

Glass nanopore

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This report describes all the steps to build the model related to the PEG study. To reproduce the no PEG model, replace all bath parameters (name ending with "...Bath") with the ones allocated to the pore in addition to the desired surface charge.

Contents

1. Global Definitions.....	3
1.1. Parameters.....	3
2. Model 1	7
2.1. Definitions.....	7
2.2. Nanopipette.....	19
2.3. Transport of Diluted Species	21
2.4. Electrostatics.....	31
2.5. Laminar Flow.....	42
2.6. Meshes.....	51
3. Results	57
3.1. Data Sets.....	57
3.2. Tables.....	57
3.3. Plot Groups.....	58

1 Global Definitions

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GLOBAL SETTINGS

Version	COMSOL Multiphysics 5.6 (Build: 401)
Unit system	SI

USED PRODUCTS

COMSOL Multiphysics
Chemical Reaction Engineering Module

1.1 PARAMETERS

PARAMETERS

Name	Expression	Value	Description
PoreAngle	7[deg]	0.12217 rad	Inner truncated hollow cone angle; estimated from SEM imaging
PoreRadius	12.5[nm]	1.25E-8 m	Inner cone aperture radius; measured from SEM imaging
PoreHeight	5[um]*SizeFactor	5E-5 m	Truncated hollow cone's height in model; measured along the axis taking the aperture as flat
PoreTopRadius	$\text{PoreRadius} + \tan(\text{PoreAngle}) * \text{PoreHeight}$	6.1517E-6 m	Estimated radius of the inner cone at $z = \text{PoreHeight}$
RadiusRatio	$\text{PoreRadius} / \text{PoreTopRadius}$	0.0020319	Ratio between the inner cone radii at the nanopipette opening and at $z = \text{PoreHeight}$
WallThickness	10 [nm]	1E-8 m	Glass thickness at the nanopipette opening; measured from SEM imaging
WallRadius	$\text{PoreRadius} + \text{WallThickness}$	2.25E-8 m	Outer cone (glass wall) radius at $z = 0$
WallTopRadius	$\text{WallRadius} / \text{RadiusRatio}$	1.1073E-5 m	Outer cone (glass

Name	Expression	Value	Description
			wall) radius at z = PoreHeight
WallAngle	$\text{atan}((\text{WallTopRadius} - \text{WallRadius})/\text{PoreHeight})$	0.21752 rad	Estimated inner cone angle of the outer cone (glass wall)
BeyondPoreRadius	$\text{PoreRadius} * 100 * \text{SizeFactor}$	1.25E-5 m	Mathematical factor for selected boundaries length
ConeApex	$-\text{PoreHeight} * \text{PoreRadius} / (\text{PoreTopRadius} - \text{PoreRadius})$	-1.018E-7 m	z value where the apex of the inner cone (if continued) would lie
SizeFactor	10	10	Scaling factor for selected boundaries dimensions
Delta	$\text{PoreRadius} / 50$	2.5E-10 m	Used for selecting geometric boundaries
T	25[degC]	298.15 K	Temperature
EpsilonR	77	77	Electric relative permittivity of bulk
EpsilonRBath	52	52	Electric relative permittivity of bath [Arnold, 1985]
BulkConductivity	1.299[S/m]	1.299 S/m	Experimental conductivity of the bulk medium
BathConductivity	0.1507 [S/m]	0.1507 S/m	Experimental conductivity of the bath medium
FluidDensity	1001.5[kg/m ³]	1001.5 kg/m ³	[Ref. Hai-Lang & Shi-Jun, 1996 for 0.0955 (mol/kg)]
FluidDensityBath	1086.2 [kg/m ³]	1086.2 kg/m ³	[Ref. Gonzalez-Tello et al., 1994 for 50% PEG 8000 in H ₂ O (kg/m ³)]
FluidViscosity	0.9[mPa*s]	9E-4 Pa·s	Experimental viscosity of the bulk medium
FluidViscosityBath	8.73125 [Pa*s]	8.7313 Pa·s	Experimental viscosity of the bath medium

Name	Expression	Value	Description
VApp	500[mV]	0.5 V	Applied voltage
PApp	0[Pa]	0 Pa	Applied pressure differential (bottom-top)
HydrostaticPressure	FluidDensity*9.81[m/s ²]*PoreHeight	0.49124 Pa	Hydrostatic pressure at the cone aperture
PoreSurfaceCharge	0[mC/m ²]	0 C/m ²	Surface charge of quartz glass wall
cb	100[mol/m ³]	100 mol/m ³	Experimental bulk concentration
cbath	cb	100 mol/m ³	Estimated outer bath concentration
DK	$0.49 * \text{BulkConductivity} * (\text{R_const} * \text{T}) / (\text{F_const}^2 * \text{cb})$	1.6949E-9 m ² /s	Analytical and Physical Electrochemistry (Girault, 2004)
DCI	$0.51 * \text{BulkConductivity} * (\text{R_const} * \text{T}) / (\text{F_const}^2 * \text{cb})$	1.7641E-9 m ² /s	Analytical and Physical Electrochemistry (Girault, 2004)
DKBath	$0.35 * \text{BathConductivity} * (\text{R_const} * \text{T}) / (\text{F_const}^2 * \text{cbath})$	1.4045E-10 m ² /s	Estimated diffusion coefficient of cations in bath (50% PEG)
DCIBath	$0.65 * \text{BathConductivity} * (\text{R_const} * \text{T}) / (\text{F_const}^2 * \text{cbath})$	2.6084E-10 m ² /s	Estimated diffusion coefficient of anions in bath (50% PEG)
DebyeLength	$\text{sqrt}((\text{EpsilonR} * \text{epsilon0_const} * \text{R_const} * \text{T}) / (2 * \text{cb} * \text{F_const}^2))$	9.5275E-10 m	Debye Length (pore)
DebyeLengthBath	$\text{sqrt}((\text{EpsilonRBath} * \text{epsilon0_const} * \text{R_const} * \text{T}) / (2 * \text{cbath} * \text{F_const}^2))$	7.8295E-10 m	Debye Length (bath)
GCSurfacePotential	$\text{asinh}(\text{PoreSurfaceCharge} / \text{sqrt}(8 * \text{cb} * \text{N_A_const} * \text{EpsilonR} * \text{epsilon0_const} * \text{k_B_const} * \text{T})) * (2 * \text{k_B_const} * \text{T}) / (1 * \text{e_const})$	0 V	Surface potential difference from Gouy-Chapman (pore)
GCSurfacePotentialBath	$\text{asinh}(\text{PoreSurfaceCharge} / \text{sqrt}(8 * \text{cbath} * \text{N_A_const} * \text{EpsilonRBath} * \text{epsilon0_const} * \text{k_B_const} * \text{T})) * (2 * \text{k_B_const} * \text{T}) / (1 * \text{e_const})$	0 V	Surface potential difference from Gouy-Chapman (bath)
gamma	$(\text{exp}(1 * \text{e_const} * \text{GCSurfacePotential} / (2 * \text{k_B_const} * \text{T})) -$	0	Helper for Gouy-

Name	Expression	Value	Description
	$1)/(\exp(1 \cdot e_{\text{const}} \cdot \text{GCSurfacePotential}/(2 \cdot k_{\text{B_const}} \cdot T)) + 1)$		Chapman (pore)
gammaBath	$(\exp(1 \cdot e_{\text{const}} \cdot \text{GCSurfacePotentialBath}/(2 \cdot k_{\text{B_const}} \cdot T)) - 1)/(\exp(1 \cdot e_{\text{const}} \cdot \text{GCSurfacePotentialBath}/(2 \cdot k_{\text{B_const}} \cdot T)) + 1)$	0	Helper for Gouy-Chapman (bath)
RAccessBottom	$1/(4 \cdot \text{BulkConductivity} \cdot \text{PoreRadius})$	1.5396E7 Ω	Analytical Access Resistance
RPore	$1/(\text{BulkConductivity} \cdot \pi \cdot \text{PoreRadius} \cdot \tan(\text{PoreAngle}))$	1.5966E8 Ω	Analytical Resistance inside the pore
RTot	$\text{RAccessBottom} + \text{RPore}$	1.7505E8 Ω	Total Resistance
VBottom	$\text{VApp} \cdot \text{RAccessBottom} / \text{RTot}$	0.043977 V	Potential drop outside the pore

2 Model 1

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SETTINGS

Description	Value
Unit system	Same as global system (SI)
Geometry shape function	Automatic
Avoid inverted elements by curving interior domain elements	Off

SPATIAL FRAME COORDINATES

First	Second	Third
r	phi	z

MATERIAL FRAME COORDINATES

First	Second	Third
R	PHI	Z

GEOMETRY FRAME COORDINATES

First	Second	Third
Rg	PHIg	Zg

MESH FRAME COORDINATES

First	Second	Third
Rm	PHIm	Zm

2.1 DEFINITIONS

2.1.1 Variables

Excess Charge

SELECTION

Geometric entity level	Domain
Selection	Geometry geom1: Dimension 2: Domains 1–3

Name	Expression	Unit	Description
ExcessCharge	$F_const \cdot (cK - cCl)$	C/m ³	

Distance from glass (internal electrode)

SELECTION

Geometric entity level	Boundary
------------------------	----------

Name	Internal Electrode
Selection	Named sel3: Geometry geom1: Dimension 1: Boundary 4

Name	Expression	Unit	Description
dGlass	$(\text{PoreTopRadius} - r) \cdot \sin(90[\text{deg}] - \text{PoreAngle})$	m	

Distance from glass (external electrode, upper part)

SELECTION

Geometric entity level	Boundary
Selection	Geometry geom1: Dimension 1: Boundaries 10–11

Name	Expression	Unit	Description
dGlass	$\cos(\text{WallAngle}) \cdot (r - \text{WallRadius} - z \cdot \tan(\text{WallAngle}))$	m	

Distance from glass (external electrode, bottom part)

SELECTION

Geometric entity level	Boundary
Selection	Geometry geom1: Dimension 1: Boundary 9

Name	Expression	Unit	Description
dGlass	$(r < \text{PoreRadius}) \cdot (\sqrt{(r - \text{PoreRadius})^2 + z^2}) + (-z) \cdot (r \geq \text{PoreRadius}) \cdot (r < \text{WallRadius}) + (r \geq \text{WallRadius}) \cdot (\sqrt{(r - \text{WallRadius})^2 + z^2})$	m	

Analytical Potential, No Charge (Bath)

SELECTION

Geometric entity level	Domain
Selection	Geometry geom1: Dimension 2: Domains 1, 3

Name	Expression	Unit	Description
AnalyticalPotentialNoCharge	$\text{DiskElec}(r, -z, \text{PoreRadius}) \cdot V_{\text{Bottom}}$	V	

Analytical Potential, No Charge (Pore)

SELECTION

Geometric entity level	Domain
Selection	Geometry geom1: Dimension 2: Domain 2

Name	Expression	Unit	Description
AnalyticalPotentialNoCharge	$V_{\text{Bottom}} + (V_{\text{App}} -$	V	

Name	Expression	Unit	Description
	$V_{\text{Bottom}} * 1 / (\text{BulkConductivity} * \pi) * z / (\text{PoreRadius} * (\text{PoreRadius} + z / \text{PoreHeight} * (\text{PoreTopRadius} - \text{PoreRadius}))) / R_{\text{Pore}}$		

Domain Expressions Gouy-Chapman

SELECTION

Geometric entity level	Entire model
------------------------	--------------

Name	Expression	Unit	Description
cCl_GC	c_GC(WallDistance, -1)	mol/m ³	
cK_GC	c_GC(WallDistance, 1)	mol/m ³	
Potential_GC	E_GC(WallDistance)	V	
cCl_GCBath	c_GCBath(WallDistance, -1)	mol/m ³	
cK_GCBath	c_GCBath(WallDistance, 1)	mol/m ³	
Potential_GCBath	E_GCBath(WallDistance)	V	

Wall Distance (Pore)

SELECTION

Geometric entity level	Domain
Selection	Geometry geom1: Dimension 2: Domain 2

Name	Expression	Unit	Description
lambda	$(r * \text{PoreRadius} - z * \text{ConeApex} + \text{ConeApex}^2) / (\text{PoreRadius}^2 + \text{ConeApex}^2)$		helper value for point of nearest wall
WallDistance	$(\text{lambda} \geq 1) * \sqrt{(r - \text{lambda} * \text{PoreRadius})^2 + (z - (\text{ConeApex} - \text{lambda} * \text{ConeApex}))^2} + (\text{lambda} < 1) * \sqrt{(r - \text{PoreRadius})^2 + z^2}$	m	

Wall Distance (Bath, bottom part)

SELECTION

Geometric entity level	Domain
Selection	Geometry geom1: Dimension 2: Domain 1

Name	Expression	Unit	Description
WallDistance	$(r < \text{PoreRadius}) * \sqrt{(r - \text{PoreRadius})^2 + z^2} + (-z) * (r \geq \text{PoreRadius}) * (r < \text{WallRadius}) + (r \geq \text{WallRadius}) * \sqrt{(r - \text{WallRadius})^2 + z^2}$	m	

Wall Distance (Bath, upper part)

