Approach Curve COMSOL Report File

Contents

1. Global Definitions

1.1. Parameters 1

Parameters

Name	Expression	Description
W_Tip	315[um]	
R_Ins	300[um]	
R_Sub	1[mm]	
R_Cell	5[mm]	
H_Cell	5[mm]	
D_O	7.9E-5[cm^2/s]	
D_R	4.5E-5[cm^2/s]	
C_O	10^-2.3[mol/L]	
C_R	0[mol/L]	
n	1	
F	96485[C/mol]	
Tip_Area	W_Tip*L_Tip	
k_Step	700 [um]	
time_Step	15 [s]	
L_Tip	345 [um]	

2. Model 1 (mod1)

2.1. Definitions

2.1.1. Variables

Tip Variables

Selection

Geometric entity level	Point
Selection	Point 18

Name	Expression	Description
i_Tip	-intop1(n*F*D_O*Oz)+intop3(n*F*chds.tfluxMag_O)	

Sub Variables

Selection

Geometric entity level	Point
Selection	Point 17

Name	Expression	Description
i_Sub	-intop2(2*n*F*D_R*Rz)	

2.1.2. Model Couplings

Tip_Integration

Coupling type	Integration
Operator name	intop1

Source selection

Geometric entity level	Boundary
Selection	Boundary 12

Sub Integration

Coupling type	Integration
Operator name	intop2

Source selection

Geometric entity level	Boundary
Selection	Boundary 5

Tip_Side

Coupling type	Integration
Operator name	intop3

Source selection

Geometric entity level	Boundary
Selection	Boundaries 10-11, 17, 23

2.1.3. Coordinate Systems

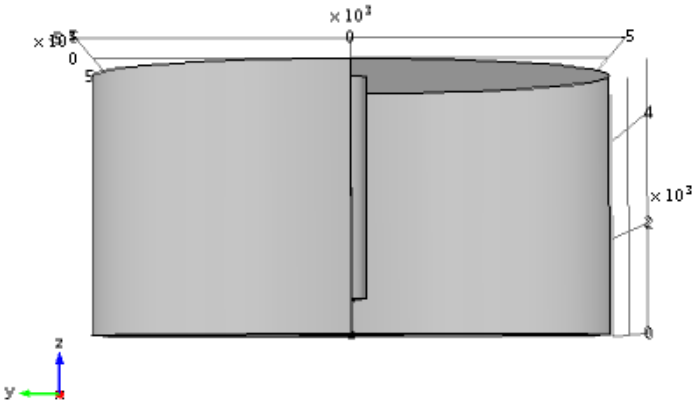
Boundary System 1

Coordinate system type	Boundary system
Identifier	sys1

Settings

Name	Value
Coordinate names	{t1, t2, n}
Create first tangent direction from	Global Cartesian

2.2. Geometry 1



Geometry

units

Length unit	μm
Angular unit	deg

Geometry statistics

Property	Value
Space dimension	3
Number of domains	4
Number of boundaries	24
Number of edges	48
Number of vertices	34

2.2.1. Cell Domain (cyl1)

Settings

Name	Value
Position	{0, 0, 0}
Axis	{0, 0, 1}
Axis	{0, 0, 1}
Radius	R_Cell
Height	H_Cell

2.2.2. Square Tip (blk1)

Settings

Name	Value
Position	{0, 0, 0.5*(H_Cell-k_Step)+k_Step}
z	0.5*(H_Cell-k_Step)+k_Step

Axis	{0, 0, 1}
Axis	{0, 0, 1}
Base	Center
Width	W_Tip
Depth	L_Tip
Height	H_Cell - k_Step
Size	{W_Tip, L_Tip, H_Cell - k_Step}

2.2.3. Insulation (cyl2)

Settings

Name	Value
Position	{0, 0, k_Step+10[um]}
z	k_Step+10[um]
Axis	{0, 0, 1}
Axis	{0, 0, 1}
Radius	R_Ins
Height	H_Cell - k_Step-10[um]

