Supporting Information

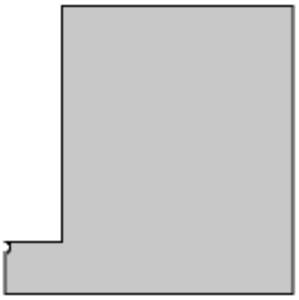
File 2

Tunneling Ultramicroelectrode (T-UME): Nanoelectrodes and Nanoparticle Collisions

Jiyeon Kim, Byung-Kwon Kim, Sung-Ki Cho and Allen J. Bard*

Center for Electrochemistry, Department of Chemistry, The University of Texas at Austin, Austin, Texas, 78712

COMSOL Model Report



Date	Dec 10, 2013 8:35:43 PM

Contents

1. Global Definitions

1.1. PARAMETERS 1

PARAMETERS

Name	Expression	Description
RG	10	
a	1	
distance	9.1	
width	100	
height	100	

1.2. VARIABLES

1.2.1. Variables 1

SELECTION

Geometric entity level	Entire model

Name	Expression	Description
K	100	

2. Model 1 (mod1)

2.1. DEFINITIONS

2.1.1. Coordinate Systems

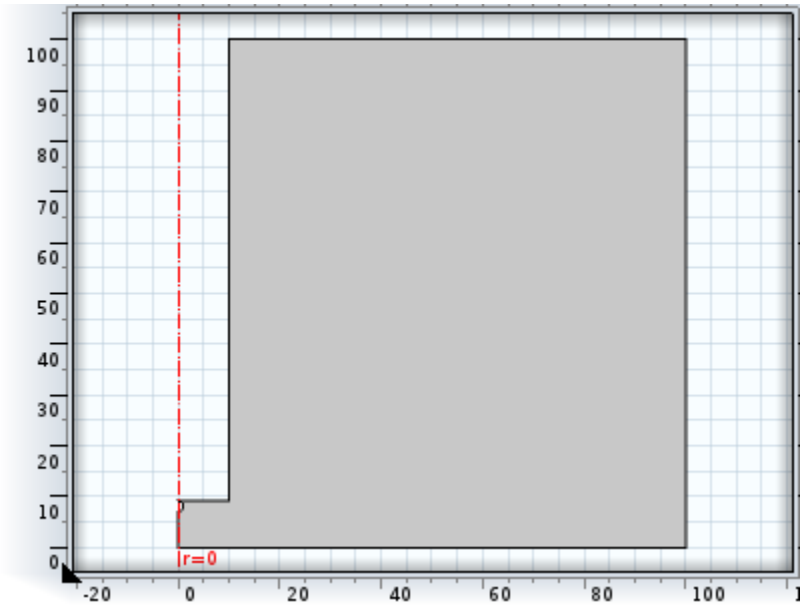
Boundary System 1

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

UNITS

Length unit	m
Angular unit	deg

GEOMETRY STATISTICS

Property	Value
Space dimension	2
Number of domains	1

Number of boundaries	8

2.2.1. Rectangle 1 (r1)

SETTINGS

Name	Value
Position	{0, 0}
Width	width
Height	height
Size	{width, height}

2.2.2. Polygon 1 (pol1)

SETTINGS

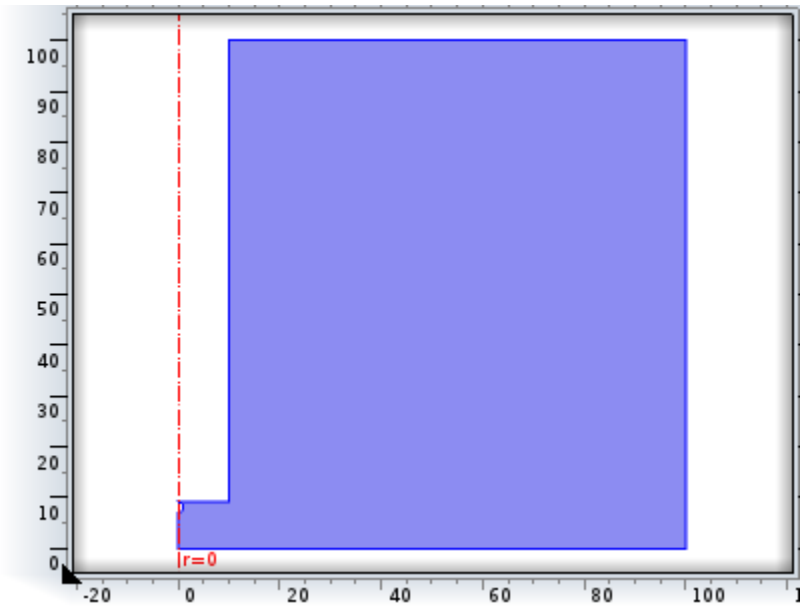
Name	Value
r	{0, 0, 10, 10}
z	{50, 30, 30, 50}

