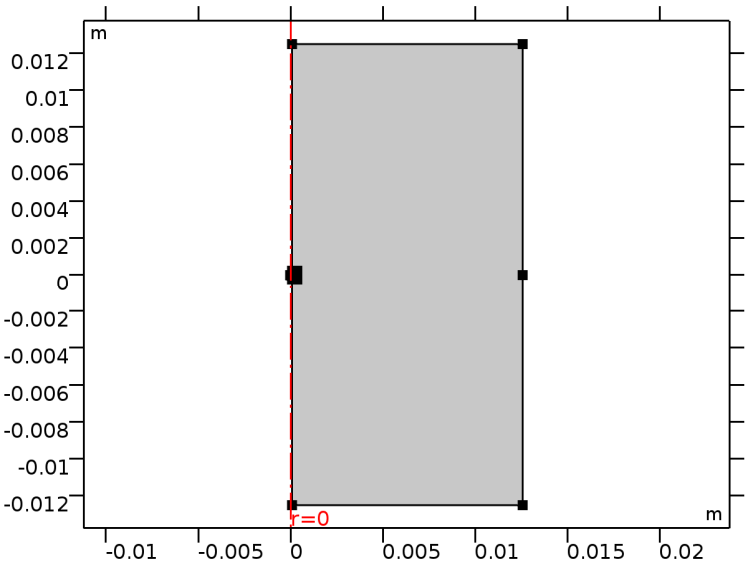
Size 1

SETTINGS

Description	Value
Maximum element size	9.25E-4

Description	Value
Minimum element size	3.13E-6
Curvature factor	0.25
Maximum element growth rate	1.25
Predefined size	Finer

2.5.2 Mesh 2



Mesh 2

Size (size)

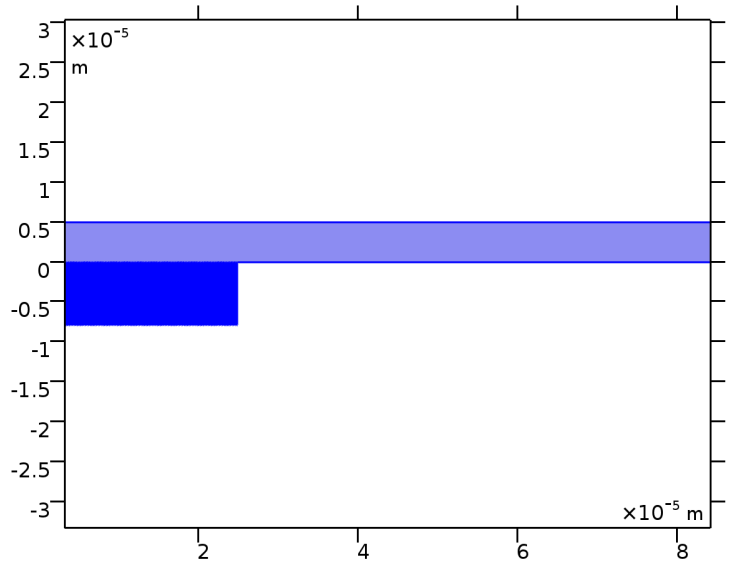
SETTINGS

Description	Value
Maximum element size	2.5E-4
Minimum element size	5.0E-7
Curvature factor	0.2
Predefined size	Extremely fine

Free Triangular 1 (ftri1)

SELECTION

Geometric entity level	Domain
Selection	Domain 1

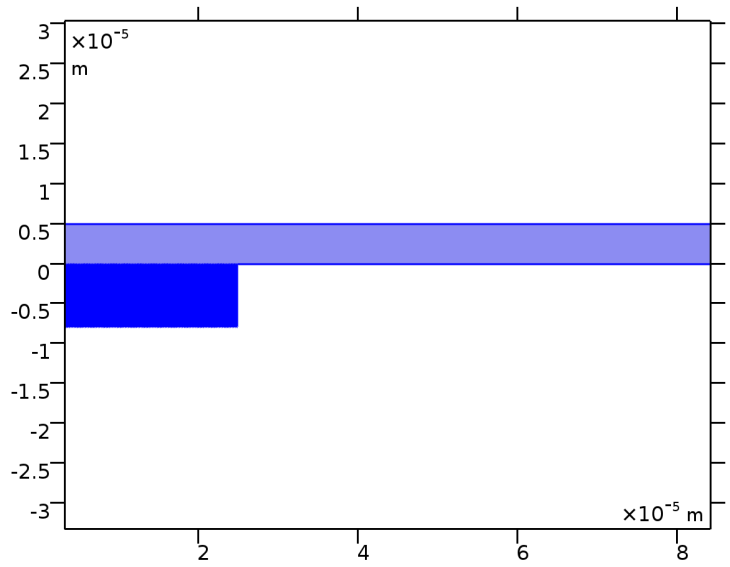


Free Triangular 1

Size 1 (size1)