SELECTION

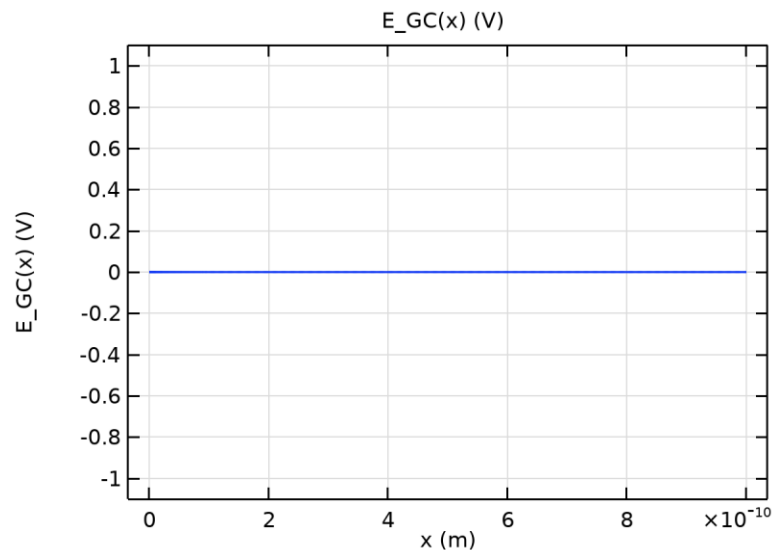
Geometric entity level	Domain
Selection	Geometry geom1: Dimension 2: Domain 3

Name	Expression	Unit	Description
WallDistance	$\cos(\text{WallAngle}) \cdot (r - \text{WallRadius} - z \cdot \tan(\text{WallAngle}))$	m	

2.1.2 Functions

Gouy-Chapman Potential (Pore)

Function name	E_GC
Function type	Analytic



Gouy-Chapman Potential (Pore)

DEFINITION

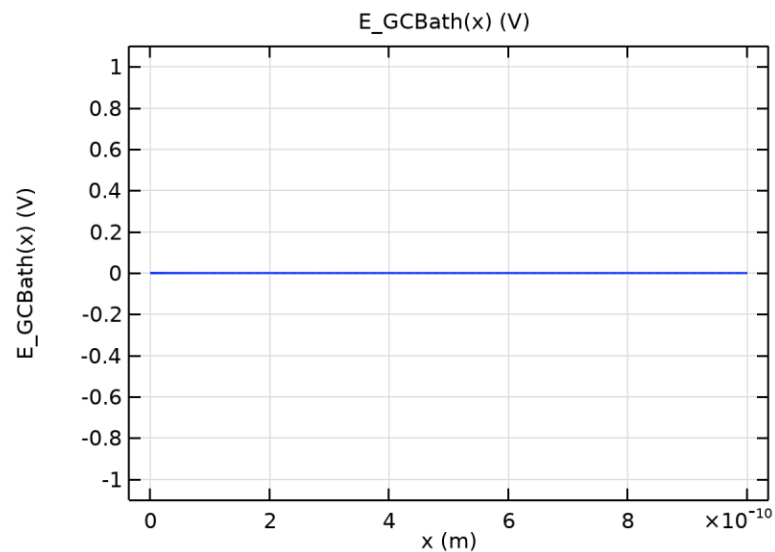
Description	Value
Expression	$(2 \cdot k_B \cdot \text{const} \cdot T / e_{\text{const}}) \cdot \log\left(\frac{1 + \gamma \cdot \exp(-x/\text{DebyeLength})}{1 - \gamma \cdot \exp(-x/\text{DebyeLength})}\right)$
Arguments	x

UNITS

Description	Value
Arguments	m
Function	V

Gouy-Chapman Potential (Bath)

Function name	E_GCBath
Function type	Analytic



Gouy-Chapman Potential (Bath)

DEFINITION

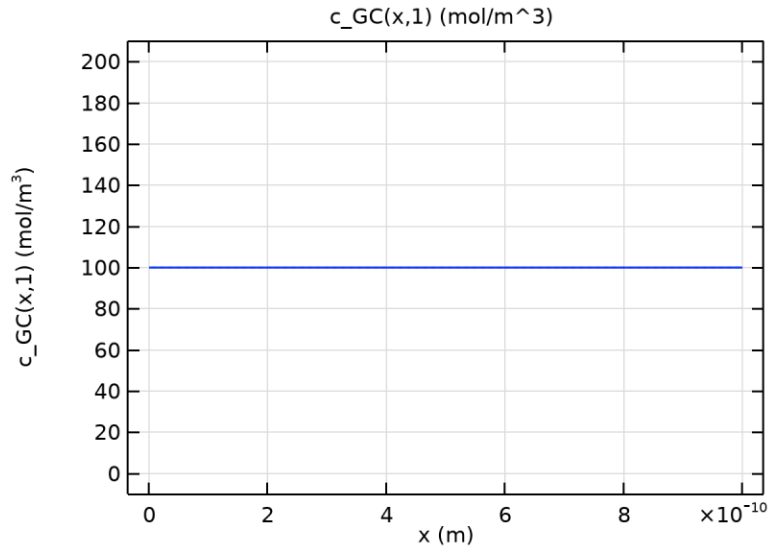
Description	Value
Expression	$((2 * k_B * \text{const} * T / e_{\text{const}}) * \log((1 + \text{gammaBath} * \exp(-x / \text{DebyeLengthBath})) / (1 - \text{gammaBath} * \exp(-x / \text{DebyeLengthBath}))))$
Arguments	x

UNITS

Description	Value
Arguments	m
Function	V

Gouy-Chapman Concentration (Pore)

Function name	c_GC
Function type	Analytic



Gouy-Chapman Concentration (Pore)

DEFINITION

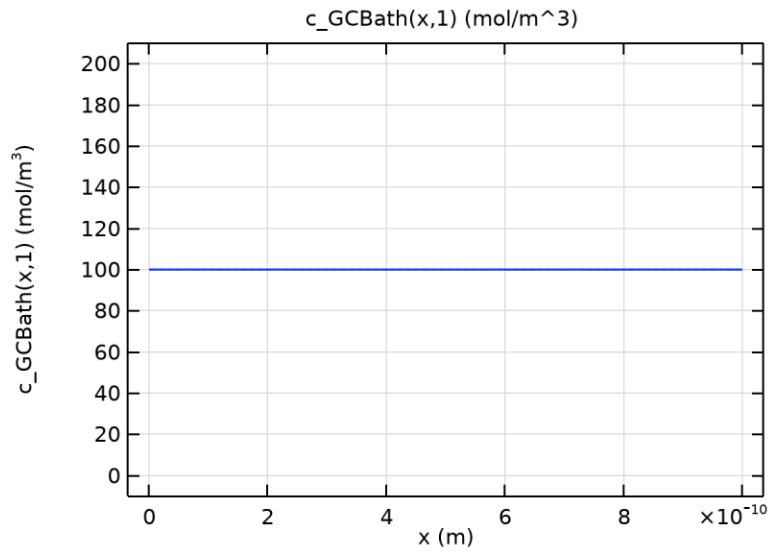
Description	Value
Expression	$cb \cdot \exp(-z \cdot e_{\text{const}} \cdot E_{\text{GC}}(x) / (k_{\text{B_const}} \cdot T))$
Arguments	{x, z}

UNITS

Description	Value
Arguments	m, 1
Function	mol/m ³

Gouy-Chapman Concentration (Bath)

Function name	c_GC Bath
Function type	Analytic



Gouy-Chapman Concentration (Bath)

DEFINITION

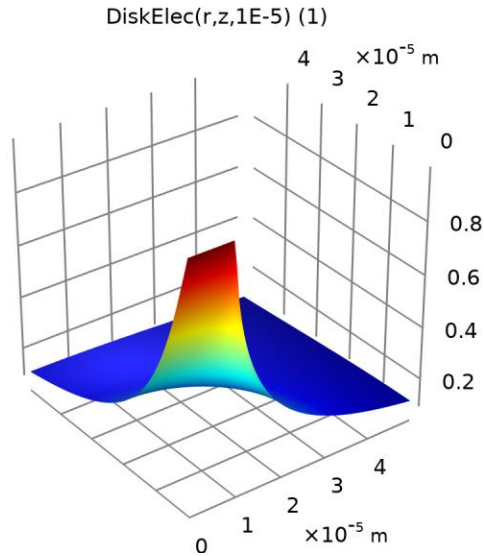
Description	Value
Expression	$cbath \cdot \exp(-z \cdot e_{\text{const}} \cdot E_{\text{GCBath}}(x) / (k_{\text{B_const}} \cdot T))$
Arguments	{x, z}

UNITS

Description	Value
Arguments	m, 1
Function	mol/m ³

Disk Electrode (Normalized Distribution)

Function name	DiskElec
Function type	Analytic



Disk Electrode (Normalized Distribution)

DEFINITION

Description	Value
Expression	$2/\pi * \text{asin}(2*a/(\text{sqrt}((z + \text{eps})^2 + (a + \text{eps} + r)^2) + \text{sqrt}((z + \text{eps})^2 + (a + \text{eps} - r)^2)))$
Arguments	{r, z, a}

UNITS

Description	Value
Arguments	m, m, m
Function	1

2.1.3 Selections

Symmetry Axis

Selection type
Box

Selection
Boundaries 1–2

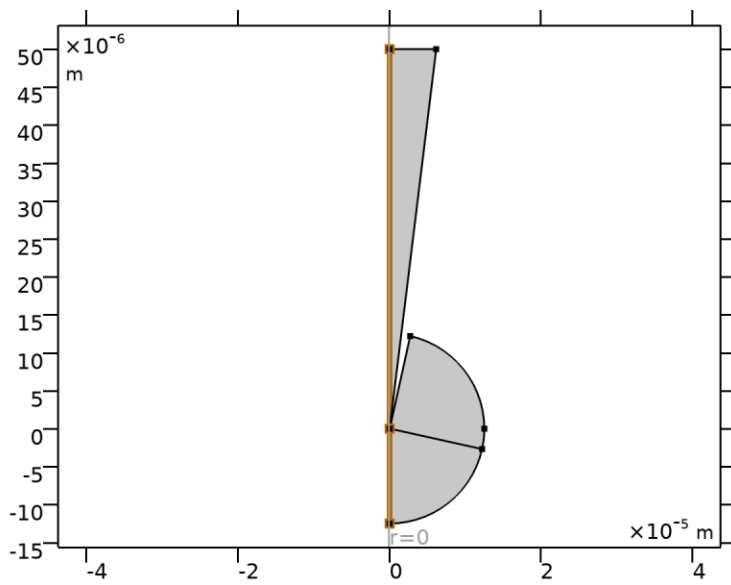
GEOMETRIC ENTITY LEVEL

Description	Value
Level	Boundary

OUTPUT ENTITIES

Description	Value
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Description	Value
Include entity if	All vertices inside box