2.2.3. Circle 1 (c1)

SETTINGS

Name	Value
Position	{0, distance-a}
z	distance-a
Radius	a

2.3. TRANSPORT OF DILUTED SPECIES (CHDS)



Transport of Diluted Species

SELECTION

Geometric entity level	Domain
Selection	Domain 1

EQUATIONS

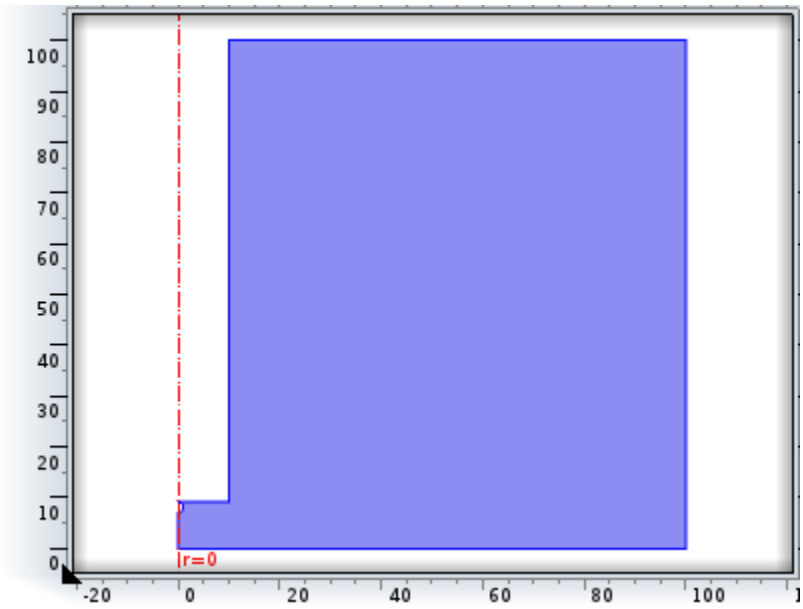
$$\nabla \cdot \left(-D_i \nabla c_i\right) = R_i$$

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

SETTINGS

Description	**Value**
Convection	0
Show equation assuming	std1/stat

2.3.1. Diffusion



Diffusion

SELECTION

Geometric entity level	Domain
Selection	Domain 1

Equations

$$\nabla \cdot \left(-D_i \nabla c_i\right) = R_i$$

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

Settings

SETTINGS

Description	Value
Diffusion coefficient	{{1, 0, 0}, {0, 1, 0}, {0, 0, 1}}

Variables

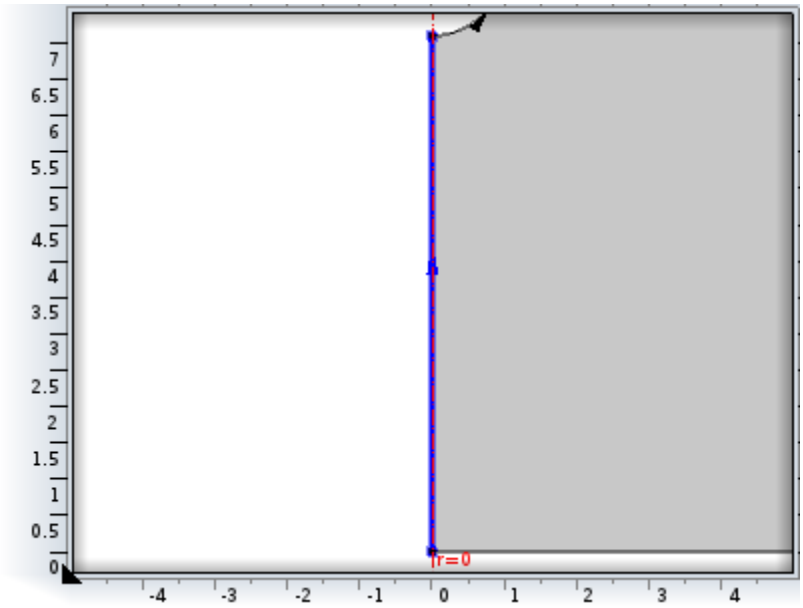
Name	Expression	Unit	Description	Selection
chds.Drr_c	1	m^2/s	Diffusion coefficient, rr component	Domain 1
chds.Dphir	0	m^2/s	Diffusion	Domain 1

