Supporting Information

Electrochemically Probing Exciton Transport in Monolayers of Two-Dimensional Semiconductors

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Additional Experimental Data

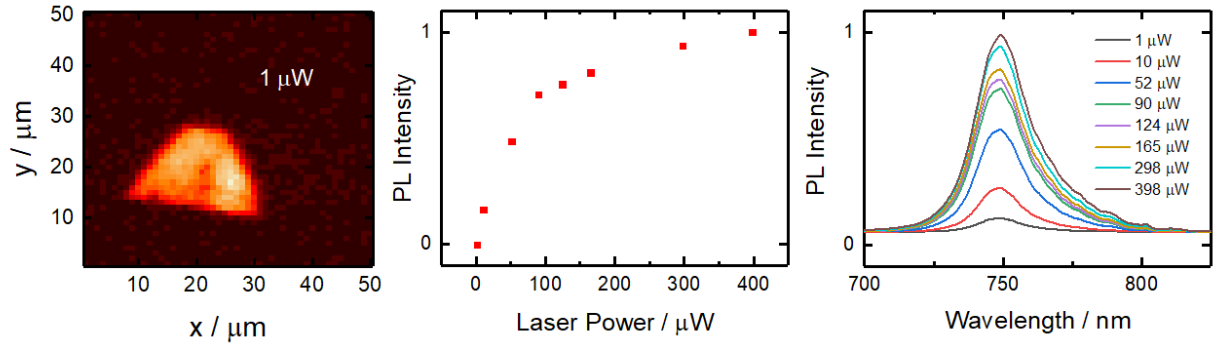


Figure S1. (a) Photoluminescence (PL) image of a WSe_2 monolayer. (b) PL intensity and spectra as a function of laser power. Nonlinear behavior is observed at higher laser intensities due to second order exciton-exciton interactions.

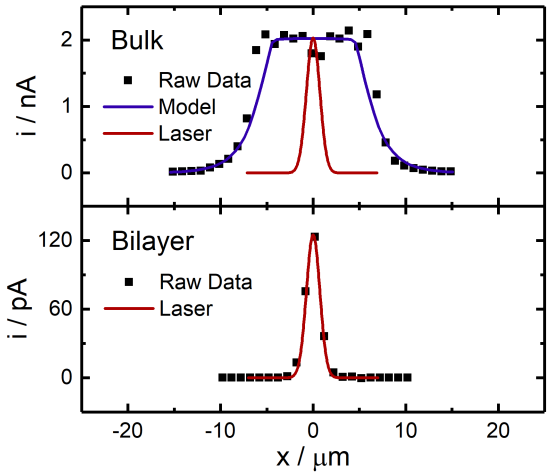


Figure S2. CG-TC SECCM profiles observed at bulk (top) and bilayer (bottom) WSe_2 structures. The blue line in the bulk example depicts a finite element simulation of the CG-TC SECCM experiment for L_{xy} = 2.1 μm. The red line represents the excitation laser profile, which is gaussian in shape with a standard deviation of 0.725 μm. In the bilayer case, the photocurrent profile essentially overlaps with the excitation, indicating extremely limited exciton diffusion.

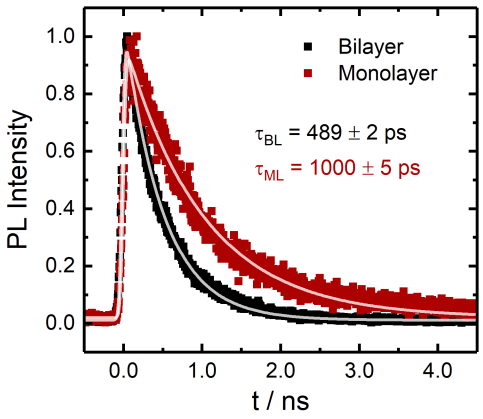


Figure S3. PL lifetimes observed at monolayer and bilayer WSe_2 samples. Squares depict raw TCSPC data, and lines represent single exponential fits convoluted with the laser pulse profile. The laser power employed was 10 μW.

Details on Finite Element Simulations

Theoretical Framework

Finite element simulations of carrier generation and transport were carried out using COMSOL Multiphysics. Steady-state solutions were found to Poisson's equation, to determine potentials within the WSe_2 material, as well as the drift-diffusion equation which governs carrier transport. These equations can be summarized as:

$$\nabla \cdot (\boldsymbol{\epsilon} \nabla \varphi) = \frac{q_e n_D}{\epsilon_0}\left[1 - e^{-\frac{q_e \varphi}{k_b T}}\right] \quad S1$$

$$\nabla \cdot \left(\boldsymbol{D}\nabla C + \frac{q\boldsymbol{D}\nabla\varphi}{k_b T} C\right) - \frac{C}{t_c} + \frac{\alpha P_0}{2\pi\sigma_0^2 h\nu} e^{-\frac{(x-x_g)^2+(y-y_g)^2}{2\sigma_0^2}} e^{-\alpha z} = 0 \quad S2$$

In these equations, $\boldsymbol{\epsilon}$ is the dielectric constant (a tensor quantity due to the anisotropy of the 2D material), φ is the electric potential, n_D is the density of dopants within the semiconductor, ϵ_0 is the vacuum dielectric constant, and $k_b T$ is Boltzmann's constant times temperature. $\boldsymbol{D}$ is the diffusion coefficient (again a tensor), t_c is the carrier lifetime, α is the absorption coefficient of the semiconductor, P_0 is the power in the gaussian excitation beam, σ_0 is the beam standard deviation, x_g/y_g denote the excitation centroid, and z denotes the vertical coordinate within the WSe_2 structure.

These equations were implemented within COMSOL using general PDE interfaces. WSe_2 samples were approximated as an oblate cylinder with a radius of 30 μm. The following boundary conditions were employed to find solutions to Poisson's equation:

$$\varphi(z = 0) = 0 \quad S3$$

$$\varphi\left(\left[x - x_p\right]^2 + \left[y - y_p\right]^2 < r_0^2, \quad z = w\right) = E_{fb} - E \quad S4$$

Here, w is the WSe_2 thickness, r_0 is the pipet radius, x_p/y_p denote the lateral pipet location, and $E_{fb} - E$ represents the applied potential with respect to the flatband potential. For the drift-diffusion equations, boundary conditions were employed at the pipet and defect interfaces:

$$C\left(\left[x - x_p\right]^2 + \left[y - y_p\right]^2 < r_0^2, z = w\right) = 0 \quad S5$$

$$C(x = 0, w_2 > z > w_1) = 0 \quad S6$$

Results from these simulations were used to calculate a carrier transport-limited current, i_{CT}. This can be used to estimate the experimental response in CG-TC SECCM using the following equation:

$$i = \frac{(i_{CT} + i_{MT} + \beta) \pm \sqrt{(i_{CT} + i_{MT} + \beta)^2 - 4 i_{CT} i_{MT}}}{2} \quad S7$$

where i_{MT} is the mass transfer limited current dictated by the SECCM probe and β is an adjustable kinetic parameter that does not play a significant role in the shape of the CG-TC response. For diffusion controlled transport, i_{MT} can be estimated as:

$$i_{MT} \approx \frac{2\pi n q_e D_r C_r^* r_0 \left[1 - \cos\theta_p\right]}{\tan\theta_p} \quad S8$$

where n is the number of electrons transferred in the reaction, q_e is the electronic charge, D_r is the diffusion constant of the redox-active species, C_r^* is the bulk concentration of this species, r_0 is the pipet radius, and θ_p is the half-angle of the pipet. More information on this model can be found in our previous report.[1]

Values of Physical Constants Employed in Finite Element Simulations

Table S1. Values of physical constants employed in finite element simulations. Subscript *z*'s and *xy*'s denote out-of-plane and in-plane quantities, respectively. Values were selected to match well to experimental measurements or typical literature values.[2–5]

Quantity	Value	Quantity	Value
ϵ_z	8	α	9×10^4 cm^{-1}
ϵ_{xy}	16	n_D	1×10^{17} cm^{-3}
ϵ_0	8.854×10^{-12} F m^{-1}	q	1.6×10^{-19} C
$E - E_{fb}$	0.5 V	$k_b T$	0.026 eV

References

(1) Hill, J. W.; Hill, C. M. Directly Visualizing Carrier Transport and Recombination at Individual Defects within 2D Semiconductors. *Chem. Sci.* **2021**, *12* (14), 5102–5112.

(2) Frindt, R. F. The Optical Properties of Single Crystals of WSe_2 and $MoTe_2$. *J. Phys. Chem. Solids* **1963**, *24* (9), 1107–1108.

(3) Yu, X.; Sivula, K. Photogenerated Charge Harvesting and Recombination in Photocathodes of Solvent-Exfoliated WSe_2. *Chem. Mater.* **2017**, *29* (16), 6863–6875.

(4) Jakubowicz, A.; Mahalu, D.; Wolf, M.; Wold, A.; Tenne, R. WSe_2: Optical and Electrical Properties as Related to Surface Passivation of Recombination Centers. *Phys. Rev. B* **1989**, *40* (5), 2992–3000.

(5) Laturia, A.; Van de Put, M. L.; Vandenberghe, W. G. Dielectric Properties of Hexagonal Boron Nitride and Transition Metal Dichalcogenides: From Monolayer to Bulk. *npj 2D Mater. Appl.* **2018**, *2* (1), 6.