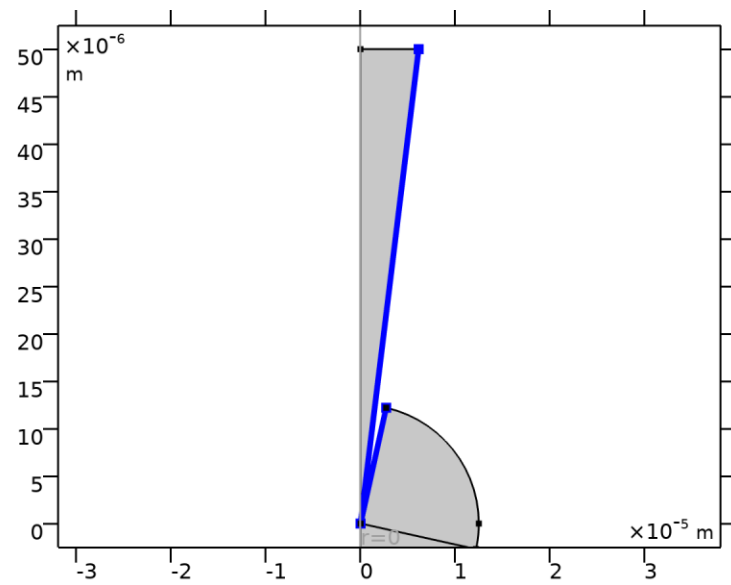


Symmetry Axis

Glass Wall

Selection type
Explicit

Selection
Boundaries 5-7



Glass Wall

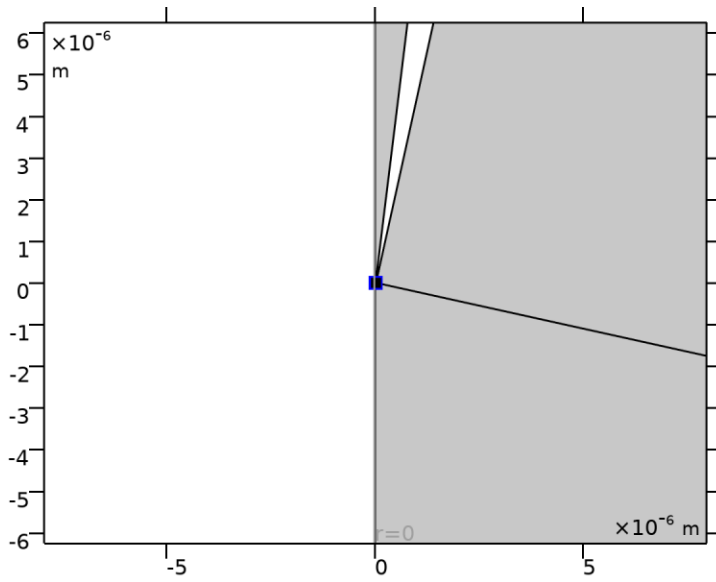
Aperture point

Selection type

Explicit

Selection

Point 4



Aperture point

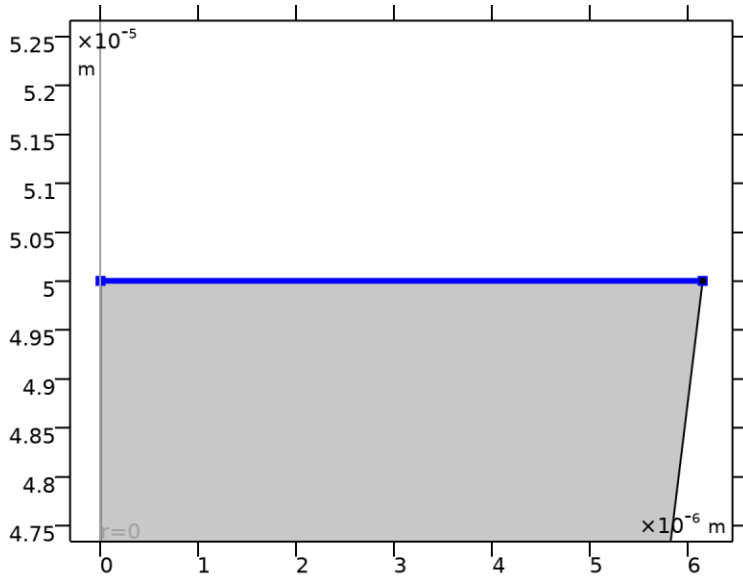
Internal Electrode

Selection type

Explicit

Selection

Boundary 4

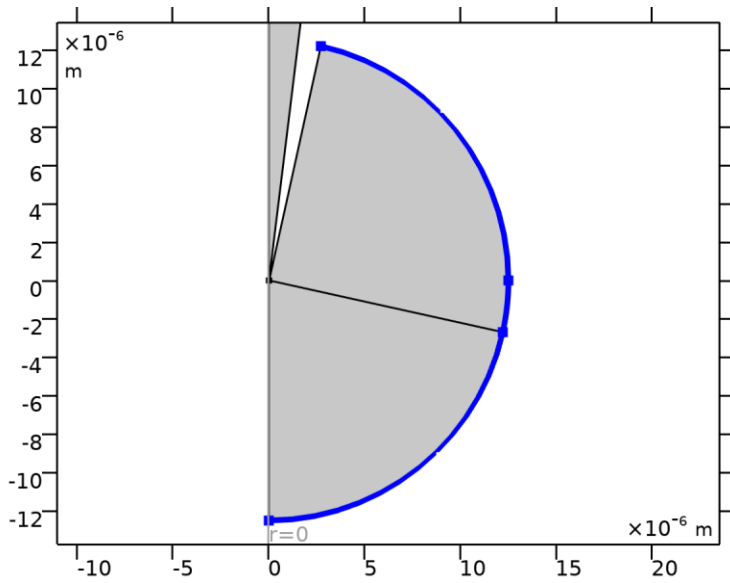


Internal Electrode

External Electrode

Selection type
Explicit

Selection
Boundaries 9–11



External Electrode

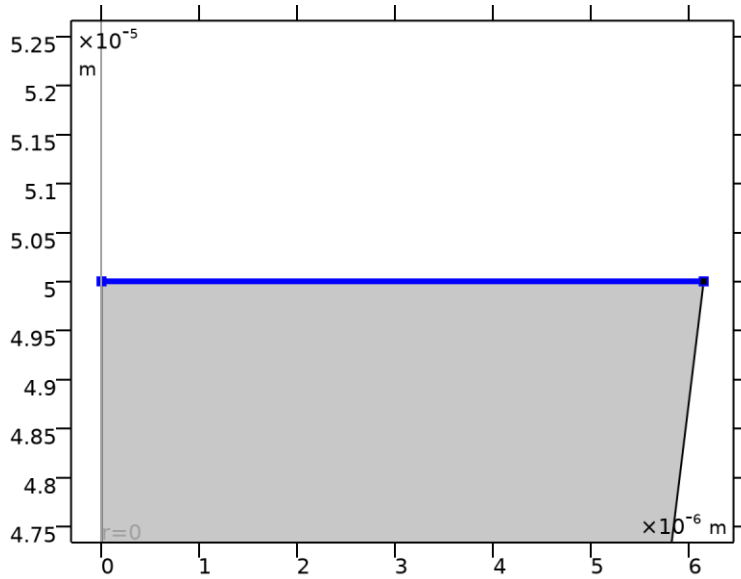
2.1.4 Probes

Current (internal electrode)

Probe type	Boundary probe
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SELECTION

Geometric entity level	Boundary
Selection	Geometry geom1: Dimension 1: Boundary 4



Selection

PROBE TYPE

Description	Value
Type	Integral

EXPRESSION

Description	Value
Expression	$-F_{\text{const}} \cdot (\text{chds.bndFlux}_{\text{cK}} - \text{chds.bndFlux}_{\text{cCl}}) \cdot 2 \cdot \pi \cdot r$
Table and plot unit	nA
Description	Current (internal)

TABLE AND WINDOW SETTINGS

Description	Value
Output table	Probe Table
Plot window	Probe Plot 3

2.1.5 Coordinate Systems

Boundary System 1

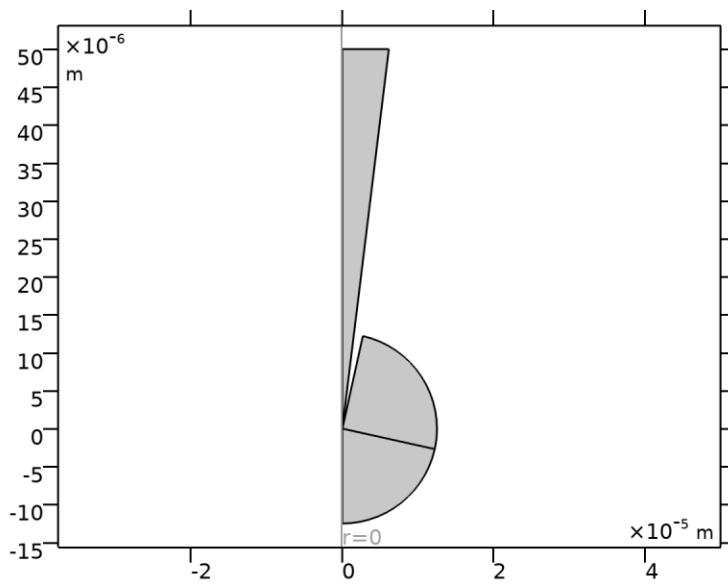
Coordinate system type	Boundary system
Tag	sys1

COORDINATE NAMES

First	Second	Third
t1	to	n

2.2 NANOPIPETTE

Pore with glass of infinite width



Nanopipette

UNITS

Length unit	m
Angular unit	deg

GEOMETRY STATISTICS

Description	Value
Space dimension	2
Number of domains	3
Number of boundaries	11
Number of vertices	9

2.2.1 Pore (b5)

POLYGON SEGMENTS

Description	Value
Control points	{{0, 0, PoreTopRadius, PoreRadius, 0}, {0, PoreHeight, PoreHeight, 0, 0}}
Degree	{1, 1, 1, 1}
Weights	{1, 1, 1, 1, 1, 1, 1, 1}
Type	Solid

2.2.2 Wall (pol1)

OBJECT TYPE

Description	Value
Type	Open curve

COORDINATES

Description	Value
Data source	Table

COORDINATES

r (m)	z (m)
PoreRadius	0
WallRadius	0
WallTopRadius	PoreHeight

2.2.3 Bath (c1)

SELECTIONS OF RESULTING ENTITIES

Description	Value
Resulting objects selection	On

POSITION

Description	Value
Position	{0, 0}

ROTATION ANGLE

Description	Value
Rotation	-90

SIZE AND SHAPE

Description	Value
Radius	BeyondPoreRadius

Description	Value
Sector angle	180

2.2.4 Difference Bath from Pipette & Wall (dif1)

SETTINGS

Description	Value
Keep input objects	On

2.2.5 Rectangle for dGlass (r1)

POSITION

Description	Value
Position	{WallRadius, 0}

ROTATION ANGLE

Description	Value
Rotation	-WallAngle

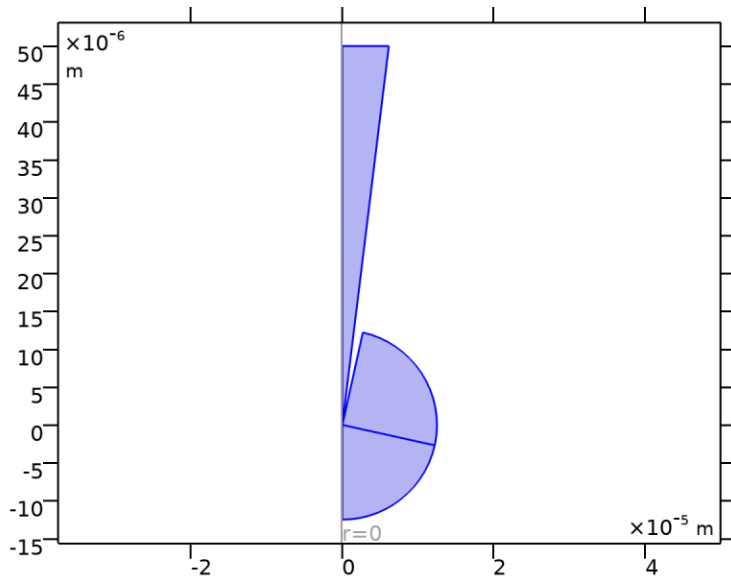
SIZE

Description	Value
Width	BeyondPoreRadius
Height	BeyondPoreRadius

2.3 TRANSPORT OF DILUTED SPECIES

USED PRODUCTS

COMSOL Multiphysics
Chemical Reaction Engineering Module



Transport of Diluted Species

SELECTION

Geometric entity level	Domain
Selection	Geometry geom1: Dimension 2: All domains

EQUATIONS

$$\nabla \cdot (\mathbf{J}_j + \mathbf{u}c_j) = R_j$$

$$\mathbf{J}_j = -D_j \nabla c_j - z_j \mu_{mj} F c_j \nabla V$$

2.3.1 Interface Settings

Discretization

SETTINGS

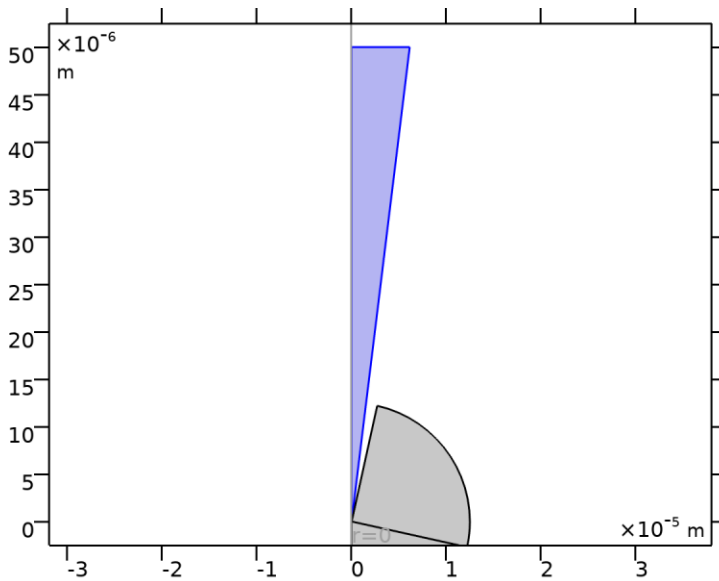
Description	Value
Concentration	Quadratic

Transport Mechanisms

SETTINGS

Description	Value
Convection	On
Migration in electric field	On
Mass transfer in porous media	Off

2.3.2 Convection, Diffusion, and Migration (Pore)



Convection, Diffusion, and Migration (Pore)

SELECTION

Geometric entity level	Domain
Selection	Geometry geom1: Dimension 2: All domains

EQUATIONS

$$\nabla \cdot (\mathbf{J}_i + \mathbf{u}c_i) = R_i$$

.....

$$\mathbf{J}_i = -D_i \nabla c_i - z_i \mu_{mj} F c_i \nabla V$$

Convection

SETTINGS

Description	Value
Velocity field	Velocity field (spf)

Diffusion

SETTINGS

Description	Value
Source	Material
Material	None
Diffusion coefficient	User defined
Diffusion coefficient	{{DK, 0, 0}, {0, DK, 0}, {0, 0, DK}}
Diffusion coefficient	User defined
Diffusion coefficient	{{DCI, 0, 0}, {0, DCI, 0}, {0, 0, DCI}}

Migration in Electric Field

SETTINGS

Description	Value
Electric potential	Electric potential (es)
Mobility	Nernst - Einstein relation
Charge number	{1, -1}