_c			coefficient, phir component	
chds.Dzr_c	0	m^2/s	Diffusion coefficient, zr component	Domain 1
chds.Drphi_c	0	m^2/s	Diffusion coefficient, rphi component	Domain 1
chds.Dphiphi_c	1	m^2/s	Diffusion coefficient, phiphi component	Domain 1
chds.Dzphi_c	0	m^2/s	Diffusion coefficient, zphi component	Domain 1
chds.Drz_c	0	m^2/s	Diffusion coefficient, rz component	Domain 1
chds.Dphiz_c	0	m^2/s	Diffusion coefficient, phiz component	Domain 1
chds.Dzz_c	1	m^2/s	Diffusion coefficient, zz component	Domain 1
chds.Dav_c	0.5*(chds.Drr_c+chds.Dzz_c)	m^2/s	Average diffusion coefficient	Domain 1
chds.tfluxr_c	-chds.Drr_c*cr-chds.Drz_c*cz	mol/(m^2*s)	Total flux, r component	Domain 1

chds.tfluxphi_c	-chds.Dphir_c*cr-chds.Dphiz_c*cz	mol/(m^2*s)	Total flux, phi component	Domain 1
chds.tfluxz_c	-chds.Dzr_c*cr-chds.Dzz_c*cz	mol/(m^2*s)	Total flux, z component	Domain 1
chds.dfluxr_c	-chds.Drr_c*cr-chds.Drz_c*cz	mol/(m^2*s)	Diffusive flux, r component	Domain 1
chds.dfluxphi_c	-chds.Dphir_c*cr-chds.Dphiz_c*cz	mol/(m^2*s)	Diffusive flux, phi component	Domain 1
chds.dfluxz_c	-chds.Dzr_c*cr-chds.Dzz_c*cz	mol/(m^2*s)	Diffusive flux, z component	Domain 1
chds.gradr_c	cr	mol/m^4	Concentration gradient, r component	Domain 1
chds.gradphi_c	0	mol/m^4	Concentration gradient, phi component	Domain 1
chds.gradz_c	cz	mol/m^4	Concentration gradient, z component	Domain 1
chds.ntflux_c	chds.nr*chds.tfluxr_c+chds.nphi*chds.tfluxphi_c+chds.nz*chds.tfluxz_c	mol/(m^2*s)	Normal total flux	Boundaries 1-8
chds.ndflux_c	chds.nr*chds.dfluxr_c+chds.nphi*chds.dfluxphi_c+chds.nz*chds.dfluxz_c	mol/(m^2*s)	Normal diffusive flux	Boundaries 1-8
chds.dfluxMag_c	sqrt(chds.dfluxr_c^2+chds.dfluxphi_c^2+chds.dfluxz_c^2)	mol/(m^2*s)	Diffusive flux magnitude	Domain 1

chds.tflux Mag_c	sqrt(chds.tfluxr_c^2+chds.tfluxphi_c^2+chds.tfluxz_c^2)	mol/(m^2*s)	Total flux magnitude	Domain 1
chds.helem	h	m	Element size	Domain 1
chds.glim	0.1[mol/m^3]/chds.helem	mol/m^4	Lower gradient limit	Domain 1
chds.Res_c	-chds.R_c	mol/(m^3*s)	Equation residual	Domain 1

