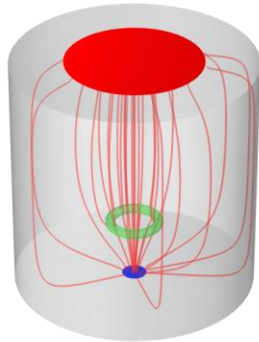


Electrode Model CPE RC



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1 Global Definitions

GLOBAL SETTINGS

Name	Electrode Model CPE RC.mph
Version	COMSOL Multiphysics 6.0 (Build: 312)
Unit system	SI

USED PRODUCTS

COMSOL Multiphysics
AC/DC Module

1.1 PARAMETERS

PARAMETERS 1

Name	Expression	Value	Description
sigma	1.5	1.5	Electrolyte conductivity [S/m]
epsilon_r	77	77	Electrolyte relative permittivity
a	$\sqrt{3.25/\pi}$	1.0171	Electrode radius [mm]
V_P	-0.6	-0.6	Command voltage [V]
deltat	$2.5 \cdot 10^{-5}$	2.5E-5	CPE time resolution [s]
CPE	1	1	Choose CPE or RC, 1 for CPE, 0 for RC
R_s	150	150	Additional series resistance in the circuit (put 0 if none) [Ω]

2 Component 2

2.1 DEFINITIONS

2.1.1 Variables

Variables 1

SELECTION

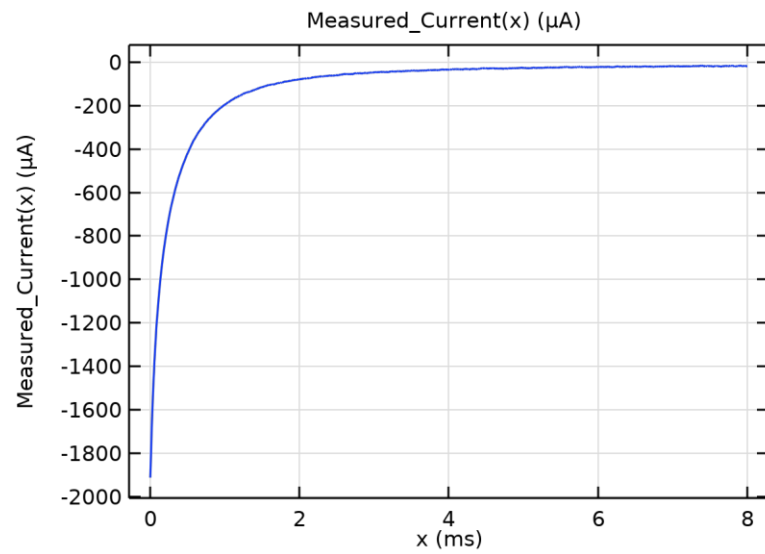
Geometric entity level	Boundary
Selection	Geometry geom3: Dimension 1: Boundary 4

Name	Expression	Unit	Description
ChargeDensityCPE	$(\text{Integral_First_Part} + \text{Integral_Second_Part}) \cdot 1 [\text{C}/\text{m}^2]$	C/m^2	
CurrentDensityCPE	$(V_W - V) \cdot \sigma_1(V_W - V) [\text{mS}/\text{cm}^2] + d(\text{ChargeDensityCPE}, t)$	A/m^2	
ChargeDensityRC	$C_1(V_W - V) [\text{uF}/\text{cm}^2] \cdot (V_W - V)$	C/m^2	
CurrentDensityRC	$(V_W - V) \cdot \sigma_1(V_W - V) [\text{mS}/\text{cm}^2] + d(\text{ChargeDensityRC}, t)$	A/m^2	
CurrentDensity	$\text{if}(\text{CPE} == 1, \text{CurrentDensityCPE}, \text{CurrentDensityRC})$	A/m^2	
Integral_First_Part	$\text{linproj1}(Q(u_2)/\gamma(1 - \alpha(u_2)) \cdot u_2/1 [\text{V}] / (-z/1 [\text{m}])^{\alpha(u_2)} \cdot (-z/1 [\text{m}] < t/1 [\text{s}]) \cdot (-z/1 [\text{m}] > \text{deltat})) / 1 [\text{m}]$		
Integral_Second_Part	$Q(V_W - V) / \gamma(1 - \alpha(V_W - V)) \cdot (V_W - V) / 1 [\text{V}] \cdot (\text{deltat})^{(1 - \alpha(V_W - V))} / (1 - \alpha(V_W - V))$		

2.1.2 Functions

Measured Current

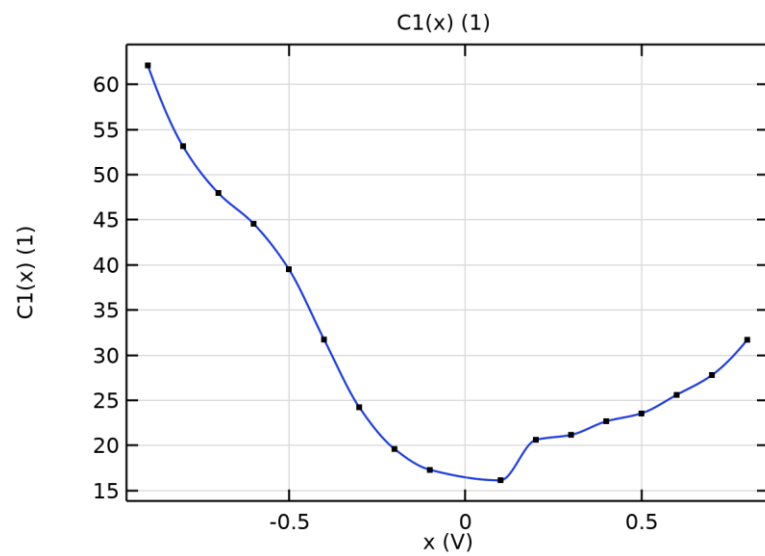
Function names	Measured_Current
Function type	Interpolation