COMSOL Model Report

GLOBAL DEFINITIONS

Date	Oct 16, 2020 5:03:50 PM

GLOBAL SETTINGS

Name	Sheet Diffusion Model.mph
Path	Y:\Sheet_Diffusion_Model.mph
Version	COMSOL 5.3 (Build: 316)

USED PRODUCTS

COMSOL Multiphysics

1.1 PARAMETERS

PARAMETERS 1

Name	Expression	Value	Description
rp	150[nm]	1.5E−7 m	
w	20[nm]	2E−8 m	
nD	1e17[1/cm^3]	1E23 1/m³	
kbT	0.0257[eV]	4.1176E−21 J	
rs	30[um]	3E−5 m	
epxy	16	16	
epz	8	8	
dPhi	0.5[V]	0.5 V	
Lxy	2.8[um]	2.8E−6 m	
RL	500	500	
Lz	Lxy/RL	5.6E−9 m	
tau	1[ns]	1E−9 s	
Dxy	Lxy^2/tau	0.00784 m²/s	
Dz	Lz^2/tau	3.136E−8 m²/s	
S	0.725[um]	7.25E−7 m	
P0	1.12[uW]	1.12E−6 W	
wl	633[nm]	6.33E−7 m	
Ep	1240[nm*eV]/wl	3.1385E−19 J	
N0	P0/Ep	3.5685E12 1/s	
alpha	9e4[1/cm]	9E6 1/m	
xp	1.5[um]	1.5E−6 m	
h0	0.1[nm]	1E−10 m	

Name	Expression	Value	Description
beta	0.5	0.5	
Nh	ceil(1/beta*log(1 + w/h0*(exp(beta) - 1)))	10	

2 Component 1

SETTINGS

Description	Value
Unit system	Same as global system
Avoid inverted elements by curving interior domain elements	Off

2.1 DEFINITIONS

2.1.1 Variables

Variables 1

SELECTION

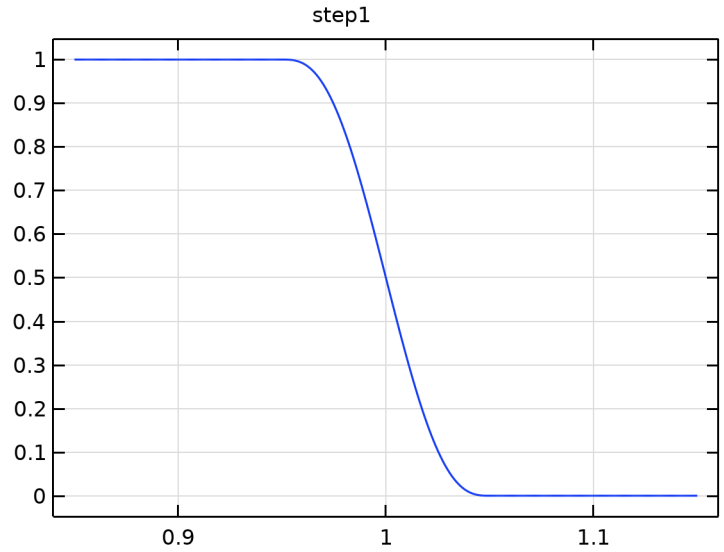
Geometric entity level	Entire model

Name	Expression	Unit	Description
Rg	N0*alpha*exp(-alpha*z)/(2*pi*S^2)*exp(-1*(x^2 + y^2)/(2*S^2))	1/(m³·s)	
phi0	-dPhi*step1(((x - xp)^2 + y^2)/rp^2)	V	

2.1.2 Functions

Step 1

Function name	step1
Function type	Step



Step 1

PARAMETERS

Description	Value
Location	1
From	1
To	0

2.1.3 Coordinate Systems

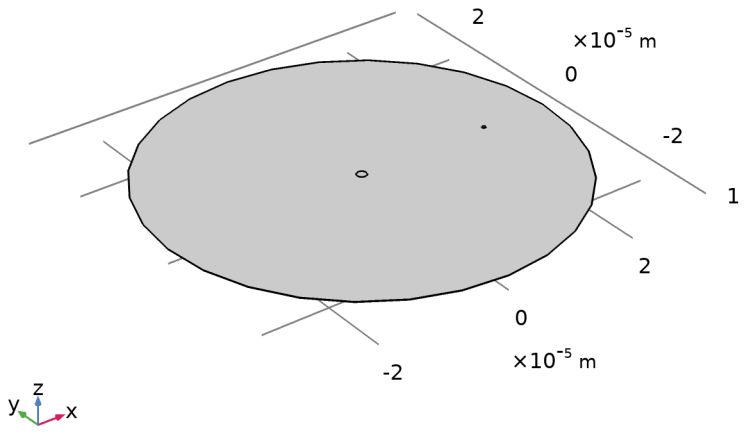
Boundary System 1

Coordinate system type	Boundary system
Tag	sys1

COORDINATE NAMES

First	Second	Third
t1	t2	n

2.2 GEOMETRY 1



Geometry 1

UNITS

Length unit	m
Angular unit	deg

GEOMETRY STATISTICS

Description	Value
Space dimension	3
Number of domains	5
Number of boundaries	28

Description	Value
Number of edges	52
Number of vertices	32

2.2.1 Cylinder 1 (cyl1)

POSITION

Description	Value
Position	{xp, 0, 0}

AXIS

Description	Value
Axis type	z - axis

SIZE AND SHAPE

Description	Value
Radius	rp
Height	w

2.2.2 Cylinder 2 (cyl2)

POSITION

Description	Value
Position	{xp, 0, 0}

AXIS

Description	Value
Axis type	z - axis

SIZE AND SHAPE

Description	Value
Radius	rp + w
Height	w

2.2.3 Work Plane 1 (wp1)

PLANE DEFINITION

Description	Value
Plane	xz - plane

UNITE OBJECTS

Description	Value
Unite objects	On

Plane Geometry (sequence2D)

2.2.4 Partition Domains 1 (pard1)

SETTINGS

Description	Value
Work plane	Work Plane 1

2.2.5 Cylinder 3 (cyl3)

POSITION

Description	Value
Position	{0, 0, 0}

AXIS

Description	Value
Axis type	z - axis

SIZE AND SHAPE

Description	Value
Radius	rs
Height	w

2.2.6 Cylinder 4 (cyl4)

POSITION

Description	Value
Position	{0, 0, 0}

AXIS

Description	Value
Axis type	z - axis

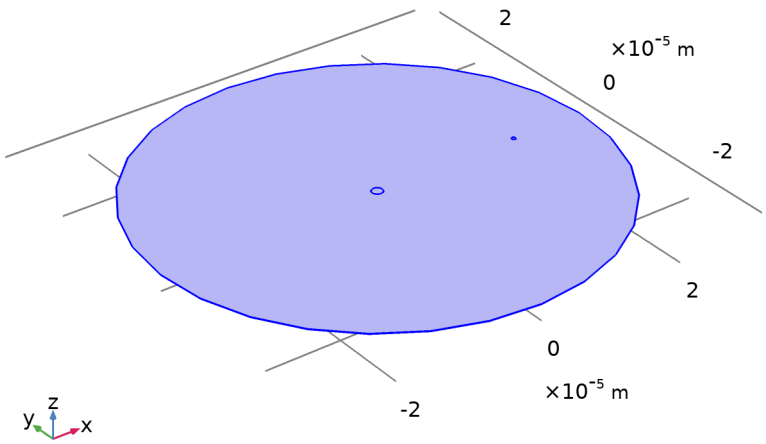
SIZE AND SHAPE

Description	Value
Radius	S
Height	w

2.3 POISSON-BOLTZMANN

USED PRODUCTS

COMSOL Multiphysics



Poisson-Boltzmann

SELECTION

Geometric entity level	Domain
Selection	Geometry geom1: Dimension 3: All domains

2.3.1 Interface settings

Discretization

SETTINGS

Description	Value
Shape function type	Lagrange
Element order	Quadratic
Frame	Spatial

Units

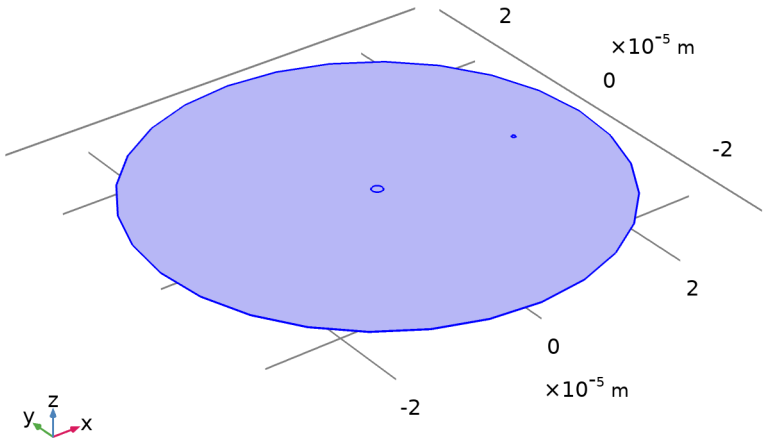
Dependent variable quantity	Unit
Electric potential	V

Source term quantity	Unit
Custom unit	C/m^3

2.3.2 Variables

Name	Expression	Unit	Description	Selection	Details
p.nx	nx		Normal vector, x component	Boundaries 1–28	Meta
p.ny	ny		Normal vector, y component	Boundaries 1–28	Meta
p.nz	nz		Normal vector, z component	Boundaries 1–28	Meta
p.nxmesh	nxmesh		Normal vector (mesh), x component	Boundaries 1–28	Meta
p.nymesh	nymesh		Normal vector (mesh), y component	Boundaries 1–28	Meta
p.nzmesh	nzmesh		Normal vector (mesh), z component	Boundaries 1–28	Meta

2.3.3 Coefficient Form PDE 1



Coefficient Form PDE 1

SELECTION

Geometric entity level	Domain
Selection	Geometry geom1: Dimension 3: All domains

EQUATIONS

$$e_a\frac{\partial^2 phi}{\partial t^2}+d_a\frac{\partial phi}{\partial t}+\nabla\cdot(-c\nabla phi - \alpha phi+\gamma)+\beta\cdot\nabla phi+aphi=f$$

$$\nabla=[\frac{\partial}{\partial x},\frac{\partial}{\partial y},\frac{\partial}{\partial z}]$$

SETTINGS

Description	Value
Absorption coefficient	0
Diffusion coefficient	{{epxy*epsilon0_const, 0, 0}, {0, epxy*epsilon0_const, 0}, {0, 0, epz*epsilon0_const}}
Convection coefficient	{0, 0, 0}
Source term	e_const*nD*(1 - exp(e_const*phi/kbT))
Conservative flux source	{0, 0, 0}
Conservative flux convection coefficient	{0, 0, 0}
Mass coefficient	0
Damping or mass coefficient	0

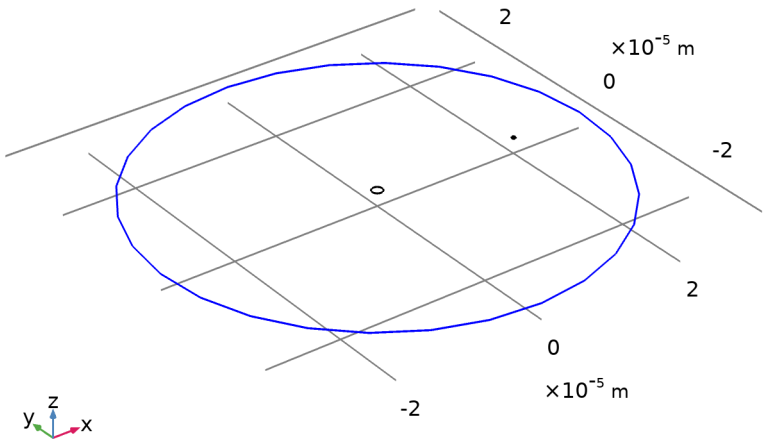
Variables

Name	Expression	Unit	Description	Selection
domflux.phix	-epxy*epsilon0_const*phix	C/m²	Domain flux, x component	Domains 1–5
domflux.phiy	-epxy*epsilon0_const*phiy	C/m²	Domain flux, y component	Domains 1–5
domflux.phiz	-epz*epsilon0_const*phiz	C/m²	Domain flux, z component	Domains 1–5

Shape functions

Name	Shape function	Unit	Description	Shape frame	Selection
phi	Lagrange (Quadratic)	V	Dependent variable phi	Spatial	Domains 1–5