2.2.4. Center Sub (pt1)

Settings

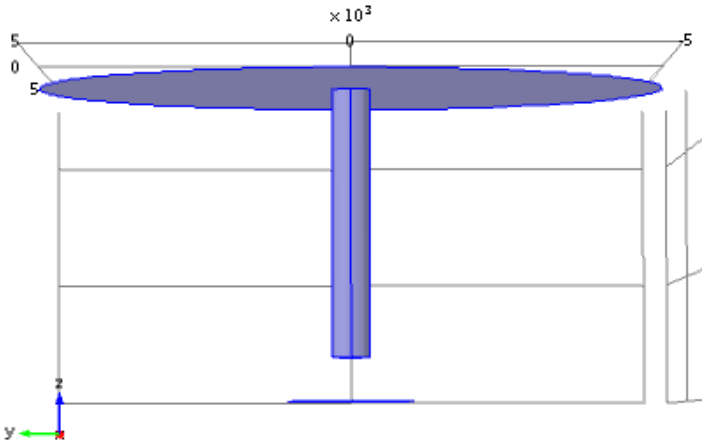
Name	Value
Point coordinate	{0, 0, 0}

2.2.5. Center Tip (pt2)

Settings

Name	Value
Point coordinate	{0, 0, k_Step}

2.3. Transport of Diluted Species (chds)



Transport of Diluted Species

Selection

Geometric entity level	Domain
Selection	Domain 1

Equations

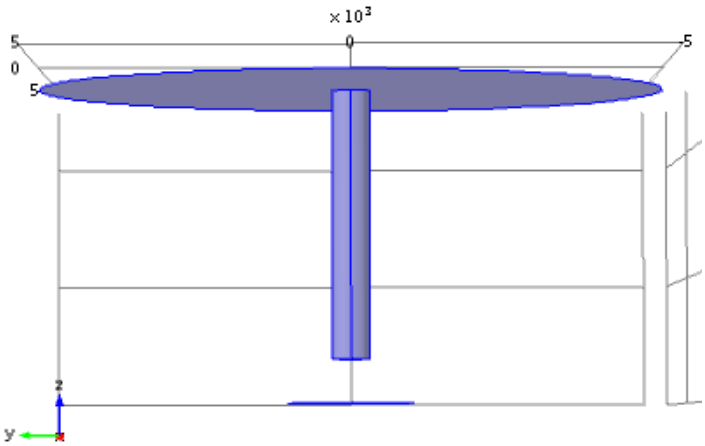
$$\frac{\partial c_i}{\partial t} + \nabla \cdot (-D_i \nabla c_i) = R_i$$

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

Settings

Description	Value
Convection	0
Show equation assuming	std1/time

2.3.1. Diffusion



Diffusion

Selection

Geometric entity level	Domain
Selection	Domain 1

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

Settings

Description	Value
Diffusion coefficient	{{D_O, 0, 0}, {0, D_O, 0}, {0, 0, D_O}}
Diffusion coefficient	{{D_R, 0, 0}, {0, D_R, 0}, {0, 0, D_R}}