Measured Current

Capacitance

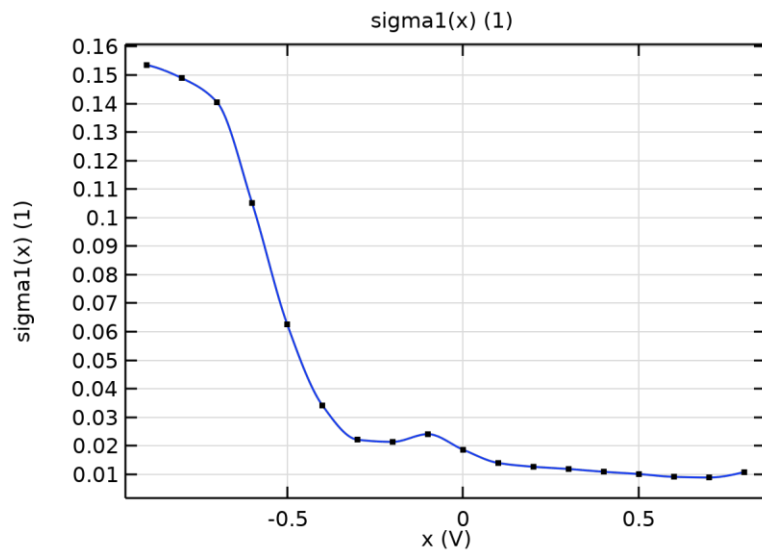
Function names	C1
Function type	Interpolation



Capacitance

Conductance

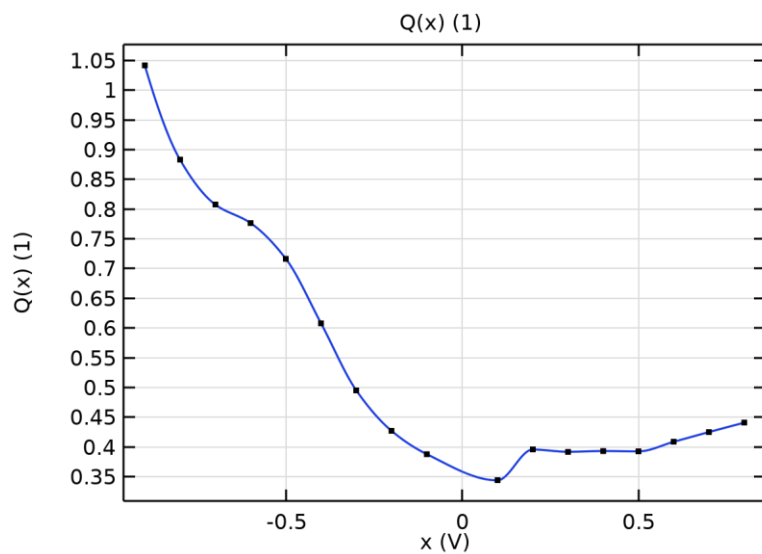
Function names	sigma1
Function type	Interpolation



Conductance

CPE parameter

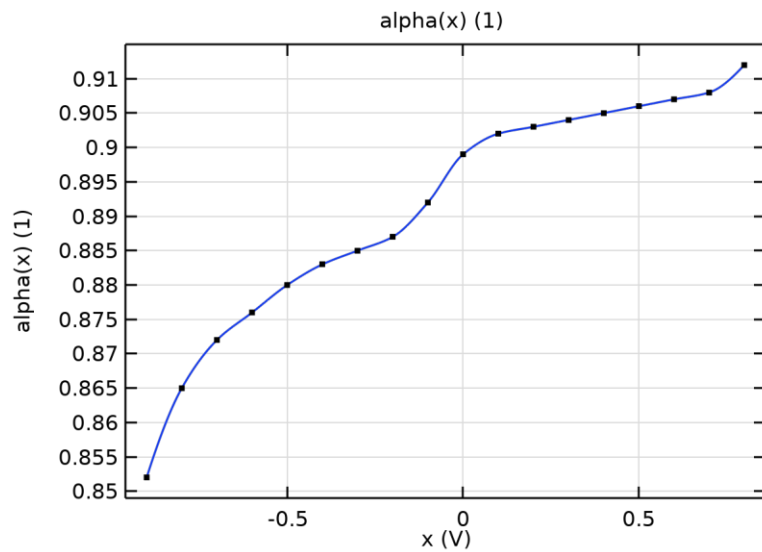
Function names	Q
Function type	Interpolation



CPE parameter

CPE exponent

Function names	alpha
Function type	Interpolation



CPE exponent

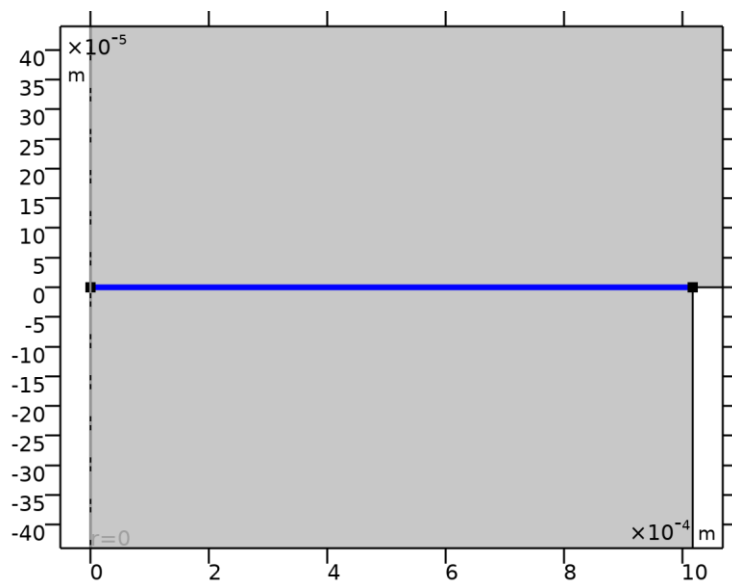
2.1.3 Probes

Total Current

Probe type	Boundary probe
------------	----------------

SELECTION

Geometric entity level	Boundary
Selection	Geometry geom3: Dimension 1: Boundary 4