Coordinate System Selection

SETTINGS

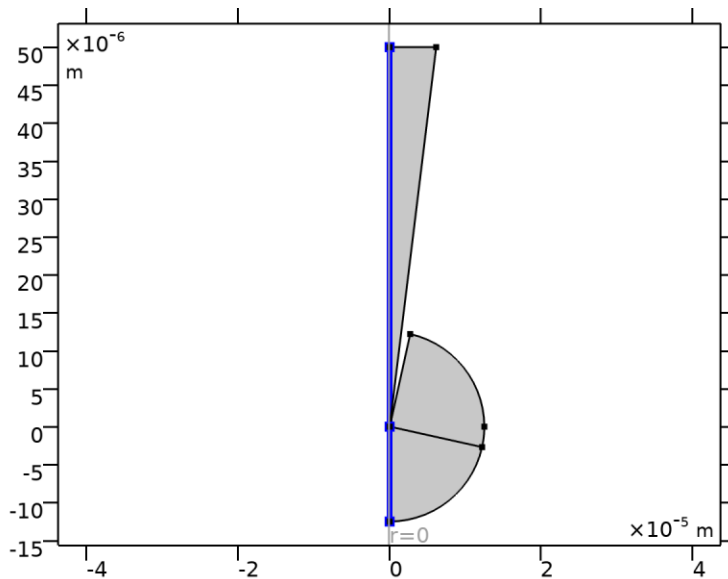
Description	Value
Coordinate system	Global coordinate system

Model Input

SETTINGS

Description	Value
Temperature	User defined
Temperature	T

2.3.3 Axial Symmetry

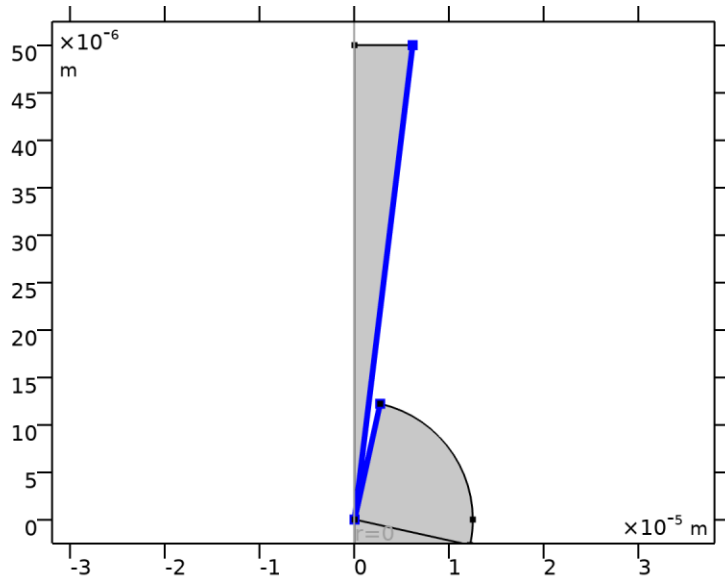


Axial Symmetry

SELECTION

Geometric entity level	Boundary
Selection	Geometry geom1: Dimension 1: All boundaries

2.3.4 No Flux (Glass Wall)



No Flux (Glass Wall)

SELECTION

Geometric entity level	Boundary
Selection	Geometry geom1: Dimension 1: All boundaries

EQUATIONS

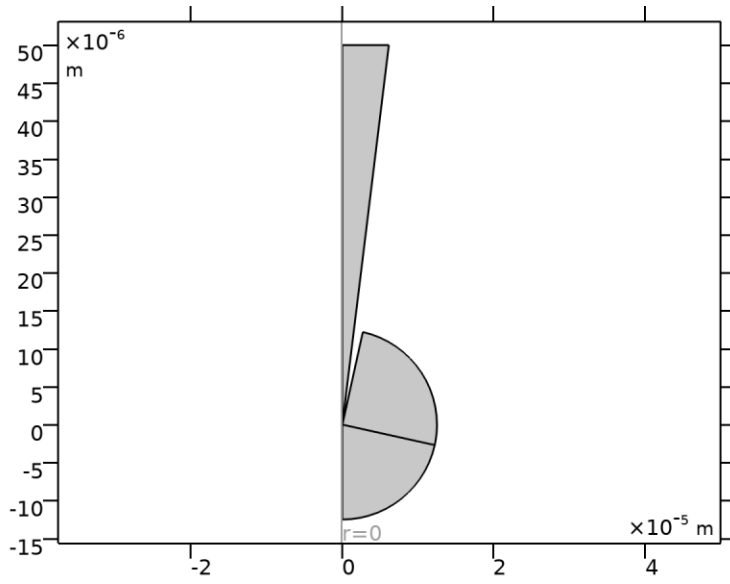
$$-\mathbf{n} \cdot \mathbf{J}_i = 0$$

Convection

SETTINGS

Description	Value
Include	Off

2.3.5 Initial Values



Initial Values

SELECTION

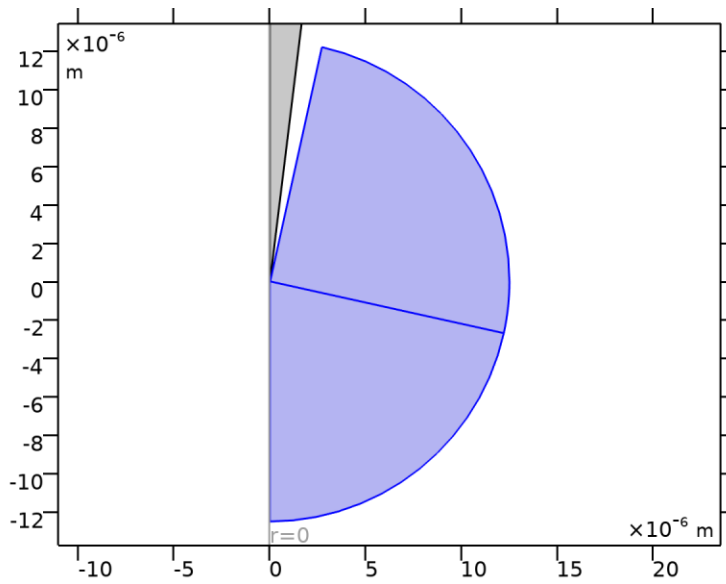
Geometric entity level	Domain
Selection	Geometry geom1: Dimension 2: All domains

Initial Values

SETTINGS

Description	Value
Concentration	{cb, cb}

2.3.6 Convection, Diffusion, and Migration (Bath)



Convection, Diffusion, and Migration (Bath)

SELECTION

Geometric entity level	Domain
Selection	Geometry geom1: Dimension 2: Domains 1, 3

EQUATIONS

$$\nabla \cdot (\mathbf{J}_i + \mathbf{u}c_i) = R_i$$

.....

$$\mathbf{J}_i = -D_i \nabla c_i - z_i \mu_{mj} F c_i \nabla V$$

Convection

SETTINGS

Description	Value
Velocity field	Velocity field (spf)

Diffusion

SETTINGS

Description	Value
Source	Material
Material	None
Diffusion coefficient	User defined
Diffusion coefficient	{{DKBath, 0, 0}, {0, DKBath, 0}, {0, 0, DKBath}}
Diffusion coefficient	User defined
Diffusion coefficient	{{DCIBath, 0, 0}, {0, DCIBath, 0}, {0, 0, DCIBath}}

Migration in Electric Field

SETTINGS

Description	Value
Electric potential	Electric potential (es)
Mobility	Nernst - Einstein relation
Charge number	{1, -1}

Coordinate System Selection

SETTINGS

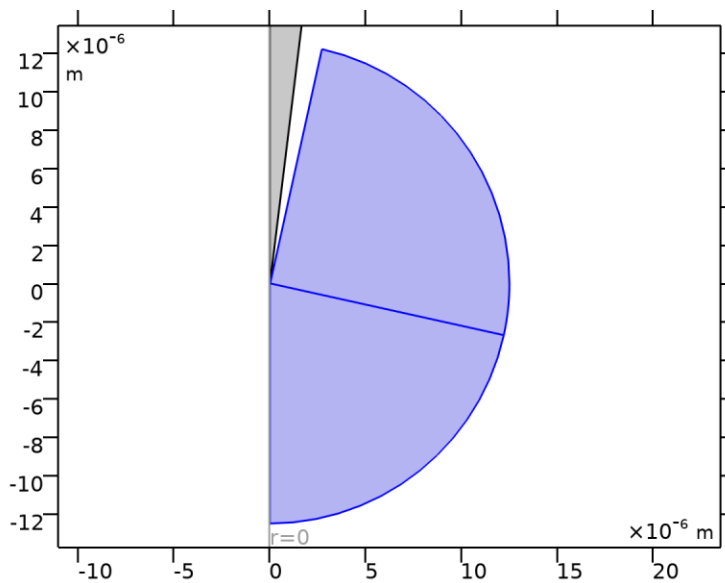
Description	Value
Coordinate system	Global coordinate system

Model Input

SETTINGS

Description	Value
Temperature	User defined
Temperature	T

2.3.7 Initial Values (Gouy-Chapman, Bath)



Initial Values (Gouy-Chapman, Bath)

SELECTION

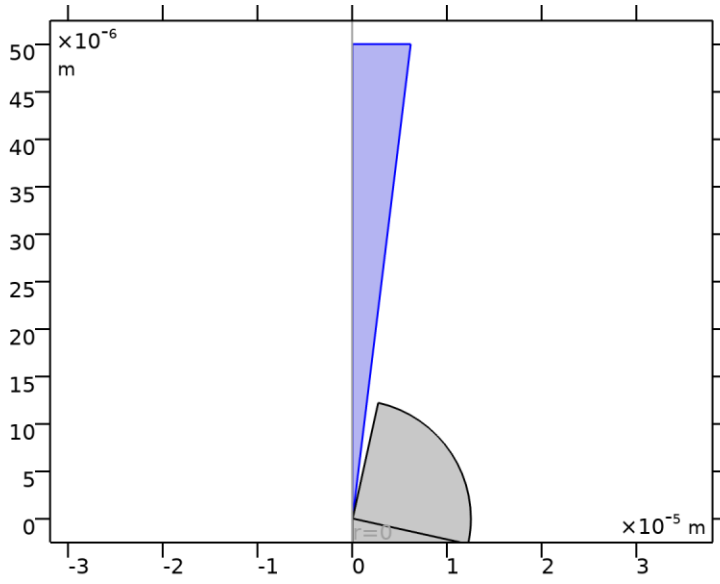
Geometric entity level	Domain
Selection	Geometry geom1: Dimension 2: Domains 1, 3

Initial Values

SETTINGS

Description	Value
Concentration	{cK_GCBath, cCl_GCBath}

2.3.8 Initial Values (Gouy-Chapman, Pore)



Initial Values (Gouy-Chapman, Pore)

SELECTION

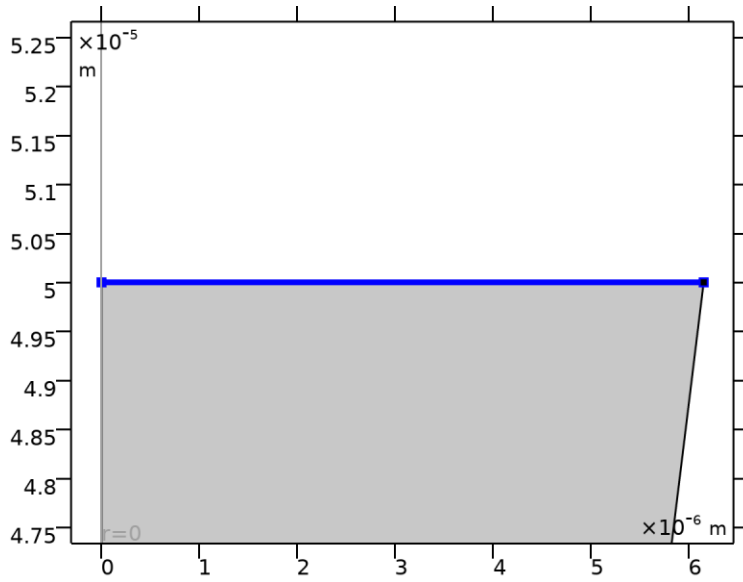
Geometric entity level	Domain
Selection	Geometry geom1: Dimension 2: Domain 2

Initial Values

SETTINGS

Description	Value
Concentration	{cK_GC, cCl_GC}

2.3.9 Concentration (Gouy-Chapman, internal electrode)



Concentration (Gouy-Chapman, internal electrode)

SELECTION

Geometric entity level	Boundary
Selection	Geometry geom1: Dimension 1: Boundary 4

EQUATIONS

$$c_i = c_{0j}$$

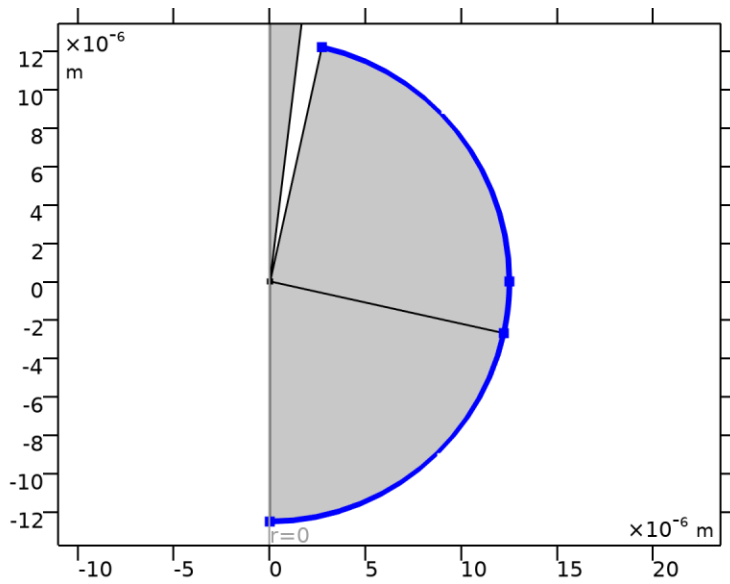
.....