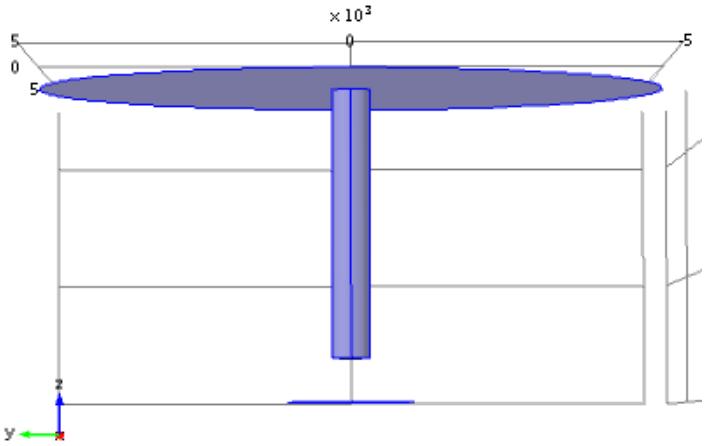
Variables

Name	Expression	Unit	Description	Selection
chds.Dxx_O	D_O	m^2/s	Diffusion coefficient, xx component	Domain 1
chds.Dyx_O	0	m^2/s	Diffusion coefficient, yx component	Domain 1
chds.Dzx_O	0	m^2/s	Diffusion coefficient, zx component	Domain 1
chds.Dxy_O	0	m^2/s	Diffusion coefficient, xy component	Domain 1
chds.Dyy_O	D_O	m^2/s	Diffusion coefficient, yy component	Domain 1
chds.Dzy_O	0	m^2/s	Diffusion coefficient, zy component	Domain 1
chds.Dxz_O	0	m^2/s	Diffusion coefficient, xz component	Domain 1
chds.Dyz_O	0	m^2/s	Diffusion coefficient, yz component	Domain 1
chds.Dzz_O	D_O	m^2/s	Diffusion coefficient, zz component	Domain 1
chds.Dav_O	(chds.Dxx_O+chds.Dyy_O+chds.Dzz_O)/3	m^2/s	Average diffusion coefficient	Domain 1
chds.tfluxx_O	-chds.Dxx_O*Ox-chds.Dxy_O*Oy-chds.Dxz_O*Oz	mol/(m^2*s)	Total flux, x component	Domain 1
chds.tfluxy_O	-chds.Dyx_O*Ox-chds.Dyy_O*Oy-chds.Dyz_O*Oz	mol/(m^2*s)	Total flux, y component	Domain 1
chds.tfluxz_O	-chds.Dzx_O*Ox-chds.Dzy_O*Oy-chds.Dzz_O*Oz	mol/(m^2*s)	Total flux, z component	Domain 1
chds.dfluxx_O	-chds.Dxx_O*Ox-chds.Dxy_O*Oy-chds.Dxz_O*Oz	mol/(m^2*s)	Diffusive flux, x component	Domain 1
chds.dfluxy_O	-chds.Dyx_O*Ox-chds.Dyy_O*Oy-chds.Dyz_O*Oz	mol/(m^2*s)	Diffusive flux, y component	Domain 1
chds.dfluxz_O	-chds.Dzx_O*Ox-chds.Dzy_O*Oy-chds.Dzz_O*Oz	mol/(m^2*s)	Diffusive flux, z component	Domain 1
chds.gradx_O	Ox	mol/m^4	Concentration gradient, x component	Domain 1
			Concentration	

chds.grady_O	Oy	mol/m^4	gradient, y component	Domain 1
chds.gradz_O	Oz	mol/m^4	Concentration gradient, z component	Domain 1
chds.ntflux_O	chds.nx*chds.tfluxx_O+chds.ny*chds.tfluxy_O+chds.nz*chds.tfluxz_O	mol/(m^2*s)	Normal total flux	Boundaries 1-8, 10-12, 17, 19-23
chds.ndflux_O	chds.nx*chds.dfluxx_O+chds.ny*chds.dfluxy_O+chds.nz*chds.dfluxz_O	mol/(m^2*s)	Normal diffusive flux	Boundaries 1-8, 10-12, 17, 19-23
chds.dfluxMag_O	sqrt(chds.dfluxx_O^2+chds.dfluxy_O^2+chds.dfluxz_O^2)	mol/(m^2*s)	Diffusive flux magnitude	Domain 1
chds.tfluxMag_O	sqrt(chds.tfluxx_O^2+chds.tfluxy_O^2+chds.tfluxz_O^2)	mol/(m^2*s)	Total flux magnitude	Domain 1
chds.Dxx_R	D_R	m^2/s	Diffusion coefficient, xx component	Domain 1
chds.Dyx_R	0	m^2/s	Diffusion coefficient, yx component	Domain 1
chds.Dzx_R	0	m^2/s	Diffusion coefficient, zx component	Domain 1
chds.Dxy_R	0	m^2/s	Diffusion coefficient, xy component	Domain 1
chds.Dyy_R	D_R	m^2/s	Diffusion coefficient, yy component	Domain 1
chds.Dzy_R	0	m^2/s	Diffusion coefficient, zy component	Domain 1
chds.Dxz_R	0	m^2/s	Diffusion coefficient, xz component	Domain 1
chds.Dyz_R	0	m^2/s	Diffusion coefficient, yz component	Domain 1
chds.Dzz_R	D_R	m^2/s	Diffusion coefficient, zz component	Domain 1
chds.Dav_R	(chds.Dxx_R+chds.Dyy_R+chds.Dzz_R)/3	m^2/s	Average diffusion coefficient	Domain 1
chds.tfluxx_R	-chds.Dxx_R*Rx-chds.Dxy_R*Ry-chds.Dxz_R*Rz	mol/(m^2*s)	Total flux, x component	Domain 1
chds.tfluxy_R	-chds.Dyx_R*Rx-chds.Dyy_R*Ry-chds.Dyz_R*Rz	mol/(m^2*s)	Total flux, y component	Domain 1