2.3.4 Zero Flux 1



Zero Flux 1

SELECTION

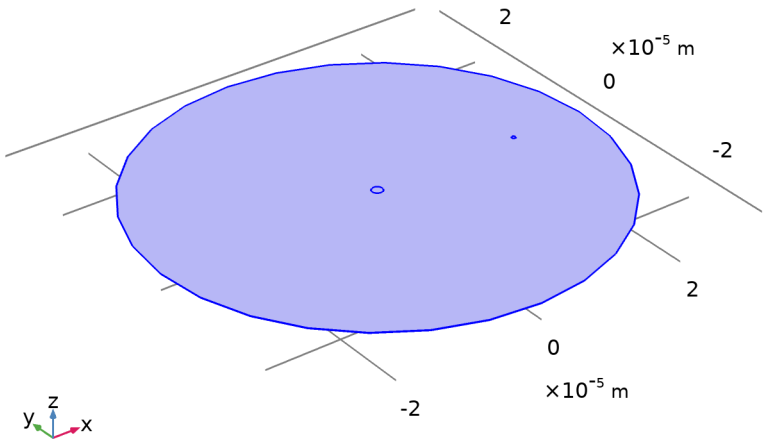
Geometric entity level	Boundary
Selection	Geometry geom1: Dimension 2: All boundaries

EQUATIONS

$$-\mathbf{n}\cdot(-c\nabla phi - \alpha phi + \gamma) = 0$$

$$\nabla = [\frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z}]$$

2.3.5 Initial Values 1



Initial Values 1

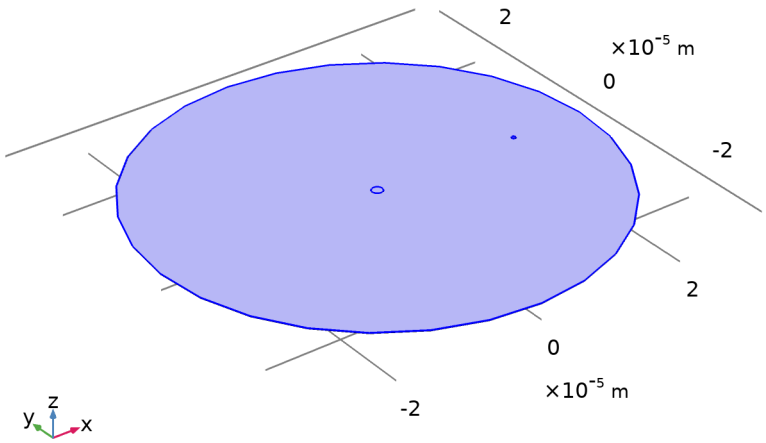
SELECTION

Geometric entity level	Domain
Selection	Geometry geom1: Dimension 3: All domains

SETTINGS

Description	Value
Initial value for phi	0
Initial time derivative of phi	0

2.3.6 Dirichlet Boundary Condition 1



Dirichlet Boundary Condition 1

SELECTION

Geometric entity level	Boundary
Selection	Geometry geom1: Dimension 2: Boundaries 4, 8, 18–19, 23

EQUATIONS

$phi = r$

$g_{reaction} = -\mu$

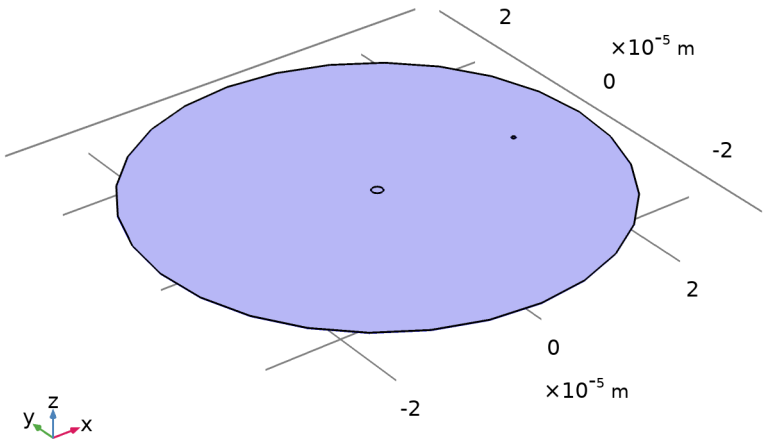
SETTINGS

Description	Value
Value on boundary	phi0
Prescribed value of phi	On

Constraints

Constraint	Constraint force	Shape function	Selection	Details
phi0-phi	-test(phi)	Lagrange (Quadratic)	Boundaries 4, 8, 18–19, 23	Elemental

2.3.7 Dirichlet Boundary Condition 2



Dirichlet Boundary Condition 2

SELECTION

Geometric entity level	Boundary
Selection	Geometry geom1: Dimension 2: Boundaries 3, 7, 16–17, 22

EQUATIONS

$phi = r$

$g_{reaction} = -\mu$

SETTINGS

Description	Value
Value on boundary	0
Prescribed value of phi	On

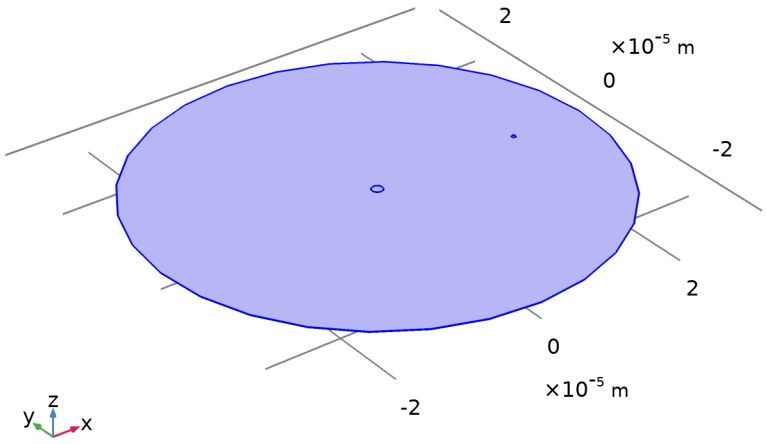
Constraints

Constraint	Constraint force	Shape function	Selection	Details
-phi	-test(phi)	Lagrange (Quadratic)	Boundaries 3, 7, 16–17, 22	Elemental

2.4 DRIFT-DIFFUSION

USED PRODUCTS

COMSOL Multiphysics



Drift-Diffusion

SELECTION

Geometric entity level	Domain
Selection	Geometry geom1: Dimension 3: All domains

2.4.1 Interface settings

Discretization

SETTINGS

Description	Value
Shape function type	Lagrange
Element order	Quadratic
Frame	Spatial

Units

Dependent variable quantity	Unit
Number density	1/m^3

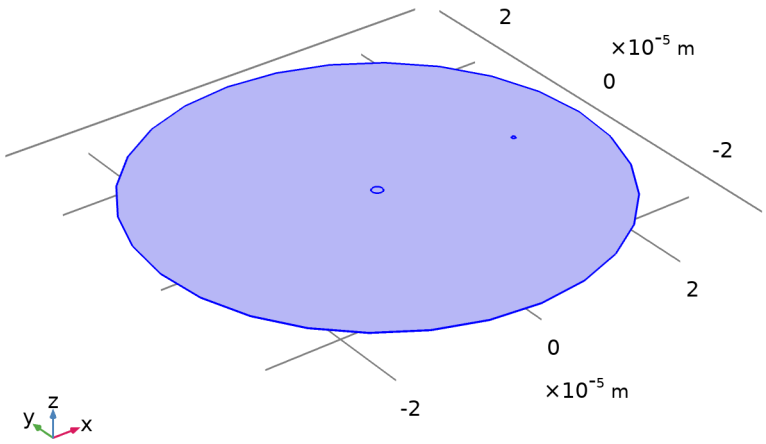
Source term quantity	Unit
Custom unit	m^-3*s^-1

2.4.2 Variables

Name	Expression	Unit	Description	Selection	Details
C.nx	nx		Normal vector, x component	Boundaries 1–28	Meta

Name	Expression	Unit	Description	Selection	Details
C.ny	ny		Normal vector, y component	Boundaries 1–28	Meta
C.nz	nz		Normal vector, z component	Boundaries 1–28	Meta
C.nxmesh	nxmesh		Normal vector (mesh), x component	Boundaries 1–28	Meta
C.nymesh	nymesh		Normal vector (mesh), y component	Boundaries 1–28	Meta
C.nzmesh	nzmesh		Normal vector (mesh), z component	Boundaries 1–28	Meta

2.4.3 Coefficient Form PDE 1



Coefficient Form PDE 1

SELECTION

Geometric entity level	Domain
Selection	Geometry geom1: Dimension 3: All domains

EQUATIONS

$$e_a\frac{\partial^2 Ch}{\partial t^2}+d_a\frac{\partial Ch}{\partial t}+\nabla\cdot(-c\nabla Ch-\alpha Ch+\gamma)+\beta\cdot\nabla Ch+aCh=f$$

$$\nabla=[\frac{\partial}{\partial x},\frac{\partial}{\partial y},\frac{\partial}{\partial z}]$$

SETTINGS

Description	Value
Absorption coefficient	1/tau

Description	Value
Diffusion coefficient	{{Dxy, 0, 0}, {0, Dxy, 0}, {0, 0, Dz}}
Convection coefficient	{0, 0, 0}
Source term	Rg
Conservative flux source	{0, 0, 0}
Conservative flux convection coefficient	{e_const*Dxy*phix/kbT, e_const*Dxy*phiy/kbT, e_const*Dz*phiz/kbT}
Mass coefficient	0
Damping or mass coefficient	1

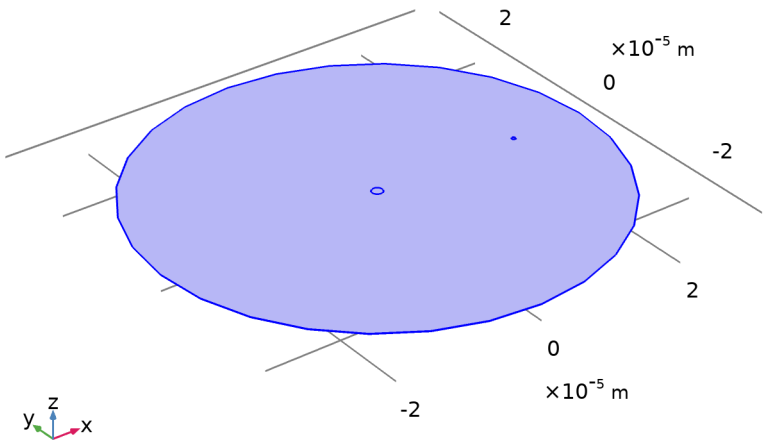
Variables

Name	Expression	Unit	Description	Selection
domflux.Chx	Dxy*(-Chx-e_const*phix*Ch/kbT)	1/(m²·s)	Domain flux, x component	Domains 1–5
domflux.Chy	Dxy*(-Chy-e_const*phiy*Ch/kbT)	1/(m²·s)	Domain flux, y component	Domains 1–5
domflux.Chz	Dz*(-Chz-e_const*phiz*Ch/kbT)	1/(m²·s)	Domain flux, z component	Domains 1–5