2.3.2. Axial Symmetry 1

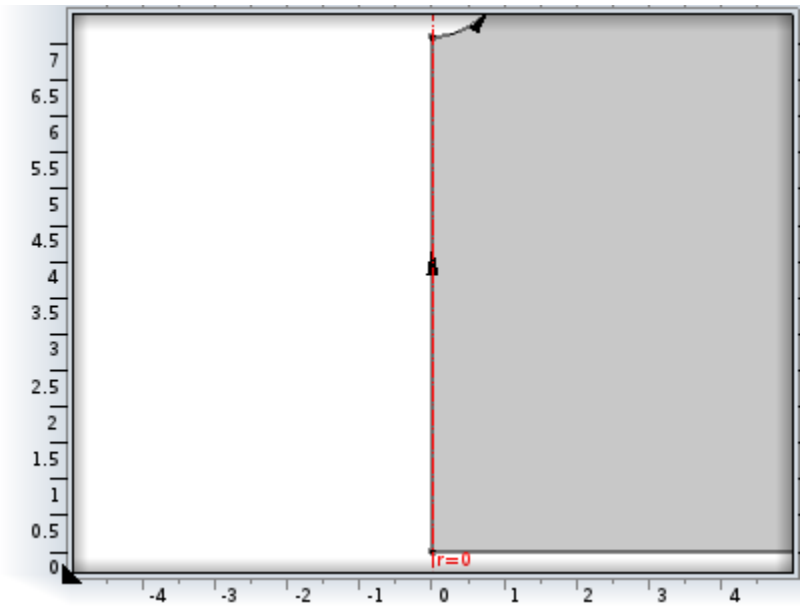


Axial Symmetry 1

SELECTION

Geometric entity level	Boundary
Selection	Boundary 1

2.3.3. No Flux 1



No Flux 1

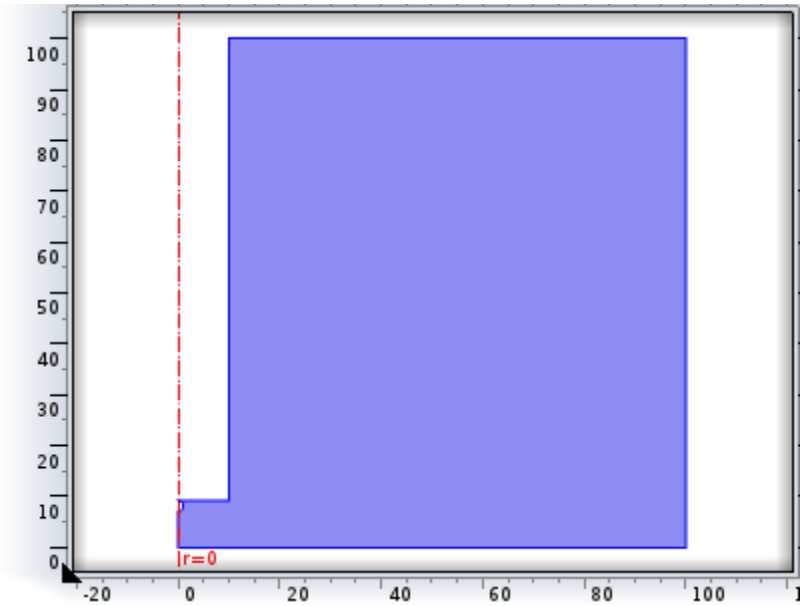
SELECTION

Geometric entity level	Boundary
Selection	No boundaries

Equations

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

2.3.4. Initial Values 1



Initial Values 1

SELECTION

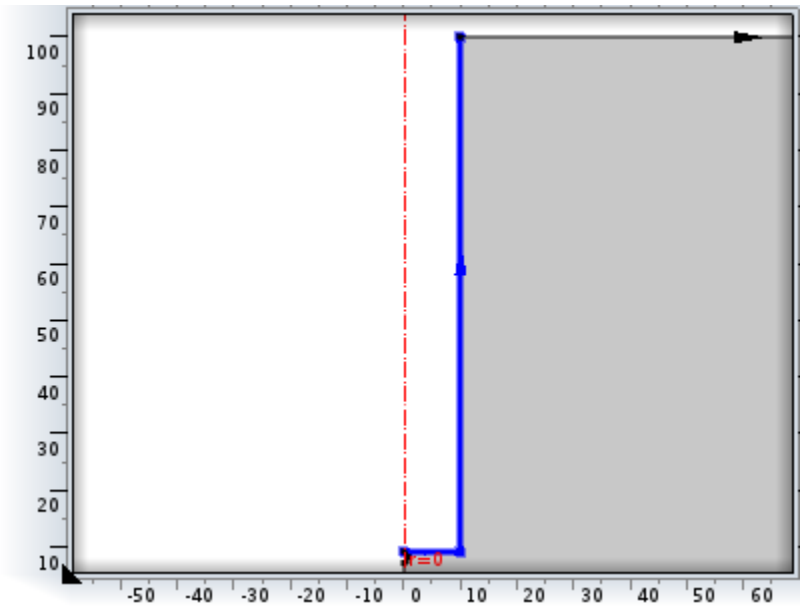
Geometric entity level	Domain
Selection	Domain 1