Concentration

SETTINGS

Description	Value
Species cK	On
Species cCl	On
Concentration	{c_GC(dGlass, 1), c_GC(dGlass, -1)}

2.3.10 Concentration (Gouy-Chapman, external electrode)



Concentration (Gouy-Chapman, external electrode)

SELECTION

Geometric entity level	Boundary
Selection	Geometry geom1: Dimension 1: Boundaries 9–11

EQUATIONS

$$c_i = c_{0j}$$

.....

Concentration

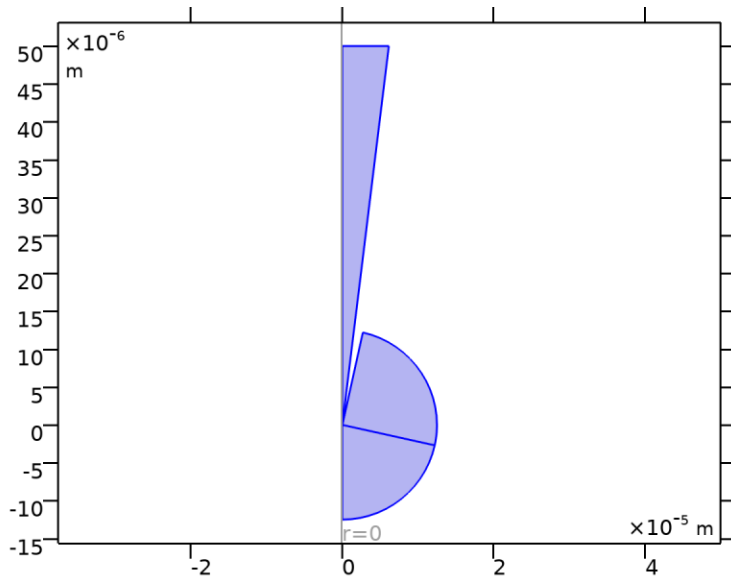
SETTINGS

Description	Value
Species cK	On
Species cCl	On
Concentration	{c_GCBath(dGlass, 1), c_GCBath(dGlass, -1)}

2.4 ELECTROSTATICS

USED PRODUCTS

COMSOL Multiphysics



Electrostatics

SELECTION

Geometric entity level	Domain
Selection	Geometry geom1: Dimension 2: All domains

EQUATIONS

$$\nabla \cdot \mathbf{D} = \rho_v$$

$$\mathbf{E} = -\nabla V$$

2.4.1 Interface Settings

Discretization

SETTINGS

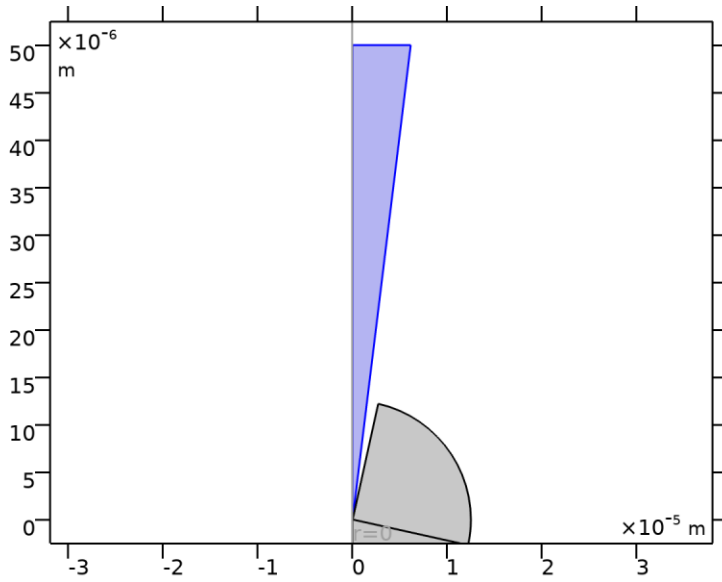
Description	Value
Electric potential	Quadratic

Manual Terminal Sweep Settings

SETTINGS

Description	Value
Use manual terminal sweep	Off
Reference impedance	50[ohm]

2.4.2 Charge Conservation (Pore)



Charge Conservation (Pore)

SELECTION

Geometric entity level	Domain
Selection	Geometry geom1: Dimension 2: All domains

EQUATIONS

$$\mathbf{E} = -\nabla V$$

$$\nabla \cdot (\epsilon_0 \epsilon_r \mathbf{E}) = \rho_v$$

Constitutive Relation D-E

SETTINGS

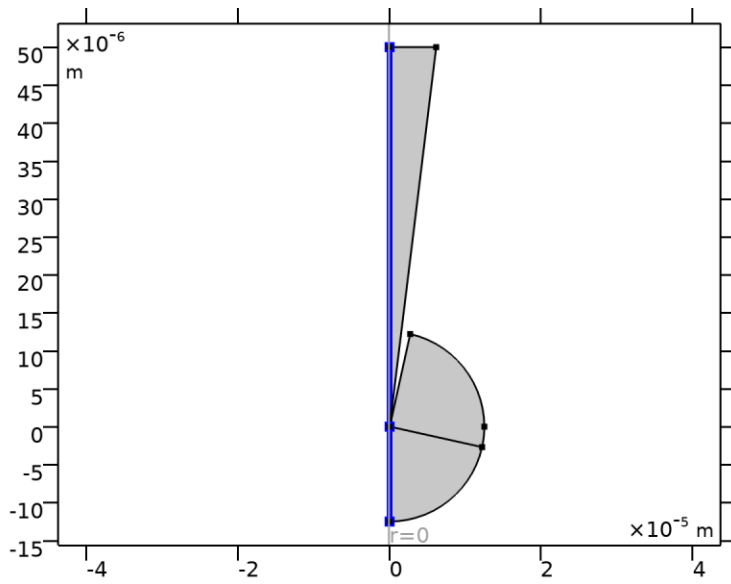
Description	Value
Dielectric model	Relative permittivity
Relative permittivity	User defined
Relative permittivity	{{EpsilonR, 0, 0}, {0, EpsilonR, 0}, {0, 0, EpsilonR}}

Coordinate System Selection

SETTINGS

Description	Value
Coordinate system	Global coordinate system

2.4.3 Axial Symmetry

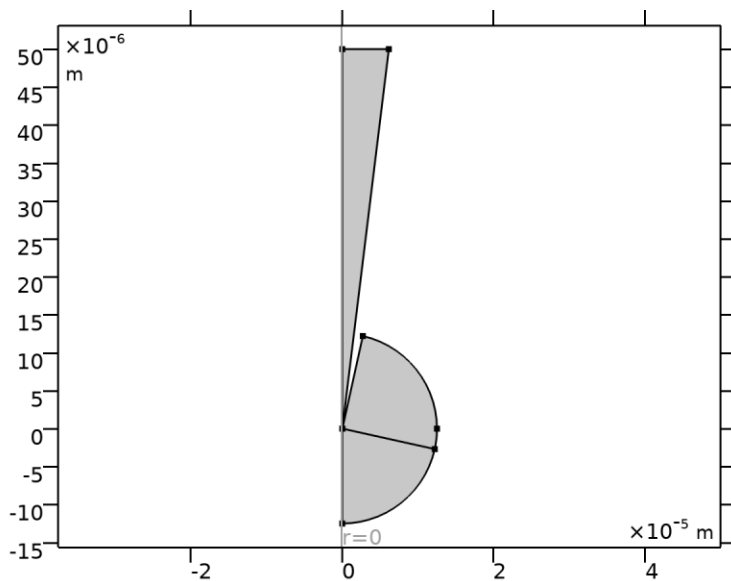


Axial Symmetry

SELECTION

Geometric entity level	Boundary
Selection	Geometry geom1: Dimension 1: All boundaries

2.4.4 Zero Charge



Zero Charge

SELECTION

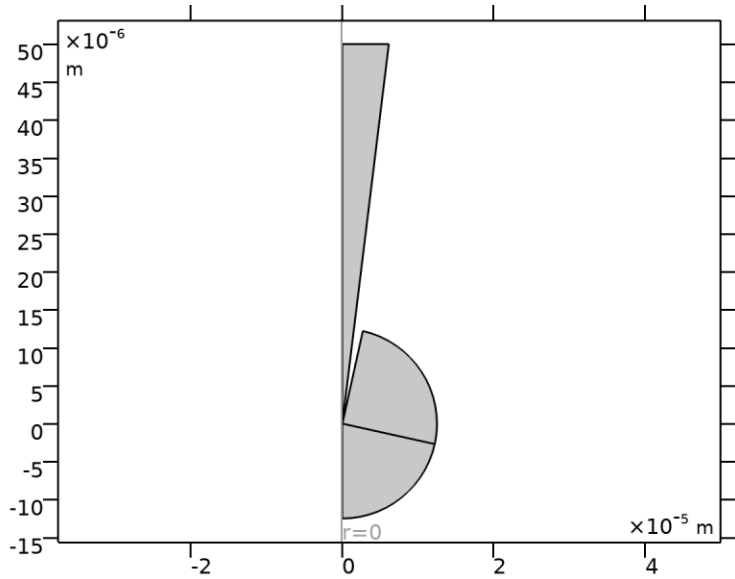
Geometric entity level	Boundary
------------------------	----------

Selection	Geometry geom1: Dimension 1: All boundaries
-----------	---

EQUATIONS

$$\mathbf{n} \cdot \mathbf{D} = 0$$

2.4.5 Initial Values



Initial Values

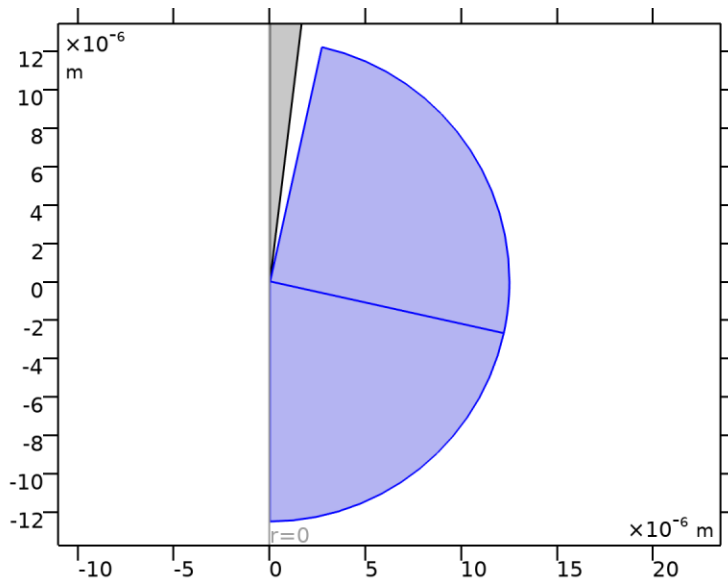
SELECTION

Geometric entity level	Domain
Selection	Geometry geom1: Dimension 2: All domains

SETTINGS

Description	Value
Electric potential	0

2.4.6 Charge Conservation (Bath)



Charge Conservation (Bath)

SELECTION

Geometric entity level	Domain
Selection	Geometry geom1: Dimension 2: Domains 1, 3

EQUATIONS

$$\mathbf{E} = -\nabla V$$

$$\nabla \cdot (\epsilon_0 \epsilon_r \mathbf{E}) = \rho_v$$

Constitutive Relation D-E

SETTINGS

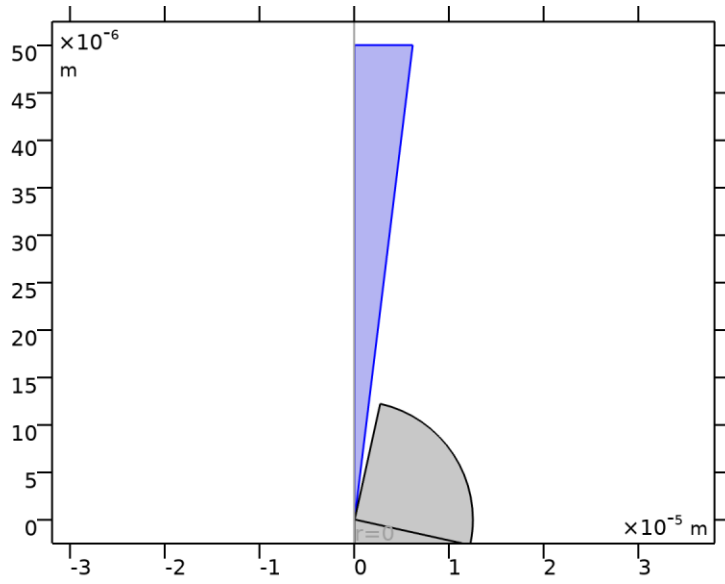
Description	Value
Dielectric model	Relative permittivity
Relative permittivity	User defined
Relative permittivity	{{EpsilonRBath, 0, 0}, {0, EpsilonRBath, 0}, {0, 0, EpsilonRBath}}