Shape functions

Name	Shape function	Unit	Description	Shape frame	Selection
Ch	Lagrange (Quadratic)	1/m³	Dependent variable Ch	Spatial	Domains 1–5

2.4.4 Zero Flux 1



Zero Flux 1

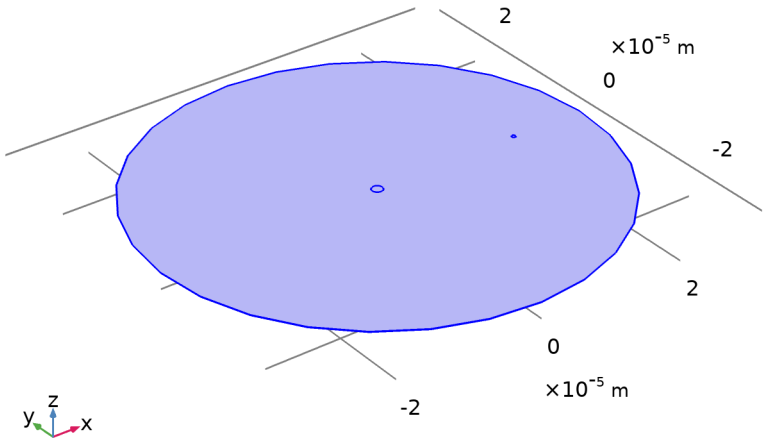
SELECTION

Geometric entity level	Boundary
Selection	Geometry geom1: Dimension 2: All boundaries

EQUATIONS

$$-\mathbf{n}\cdot(-c\nabla Ch - \alpha Ch + \gamma) = 0$$
$$\nabla = [\frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z}]$$

2.4.5 Initial Values 1



Initial Values 1

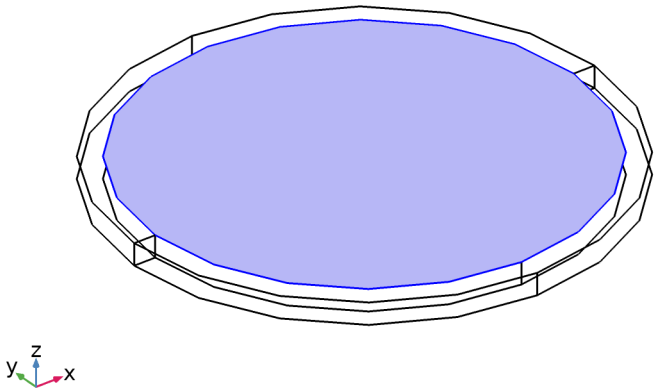
SELECTION

Geometric entity level	Domain
Selection	Geometry geom1: Dimension 3: All domains

SETTINGS

Description	Value
Initial value for Ch	Rg*tau
Initial time derivative of Ch	0

2.4.6 Dirichlet Boundary Condition 1



Dirichlet Boundary Condition 1

SELECTION

Geometric entity level	Boundary
Selection	Geometry geom1: Dimension 2: Boundary 23

EQUATIONS

$$Ch = r$$
$$g_{reaction} = -\mu$$

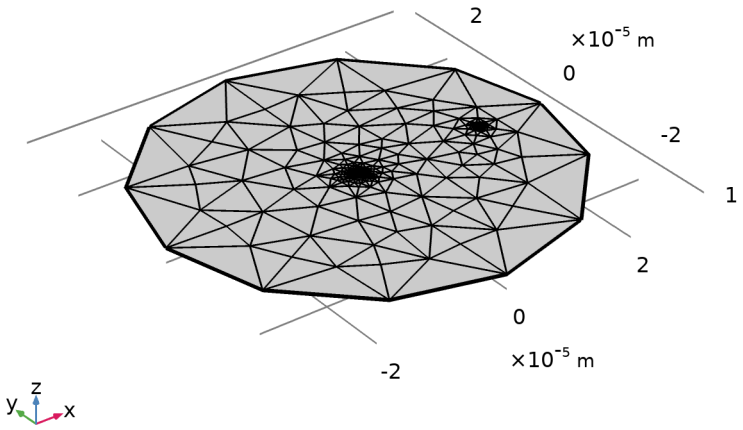
SETTINGS

Description	Value
Value on boundary	0
Prescribed value of Ch	On

Constraints

Constraint	Constraint force	Shape function	Selection	Details
-Ch	-test(Ch)	Lagrange (Quadratic)	Boundary 23	Elemental

2.5 MESH 1



Mesh 1

2.5.1 Size (size)

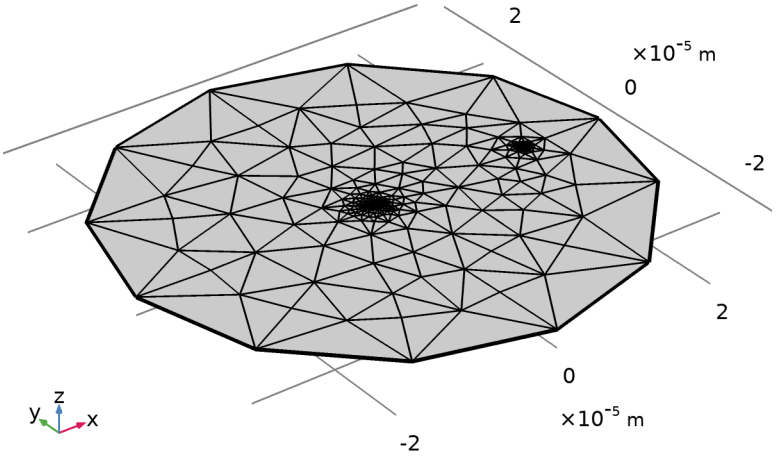
SETTINGS

Description	Value
Maximum element size	6.0E-6
Minimum element size	1.08E-6
Curvature factor	0.6
Resolution of narrow regions	0.5
Maximum element growth rate	1.5

2.5.2 Size 1 (size1)

SELECTION

Geometric entity level	Domain
Selection	Geometry geom1



Size 1

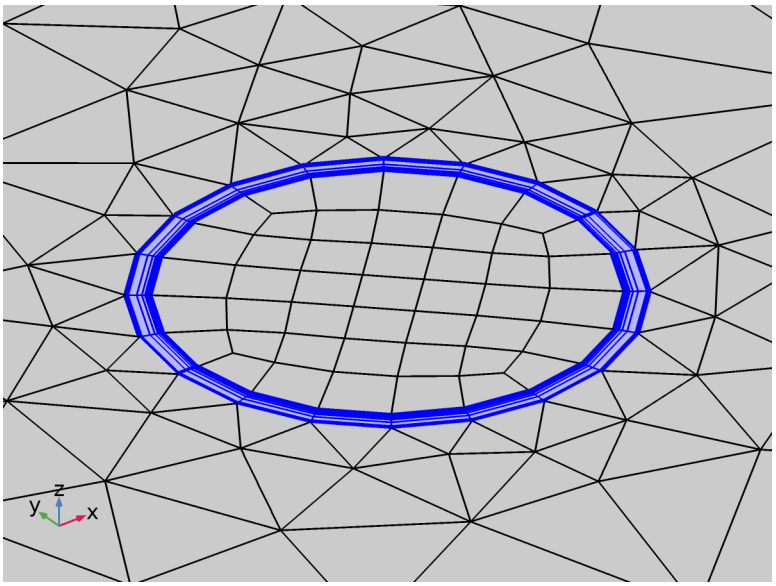
SETTINGS

Description	Value
Maximum element size	6.0E-6
Minimum element size	1.08E-6
Curvature factor	0.6
Resolution of narrow regions	0.5
Maximum element growth rate	1.5

2.5.3 Mapped 1 (map1)

SELECTION

Geometric entity level	Boundary
Selection	Geometry geom1: Dimension 2: Boundaries 18–19

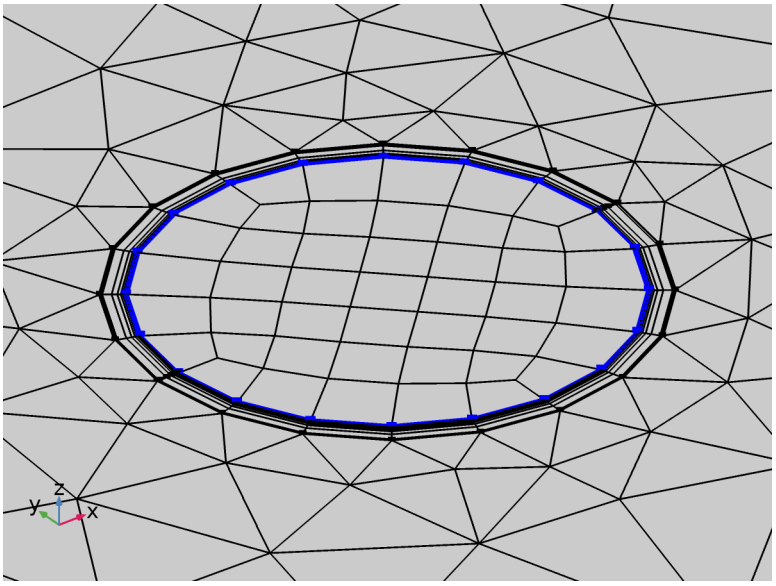


Mapped 1

Distribution 1 (dis1)

SELECTION

Geometric entity level	Edge
Selection	Geometry geom1: Dimension 1: Edges 34–35, 41, 44



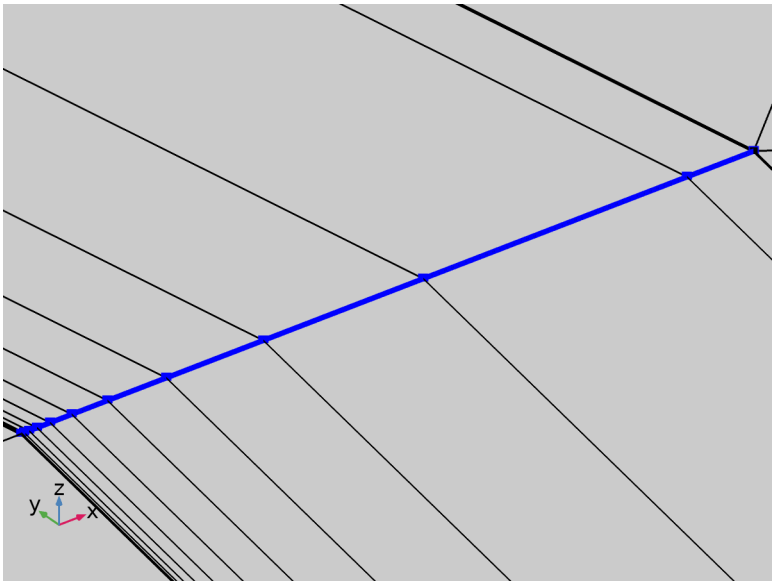
Distribution 1

Distribution 2 (dis2)