chds.tfluxz_R	-chds.Dzx_R*Rx-chds.Dzy_R*Ry-chds.Dzz_R*Rz	mol/(m^2*s)	Total flux, z component	Domain 1
chds.dfluxx_R	-chds.Dxx_R*Rx-chds.Dxy_R*Ry-chds.Dxz_R*Rz	mol/(m^2*s)	Diffusive flux, x component	Domain 1
chds.dfluxy_R	-chds.Dyx_R*Rx-chds.Dyy_R*Ry-chds.Dyz_R*Rz	mol/(m^2*s)	Diffusive flux, y component	Domain 1
chds.dfluxz_R	-chds.Dzx_R*Rx-chds.Dzy_R*Ry-chds.Dzz_R*Rz	mol/(m^2*s)	Diffusive flux, z component	Domain 1
chds.gradx_R	Rx	mol/m^4	Concentration gradient, x component	Domain 1
chds.grady_R	Ry	mol/m^4	Concentration gradient, y component	Domain 1
chds.gradz_R	Rz	mol/m^4	Concentration gradient, z component	Domain 1
chds.ntflux_R	chds.nx*chds.tfluxx_R+chds.ny*chds.tfluxy_R+chds.nz*chds.tfluxz_R	mol/(m^2*s)	Normal total flux	Boundaries 1-8, 10-12, 17, 19-23
chds.ndflux_R	chds.nx*chds.dfluxx_R+chds.ny*chds.dfluxy_R+chds.nz*chds.dfluxz_R	mol/(m^2*s)	Normal diffusive flux	Boundaries 1-8, 10-12, 17, 19-23
chds.dfluxMag_R	sqrt(chds.dfluxx_R^2+chds.dfluxy_R^2+chds.dfluxz_R^2)	mol/(m^2*s)	Diffusive flux magnitude	Domain 1
chds.tfluxMag_R	sqrt(chds.tfluxx_R^2+chds.tfluxy_R^2+chds.tfluxz_R^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_O	Ot-chds.R_O	mol/(m^3*s)	Equation residual	Domain 1
chds.Res_R	Rt-chds.R_R	mol/(m^3*s)	Equation residual	Domain 1