SELECTION

Geometric entity level	Domain
Selection	Domain 1



Size 1

SETTINGS

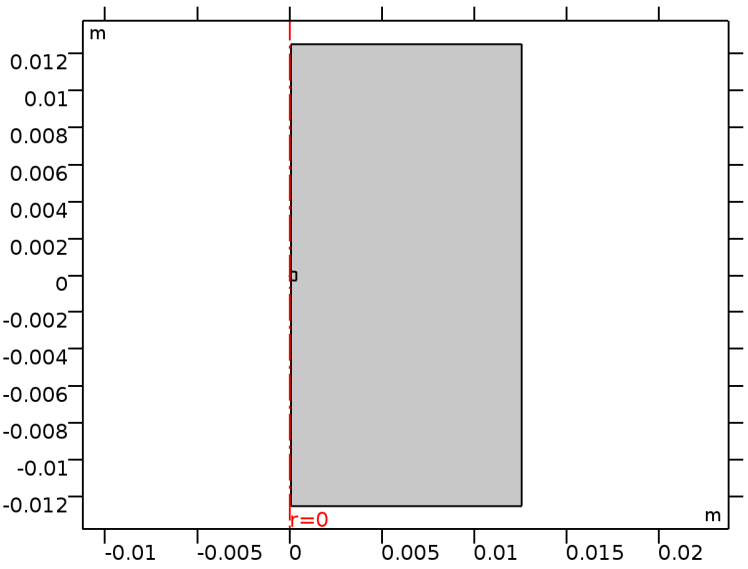
Description	Value
Maximum element size	1e-6

Description	Value
Minimum element size	3.13E-6
Minimum element size	Off
Curvature factor	0.25
Curvature factor	Off
Resolution of narrow regions	Off
Maximum element growth rate	1.25
Maximum element growth rate	Off
Predefined size	Finer
Custom element size	Custom

Free Triangular 2 (ftri2)

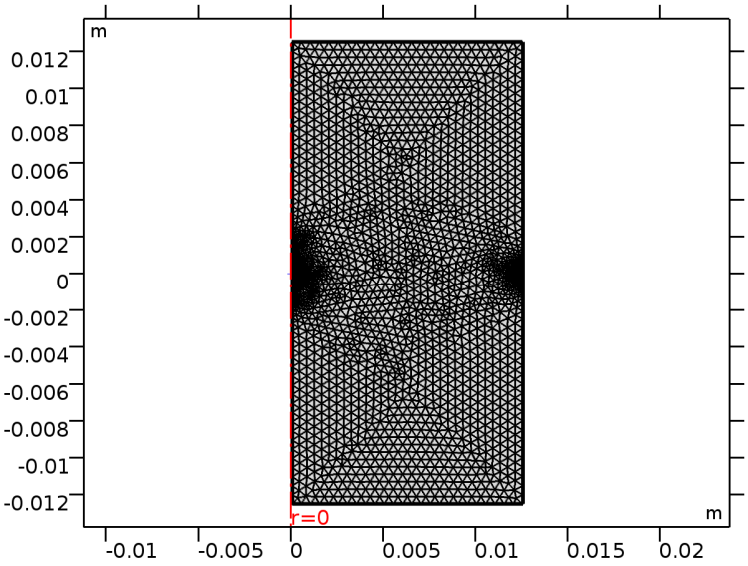
SELECTION

Geometric entity level	Remaining



Free Triangular 2

2.5.3 Mesh 3



Mesh 3

Size (size)