Coordinate System Selection

SETTINGS

Description	Value
Coordinate system	Global coordinate system

2.4.7 Initial Values (Gouy-Chapman in Pore)



Initial Values (Gouy-Chapman in Pore)

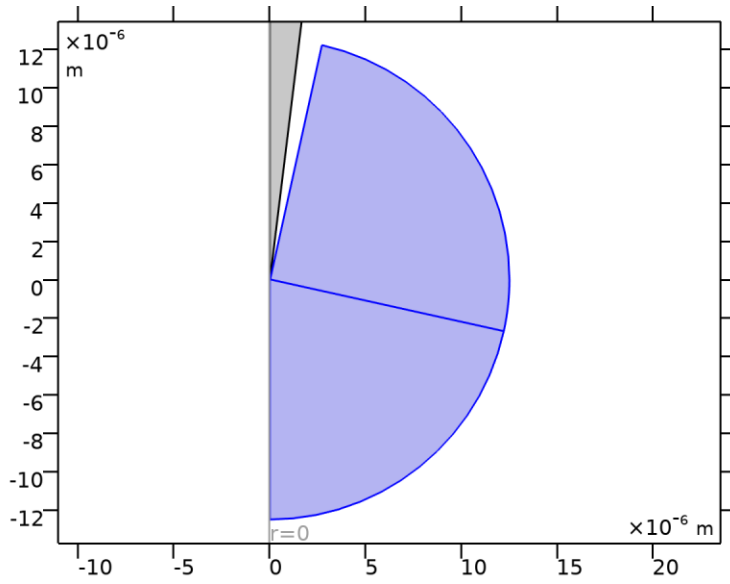
SELECTION

Geometric entity level	Domain
Selection	Geometry geom1: Dimension 2: Domain 2

SETTINGS

Description	Value
Electric potential	Potential_GC + AnalyticalPotentialNoCharge

2.4.8 Initial Values (Gouy-Chapman in Bath)



Initial Values (Gouy-Chapman in Bath)

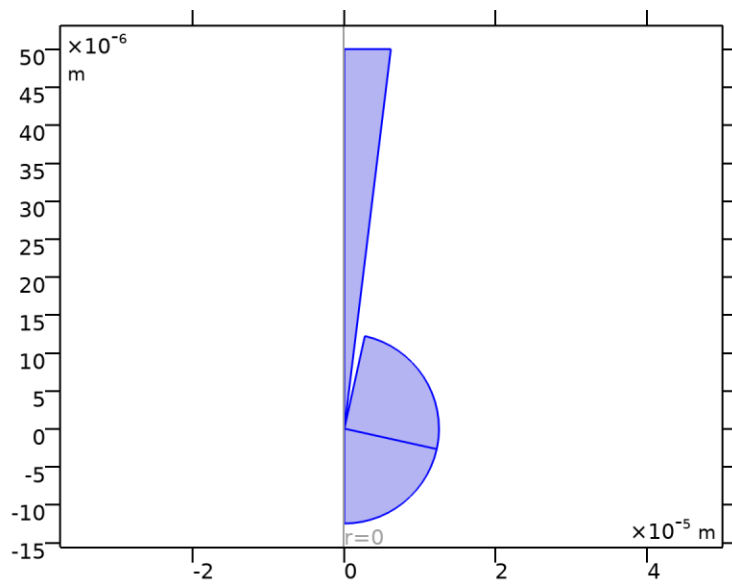
SELECTION

Geometric entity level	Domain
Selection	Geometry geom1: Dimension 2: Domains 1, 3

SETTINGS

Description	Value
Electric potential	Potential_GCBath + AnalyticalPotentialNoCharge

2.4.9 Space Charge Density



Space Charge Density

SELECTION

Geometric entity level	Domain
Selection	Geometry geom1: Dimension 2: Domains 1-3

EQUATIONS

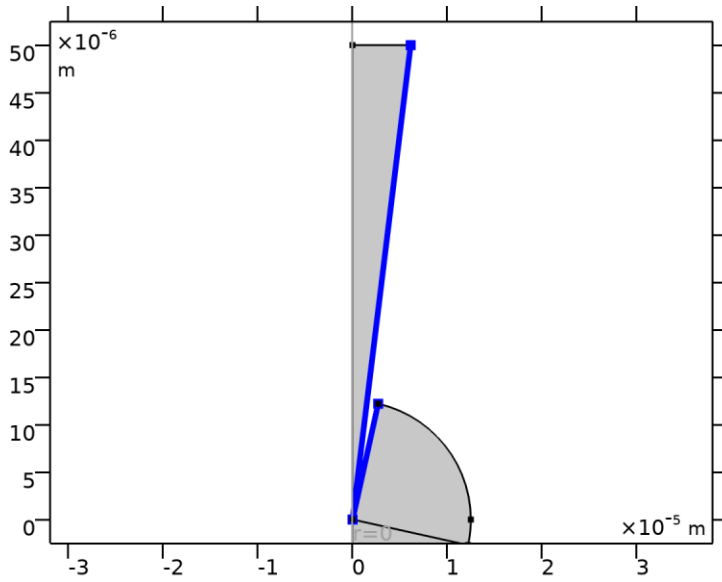
$$\nabla \cdot \mathbf{D} = \rho_v$$

Coordinate System Selection

SETTINGS

Description	Value
Coordinate system	Global coordinate system

2.4.10 Surface Charge (Glass Wall)



Surface Charge (Glass Wall)

SELECTION

Geometric entity level	Boundary
Name	Glass Wall
Selection	Named sel1: Geometry geom1: Dimension 1: Boundaries 5–7

EQUATIONS

$$\mathbf{n} \cdot (\mathbf{D}_1 - \mathbf{D}_2) = \rho_s$$

Surface Charge Density

SETTINGS

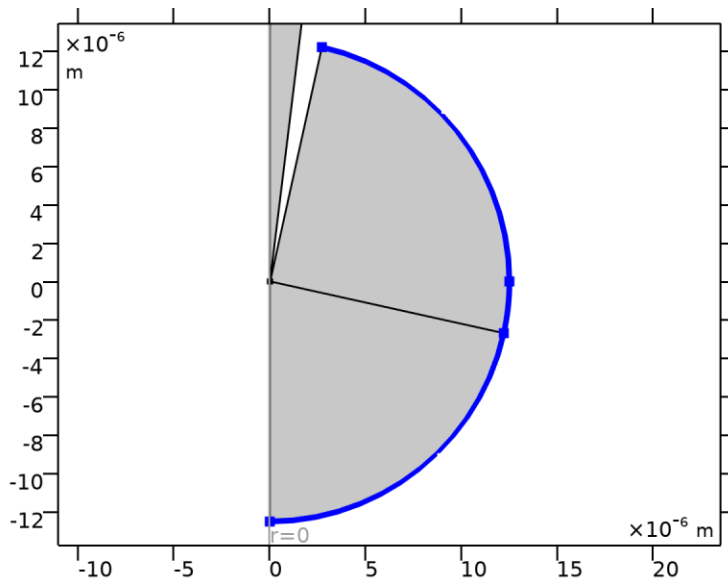
Description	Value
Surface charge density	PoreSurfaceCharge

Coordinate System Selection

SETTINGS

Description	Value
Coordinate system	Global coordinate system

2.4.11 Electric Potential (Gouy-Chapman, external electrode)



Electric Potential (Gouy-Chapman, external electrode)

SELECTION

Geometric entity level	Boundary
Name	External Electrode
Selection	Named sel4: Geometry geom1: Dimension 1: Boundaries 9–11

EQUATIONS

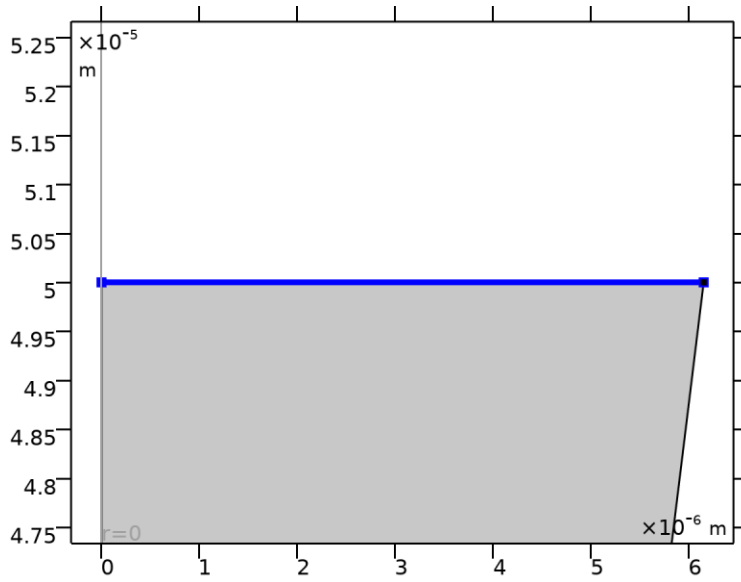
$$V = V_0$$

Electric Potential

SETTINGS

Description	Value
Electric potential	E_GCBath(dGlass)

2.4.12 Electric Potential (Gouy-Chapman, internal electrode)



Electric Potential (Gouy-Chapman, internal electrode)

SELECTION

Geometric entity level	Boundary
Name	Internal Electrode
Selection	Named sel3: Geometry geom1: Dimension 1: Boundary 4

EQUATIONS

$$V = V_0$$

Electric Potential

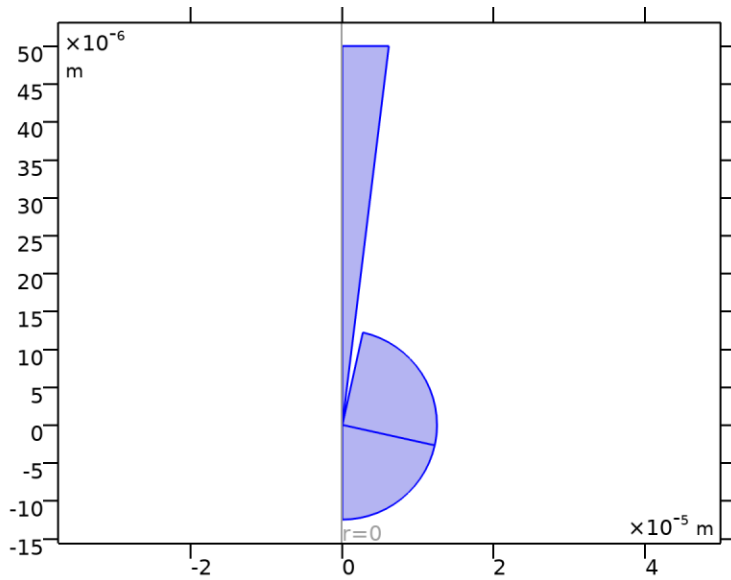
SETTINGS

Description	Value
Electric potential	VApp + E_GC(dGlass)

2.5 LAMINAR FLOW

USED PRODUCTS

COMSOL Multiphysics



Laminar Flow

SELECTION

Geometric entity level	Domain
Selection	Geometry geom1: Dimension 2: All domains

EQUATIONS

$$\rho(\mathbf{u} \cdot \nabla)\mathbf{u} = \nabla \cdot [-p\mathbf{I} + \mathbf{K}] + \mathbf{F}$$

$$\rho \nabla \cdot \mathbf{u} = 0$$

2.5.1 Interface Settings

Discretization

SETTINGS

Description	Value
Discretization of fluids	P1 + P1

Physical Model

SETTINGS

Description	Value
Neglect inertial term (Stokes flow)	Off
Compressibility	Incompressible flow
Swirl flow	Off
Enable porous media domains	Off
Include gravity	Off
Reference temperature	293.15[K]

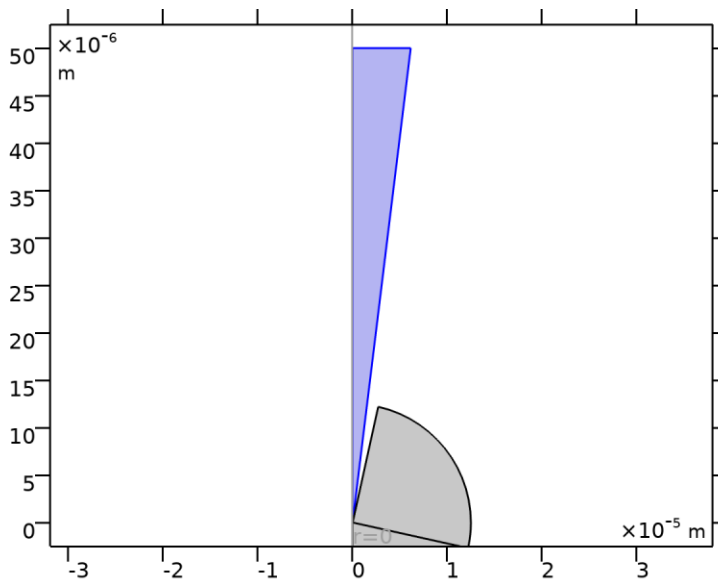
Description	Value
Reference pressure level	1[atm]
Reference temperature	User defined