Settings

SETTINGS

Description	Value
Concentration	1

2.3.5. No Flux 2



No Flux 2

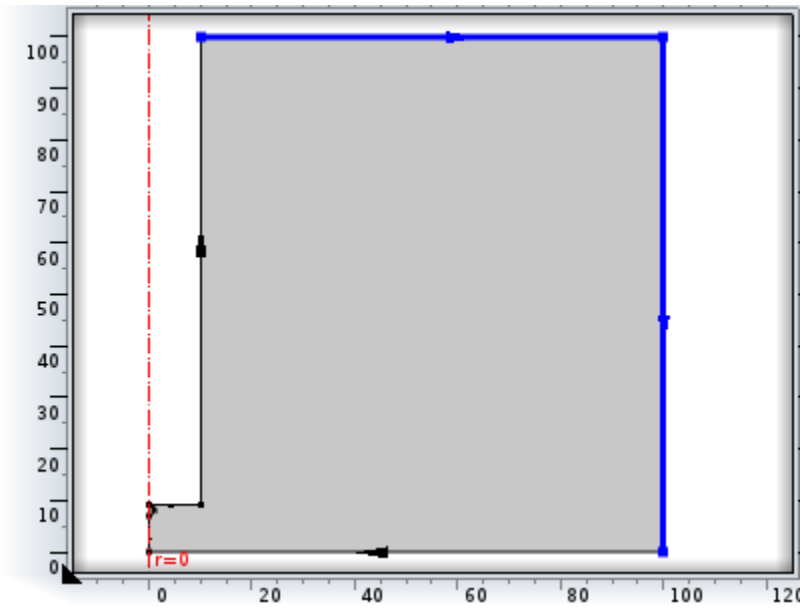
SELECTION

Geometric entity level	Boundary
Selection	Boundaries 3-4

Equations

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

2.3.6. Concentration 1



Concentration 1

SELECTION

Geometric entity level	Boundary
Selection	Boundaries 5-6

Equations

$c_i = c_{0i}$

Settings

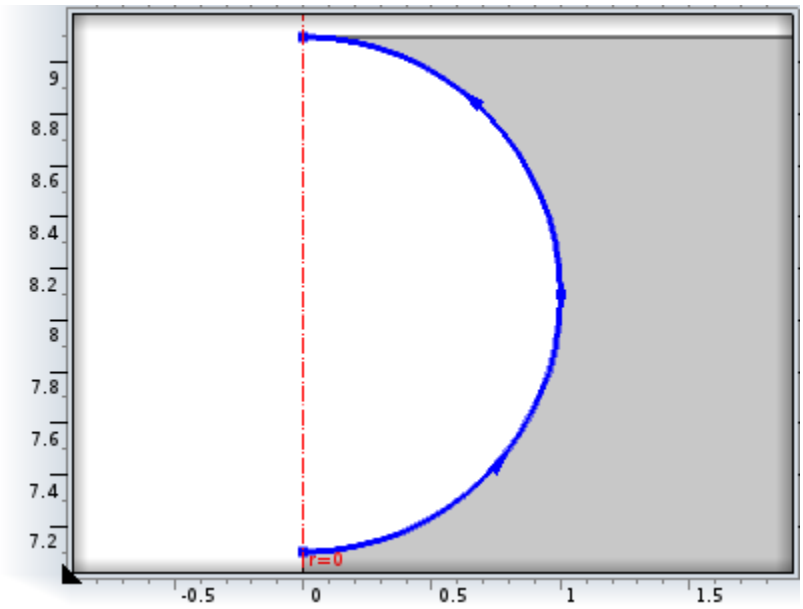
SETTINGS

Description	Value
Concentration	1
Species c	1

Variables

Name	Expression	Unit	Description	Selection
chds.c0_c	1	mol/m^3	Concentration	Boundaries 5-6