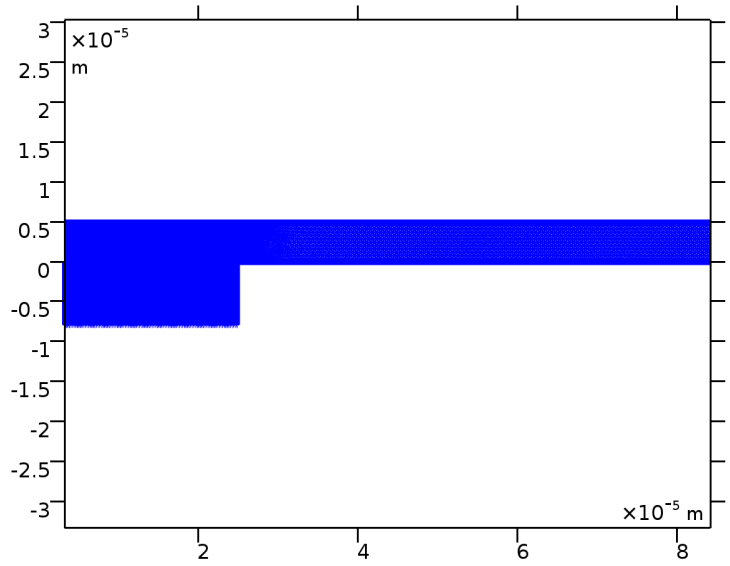
SETTINGS

Description	Value
Maximum element size	0.00168
Minimum element size	7.5E-6
Curvature factor	0.3
Maximum element growth rate	1.3

Free Triangular 1 (ftri1)

SELECTION

Geometric entity level	Domain
Selection	Domain 1

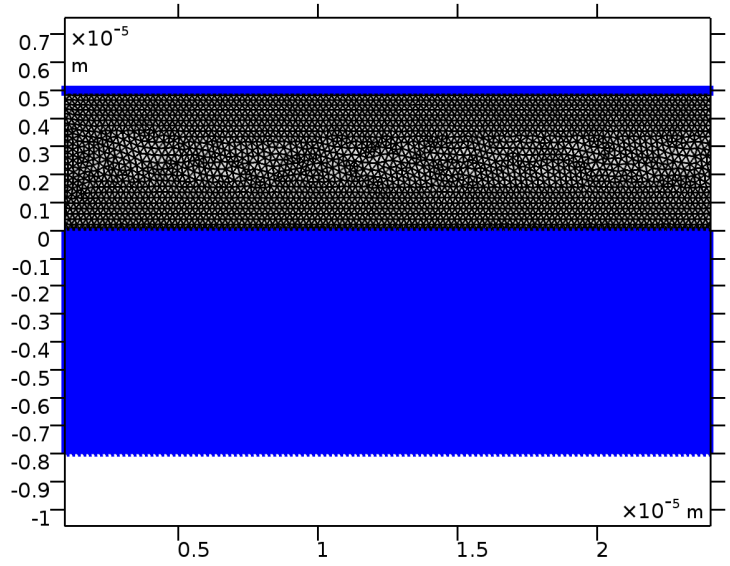


Free Triangular 1

Size 2 (size2)

SELECTION

Geometric entity level	Boundary
Selection	Boundaries 2, 4–502



Size 2

SETTINGS

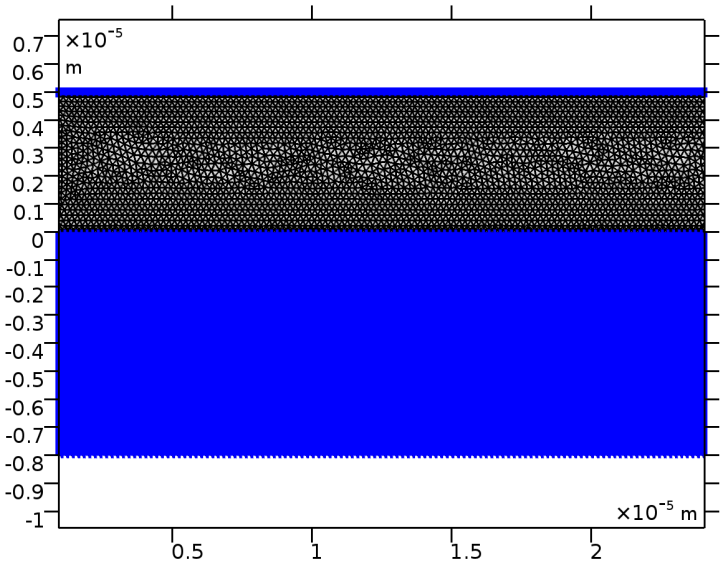
Description	Value
Maximum element size	5e-7

Description	Value
Minimum element size	5e-8
Curvature factor	0.3
Curvature factor	Off
Resolution of narrow regions	0.5
Maximum element growth rate	1.3
Maximum element growth rate	Off
Custom element size	Custom

Size 3 (size3)