Selection

PROBE TYPE

Description	Value
Type	Integral

EXPRESSION

Description	Value
Expression	CurrentDensity
Table and plot unit	A

TABLE AND WINDOW SETTINGS

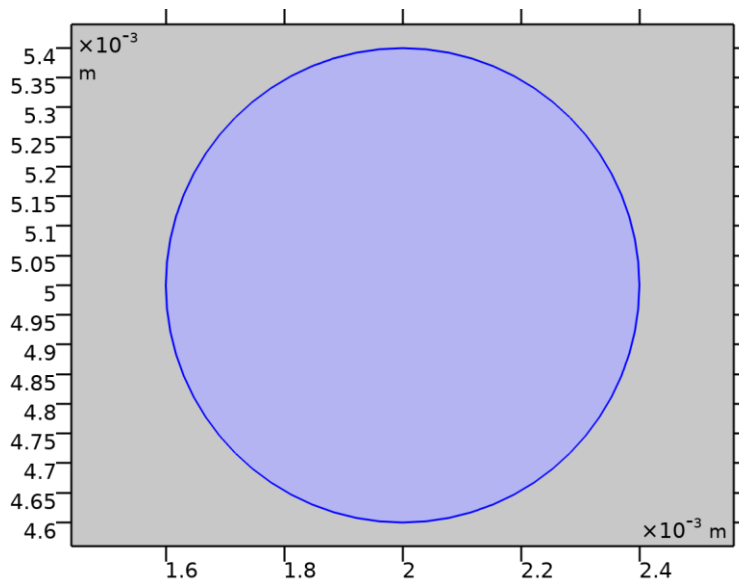
Description	Value
Output table	Probe Table 1
Plot window	Probe Plot 6