2.3.2. No Flux 1



No Flux 1

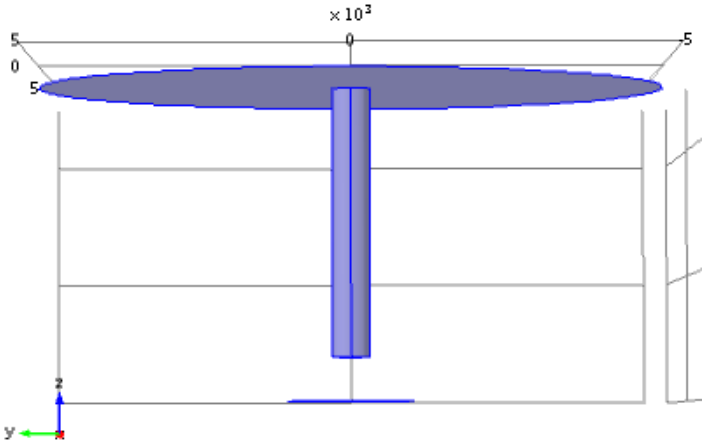
Selection

Geometric entity level	Boundary
Selection	Boundaries 1-4, 6-8, 19-22

Equations

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

2.3.3. Initial Values 1



Initial Values 1

Selection

Geometric entity level	Domain
Selection	Domain 1

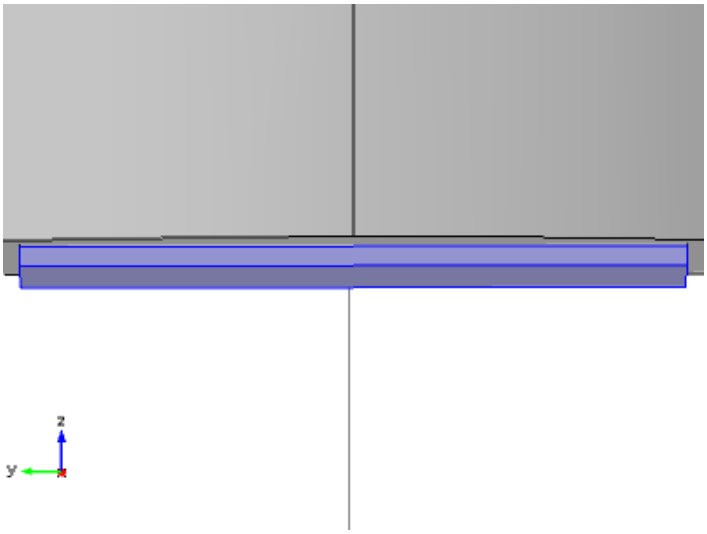
Settings

Settings

Description	Value
Concentration	C_O

Concentration	C_R

2.3.4. Concentration 1



Concentration 1

Selection

Geometric entity level	Boundary
Selection	Boundaries 10-12, 17, 23

Equations

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

Settings

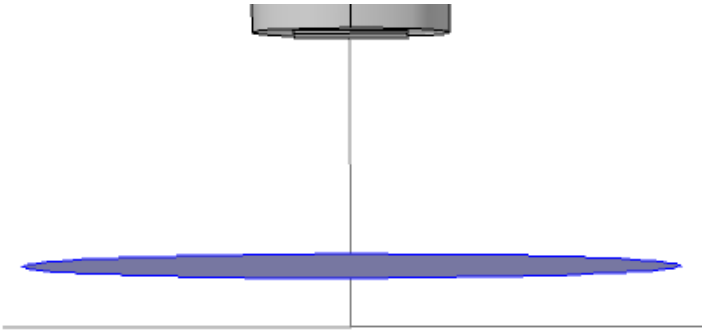
Settings

Description	Value
Concentration	{0, C_O}
Species O	1
Species R	1

Variables

Name	Expression	Unit	Description	Selection
chds.c0_O	0	mol/m^3	Concentration	Boundaries 10-12, 17, 23
chds.c0_R	C_O	mol/m^3	Concentration	Boundaries 10-12, 17, 23

2.3.5. Concentration 2



Concentration 2

Selection

Geometric entity level	Boundary
Selection	Boundary 5

Equations

$$c_i = c_{0i}$$

Settings

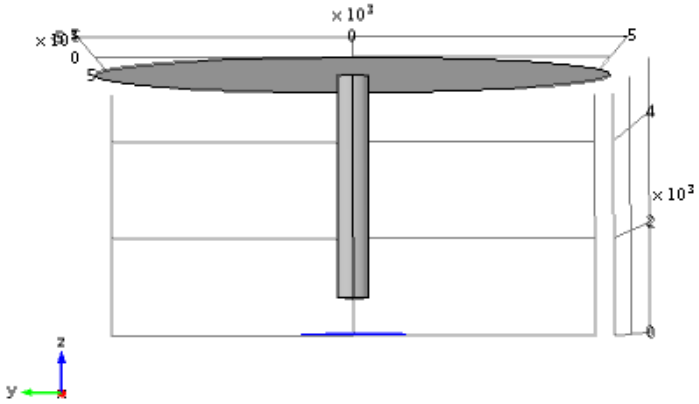
Settings

Description	Value
Concentration	{C_O, 0}
Species O	1
Species R	1

Variables

Name	Expression	Unit	Description	Selection
chds.c0_O	C_O	mol/m^3	Concentration	Boundary 5
chds.c0_R	0	mol/m^3	Concentration	Boundary 5