SELECTION

Geometric entity level	Boundary
Selection	Boundaries 1–502



Size 3

SETTINGS

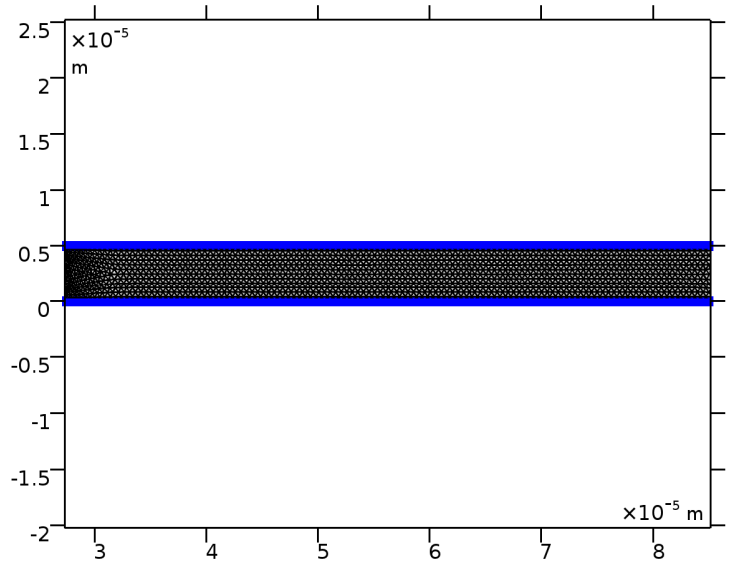
Description	Value
Maximum element size	if(d_L<1, 0.1, if(d_L>=10, d_L/2, if(d_L>=4, d_L/4, 0.4)))*2e-6
Minimum element size	5e-8
Curvature factor	0.3
Curvature factor	Off
Resolution of narrow regions	Off
Maximum element growth rate	1.3
Maximum element growth rate	Off

Description	Value
Custom element size	Custom

Size 4 (size4)

SELECTION

Geometric entity level	Boundary
Selection	Boundaries 503–504



Size 4

SETTINGS

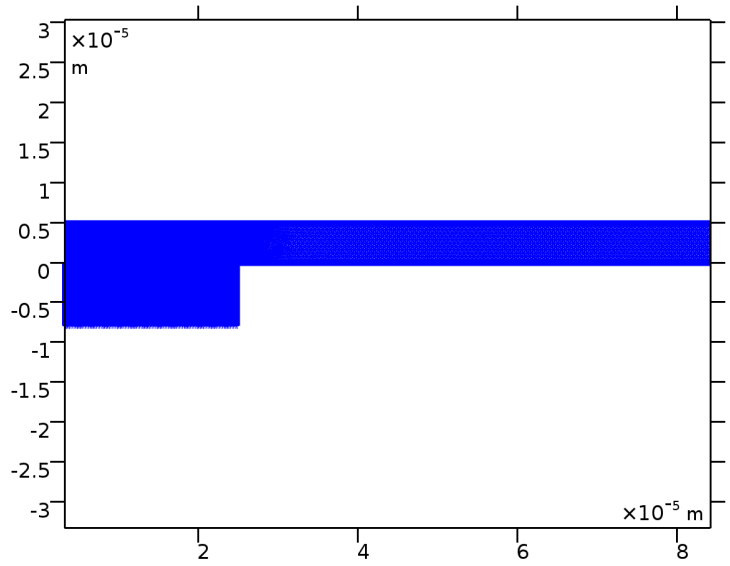
Description	Value
Maximum element size	5e-7
Minimum element size	7.5E-6
Minimum element size	Off
Curvature factor	0.3
Curvature factor	Off
Resolution of narrow regions	Off
Maximum element growth rate	1.3
Maximum element growth rate	Off
Custom element size	Custom

Size 5 (size5)