2.3.7. Concentration 2



Concentration 2

SELECTION

Geometric entity level	Boundary
Selection	Boundaries 7-8

Equations

$c_i = c_{0i}$

Settings

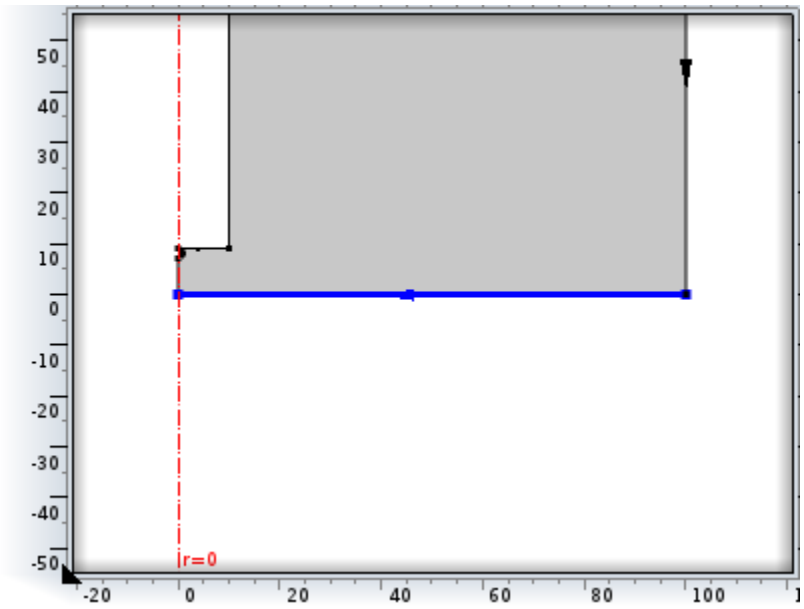
SETTINGS

Description	Value
Species c	1

Variables

Name	Expression	Unit	Description	Selection
chds.c0_c	0	mol/m^3	Concentration	Boundaries 7-8

2.3.8. Flux 1



Flux 1

SELECTION

Geometric entity level	Boundary
Selection	Boundary 2

Equations

$$-\mathbf{n} \cdot \mathbf{N}_i = k_{c,i}(c_{b,i} - c_i)$$

Settings

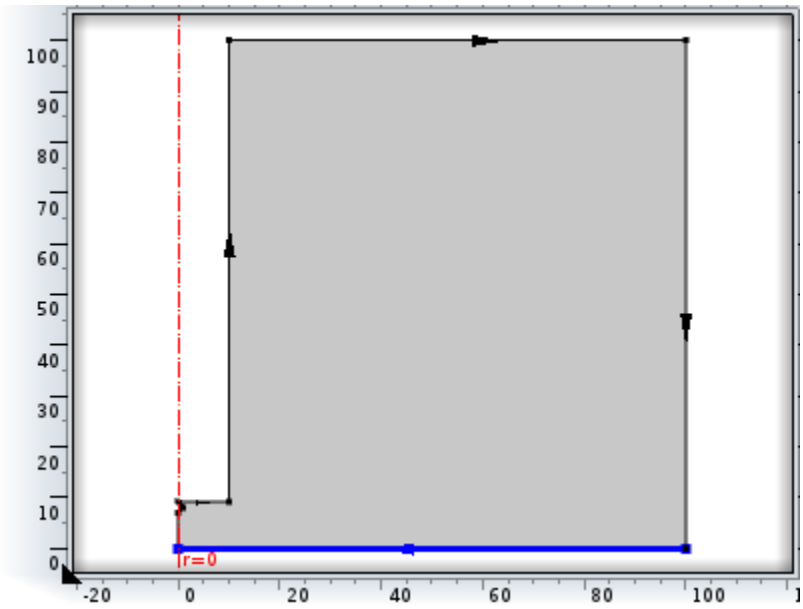
SETTINGS

Description	Value
Species c	1
Flux type	External forced convection

Variables

Name	Expression	Unit	Description	Selection
chds.cb_c	1	mol/m^3	Bulk concentration	Boundary 2
chds.kc_c	K	m/s	Mass transfer coefficient	Boundary 2

2.4. MESH 1



Mesh 1

2.4.1. Size (size)

SETTINGS

Name	Value
Maximum element size	5.3
Minimum element size	0.03
Resolution of curvature	0.3
Maximum element growth rate	1.3
Predefined size	Fine

3. Study 1

3.1. PARAMETRIC SWEEP

Parameter name: distance

Parameters: range(6.1,1,9.1)

3.2. STATIONARY

MESH SELECTION

Geometry	Mesh
Geometry 1 (geom1)	mesh1

PHYSICS SELECTION

Physics interface	Discretization
Transport of Diluted Species (chds)	physics

3.3. SOLVER CONFIGURATIONS

3.3.1. Solver 1

Compile Equations: Stationary (st1)

SETTINGS

Name	Value
Use study	Study 1
Use study step	Stationary

Dependent Variables 1 (v1)

SETTINGS

Name	Value
Defined by study step	Stationary
Solution	Zero
Solution	Zero

Mod1.c (mod1_c)

SETTINGS

Name	Value
Field components	mod1.c

Stationary Solver 1 (s1)

SETTINGS

Name	Value
Defined by study step	Stationary

Fully Coupled 1 (fc1)