Turbulence

SETTINGS

Description	Value
Turbulence model type	None

2.5.2 Fluid Properties Bulk



Fluid Properties Bulk

SELECTION

Geometric entity level	Domain
Selection	Geometry geom1: Dimension 2: All domains

EQUATIONS

$$\rho(\mathbf{u} \cdot \nabla)\mathbf{u} = \nabla \cdot [-p\mathbf{I} + \mathbf{K}] + \mathbf{F}$$

$$\rho \nabla \cdot \mathbf{u} = 0$$

$$\mathbf{K} = \mu(\nabla\mathbf{u} + (\nabla\mathbf{u})^T)$$

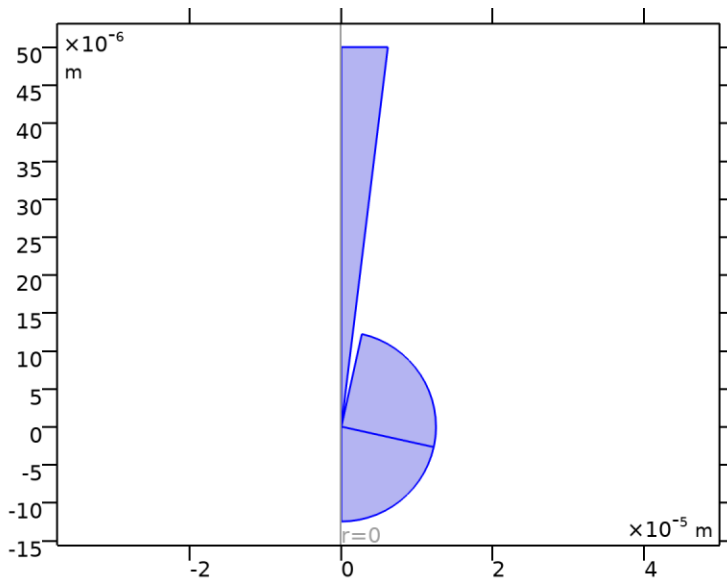
Fluid Properties

SETTINGS

Description	Value
Density	User defined

Description	Value
Density	FluidDensity
	Newtonian
Dynamic viscosity	User defined
Dynamic viscosity	FluidViscosity

2.5.3 Initial Values



Initial Values

SELECTION

Geometric entity level	Domain
Selection	Geometry geom1: Dimension 2: All domains

Initial Values

SETTINGS

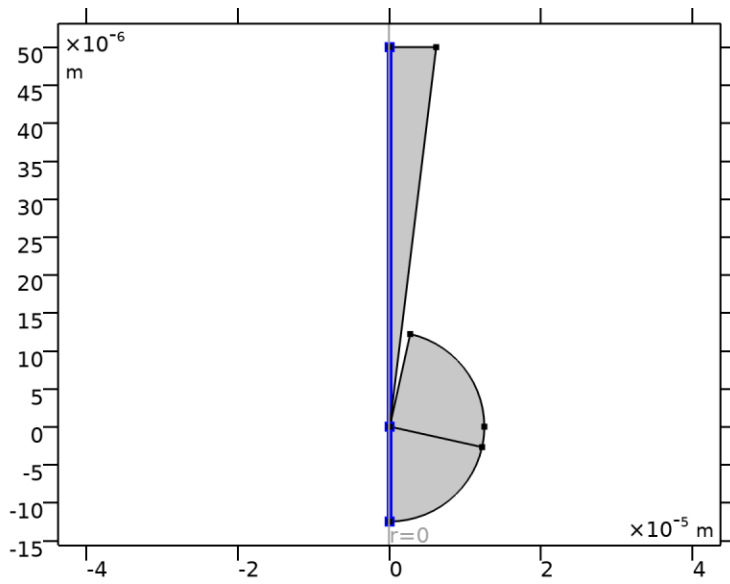
Description	Value
Velocity field, r component	0
Velocity field, phi component	0
Velocity field, z component	0
Pressure	0

Coordinate System Selection

SETTINGS

Description	Value
Coordinate system	Global coordinate system

2.5.4 Axial Symmetry

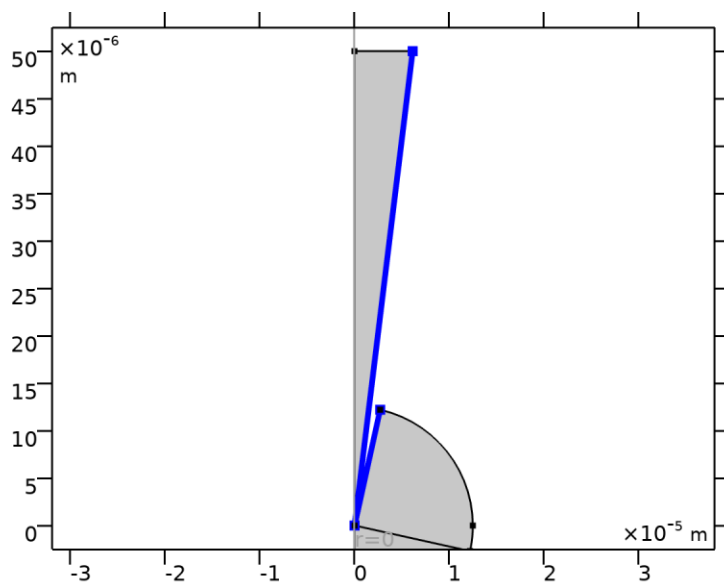


Axial Symmetry

SELECTION

Geometric entity level	Boundary
Selection	Geometry geom1: Dimension 1: All boundaries

2.5.5 Wall (Glass)



Wall (Glass)

SELECTION

Geometric entity level	Boundary
------------------------	----------

Selection	Geometry geom1: Dimension 1: All boundaries
-----------	---

EQUATIONS

$$\underline{\mathbf{u}} = \mathbf{0}$$

Boundary Condition

SETTINGS

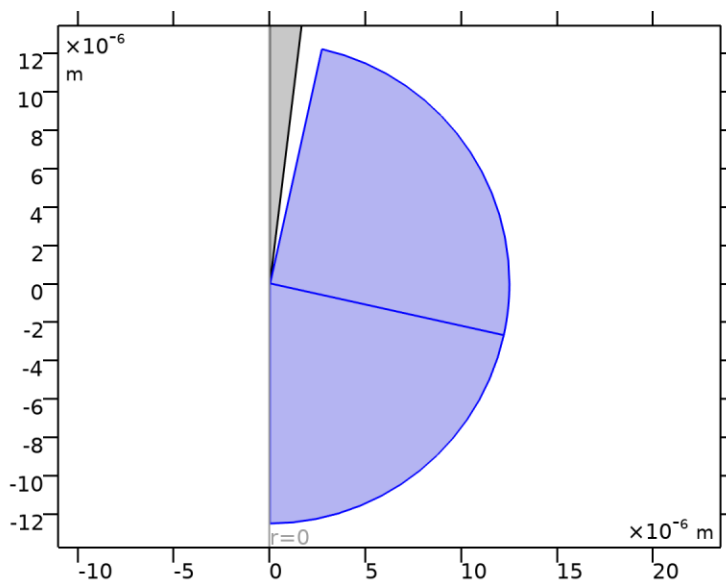
Description	Value
Wall condition	No slip

Wall Movement

SETTINGS

Description	Value
Translational velocity	Automatic from frame
Sliding wall	Off

2.5.6 Fluid Properties Bath



Fluid Properties Bath

SELECTION

Geometric entity level	Domain
Selection	Geometry geom1: Dimension 2: Domains 1, 3

EQUATIONS

$$\rho(\underline{\mathbf{u}} \cdot \nabla) \underline{\mathbf{u}} = \nabla \cdot [-p\mathbf{I} + \mathbf{K}] + \mathbf{F}$$

$$\rho \nabla \cdot \underline{\mathbf{u}} = 0$$

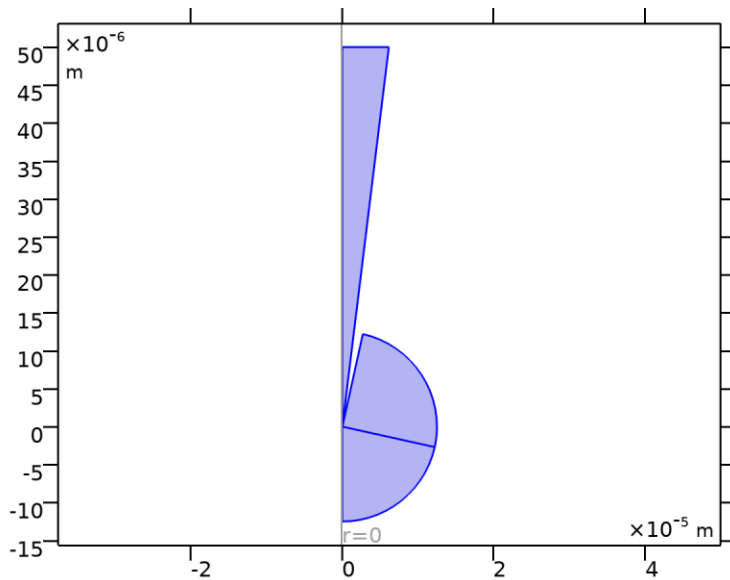
$$\mathbf{K} = \mu(\nabla\mathbf{u} + (\nabla\mathbf{u})^T)$$

Fluid Properties

SETTINGS

Description	Value
Density	User defined
Density	FluidDensityBath
	Newtonian
Dynamic viscosity	User defined
Dynamic viscosity	FluidViscosityBath

2.5.7 Volume Force



Volume Force

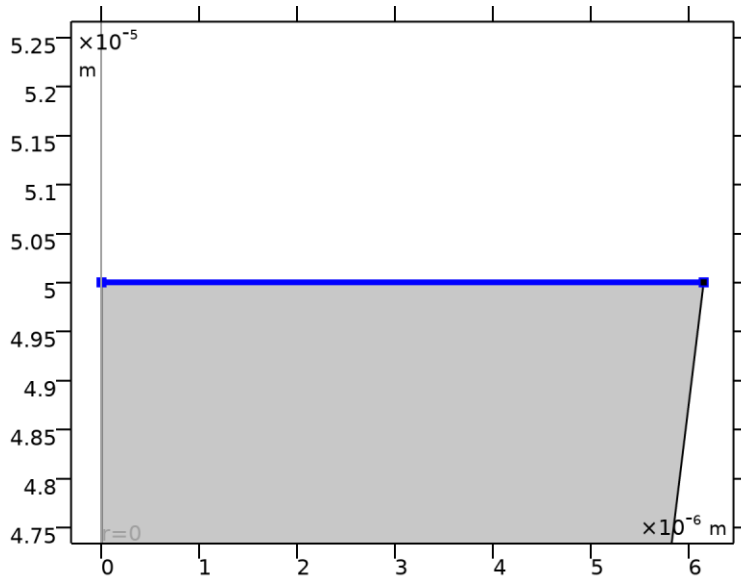
SELECTION

Geometric entity level	Domain
Selection	Geometry geom1: Dimension 2: Domains 1-3

EQUATIONS

$$\rho(\mathbf{u} \cdot \nabla)\mathbf{u} = \nabla \cdot [-p\mathbf{I} + \mathbf{K}] + \mathbf{F}$$

2.5.8 Inlet



Inlet

SELECTION

Geometric entity level	Boundary
Name	Internal Electrode
Selection	Named sel3: Geometry geom1: Dimension 1: Boundary 4

EQUATIONS

$$\mathbf{n}^T[-p\mathbf{I} + \mathbf{K}]\mathbf{n} = -p_0$$

$$\mathbf{u} \cdot \mathbf{t} = 0$$

Boundary Condition

SETTINGS

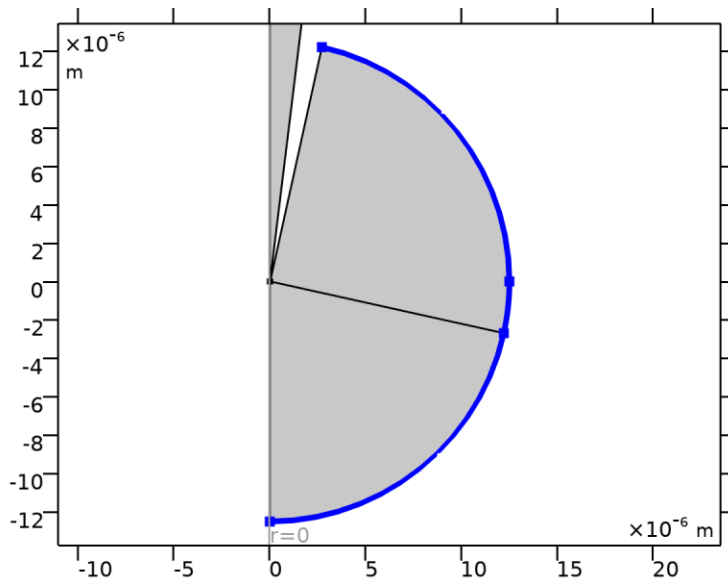
Description	Value
Boundary condition	Pressure