SELECTION

Geometric entity level	Domain

Selection	Domain 1



Size 5

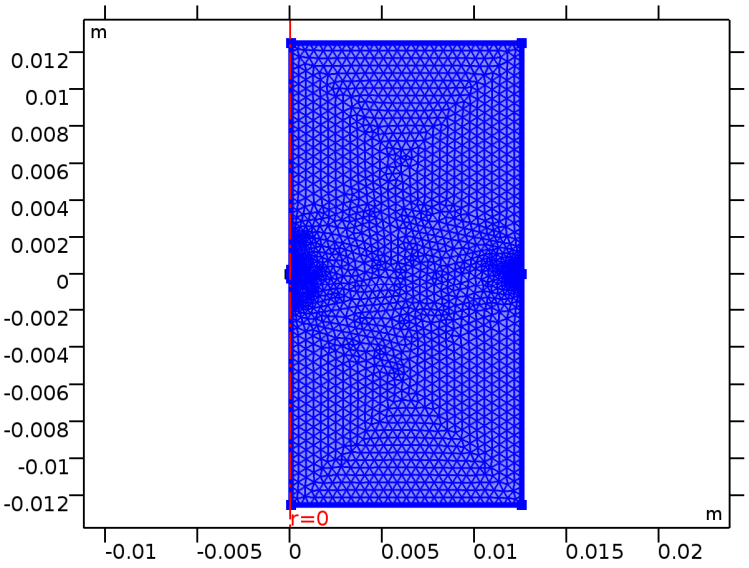
SETTINGS

Description	Value
Maximum element size	if(d_L>=10, d_L, if(d_L>=4, d_L/2, 1))*2e-5
Minimum element size	7.5E-6
Minimum element size	Off
Curvature factor	0.3
Curvature factor	Off
Resolution of narrow regions	0.4
Maximum element growth rate	1.05
Custom element size	Custom

Free Triangular 2 (ftri2)

SELECTION

Geometric entity level	Domain
Selection	Remaining

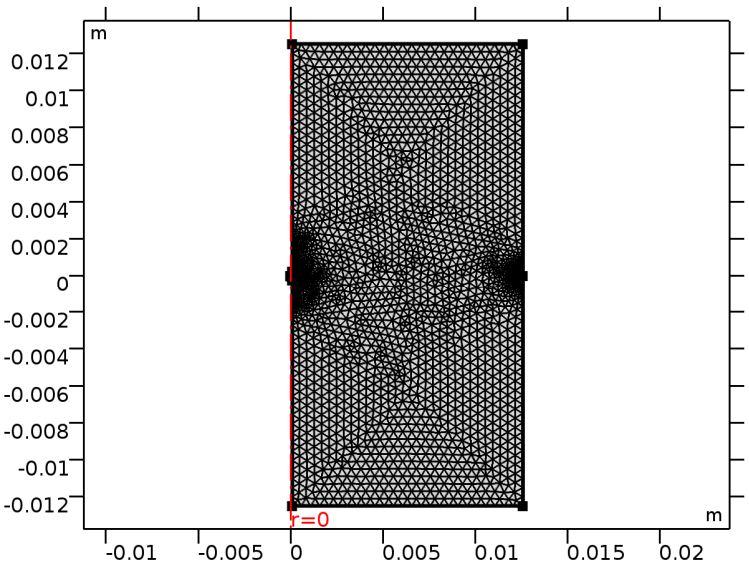


Free Triangular 2

Size 1 (size1)

SELECTION

Geometric entity level	Domain
Selection	Geometry geom1



Size 1

SETTINGS

Description	Value
Maximum element size	5.0E-4

Description	Value
Minimum element size	1.88E-6
Curvature factor	0.25
Maximum element growth rate	1.2
Predefined size	Extra fine

3 Study 1

COMPUTATION INFORMATION

Computation time	8 min 53 s
CPU	Intel(R) Xeon(R) CPU E3-1271 v3 @ 3.60GHz, 4 cores
Operating system	Windows 7

3.1 PARAMETRIC SWEEP

Parameter name	Parameter value list	Parameter unit
q10	2*q1ML,2*q1ML	C
q20	1*q1ML,1*q1ML	C
k_ox1	0.0001,0.00001	m/s
k_ox2	0.00001,0.0001	m/s
Dcs1	Dcs1,Dcs1	m^2/s

STUDY SETTINGS

Description	Value
Sweep type	Specified combinations
Parameter name	{q10, q20, k_ox1, k_ox2, Dcs1}
Parameter value list	{2*q1ML, 2*q1ML, 1*q1ML, 1*q1ML, 0.0001, 0.00001, 0.00001, 0.0001, Dcs1, Dcs1}
Unit	{C, C, m/s, m/s, m^2/s}

3.2 TIME DEPENDENT

Times	Unit
range(0,0.1,45)	s

STUDY SETTINGS

Description	Value
Include geometric nonlinearity	Off

STUDY SETTINGS

Description	Value
Tolerance	User controlled
Relative tolerance	0.001

PHYSICS AND VARIABLES SELECTION

Physics interface	Discretization
Transport of Diluted Species (tds)	physics

Physics interface	Discretization
Surface Reactions (sr)	physics

MESH SELECTION

Geometry	Mesh
Geometry 1 (geom1)	mesh3

3.3 SOLVER CONFIGURATIONS

3.3.1 Solution 1

Compile Equations: Time Dependent (st1)