V REF

Probe type	Domain probe
------------	--------------

SELECTION

Geometric entity level	Domain
Selection	Geometry geom3: Dimension 2: Domain 3



Selection

EXPRESSION

Description	Value
Expression	V
Table and plot unit	V

Description	Value
Description	Electric potential

TABLE AND WINDOW SETTINGS

Description	Value
Output table	Probe Table 1
Plot window	Probe Plot 8

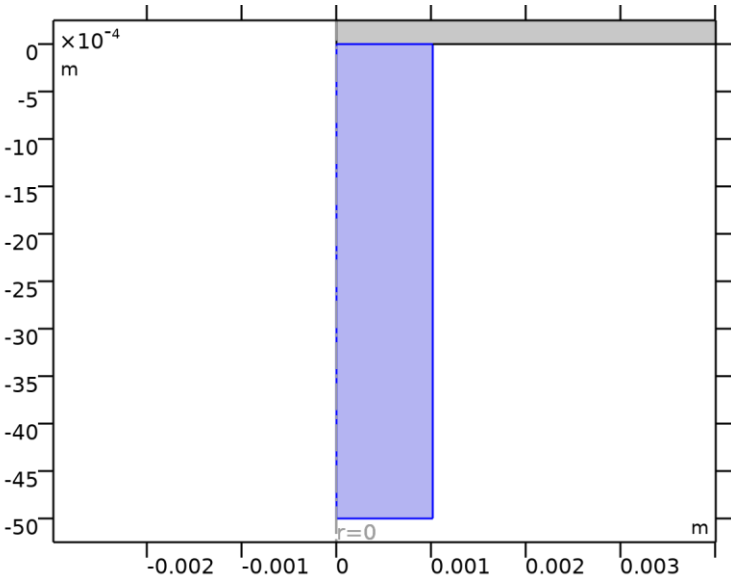
2.1.4 Nonlocal Couplings

Integration

Coupling type	Linear projection
Operator name	linproj1

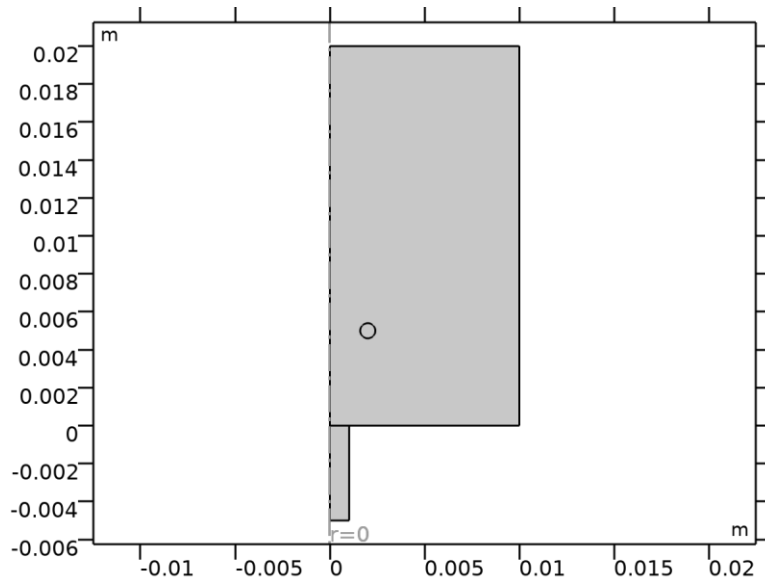
SELECTION

Geometric entity level	Domain
Selection	Geometry geom3: Dimension 2: Domain 1



Selection

2.2 GEOMETRY



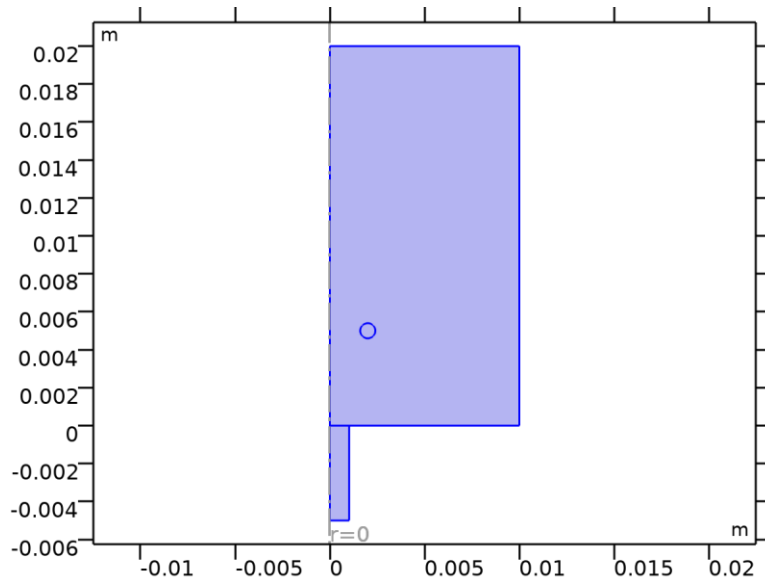
Geometry

UNITS

Length unit	m
Angular unit	deg

2.3 MATERIALS

2.3.1 1x PBS



1x PBS

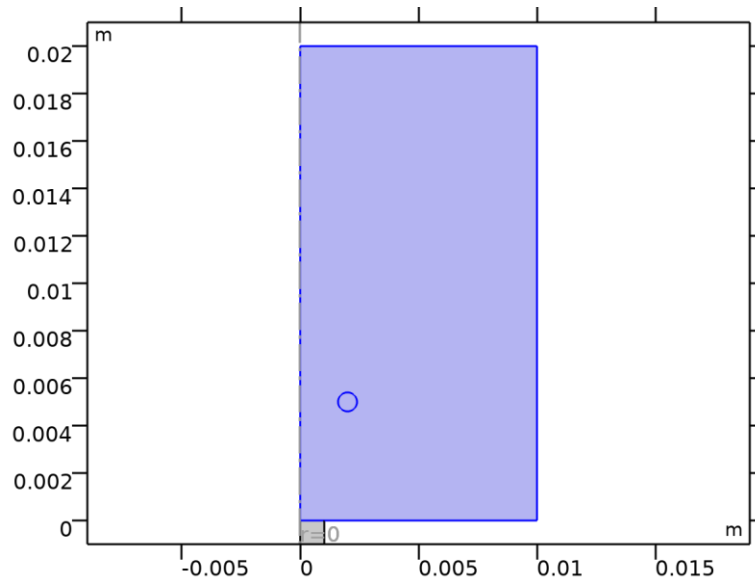
SELECTION

Geometric entity level	Domain
Selection	Geometry geom3: Dimension 2: All domains

MATERIAL PARAMETERS

Name	Value	Unit
Electrical conductivity	sigma	S/m
Relative permittivity	epsilononr	1

2.4 ELECTRIC CURRENTS 2



Electric Currents 2

EQUATIONS

$$\nabla \cdot \mathbf{J} = Q_{j,v}$$

$$\mathbf{J} = \sigma \mathbf{E} + \frac{\partial \mathbf{D}}{\partial t} + \mathbf{J}_e$$

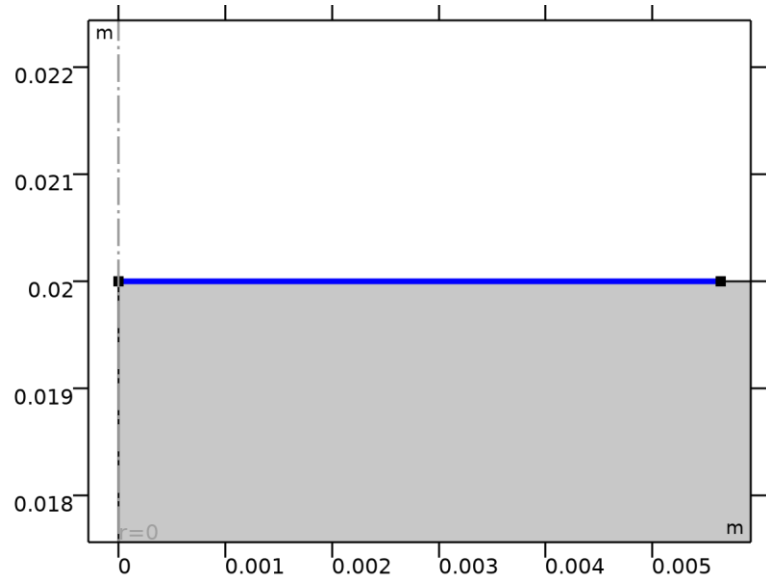
$$\mathbf{E} = -\nabla V$$

FEATURES

Name	Level
Current Conservation 1	Domain
Axial Symmetry 1	Boundary
Electric Insulation 1	Boundary
Initial Values 1	Domain
Terminal CE	Boundary
Normal Current Density WE	Boundary

Name	Level
Terminal REF	Domain
Global Equations 1	Point

2.4.1 Terminal CE



Terminal CE

EQUATIONS

$$V = V_0$$

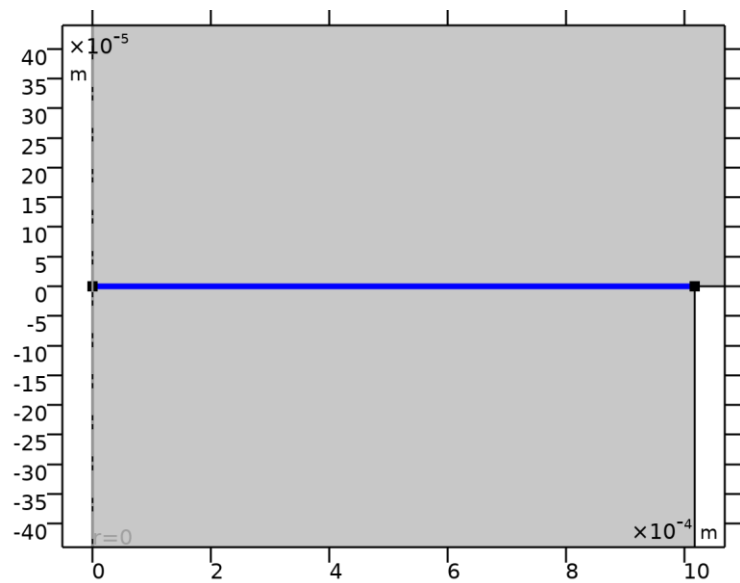
.....