2.4. Mesh 1



Mesh 1

2.4.1. Size (size)

Settings

Name	Value
Maximum element size	557
Minimum element size	40.5
Resolution of curvature	0.4
Resolution of narrow regions	0.7
Maximum element growth rate	1.4
Predefined size	Finer

3. Study 1

3.1. Parametric Sweep

Parameter name: k_Step

Parameters: 700 [um], 500 [um], 300 [um], 200 [um], 170 [um], 140 [um], 120 [um], 100 [um], 80 [um], 70 [um], 60 [um], 55 [um], 50 [um]

3.2. Time Dependent

Times: time_Step

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: Time Dependent (st1)

Settings

Name	Value
Use study	Study 1
Use study step	Time Dependent

Dependent Variables 1 (v1)

Settings

Name	Value
Defined by study step	Time Dependent
Solution	Zero
Solution	Zero

Mod1.R (mod1_R)

Settings

Name	Value
Field components	mod1.R

Mod1.O (mod1_O)

Settings

Name	Value
Field components	mod1.O

Time-Dependent Solver 1 (t1)

Settings

Name	Value
Defined by study step	Time Dependent
Time	15
Maximum BDF order	2

Fully Coupled 1 (fc1)

Settings

Name	Value
Linear solver	Iterative 1
Jacobian update	Once per time step
Maximum number of iterations	5

Iterative 1 (i1)

Settings

Name	Value
Factor in error estimate	20

Multigrid 1 (mg1)

Settings

Name	Value
Use hierarchy in geometries	Geometry 1

Presmoother (pr)

SOR Line 1 (sl1)

Settings

Name	Value
Relaxation factor	0.4
Relaxation factor	0.3

Postsmoother (po)

SOR Line 1 (sl1)

Settings

Name	Value
Relaxation factor	0.4
Number of secondary iterations	2
Relaxation factor	0.5

Coarse Solver (cs)

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

Store Solution 7 (su5)

Settings

Name	Value
Solution	Store Solution 7

Store Solution 8 (su6)

Settings

Name	Value
Solution	Store Solution 8

Store Solution 9 (su7)

Settings

Name	Value
Solution	Store Solution 9

Store Solution 10 (su8)

Settings

Name	Value
Solution	Store Solution 10

Store Solution 11 (su9)

Settings

Name	Value
Solution	Store Solution 11

Store Solution 12 (su10)

Settings

Name	Value
Solution	Store Solution 12

Store Solution 13 (su11)

Settings

Name	Value
Solution	Store Solution 13

Store Solution 14 (su12)

Settings

Name	Value
Solution	Store Solution 14

Settings

Name	Value
Solution	Store Solution 15

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. Solution 2

Selection

Geometric entity level	Domain
Selection	Geometry geom1

Settings

Name	Value
Solution	Parametric 2
Model	Save Point Geometry 1

4.2. Tables

4.2.1. Table 1

Surface Integration 1 (n*F*chds.tfluxz_O)