STUDY AND STEP

Description	Value
Use study	Study 1
Use study step	Time Dependent

Dependent Variables 1 (v1)

GENERAL

Description	Value
Defined by study step	Time Dependent

INITIAL VALUE CALCULATION CONSTANTS

Description	Value
Parameter initial value list	range(0, 0.1, 45)

Surface concentration (mod1.cs1) (mod1_cs1)

GENERAL

Description	Value
Field components	mod1.cs1

Surface concentration (mod1.cs2) (mod1_cs2)

GENERAL

Description	Value
Field components	mod1.cs2

Concentration (mod1.o1) (mod1_o1)

GENERAL

Description	Value
Field components	mod1.o1

Concentration (mod1.r1) (mod1_r1)

GENERAL

Description	Value
Field components	mod1.r1

Time-Dependent Solver 1 (t1)

TIME STEPPING

Description	Value
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

Direct 1 (d1)

GENERAL

Description	Value
Solver	PARDISO

3.3.2 Parametric Solutions 1

q10=1.2203E-6, q20=6.1015E-7, k_ox1=1E-4, k_ox2=1E-5, Dcs1=5.5E-8 (su1)

GENERAL

Description	Value
Solution	q10=1.2203E-6, q20=6.1015E-7, k_ox1=1E-4, k_ox2=1E-5, Dcs1=5.5E-8

q10=1.2203E-6, q20=6.1015E-7, k_ox1=1E-5, k_ox2=1E-4, Dcs1=5.5E-8 (su2)

GENERAL

Description	Value
Solution	q10=1.2203E-6, q20=6.1015E-7, k_ox1=1E-5, k_ox2=1E-4, Dcs1=5.5E-8

4 Results

4.1 DATA SETS

4.1.1 Study 1/Solution 1

SOLUTION

Description	Value
Solution	Solution 1
Component	Save Point Geometry 1

Data set: Study 1/Solution 1

4.2 DERIVED VALUES

4.2.1 Line Integration 1

SELECTION

Geometric entity level	Boundary
Name	Substrate
Selection	Substrate

DATA

Description	Value
Data set	Study 1/Solution 1

EXPRESSIONS

Expression	Unit	Description
2*pi*r	mm^2	

OUTPUT

Evaluated in	Table 2 {tbl2}

4.3 TABLES

4.3.1 Table 1

4.3.2 Table 2

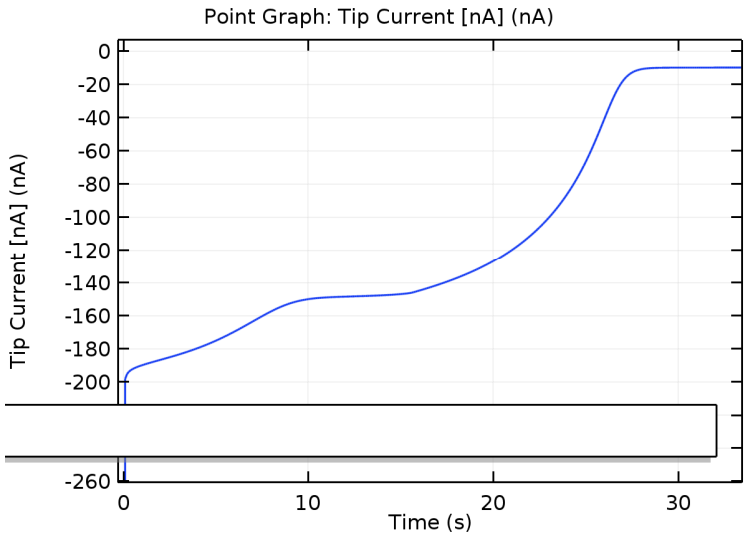
Line Integration 1 {int1} (2*pi*r)

TABLE 2

Time (s)	2*pi*r (m^2)	2*pi*r (cm^2)	2*pi*r (cm^2)	2*pi*r (cm^2)	2*pi*r (mm^2)
0.0000	3.1549E-7	0.0031549	1.3873E-4	0.0015645	0.15645

4.4 PLOT GROUPS

4.4.1 Current



Point Graph: Tip Current [nA] (nA)