SELECTION

Geometric entity level	Edge

Selection	Geometry geom1: Dimension 1: Edge 50



Distribution 2

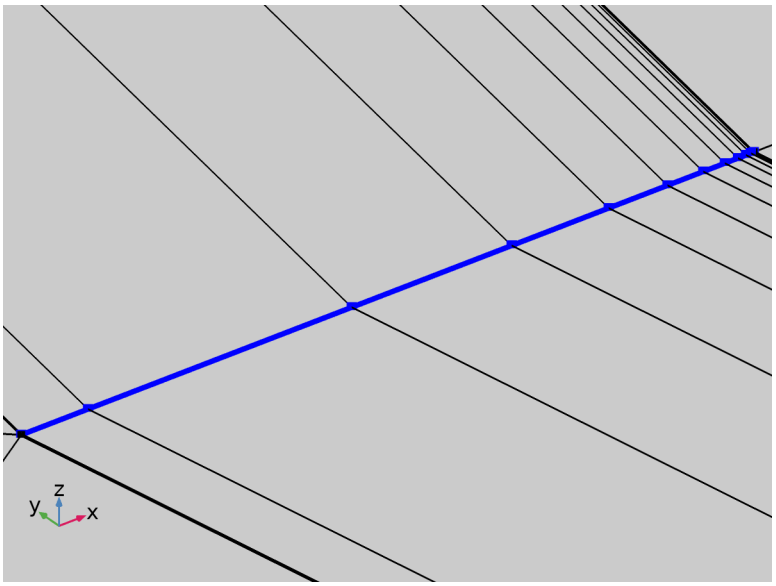
SETTINGS

Description	Value
Distribution type	Explicit
Relative placement of vertices along edge	{0, 0.005000000000000001, 0.01324360635350064, 0.026835015495795866, 0.04924346084748619, 0.08618874134213945, 0.14710121114565683, 0.24752889576159512, 0.4131061555550567, 0.6860969057207779, 1}

Distribution 3 (dis3)

SELECTION

Geometric entity level	Edge
Selection	Geometry geom1: Dimension 1: Edge 28



Distribution 3

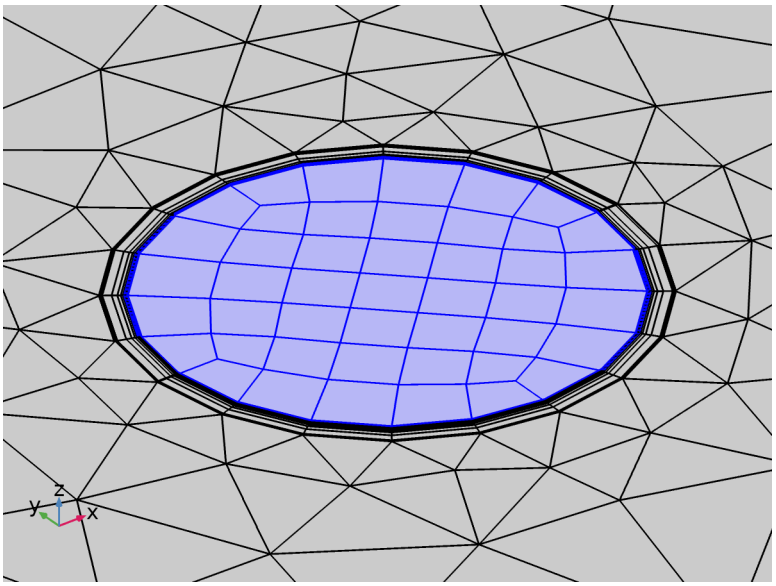
SETTINGS

Description	Value
Distribution type	Explicit
Relative placement of vertices along edge	{0, 0.005000000000000001, 0.01324360635350064, 0.02683501549579586, 0.04924346084748619, 0.0861887413421394, 0.14710121114565683, 0.24752889576159512, 0.4131061555550567, 0.6860969057207779, 1}
Reverse direction	On

2.5.4 Free Quad 1 (fq1)

SELECTION

Geometric entity level	Boundary
Selection	Geometry geom1: Dimension 2: Boundary 23



Free Quad 1

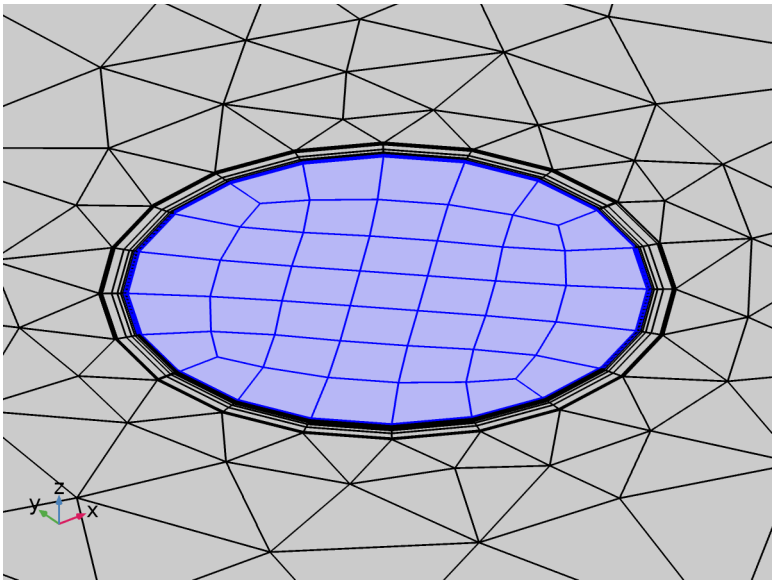
SETTINGS

Description	Value
Method	Legacy version 5.4

Size 1 (size1)

SELECTION

Geometric entity level	Boundary
Selection	Geometry geom1: Dimension 2: Boundary 23



Size 1

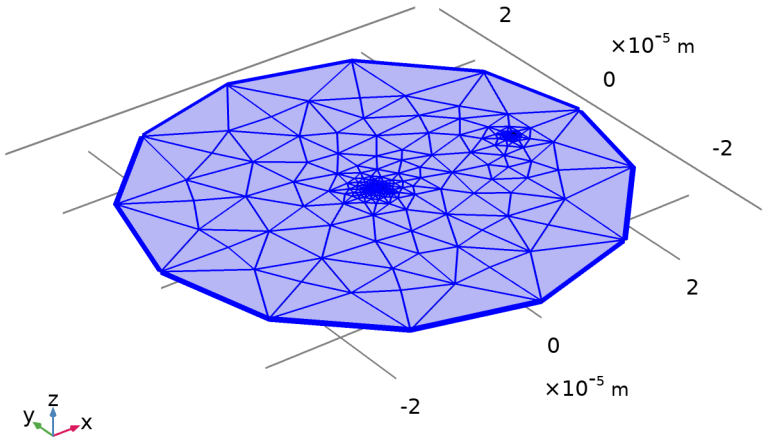
SETTINGS

Description	Value
Maximum element size	rp/20
Minimum element size	1.08E-6
Minimum element size	Off
Curvature factor	0.6
Curvature factor	Off
Resolution of narrow regions	0.5
Resolution of narrow regions	Off
Maximum element growth rate	1.5
Maximum element growth rate	Off
Custom element size	Custom

2.5.5 Free Triangular 1 (ftri1)

SELECTION

Geometric entity level	Boundary
Selection	Geometry geom1: Dimension 2: Boundaries 4, 8

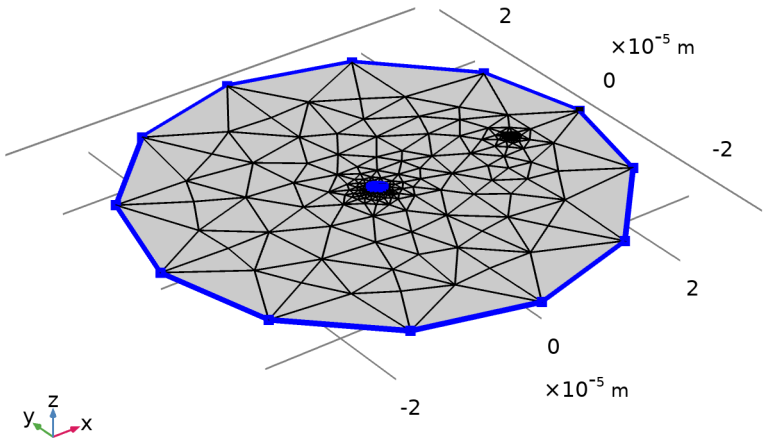


Free Triangular 1

Distribution 1 (dis1)

SELECTION

Geometric entity level	Edge
Selection	Geometry geom1: Dimension 1: Edges 4–5, 7, 9–10, 13, 16, 18–19, 22



Distribution 1

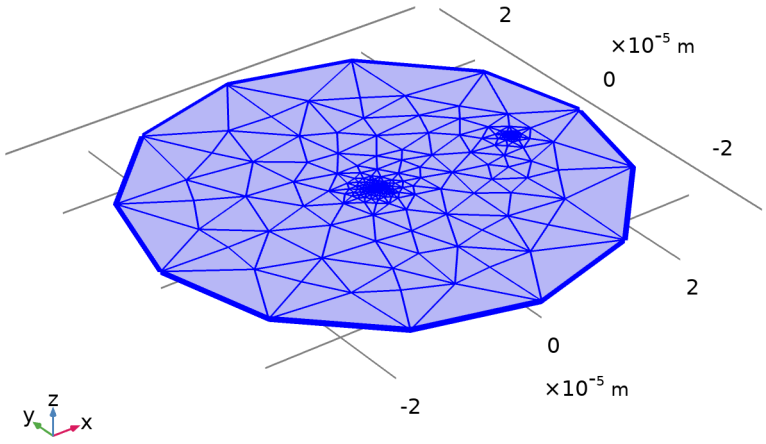
SETTINGS

Description	Value
Number of elements	3

2.5.6 Swept 1 (swe1)

SELECTION

Geometric entity level	Domain
Selection	Remaining



Swept 1

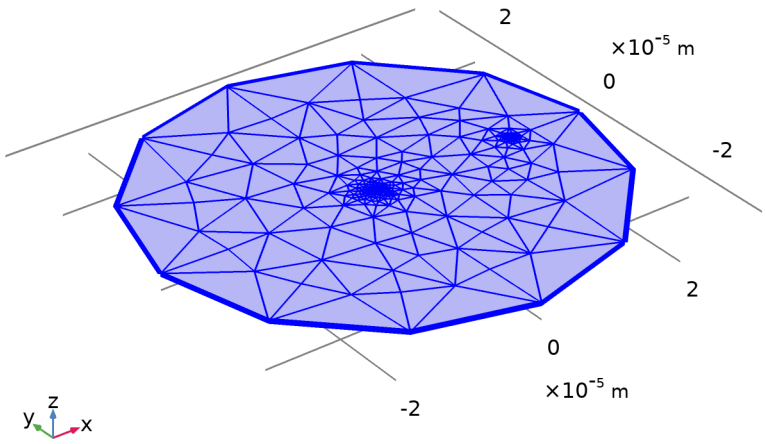
SETTINGS

Description	Value
Face meshing method	Quadrilateral (legacy version 5.4)