Terminal

SETTINGS

Description	Value
Terminal name	1
Terminal type	Voltage
Voltage	V_CE

2.4.2 Normal Current Density WE



Normal Current Density WE

EQUATIONS

$$-\mathbf{n} \cdot \mathbf{J} = j_n$$

Normal Current Density

SETTINGS

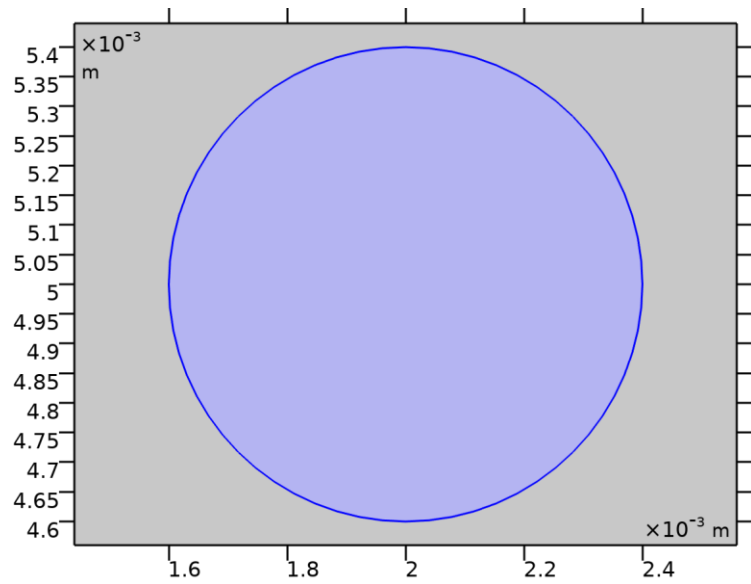
Description	Value
Type	Inward current density
Normal current density	CurrentDensity

Coordinate System Selection

SETTINGS

Description	Value
Coordinate system	Global coordinate system

2.4.3 Terminal REF



Terminal REF

EQUATIONS

$$\int_{\partial\Omega} \mathbf{J} \cdot \mathbf{n} dS = I_0$$

Terminal

SETTINGS

Description	Value
Terminal name	2
Terminal type	Current
Current	0

2.4.4 Global Equations 1

Global Equations

Name	f(u,ut,utt,t)	Initial value (u_0)	Initial value (u_t0)	Description
V_CE	V_REF+V_P[V]	0	0	
V_W	V_W+TotalCurrent*Rs[Ω]	0	0	
		0	0	

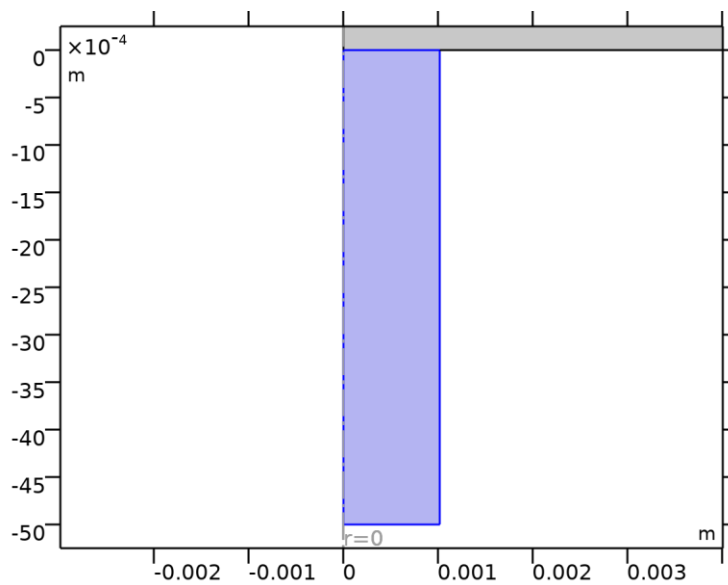
Units

Dependent variable quantity	Unit
-----------------------------	------

Dependent variable quantity	Unit
Custom unit	V

Source term quantity	Unit
Custom unit	V

2.5 STABILIZED CONVECTION-DIFFUSION EQUATION



Stabilized Convection-Diffusion Equation

EQUATIONS

$$d_a \frac{\partial u_2}{\partial t} + \nabla \cdot (-c \nabla u_2 + \alpha u_2) + \beta \cdot \nabla u_2 + a u_2 = f$$

FEATURES

Name	Level
Convection-Diffusion Equation 1	Domain
Initial Values 1	Domain
Axial Symmetry 1	Boundary
No Diffusive Flux 1	Boundary
Dirichlet Boundary Condition 1	Boundary

2.5.1 Convection-Diffusion Equation 1

EQUATIONS

$$d_a \frac{\partial u_2}{\partial t} + \nabla \cdot (-c \nabla u_2 + \alpha u_2) + \beta \cdot \nabla u_2 + a u_2 = f$$

Damping or Mass Coefficient

SETTINGS

Description	Value
Damping or mass coefficient	1

Diffusion Coefficient

SETTINGS

Description	Value
Diffusion coefficient, rr component	{{0, 0, 0}, {0, 0, 0}, {0, 0, 0}}

Conservative Flux Convection Coefficient

SETTINGS

Description	Value
Conservative flux convection coefficient, r component	0
Conservative flux convection coefficient, phi component	0
Conservative flux convection coefficient, z component	0

Convection Coefficient

SETTINGS

Description	Value
Convection coefficient, r component	0
Convection coefficient, phi component	0
Convection coefficient, z component	-1