SETTINGS

Name	Value
Linear solver	Direct 1
Initial damping factor	0.01
Minimum damping factor	1.0E-6
Maximum number of iterations	50

Direct 1 (d1)

SETTINGS

Name	Value
Solver	pardiso

3.3.2. Parametric 2

Store Solution 3 (su1)

SETTINGS

Name	Value
Solution	Store Solution 3

Store Solution 4 (su2)

SETTINGS

Name	Value
Solution	Store Solution 4

Store Solution 5 (su3)

SETTINGS

Name	Value
Solution	Store Solution 5

Store Solution 6 (su4)

SETTINGS

Name	Value

Solution	Store Solution 6

4. Results

4.1. DATA SETS

4.1.1. Solution 1

SELECTION

Geometric entity level	Domain
Selection	Geometry geom1

SETTINGS

Name	Value
Solution	Solver 1
Model	Save Point Geometry 1

4.1.2. Revolution 2D 1

SETTINGS

Name	Value
Data set	Solution 1
Points	{{0, 0}, {0, 1}}
Start angle	-90
Revolution angle	225

4.1.3. Solution 2

SELECTION

Geometric entity level	Domain
Selection	Geometry geom1

SETTINGS

Name	Value
Solution	Parametric 2

Model	Save Point Geometry 1

4.1.4. Revolution 2D 2

SETTINGS

Name	Value
Data set	Solution 2
Points	{{0, 0}, {0, 1}}
Start angle	-90
Revolution angle	225

4.2. DERIVED VALUES

4.2.1. Line Integration 1

SELECTION

Geometric entity level	Boundary
Selection	Boundaries 7-8

SETTINGS

Name	Value
Data set	Solution 1
Expression	chds.tfluxMag_c
Unit	mol/(m*s)
Description	Total flux magnitude

4.2.2. Line Integration 2

SELECTION

Geometric entity level	Boundary
Selection	Boundaries 7-8

SETTINGS

Name	Value

Data set	Solution 2
Expression	chds.tfluxMag_c
Unit	mol/(m*s)
Description	Total flux magnitude

4.3. TABLES

4.3.1. Table 1

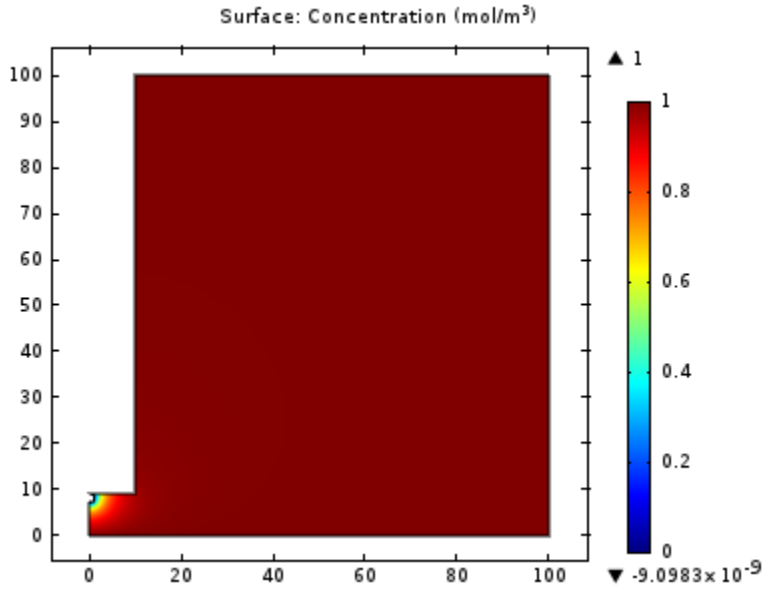
Line Integration 2 (chds.tfluxMag_c)

TABLE 1

distance	Total flux magnitude (mol/(m*s))
6.1	2.36218
7.1	2.29753
8.1	2.25145
9.1	2.22116