Pressure Conditions

SETTINGS

Description	Value
Pressure	Static
Pressure	PApp
Suppress backflow	Off
Flow direction	Normal flow

2.5.9 Outlet



Outlet

SELECTION

Geometric entity level	Boundary
Name	External Electrode
Selection	Named sel4: Geometry geom1: Dimension 1: Boundaries 9–11

EQUATIONS

$$[-\rho \mathbf{I} + \mathbf{K}] \mathbf{n} = -\hat{p}_0 \mathbf{n}$$

$$\hat{p}_0 \leq p_0,$$

Boundary Condition

SETTINGS

Description	Value
Boundary condition	Pressure

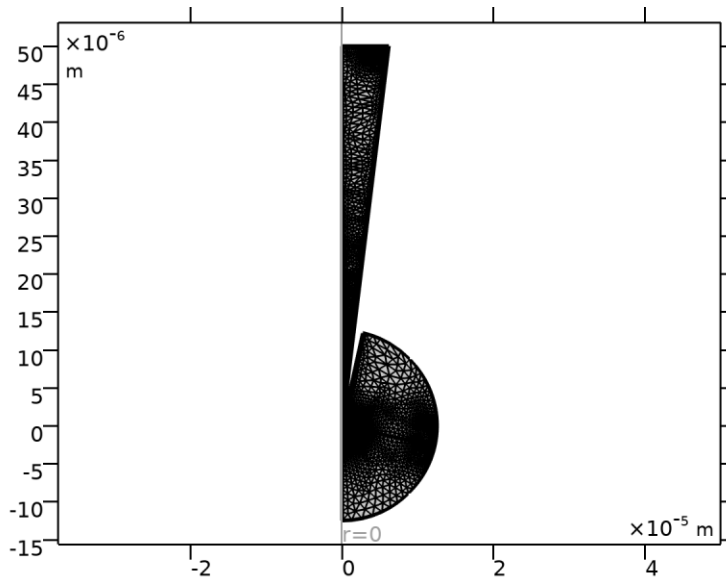
Pressure Conditions

SETTINGS

Description	Value
Pressure	Static
Pressure	0
Normal flow	Off
Suppress backflow	On

2.6 MESHES

2.6.1 Final Mesh



Final Mesh

MESH STATISTICS

Description	Value
Minimum element quality	1.781E-4
Average element quality	0.6325
Triangle	18724
Quad	6960
Edge element	1332
Vertex element	9

Size Overall (size)

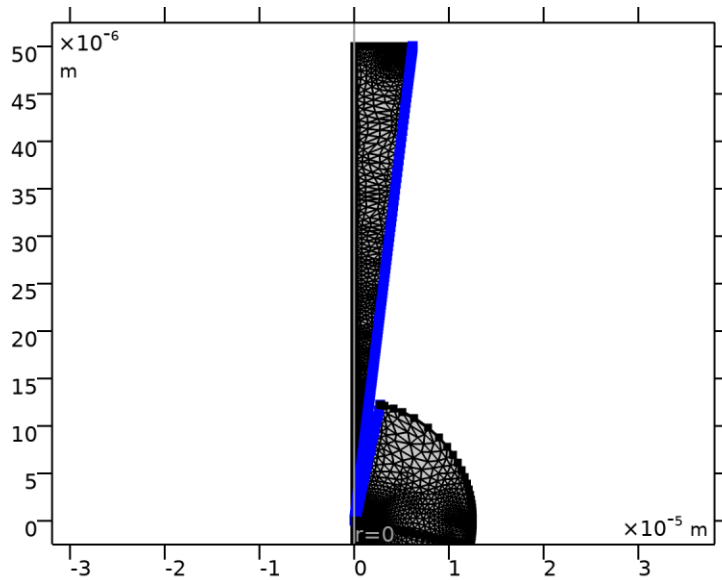
SETTINGS

Description	Value
Maximum element size	200E-7
Minimum element size	5E-10
Curvature factor	0.2
Resolution of narrow regions	10
Predefined size	Extremely fine
Custom element size	Custom

Size for Glass Wall (size2)

SELECTION

Geometric entity level	Boundary
Name	Glass Wall
Selection	Named sel1: Geometry geom1: Dimension 1: Boundaries 5–7



Size for Glass Wall

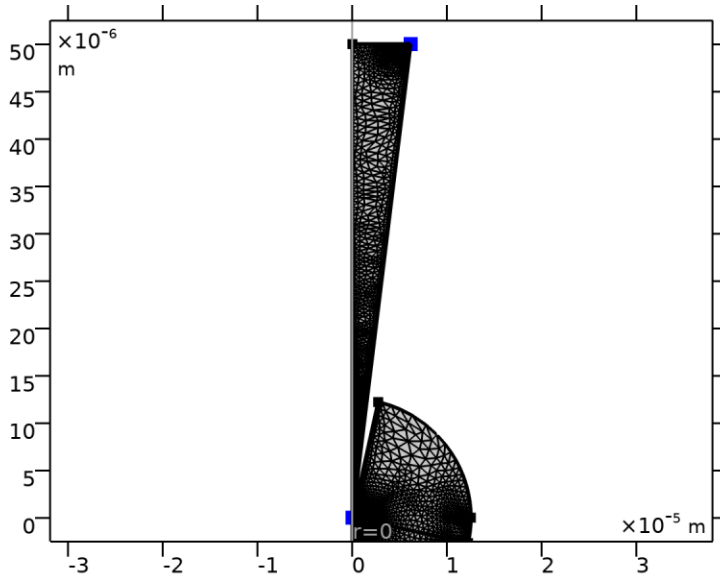
SETTINGS

Description	Value
Maximum element size	6.25E-7
Minimum element size	1.25E-9
Curvature factor	0.2
Predefined size	Extremely fine

Size Aperture Points (size1)

SELECTION

Geometric entity level	Point
Selection	Geometry geom1: Dimension 0: Points 4–5, 7



Size Aperture Points

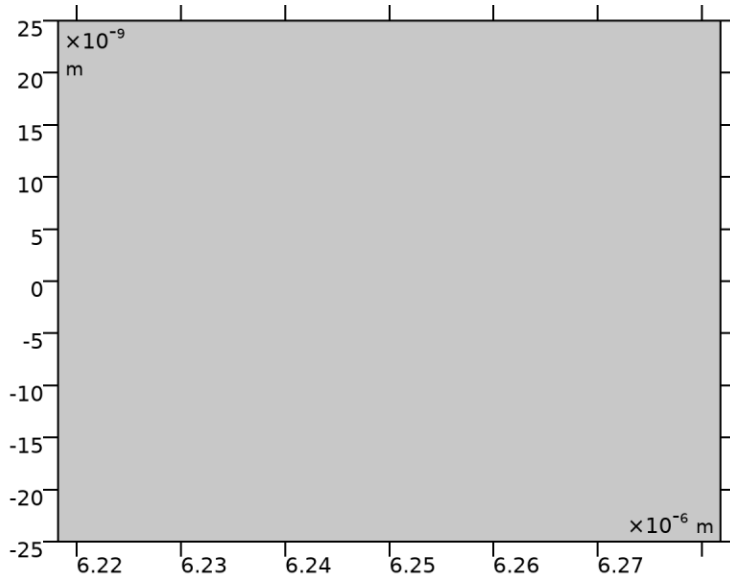
SETTINGS

Description	Value
Maximum element size	PoreRadius/100
Minimum element size	6.45E-10
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

Boundary Layers (bl1)

SELECTION

Geometric entity level	Domain
Selection	Geometry geom1



Boundary Layers

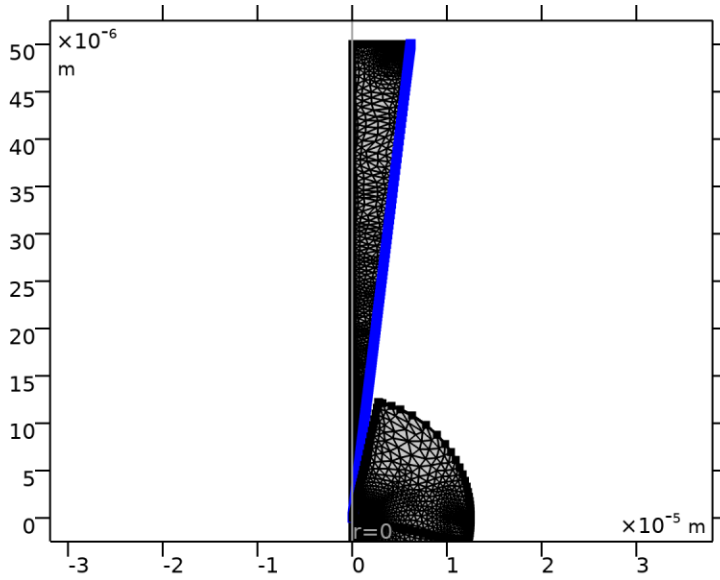
SETTINGS

Description	Value
Number of iterations	30
Maximum element depth to process	30

Boundary Layer Properties (Internal) (blp)

SELECTION

Geometric entity level	Boundary
Selection	Geometry geom1: Dimension 1: Boundary 6



Boundary Layer Properties (Internal)

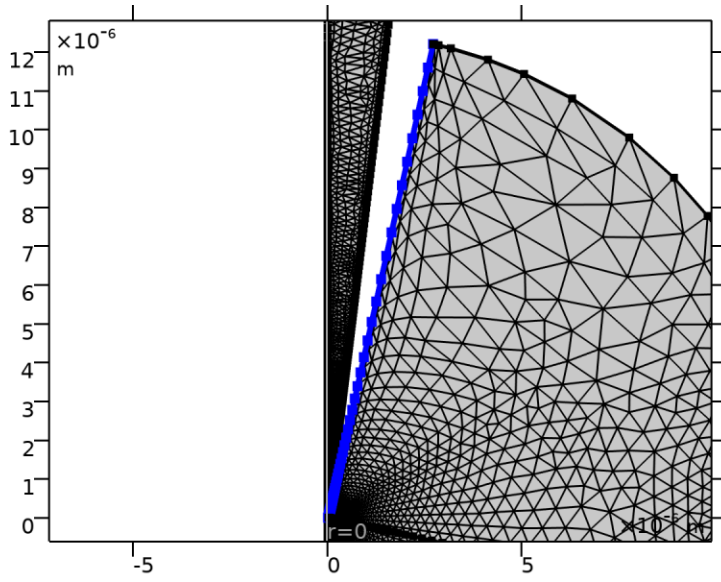
SETTINGS

Description	Value
Number of boundary layers	12
Thickness of first layer	Manual
Thickness	DebyeLength/10

Boundary Layer Properties (External) (blp1)

SELECTION

Geometric entity level	Boundary
Selection	Geometry geom1: Dimension 1: Boundaries 5, 7



Boundary Layer Properties (External)

SETTINGS

Description	Value
Number of boundary layers	12
Thickness of first layer	Manual
Thickness	DebyeLengthBath/10

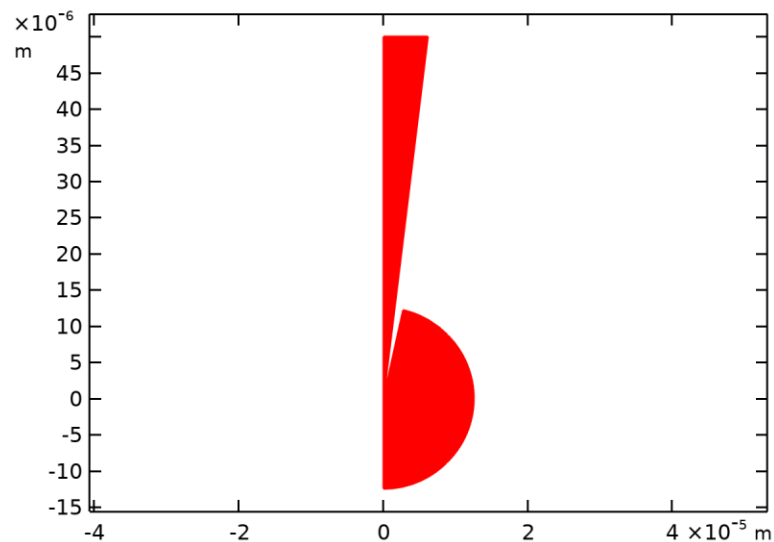
3 Results

3.1 DATA SETS

3.1.1 Mesh 2

MESH

Description	Value
Mesh	Final Mesh



Dataset: Mesh 2

3.2 TABLES

3.2.1 Probe Table

VApp (V)	Current (internal) (nA), Current (internal electrode)
-0.50000	-0.94006
-0.40000	-0.84128
-0.30000	-0.71025
-0.20000	-0.53473
-0.10000	-0.30131
0.0000	0.0079452
0.10000	0.41726
0.20000	0.95828
0.30000	1.6723
0.40000	2.6134

VApp (V)	Current (internal) (nA), Current (internal electrode)
0.50000	3.8527

3.3 PLOT GROUPS

3.3.1 Current Probe Plot