Absorption Coefficient

SETTINGS

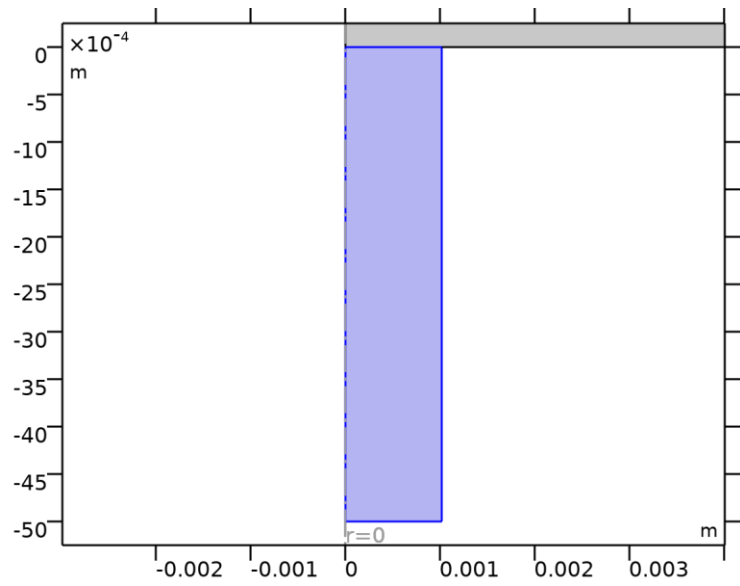
Description	Value
Absorption coefficient	0

Source Term

SETTINGS

Description	Value
Source term	0

2.5.2 Initial Values 1

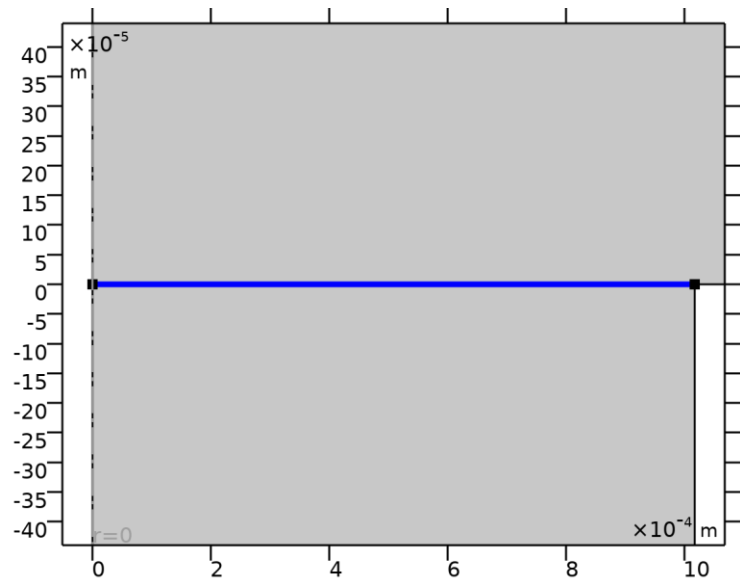


Initial Values 1

SETTINGS

Description	Value
Initial value	0

2.5.3 Dirichlet Boundary Condition 1



Dirichlet Boundary Condition 1

EQUATIONS

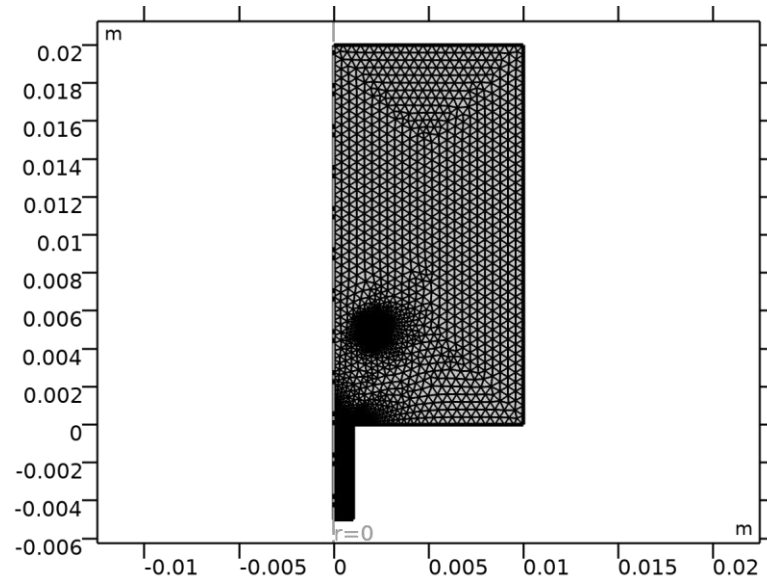
$u_2 = r$

Value on Boundary

SETTINGS

Description	Value
Value on boundary	$V_W - V$

2.6 MESH



Mesh

2.6.1 Size (size)

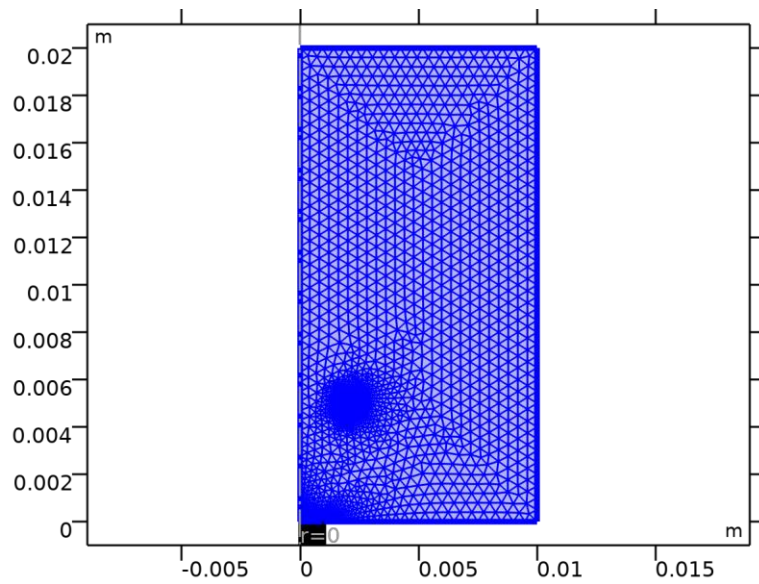
SETTINGS

Description	Value
Maximum element size	5.0E-4
Minimum element size	1.88E-6
Curvature factor	0.25
Maximum element growth rate	1.2
Predefined size	Extra fine