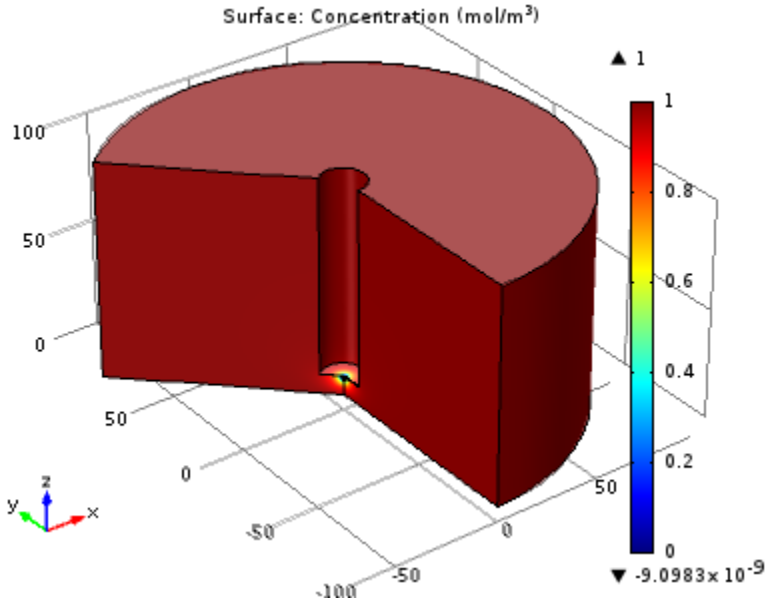
4.4. PLOT GROUPS

4.4.1. Concentration (chds)



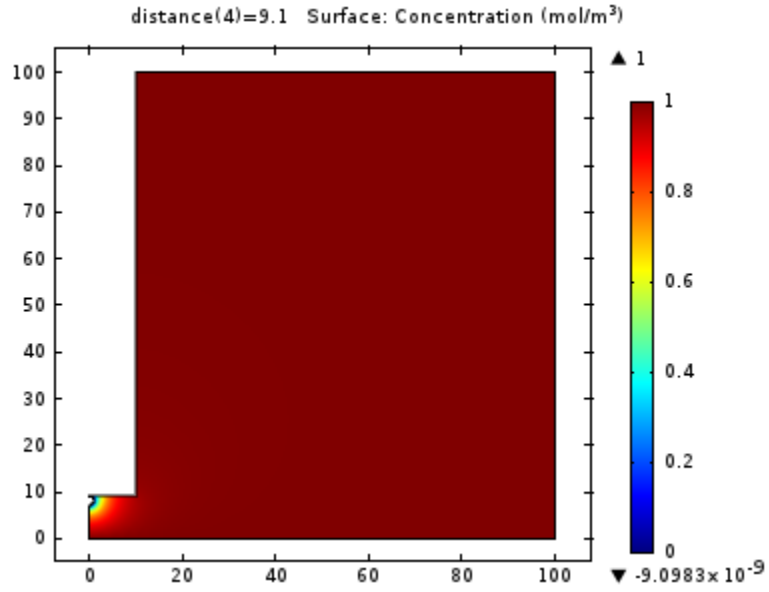
Surface: Concentration (mol/m³)

4.4.2. Concentration, 3D (chds)



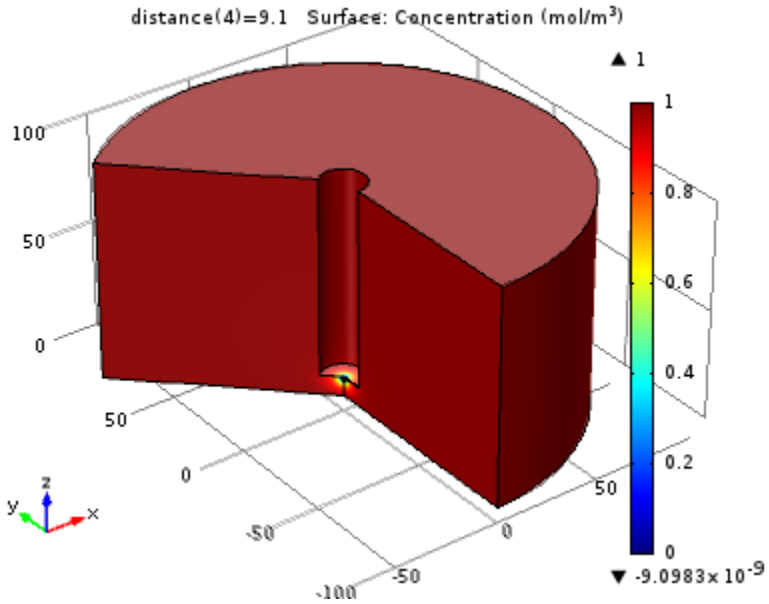
Surface: Concentration (mol/m³)

4.4.3. Concentration (chds) 1



distance(4)=9.1 Surface: Concentration (mol/m³)

4.4.4. Concentration, 3D (chds) 1



distance(4)=9.1 Surface: Concentration (mol/m^3)