Distribution 1 (dis1)

SELECTION

Geometric entity level	Domain
Selection	Geometry geom1: Dimension 3: All domains



Distribution 1

SETTINGS

Description	Value
Distribution type	Explicit
Relative placement of vertices along edge	{0, 0.005000000000000001, 0.01324360635350064, 0.026835015495795866, 0.04924346084748619, 0.08618874134213945, 0.14710121114565683, 0.24752889576159512, 0.4131061555550567, 0.6860969057207779, 1}

3 Study 1

COMPUTATION INFORMATION

Computation time	1 h 6 min 55 s
CPU	Intel64 Family 6 Model 85 Stepping 4, 4 cores
Operating system	Windows 10

3.1 EXPERIMENTAL SWEEP

Parameter name	Parameter value list	Parameter unit
rp	250	nm
w	25	nm

STUDY SETTINGS

Description	Value
Sweep type	Specified combinations
Parameter name	{rp, w}
Unit	{nm, nm}

PARAMETERS

Parameter name	Parameter value list	Parameter unit
rp	250	nm
w	25	nm

3.2 PIPET TRANSLATION

Parameter name	Parameter value list	Parameter unit
xp	range(1.5,0.5,20)	um

STUDY SETTINGS

Description	Value
Sweep type	Specified combinations
Parameter name	xp
Unit	um

PARAMETERS

Parameter name	Parameter value list	Parameter unit
xp	range(1.5,0.5,20)	um

3.3 STATIONARY

STUDY SETTINGS

Description	Value
Include geometric nonlinearity	Off

STUDY EXTENSIONS

Description	Value
Auxiliary sweep	On
Sweep type	Specified combinations

PARAMETERS

Parameter name	Parameter value list	Parameter unit
Lxy	1 1.5 2 2.5 3 3.5 4 4.5 5	um

PHYSICS AND VARIABLES SELECTION

Physics interface	Discretization
Poisson-Boltzmann (p)	physics
Drift-Diffusion (C)	physics

MESH SELECTION

Geometry	Mesh
Geometry 1 (geom1)	mesh1

3.3.1 Study extensions

STUDY EXTENSIONS

Description	Value
Auxiliary sweep	On
Sweep type	Specified combinations

PARAMETERS

Parameter name	Parameter value list	Parameter unit
Lxy	1 1.5 2 2.5 3 3.5 4 4.5 5	um

3.4 SOLVER CONFIGURATIONS

3.4.1 Solution 1

Compile Equations: Stationary (st1)

STUDY AND STEP

Description	Value
Use study	Study 1
Use study step	Stationary

Dependent Variables 1 (v1)

GENERAL

Description	Value
Defined by study step	Stationary

INITIAL VALUE CALCULATION CONSTANTS

Constant name	Initial value source
Lxy	1[um] 1.5[um] 2[um] 2.5[um] 3[um] 3.5[um] 4[um] 4.5[um] 5[um]

Dependent variable Ch (comp1.Ch) (comp1_Ch)

GENERAL

Description	Value
Field components	comp1.Ch
Internal variables	{comp1.uflux.Ch, comp1.dflux.Ch}

Dependent variable phi (comp1.phi) (comp1_phi)

GENERAL

Description	Value
Field components	comp1.phi
Internal variables	{comp1.uflux.phi, comp1.dflux.phi}

Stationary Solver 1 (s1)

GENERAL

Description	Value
Defined by study step	Stationary
Relative tolerance	1e-6

RESULTS WHILE SOLVING

Description	Value
Probes	None

Parametric 1 (p1)

GENERAL

Description	Value
Defined by study step	Stationary

PARAMETERS

Parameter name	Parameter value list	Parameter unit
Lxy	1 1.5 2 2.5 3 3.5 4 4.5 5	um

Segregated 1 (se1)

Segregated Step 1 (ss1)

GENERAL

Description	Value
Variables	Dependent variable Ch (comp1.Ch)
Linear solver	Direct

Segregated Step 2 (ss2)

GENERAL

Description	Value
Variables	Dependent variable phi (comp1.phi)
Linear solver	Direct

3.4.2 Parametric Solutions 1

rp=250, w=25, xp=1.5 (su1)

GENERAL

Description	Value
Solution	rp=250, w=25, xp=1.5

rp=250, w=25, xp=2 (su2)

GENERAL

Description	Value
Solution	rp=250, w=25, xp=2

rp=250, w=25, xp=2.5 (su3)

GENERAL

Description	Value
Solution	rp=250, w=25, xp=2.5

rp=250, w=25, xp=3 (su4)

GENERAL

Description	Value
Solution	rp=250, w=25, xp=3

rp=250, w=25, xp=3.5 (su5)

GENERAL

Description	Value
Solution	rp=250, w=25, xp=3.5

rp=250, w=25, xp=4 (su6)

GENERAL

Description	Value
Solution	rp=250, w=25, xp=4

rp=250, w=25, xp=4.5 (su7)

GENERAL

Description	Value
Solution	rp=250, w=25, xp=4.5

rp=250, w=25, xp=5 (su8)

GENERAL

Description	Value
Solution	rp=250, w=25, xp=5

rp=250, w=25, xp=5.5 (su9)

GENERAL

Description	Value
Solution	rp=250, w=25, xp=5.5

rp=250, w=25, xp=6 (su10)

GENERAL

Description	Value
Solution	rp=250, w=25, xp=6

rp=250, w=25, xp=6.5 (su11)

GENERAL

Description	Value
Solution	rp=250, w=25, xp=6.5

rp=250, w=25, xp=7 (su12)

GENERAL

Description	Value
Solution	rp=250, w=25, xp=7

rp=250, w=25, xp=7.5 (su13)

GENERAL

Description	Value
Solution	rp=250, w=25, xp=7.5

rp=250, w=25, xp=8 (su14)

GENERAL

Description	Value
Solution	rp=250, w=25, xp=8

rp=250, w=25, xp=8.5 (su15)

GENERAL

Description	Value
Solution	rp=250, w=25, xp=8.5

rp=250, w=25, xp=9 (su16)

GENERAL

Description	Value
Solution	rp=250, w=25, xp=9

rp=250, w=25, xp=9.5 (su17)

GENERAL

Description	Value
Solution	rp=250, w=25, xp=9.5

rp=250, w=25, xp=10 (su18)

GENERAL

Description	Value
Solution	rp=250, w=25, xp=10

rp=250, w=25, xp=10.5 (su19)

GENERAL

Description	Value
Solution	rp=250, w=25, xp=10.5

rp=250, w=25, xp=11 (su20)

GENERAL

Description	Value
Solution	rp=250, w=25, xp=11

rp=250, w=25, xp=11.5 (su21)

GENERAL

Description	Value
Solution	rp=250, w=25, xp=11.5

rp=250, w=25, xp=12 (su22)

GENERAL

Description	Value
Solution	rp=250, w=25, xp=12

rp=250, w=25, xp=12.5 (su23)

GENERAL

Description	Value
Solution	rp=250, w=25, xp=12.5

rp=250, w=25, xp=13 (su24)

GENERAL

Description	Value
Solution	rp=250, w=25, xp=13

rp=250, w=25, xp=13.5 (su25)

GENERAL

Description	Value
Solution	rp=250, w=25, xp=13.5

rp=250, w=25, xp=14 (su26)

GENERAL

Description	Value
Solution	rp=250, w=25, xp=14

rp=250, w=25, xp=14.5 (su27)

GENERAL

Description	Value
Solution	rp=250, w=25, xp=14.5

rp=250, w=25, xp=15 (su28)

GENERAL

Description	Value
Solution	rp=250, w=25, xp=15

rp=250, w=25, xp=15.5 (su29)

GENERAL

Description	Value
Solution	rp=250, w=25, xp=15.5

rp=250, w=25, xp=16 (su30)

GENERAL

Description	Value
Solution	rp=250, w=25, xp=16

rp=250, w=25, xp=16.5 (su31)

GENERAL

Description	Value
Solution	rp=250, w=25, xp=16.5

rp=250, w=25, xp=17 (su32)

GENERAL

Description	Value
Solution	rp=250, w=25, xp=17

rp=250, w=25, xp=17.5 (su33)

GENERAL

Description	Value
Solution	rp=250, w=25, xp=17.5

rp=250, w=25, xp=18 (su34)

GENERAL

Description	Value
Solution	rp=250, w=25, xp=18

rp=250, w=25, xp=18.5 (su35)

GENERAL

Description	Value
Solution	rp=250, w=25, xp=18.5

rp=250, w=25, xp=19 (su36)

GENERAL

Description	Value
Solution	rp=250, w=25, xp=19

rp=250, w=25, xp=19.5 (su37)

GENERAL

Description	Value
Solution	rp=250, w=25, xp=19.5

rp=250, w=25, xp=20 (su38)

GENERAL

Description	Value
Solution	rp=250, w=25, xp=20

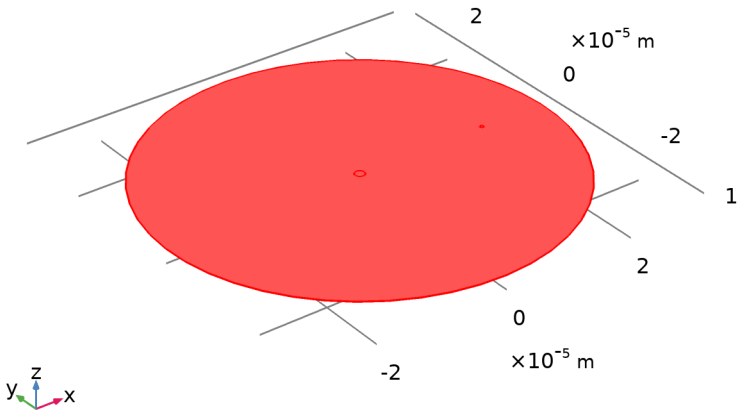
4 Results

4.1 DATA SETS

4.1.1 Study 1/Solution 1

SOLUTION

Description	Value
Solution	Solution 1
Component	Save Point Geometry 1



Dataset: Study 1/Solution 1

4.1.2 Cut Line 3D 1

DATA

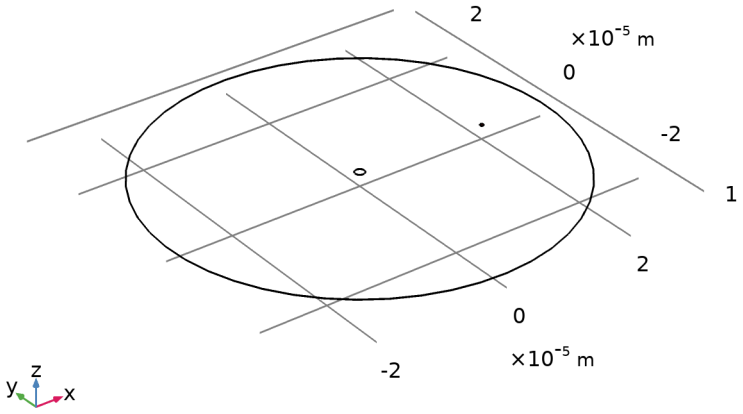
Description	Value
Dataset	Study 1/Parametric Solutions 1