2.6.2 Free Triangular 1 (ftri1)

SELECTION

Geometric entity level	Domain
Selection	Geometry geom3: Dimension 2: Domains 2–3



Free Triangular 1

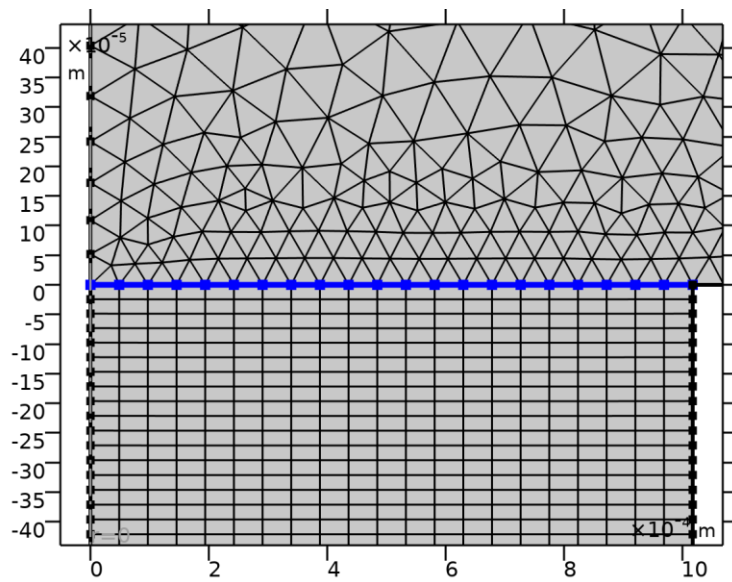
SETTINGS

Description	Value
Number of iterations	4
Maximum element depth to process	4
Last build time	0
Built with	COMSOL 6.0.0.312 (win64) 2024 - 02 - 06T14:07:18.649565100

Size 1 (size1)

SELECTION

Geometric entity level	Boundary
Selection	Geometry geom3: Dimension 1: Boundary 4



Size 1

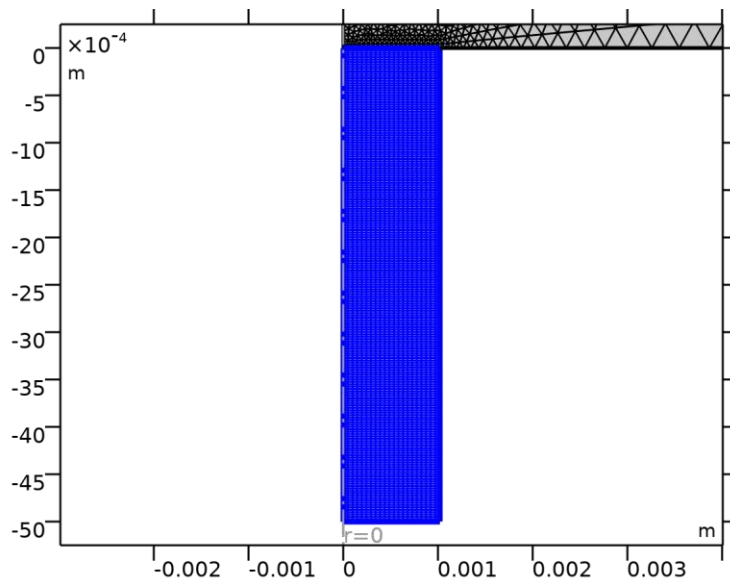
SETTINGS

Description	Value
Maximum element size	0.05 [mm]
Minimum element size	7.0E-7
Curvature factor	0.2
Predefined size	Extremely fine
Custom element size	Custom

2.6.3 Free Quad 1 (fq1)

SELECTION

Geometric entity level	Domain
Selection	Remaining



Free Quad 1

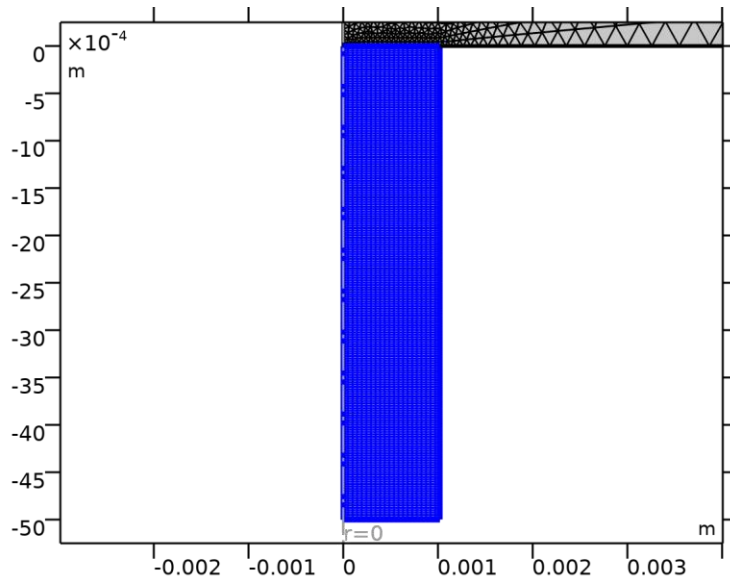
SETTINGS

Description	Value
z-direction scale	2
Number of iterations	4
Maximum element depth to process	4
Last build time	0
Built with	COMSOL 6.0.0.312 (win64) 2024 - 02 - 06T14:07:18.715390100

Size 1 (size1)