4.2.2. Evaluation 3D

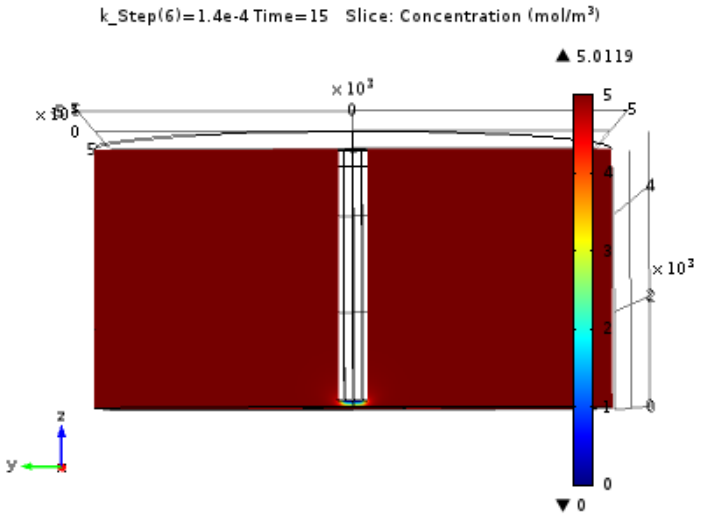
Interactive 3D values

Evaluation 3D

x	y	z	Value
0	-1615.46424	535.7382	5.01104

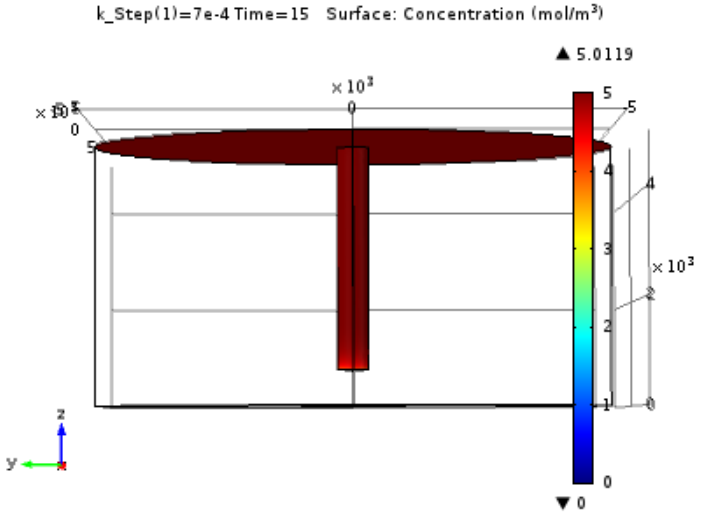
4.3. Plot Groups

4.3.1. Concentration (chds)



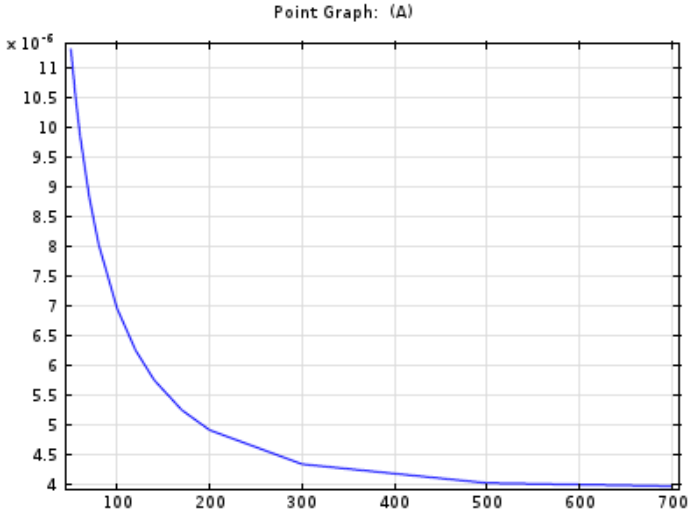
k_Step(6)=1.4e-4 Time=15 Slice: Concentration (mol/m^3)

4.3.2. Concentration (chds) 1



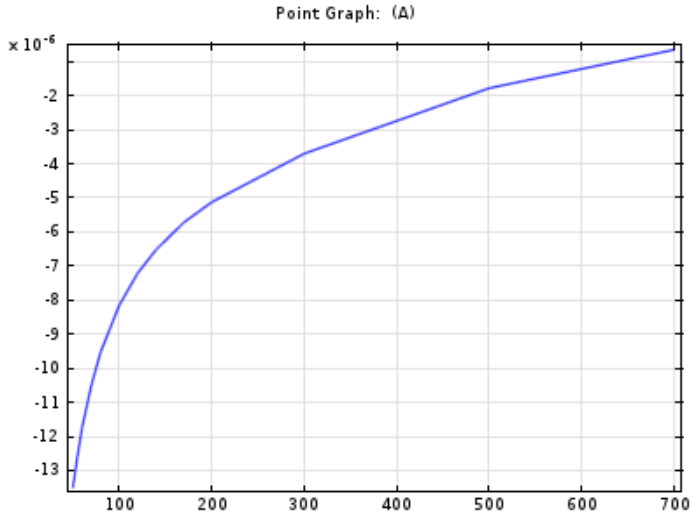
k_Step(1)=7e-4 Time=15 Surface: Concentration (mol/m^3)

4.3.3. 1D Plot Group 3



Point Graph: (A)

4.3.4. 1D Plot Group 4



Point Graph: (A)