LINE DATA

Description	Value
Line entry method	Two points
Points	{{xp, 0, w}, {xp, 0, 0}}

ADVANCED

Description	Value
Space variable	cln1x

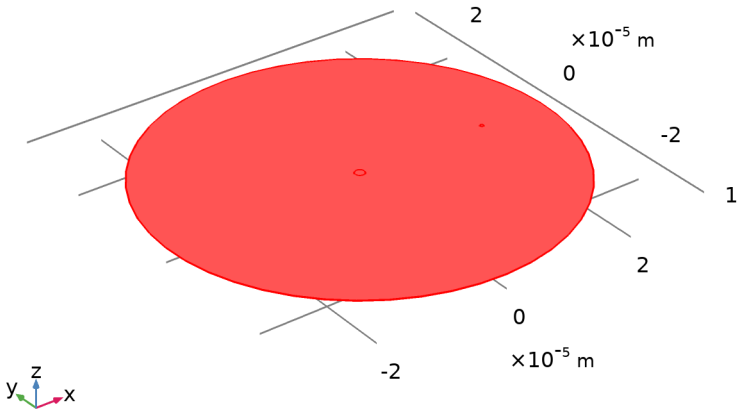


Dataset: Cut Line 3D 1

4.1.3 Study 1/Parametric Solutions 1

SOLUTION

Description	Value
Solution	Parametric Solutions 1
Component	Save Point Geometry 1



Dataset: Study 1/Parametric Solutions 1

4.2 DERIVED VALUES

4.2.1 Surface Integration 1

OUTPUT

Evaluated in	Table 8

DATA

Description	Value
Dataset	Study 1/Parametric Solutions 1
Table columns	Lxy

EXPRESSIONS

Expression	Unit	Description
-e_const*Chz*Dz	A	

INTEGRATION SETTINGS

Description	Value
Integration order	4

4.3 TABLES

4.3.1 Table 1

Point Matrix Evaluation 1 ()

4.3.2 Table 2

Surface Average 1 (phiz/dPhi)

4.3.3 Table 3

Surface Average 1 (phiz/dPhi)

4.3.4 Table 4

Surface Average 1 (phiz/dPhi)

4.3.5 Table 5

Line Average 2 (-1*dPhi/(nx*phix+ny*phiy))

4.3.6 Table 6

Line Average 2 (-1*dPhi/(nx*phix+ny*phiy))

dPhi (V)	-1*dPhi/(nx*phix+ny*phiy) (m)
0.10000	3.2140E-8
0.20000	3.5596E-8
0.30000	3.8222E-8

dPhi (V)	-1*dPhi/(nx*phix+ny*phiy) (m)
0.40000	4.0336E-8
0.50000	4.2108E-8
0.60000	4.3639E-8
0.70000	4.4987E-8

4.3.7 Table 7

Surface Integration 1 (e_const*Chz*Dz)

4.3.8 Table 8

Surface Integration 1 (-e_const*Chz*Dz)

rp (nm)	w (nm)	xp (um)	Lxy= 1E-6, -e_const*Chz*Dz (A)	Lxy= 1.5E-6, -e_const*Chz*Dz (A)	Lxy= 2E-6, -e_const*Chz*Dz (A)	Lxy= 2.5E-6, -e_const*Chz*Dz (A)	Lxy= 3E-6, -e_const*Chz*Dz (A)	Lxy= 3.5E-6, -e_const*Chz*Dz (A)	Lxy= 4E-6, -e_const*Chz*Dz (A)	Lxy= 4.5E-6, -e_const*Chz*Dz (A)	Lxy= 5E-6, -e_const*Chz*Dz (A)
250.00	25.000	1.5000	3.1677E-9	8.5491E-9	1.5191E-8	2.1574E-8	2.7119E-8	3.1775E-8	3.5663E-8	3.8927E-8	4.1693E-8
250.00	25.000	2.0000	1.8175E-9	5.6462E-9	1.0817E-8	1.6100E-8	2.0901E-8	2.5075E-8	2.8657E-8	3.1732E-8	3.4387E-8
250.00	25.000	2.5000	1.0149E-9	3.7012E-9	7.7018E-9	1.2059E-8	1.6202E-8	1.9927E-8	2.3210E-8	2.6087E-8	2.8614E-8
250.00	25.000	3.0000	5.6807E-10	2.4482E-9	5.5441E-9	9.1378E-9	1.2709E-8	1.6027E-8	1.9023E-8	2.1702E-8	2.4093E-8
250.00	25.000	3.5000	3.2105E-10	1.6368E-9	4.0342E-9	6.9984E-9	1.0074E-8	1.3023E-8	1.5751E-8	1.8235E-8	2.0486E-8
250.00	25.000	4.0000	1.8299E-10	1.1036E-9	2.9596E-9	5.4026E-9	8.0475E-9	1.0662E-8	1.3137E-8	1.5433E-8	1.7542E-8
250.00	25.000	4.5000	1.0506E-10	7.4931E-10	2.1859E-9	4.1981E-9	6.4698E-9	8.7841E-9	1.1025E-8	1.3140E-8	1.5111E-8
250.00	25.000	5.0000	6.0660E-11	5.1156E-10	1.6232E-9	3.2793E-9	5.2283E-9	7.2736E-9	9.2983E-9	1.1242E-8	1.3080E-8
250.00	25.000	5.5000	3.5186E-11	3.5075E-10	1.2104E-9	2.5720E-9	4.2417E-9	6.0461E-9	7.8719E-9	9.6550E-9	1.1363E-8
250.00	25.000	6.0000	2.0516E-11	2.4148E-10	9.0602E-10	2.0248E-9	3.4539E-9	5.0436E-9	6.6875E-9	8.3199E-9	9.9043E-9
250.00	25.000	6.5000	1.1959E-11	1.6663E-10	6.8004E-10	1.5985E-9	2.8202E-9	4.2190E-9	5.6969E-9	7.1890E-9	8.6563E-9

rp (nm)	w (nm)	xp (um)	Lxy= 1E-6, -e_const*Chz*Dz (A)	Lxy= 1.5E-6, -e_const*Chz*Dz (A)	Lxy= 2E-6, -e_const*Chz*Dz (A)	Lxy= 2.5E-6, -e_const*Chz*Dz (A)	Lxy= 3E-6, -e_const*Chz*Dz (A)	Lxy= 3.5E-6, -e_const*Chz*Dz (A)	Lxy= 4E-6, -e_const*Chz*Dz (A)	Lxy= 4.5E-6, -e_const*Chz*Dz (A)	Lxy= 5E-6, -e_const*Chz*Dz (A)
250.00	25.000	7.0000	7.0207E-12	1.1543E-10	5.1206E-10	1.2656E-9	2.3092E-9	3.5388E-9	4.8658E-9	6.2277E-9	7.5847E-9
250.00	25.000	7.5000	4.1132E-12	8.0028E-11	3.8614E-10	1.0038E-9	1.8943E-9	2.9738E-9	4.1637E-9	5.4052E-9	6.6583E-9
250.00	25.000	8.0000	2.4290E-12	5.5694E-11	2.9197E-10	7.9789E-10	1.5569E-9	2.5035E-9	3.5691E-9	4.6991E-9	5.8544E-9
250.00	25.000	8.5000	1.4513E-12	3.8880E-11	2.2128E-10	6.3561E-10	1.2824E-9	2.1121E-9	3.0659E-9	4.0938E-9	5.1583E-9
250.00	25.000	9.0000	8.3871E-13	2.6988E-11	1.6751E-10	5.0643E-10	1.0570E-9	1.7835E-9	2.6363E-9	3.5702E-9	4.5498E-9
250.00	25.000	9.5000	5.0580E-13	1.8937E-11	1.2743E-10	4.0473E-10	8.7320E-10	1.5088E-9	2.2706E-9	3.1183E-9	4.0189E-9
250.00	25.000	10.000	2.9572E-13	1.3194E-11	9.6732E-11	3.2329E-10	7.2152E-10	1.2772E-9	1.9573E-9	2.7263E-9	3.5538E-9
250.00	25.000	10.500	1.7647E-13	9.2159E-12	7.3517E-11	2.5851E-10	5.9678E-10	1.0822E-9	1.6887E-9	2.3857E-9	3.1453E-9
250.00	25.000	11.000	1.1150E-13	6.5227E-12	5.6181E-11	2.0735E-10	4.9468E-10	9.1855E-10	1.4592E-9	2.0904E-9	2.7871E-9
250.00	25.000	11.500	7.2889E-14	4.6453E-12	4.3051E-11	1.6663E-10	4.1065E-10	7.8066E-10	1.2624E-9	1.8337E-9	2.4724E-9
250.00	25.000	12.000	4.2639E-14	3.2419E-12	3.2773E-11	1.3355E-10	3.4054E-10	6.6328E-10	1.0922E-9	1.6093E-9	2.1946E-9
250.00	25.000	12.500	2.3351E-14	2.2571E-12	2.4977E-11	1.0715E-10	2.8264E-10	5.6391E-10	9.4553E-10	1.4129E-9	1.9487E-9
250.00	25.000	13.000	1.3747E-14	1.5888E-12	1.9117E-11	8.6210E-11	2.3509E-10	4.8034E-10	8.1996E-10	1.2425E-9	1.7331E-9
250.00	25.000	13.500	1.0224E-14	1.1455E-12	1.4697E-11	6.9424E-11	1.9555E-10	4.0907E-10	7.1088E-10	1.0924E-9	1.5411E-9
250.00	25.000	14.000	6.2328E-15	8.0618E-13	1.1241E-11	5.5855E-11	1.6273E-10	3.4872E-10	6.1705E-10	9.6168E-10	1.3722E-9
250.00	25.000	14.500	2.9513E-15	5.5388E-13	8.5613E-12	4.4887E-11	1.3535E-10	2.9718E-10	5.3548E-10	8.4644E-10	1.2216E-9
250.00	25.000	15.000	2.1590E-15	4.0032E-13	6.6011E-12	3.6243E-11	1.1286E-10	2.5367E-10	4.6528E-10	7.4583E-10	1.0886E-9