SELECTION

Geometric entity level	Domain
Selection	Geometry geom3: Dimension 2: Domain 1



Size 1

SETTINGS

Description	Value
Maximum element size	0.05 [mm]
Minimum element size	6.0E-7
Curvature factor	0.2
Predefined size	Extremely fine
Custom element size	Custom

3 Study 1

3.1 TIME DEPENDENT

Times	Unit
range(0 [ms],0.01 [ms],5[ms])	s

STUDY SETTINGS

Description	Value
Include geometric nonlinearity	Off

PHYSICS AND VARIABLES SELECTION

Physics interface	Discretization
Electric Currents 2 (ec2)	physics
Stabilized Convection-Diffusion Equation (scdeq)	physics

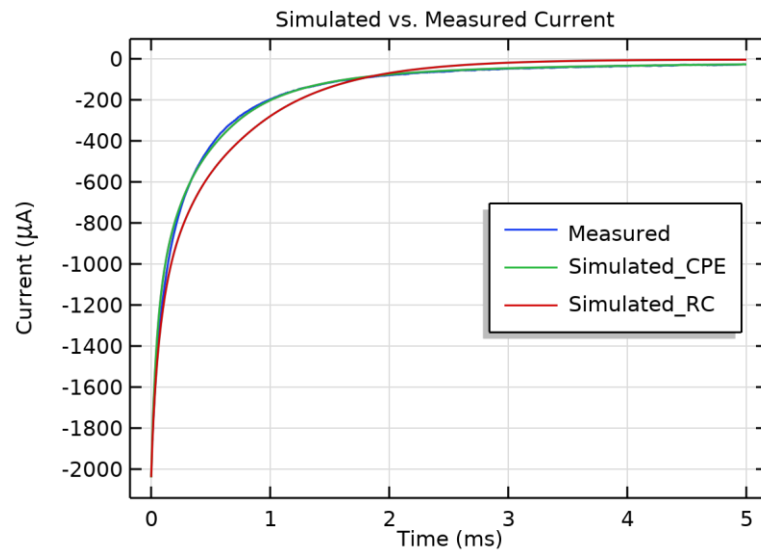
MESH SELECTION

Geometry	Mesh
Geometry (geom3)	mesh3

4 Results

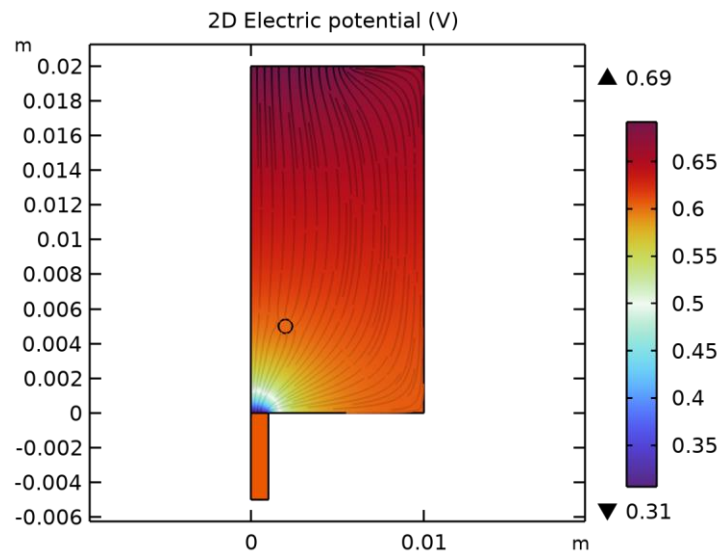
4.1 PLOT GROUPS

4.1.1 Simulated Current



Simulated vs. Measured Current

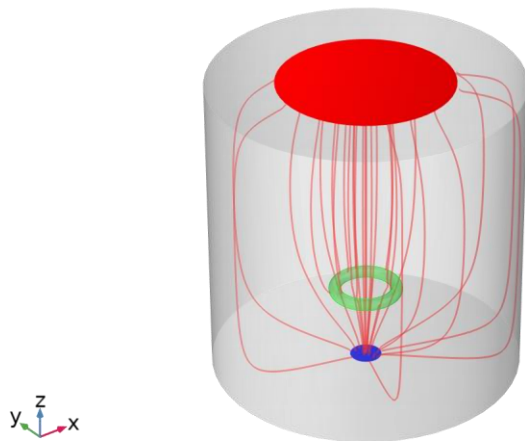
4.1.2 Electric Potential (ec2)



2D Electric potential (V)

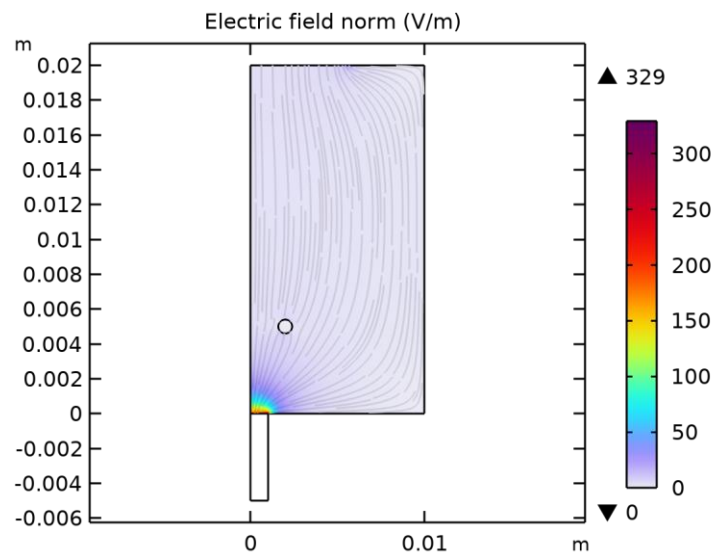
4.1.3 Revolved Geometry (ec2)

Streamline: 3D Current density



Streamline: 3D Current density

4.1.4 Electric Field Norm (ec2)



Electric field norm (V/m)