rp (nm)	w (nm)	xp (um)	Lxy= 1E-6, -e_const*Chz*Dz (A)	Lxy= 1.5E-6, -e_const*Chz*Dz (A)	Lxy= 2E-6, -e_const*Chz*Dz (A)	Lxy= 2.5E-6, -e_const*Chz*Dz (A)	Lxy= 3E-6, -e_const*Chz*Dz (A)	Lxy= 3.5E-6, -e_const*Chz*Dz (A)	Lxy= 4E-6, -e_const*Chz*Dz (A)	Lxy= 4.5E-6, -e_const*Chz*Dz (A)	Lxy= 5E-6, -e_const*Chz*Dz (A)
250.00	25.000	15.500	1.3409E-15	2.8300E-13	5.0633E-12	2.9225E-11	9.4102E-11	2.1664E-10	4.0459E-10	6.5778E-10	9.7115E-10
250.00	25.000	16.000	6.9702E-16	1.9602E-13	3.8644E-12	2.3519E-11	7.8379E-11	1.8489E-10	3.5167E-10	5.7996E-10	8.6621E-10
250.00	25.000	16.500	5.2623E-16	1.4021E-13	2.9632E-12	1.8941E-11	6.5288E-11	1.5780E-10	3.0570E-10	5.1147E-10	7.7287E-10
250.00	25.000	17.000	4.2472E-16	1.0425E-13	2.3121E-12	1.5405E-11	5.4739E-11	1.3533E-10	2.6676E-10	4.5252E-10	6.9155E-10
250.00	25.000	17.500	4.1420E-16	7.5505E-14	1.7768E-12	1.2426E-11	4.5660E-11	1.1565E-10	2.3220E-10	3.9962E-10	6.1788E-10
250.00	25.000	18.000	3.3363E-16	5.6084E-14	1.3835E-12	1.0097E-11	3.8282E-11	9.9238E-11	2.0282E-10	3.5401E-10	5.5372E-10
250.00	25.000	18.500	8.0871E-17	3.6089E-14	1.0442E-12	8.1154E-12	3.1923E-11	8.4867E-11	1.7672E-10	3.1301E-10	4.9543E-10
250.00	25.000	19.000	1.3873E-16	2.7594E-14	8.1171E-13	6.5724E-12	2.6687E-11	7.2654E-11	1.5409E-10	2.7692E-10	4.4357E-10
250.00	25.000	19.500	1.8076E-16	2.4614E-14	6.5767E-13	5.4012E-12	2.2460E-11	6.2434E-11	1.3468E-10	2.4544E-10	3.9773E-10
250.00	25.000	20.000	7.3629E-17	1.6305E-14	5.0149E-13	4.3659E-12	1.8800E-11	5.3552E-11	1.1767E-10	2.1761E-10	3.5687E-10

4.3.9 Table 9

Surface Average 1 (phi, Ch)

dPhi (V)	Dependent variable phi (V)	Ch (1/m^3)
0.0000	0.0000	1.0501E-32
0.20000	-0.18211	2.2524E-125
0.40000	-0.36422	0.0000
0.60000	-0.54633	0.0000
0.80000	-0.72845	0.0000
1.0000	-0.91056	0.0000

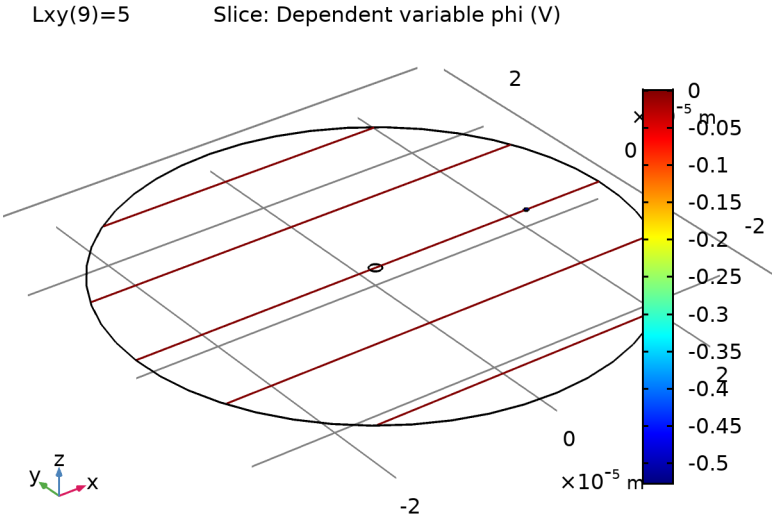
4.3.10 Table 10

Surface Integration 2 (e_const*Dxy*(nx*Chx+ny*Chy))

dPhi (V)	-e_const*Dxy*(nx*Chx+ny*Chy) (A)	-e_const^2/kbT*Dxy*Ch*(nx*phix+ny*phiy) (A)	-e_const*Dxy*(nx*Chx+ny*Chy)-e_const^2/kbT*Dxy*Ch*(nx*phix+ny*phiy) (A)
0.0000	6.0549E-10	0.0000	6.0549E-10
0.20000	-8.1254E-9	6.2148E-9	-1.9106E-9
0.40000	-4.9279E-9	2.5441E-9	-2.3837E-9
0.60000	-3.7364E-9	7.7118E-9	3.9754E-9
0.80000	-4.1578E-9	1.4928E-8	1.0770E-8
1.0000	-4.4081E-9	1.9154E-8	1.4746E-8

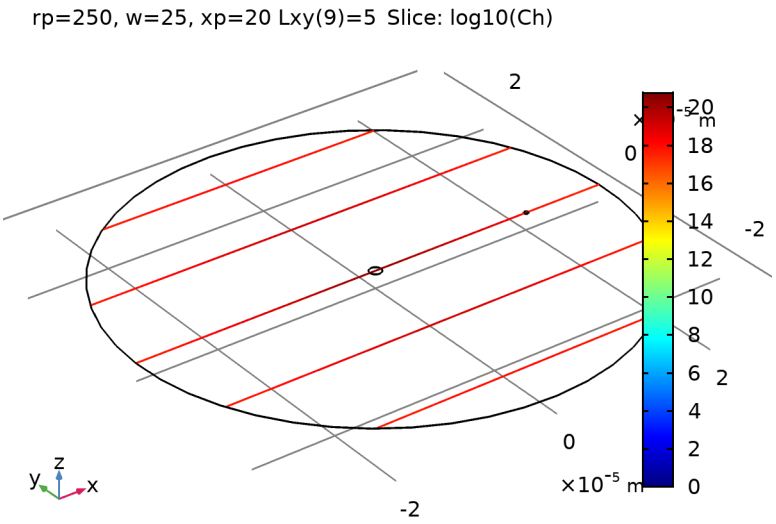
4.4 PLOT GROUPS

4.4.1 3D Plot Group 1



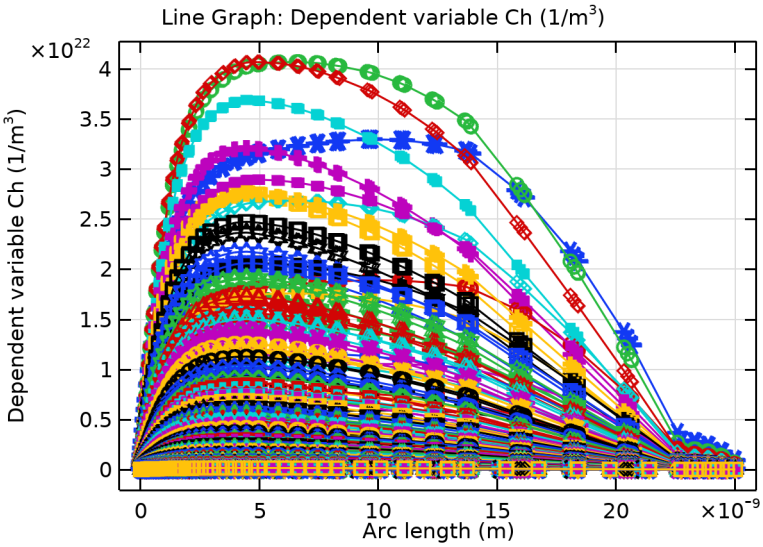
Slice: Dependent variable phi (V)

4.4.2 3D Plot Group 2



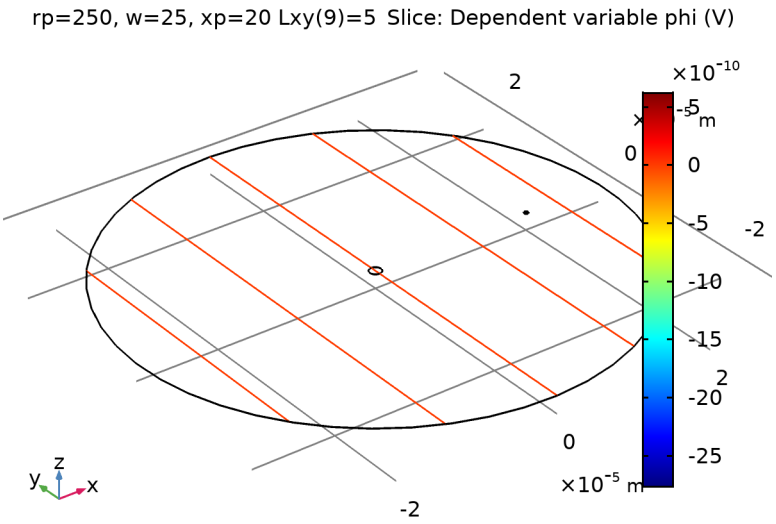
Slice: log10(Ch)

4.4.3 1D Plot Group 3



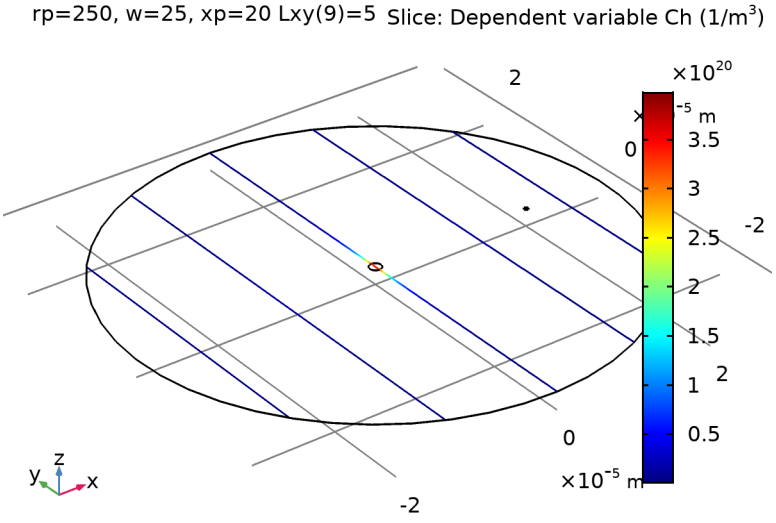
Line Graph: Dependent variable Ch (1/m³)

4.4.4 3D Plot Group 4



Slice: Dependent variable phi (V)

4.4.5 3D Plot Group 5



Slice: Dependent variable Ch (1/m^3)